



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 06:14 AM EST

PDB ID : 5V8I  
Title : Thermus thermophilus 70S ribosome lacking ribosomal protein uS17  
Authors : Gregory, S.T.; Jogl, G.  
Deposited on : 2017-03-22  
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

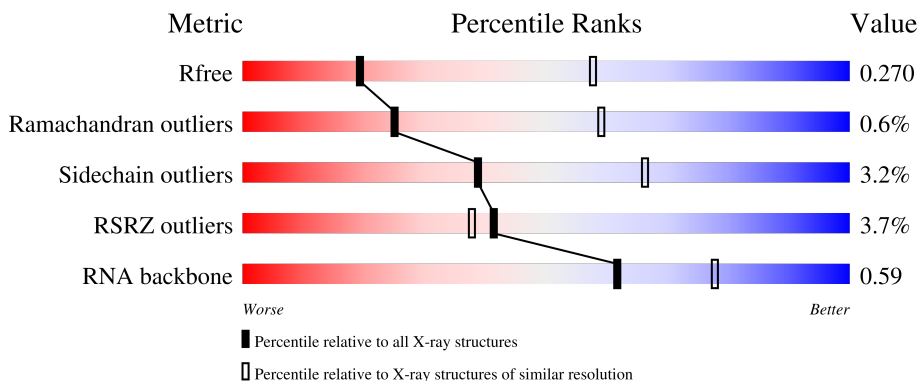
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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	2894	 3% 85% 14% .
1	2A	2894	 3% 83% 15% .
2	1B	120	 92% 7% .
2	2B	120	 2% 90% 8% ..
3	1D	276	 95% 5%

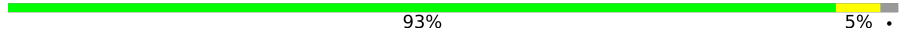
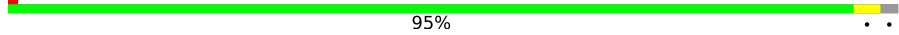
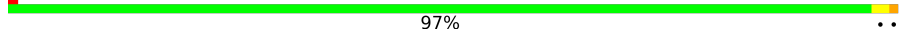
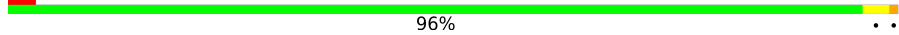
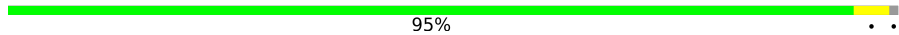
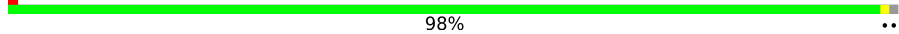
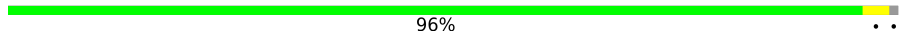
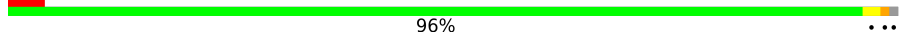
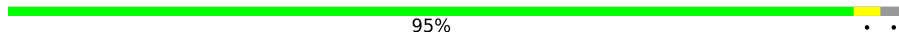
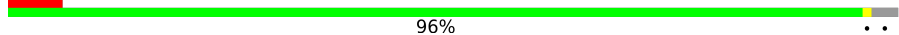
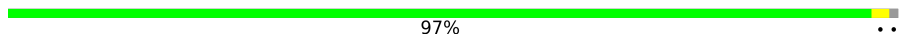
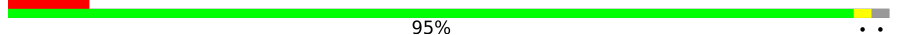



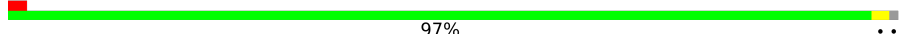



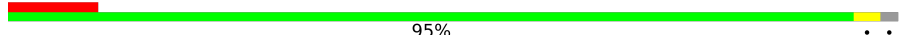


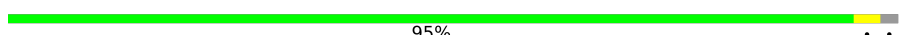
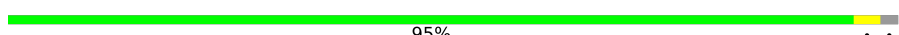
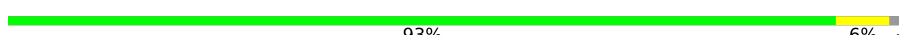
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	2D	276	96%
4	1E	206	93% 6%
4	2E	206	92% 7%
5	1F	210	93%
5	2F	210	94%
6	1G	182	2% 97%
6	2G	182	14% 96%
7	1H	180	% 93%
7	2H	180	9% 93%
8	1I	148	% 95%
8	2I	148	3% 96%
9	1N	140	% 94% 6%
9	2N	140	2% 94% 6%
10	1O	122	100%
10	2O	122	98%
11	1P	150	97%
11	2P	150	% 97%
12	1Q	141	98%
12	2Q	141	% 98%
13	1R	118	93% 7%
13	2R	118	95% 5%
14	1S	112	2% 95%
14	2S	112	9% 97%
15	1T	146	% 88% 10%
15	2T	146	87% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	1U	118	 93% 5%
16	2U	118	 95%
17	1V	101	 97%
17	2V	101	 96%
18	1W	113	 95%
18	2W	113	 98%
19	1X	96	 96%
19	2X	96	 96%
20	1Y	110	 95%
20	2Y	110	 96%
21	1Z	206	 97%
21	2Z	206	 95%
22	10	85	 87% 9%
22	20	85	 89% 9%
23	11	98	 99%
23	21	98	 97%
24	12	72	 93%
24	22	72	 93%
25	13	60	 93% 5%
25	23	60	 95%
26	14	71	 89% 6%
26	24	71	 92%
27	15	60	 95%
27	25	60	 95%
28	16	54	 93% 6%

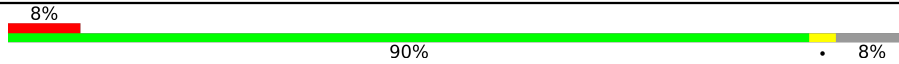
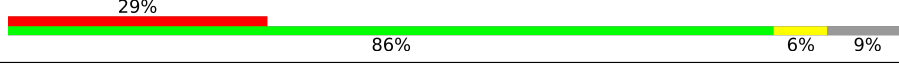
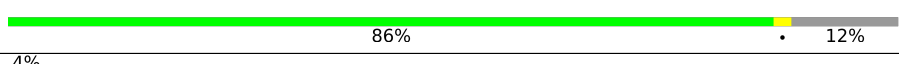

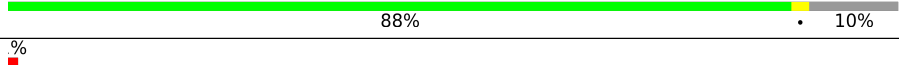
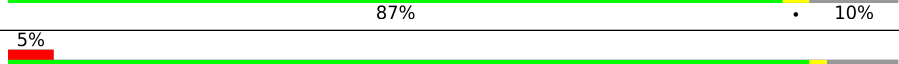
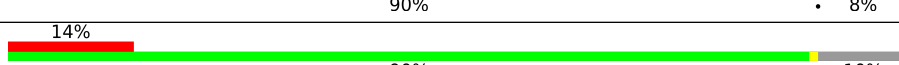
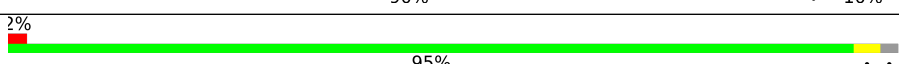
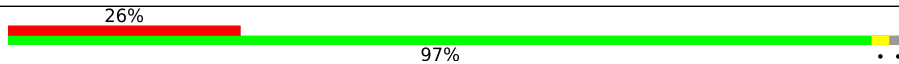
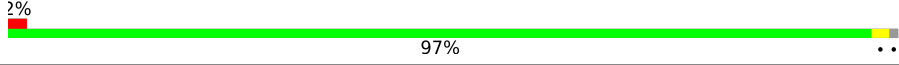
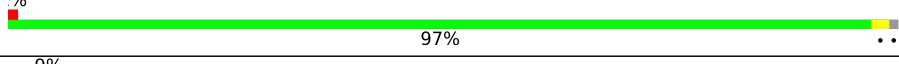
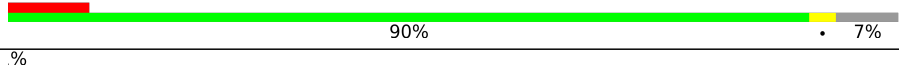
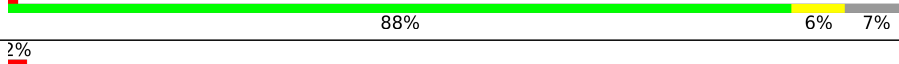

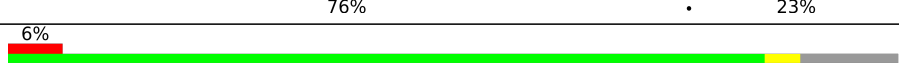


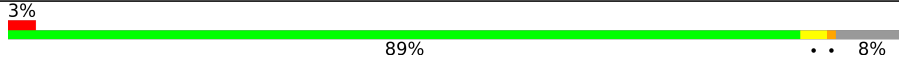

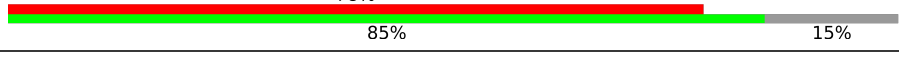



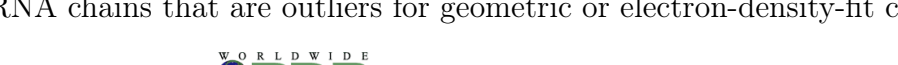
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	26	54	2% 94%
29	17	49	6% 94%
29	27	49	2% 96%
30	18	65	95%
30	28	65	97%
31	19	37	100%
31	29	37	3% 97%
32	1a	1522	2% 84% 14%
32	2a	1522	2% 83% 15%
33	1b	256	4% 84% 6% 10%
33	2b	256	10% 86% 10%
34	1c	239	% 85% 14%
34	2c	239	9% 85% 14%
35	1d	209	4% 97%
35	2d	209	97%
36	1e	162	% 90% 9%
36	2e	162	% 90% 9%
37	1f	101	% 99%
37	2f	101	% 97%
38	1g	156	3% 99%
38	2g	156	12% 97%
39	1h	138	% 96%
39	2h	138	4% 96%
40	1i	128	6% 99%
40	2i	128	29% 95%

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	135	
43	2l	135	
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	1r	88	
48	2r	88	
49	1s	93	
49	2s	93	
50	1t	106	
50	2t	106	
51	1u	27	
51	2u	27	
52	1y	113	
52	2y	113	

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	MPD	2A	3002	-	-	-	X
53	MPD	2B	201	-	-	-	X
54	MG	10	106	-	-	-	X
54	MG	19	103	-	-	-	X
54	MG	1A	3028	-	-	-	X
54	MG	1A	3030	-	-	-	X
54	MG	1A	3170	-	-	-	X
54	MG	1A	3211	-	-	-	X
54	MG	1A	3227	-	-	-	X
54	MG	1A	3260	-	-	-	X
54	MG	1A	3562	-	-	-	X
54	MG	1A	3600	-	-	-	X
54	MG	1A	3608	-	-	-	X
54	MG	1A	3637	-	-	-	X
54	MG	1A	3720	-	-	-	X
54	MG	1A	3732	-	-	-	X
54	MG	1A	3806	-	-	-	X
54	MG	1A	3834	-	-	-	X
54	MG	1A	3850	-	-	-	X
54	MG	1A	3879	-	-	-	X
54	MG	1B	1017	-	-	-	X
54	MG	1F	311	-	-	-	X
54	MG	1P	205	-	-	-	X
54	MG	1a	1650	-	-	-	X
54	MG	1a	1663	-	-	-	X
54	MG	1a	1665	-	-	-	X
54	MG	1a	1668	-	-	-	X
54	MG	1a	1694	-	-	-	X
54	MG	1a	1709	-	-	-	X
54	MG	1a	1734	-	-	-	X
54	MG	1a	1789	-	-	-	X
54	MG	1a	1821	-	-	-	X
54	MG	1a	1822	-	-	-	X
54	MG	1a	1839	-	-	-	X
54	MG	1a	1843	-	-	-	X
54	MG	1d	502	-	-	-	X
54	MG	1e	202	-	-	-	X
54	MG	1e	203	-	-	-	X
54	MG	1y	204	-	-	-	X
54	MG	23	101	-	-	-	X
54	MG	2A	3022	-	-	-	X
54	MG	2A	3045	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	2A	3055	-	-	-	X
54	MG	2A	3058	-	-	-	X
54	MG	2A	3071	-	-	-	X
54	MG	2A	3075	-	-	-	X
54	MG	2A	3077	-	-	-	X
54	MG	2A	3086	-	-	-	X
54	MG	2A	3087	-	-	-	X
54	MG	2A	3105	-	-	-	X
54	MG	2A	3114	-	-	-	X
54	MG	2A	3138	-	-	-	X
54	MG	2A	3151	-	-	-	X
54	MG	2A	3183	-	-	-	X
54	MG	2A	3187	-	-	-	X
54	MG	2A	3202	-	-	-	X
54	MG	2A	3207	-	-	-	X
54	MG	2A	3209	-	-	-	X
54	MG	2A	3213	-	-	-	X
54	MG	2A	3230	-	-	-	X
54	MG	2A	3301	-	-	-	X
54	MG	2A	3317	-	-	-	X
54	MG	2A	3452	-	-	-	X
54	MG	2A	3488	-	-	-	X
54	MG	2A	3565	-	-	-	X
54	MG	2A	3615	-	-	-	X
54	MG	2A	3630	-	-	-	X
54	MG	2B	204	-	-	-	X
54	MG	2B	205	-	-	-	X
54	MG	2B	211	-	-	-	X
54	MG	2a	1608	-	-	-	X
54	MG	2a	1617	-	-	-	X
54	MG	2a	1655	-	-	-	X
54	MG	2a	1658	-	-	-	X
54	MG	2a	1659	-	-	-	X
54	MG	2a	1663	-	-	-	X
54	MG	2a	1664	-	-	-	X
54	MG	2a	1670	-	-	-	X
54	MG	2a	1675	-	-	-	X
54	MG	2a	1690	-	-	-	X
54	MG	2a	1701	-	-	-	X
54	MG	2i	201	-	-	-	X



## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 290709 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
			Total	C	N	O	P			
1	1A	2862	Total	C	N	O	P	0	0	0
			61654	27444	11530	19819	2861			
1	2A	2858	Total	C	N	O	P	0	0	0
			61564	27404	11511	19793	2856			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	118	Total	C	N	O	P	0	0	0
			2536	1128	471	819	118			
2	2B	118	Total	C	N	O	P	0	0	0
			2536	1128	471	819	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			1586	1011	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1582	1009	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
			1427	917	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1425	913	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1095	700	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1077	688	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			932	587	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
			932	587	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
			1121	715	212	187	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	7			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	681	225	184	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	676	224	182	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			606	375	127	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			606	375	127	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			756	475	150	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			761	478	151	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	24	69	536	342	98	91	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	15	59	460	290	90	75	5	0	0	0
27	25	59	456	287	89	75	5	0	0	0

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

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

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

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

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

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

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

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

- 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
			32249	14359	5977	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32334	14397	5992	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			987	625	194	168			
40	2i	126	Total	C	N	O	0	0	0
			967	613	187	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

*Continued on next page...*



*Continued from previous page...*

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	2	0	0	0

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

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

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

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

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

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
48	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
49	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1t	96	Total	C	N	O	S	0	0	0
			731	448	157	124	2			
50	2t	98	Total	C	N	O	S	0	0	0
			732	450	154	126	2			

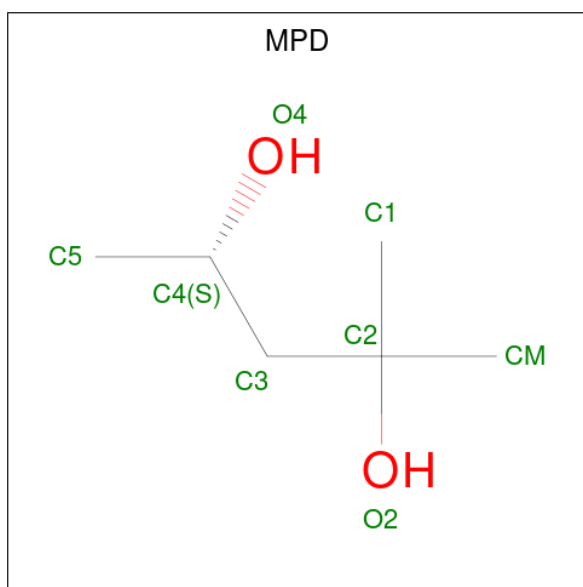
- Molecule 51 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
52	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 53 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	1A	1	Total C O 8 6 2	0	0
53	1T	1	Total C O 8 6 2	0	0
53	18	1	Total C O 8 6 2	0	0
53	1a	1	Total C O 8 6 2	0	0
53	2A	1	Total C O 8 6 2	0	0
53	2A	1	Total C O 8 6 2	0	0
53	2B	1	Total C O 8 6 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1A	900	Total Mg 900 900	0	0
54	1B	29	Total Mg 29 29	0	0
54	1D	12	Total Mg 12 12	0	0
54	1E	5	Total Mg 5 5	0	0
54	1F	12	Total Mg 12 12	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1G	4	Total 4	Mg 4	0	0
54	1H	2	Total 2	Mg 2	0	0
54	1N	3	Total 3	Mg 3	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	5	Total 5	Mg 5	0	0
54	1Q	3	Total 3	Mg 3	0	0
54	1R	7	Total 7	Mg 7	0	0
54	1T	5	Total 5	Mg 5	0	0
54	1U	3	Total 3	Mg 3	0	0
54	1V	3	Total 3	Mg 3	0	0
54	1W	4	Total 4	Mg 4	0	0
54	1X	2	Total 2	Mg 2	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	6	Total 6	Mg 6	0	0
54	11	4	Total 4	Mg 4	0	0
54	13	2	Total 2	Mg 2	0	0
54	15	3	Total 3	Mg 3	0	0
54	16	1	Total 1	Mg 1	0	0
54	17	3	Total 3	Mg 3	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	257	Total 257	Mg 257	0	0

*Continued on next page...*

*Continued from previous page...*

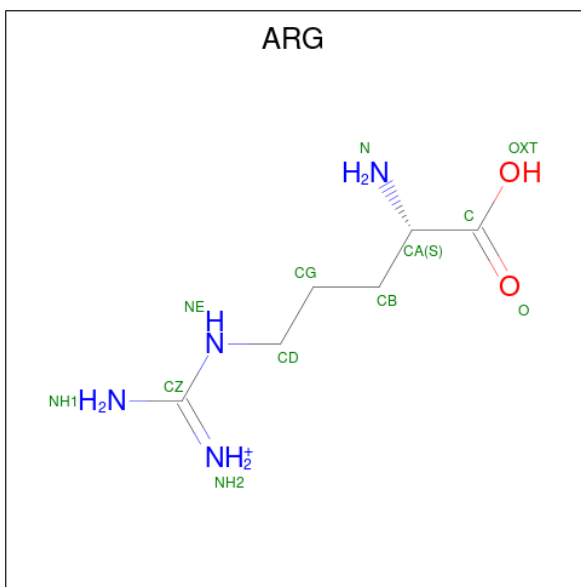
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1b	1	Total 1	Mg 1	0	0
54	1d	6	Total 6	Mg 6	0	0
54	1e	3	Total 3	Mg 3	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1n	2	Total 2	Mg 2	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1t	2	Total 2	Mg 2	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2A	641	Total 641	Mg 641	0	0
54	2B	16	Total 16	Mg 16	0	0
54	2D	6	Total 6	Mg 6	0	0
54	2E	2	Total 2	Mg 2	0	0
54	2F	2	Total 2	Mg 2	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0
54	2Q	2	Total 2	Mg 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	2R	3	Total Mg 3 3	0	0
54	2T	5	Total Mg 5 5	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	2	Total Mg 2 2	0	0
54	2X	1	Total Mg 1 1	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	1	Total Mg 1 1	0	0
54	21	4	Total Mg 4 4	0	0
54	23	1	Total Mg 1 1	0	0
54	28	1	Total Mg 1 1	0	0
54	2a	164	Total Mg 164 164	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	1	Total Mg 1 1	0	0
54	2i	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2l	2	Total Mg 2 2	0	0
54	2p	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is ARGinine (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1B	1	Total	C	N	O	0	0
			12	6	4	2		
55	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

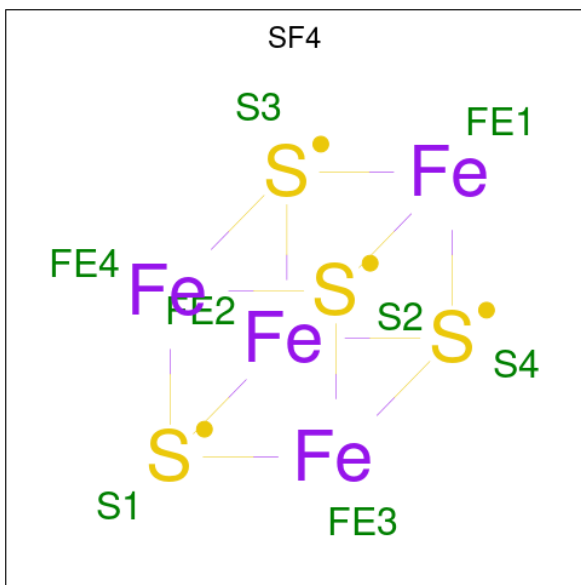
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total	Zn	0	0
			1	1		
56	14	1	Total	Zn	0	0
			1	1		
56	15	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		
56	19	1	Total	Zn	0	0
			1	1		
56	1n	1	Total	Zn	0	0
			1	1		
56	2Y	1	Total	Zn	0	0
			1	1		
56	24	1	Total	Zn	0	0
			1	1		
56	25	1	Total	Zn	0	0
			1	1		
56	26	1	Total	Zn	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	29	1	Total Zn 1 1	0	0
56	2n	1	Total Zn 1 1	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1d	1	Total Fe S 8 4 4	0	0
57	2d	1	Total Fe S 8 4 4	0	0

- Molecule 58 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1801	Total O 1801 1801	0	0
58	1B	56	Total O 56 56	0	0
58	1D	14	Total O 14 14	0	0
58	1E	17	Total O 17 17	0	0
58	1F	16	Total O 16 16	0	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1G	5	Total 5	O 5	0	0
58	1H	5	Total 5	O 5	0	0
58	1N	7	Total 7	O 7	0	0
58	1O	2	Total 2	O 2	0	0
58	1P	17	Total 17	O 17	0	0
58	1Q	5	Total 5	O 5	0	0
58	1R	5	Total 5	O 5	0	0
58	1T	8	Total 8	O 8	0	0
58	1U	6	Total 6	O 6	0	0
58	1V	5	Total 5	O 5	0	0
58	1W	2	Total 2	O 2	0	0
58	1X	6	Total 6	O 6	0	0
58	1Y	1	Total 1	O 1	0	0
58	1Z	1	Total 1	O 1	0	0
58	10	5	Total 5	O 5	0	0
58	11	3	Total 3	O 3	0	0
58	13	6	Total 6	O 6	0	0
58	15	3	Total 3	O 3	0	0
58	16	2	Total 2	O 2	0	0
58	17	1	Total 1	O 1	0	0
58	18	7	Total 7	O 7	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	19	3	Total O 3 3	0	0
58	1a	424	Total O 424 424	0	0
58	1c	1	Total O 1 1	0	0
58	1d	8	Total O 8 8	0	0
58	1e	4	Total O 4 4	0	0
58	1f	1	Total O 1 1	0	0
58	1h	1	Total O 1 1	0	0
58	1j	1	Total O 1 1	0	0
58	1l	3	Total O 3 3	0	0
58	1m	1	Total O 1 1	0	0
58	1o	3	Total O 3 3	0	0
58	1p	1	Total O 1 1	0	0
58	1t	2	Total O 2 2	0	0
58	1y	3	Total O 3 3	0	0
58	2A	1310	Total O 1310 1310	0	0
58	2B	32	Total O 32 32	0	0
58	2D	16	Total O 16 16	0	0
58	2E	10	Total O 10 10	0	0
58	2F	6	Total O 6 6	0	0
58	2G	1	Total O 1 1	0	0
58	2N	1	Total O 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2O	3	Total O 3 3	0	0
58	2P	14	Total O 14 14	0	0
58	2Q	5	Total O 5 5	0	0
58	2R	1	Total O 1 1	0	0
58	2T	4	Total O 4 4	0	0
58	2V	2	Total O 2 2	0	0
58	2W	3	Total O 3 3	0	0
58	2X	4	Total O 4 4	0	0
58	2Y	1	Total O 1 1	0	0
58	20	2	Total O 2 2	0	0
58	21	1	Total O 1 1	0	0
58	23	2	Total O 2 2	0	0
58	25	1	Total O 1 1	0	0
58	26	1	Total O 1 1	0	0
58	27	2	Total O 2 2	0	0
58	28	5	Total O 5 5	0	0
58	2a	282	Total O 282 282	0	0
58	2e	1	Total O 1 1	0	0
58	2j	2	Total O 2 2	0	0
58	2l	1	Total O 1 1	0	0
58	2t	2	Total O 2 2	0	0

*Continued on next page...*

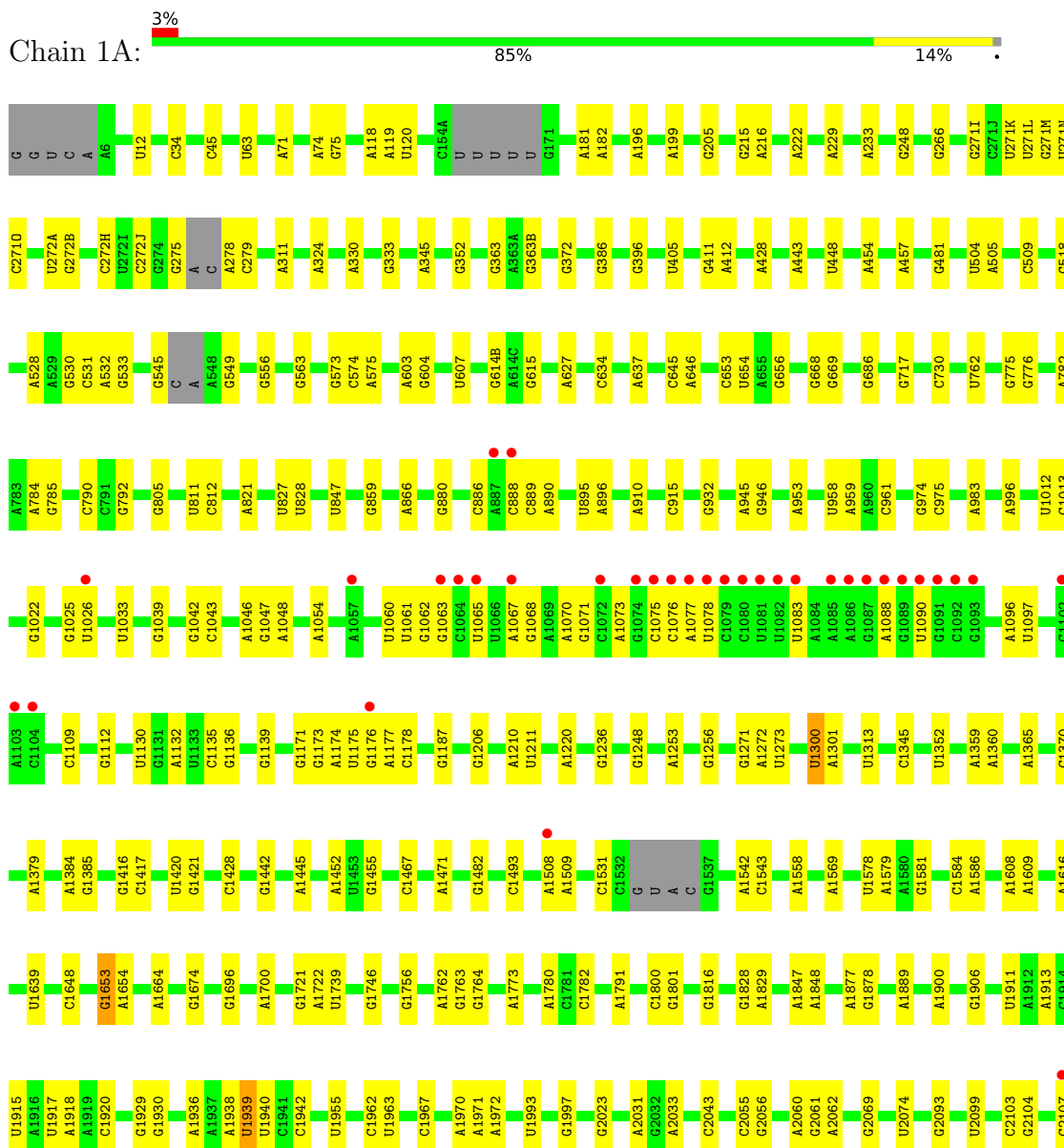
*Continued from previous page...*

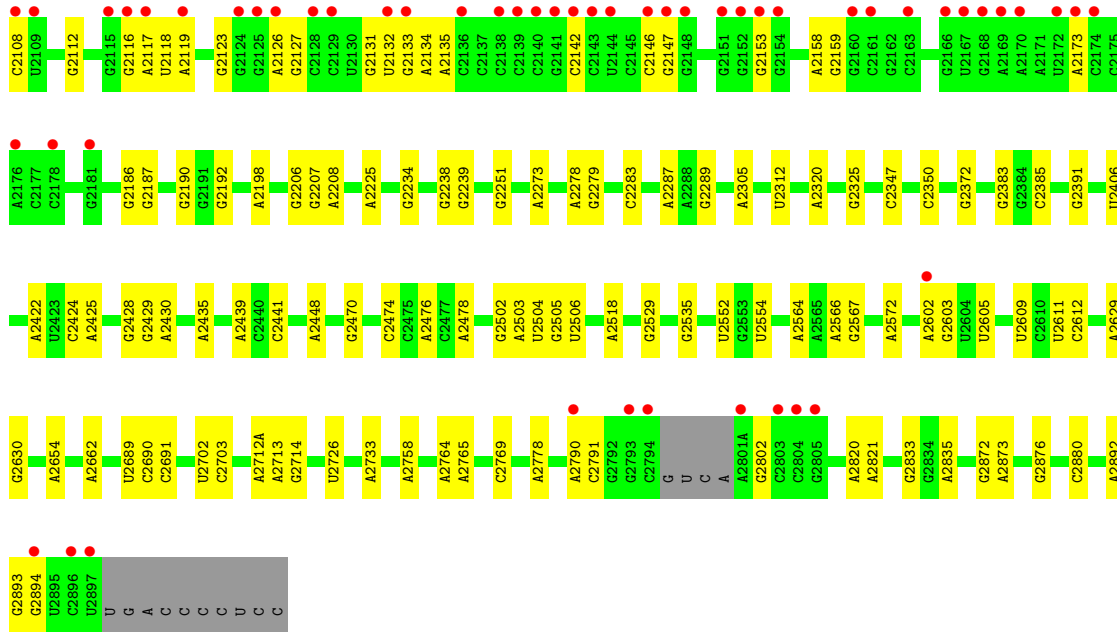
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
58	2y	3	Total	O	0	0
			3	3		

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

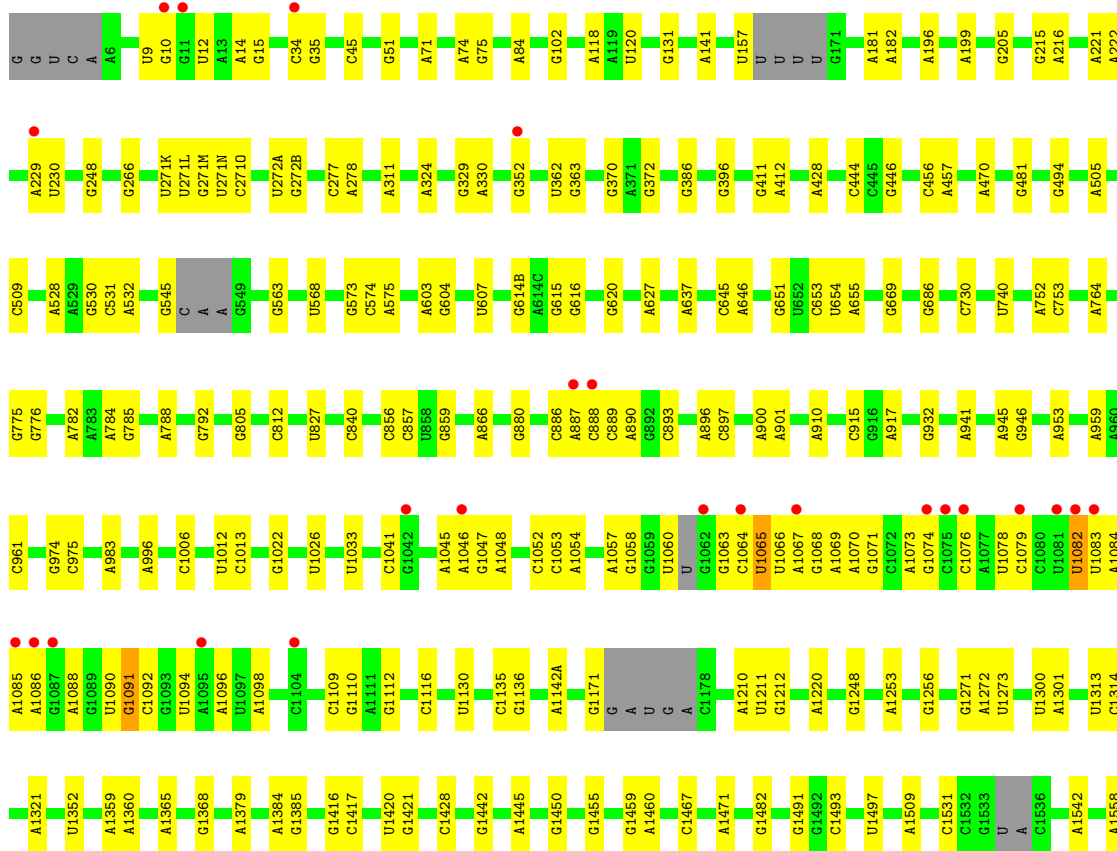
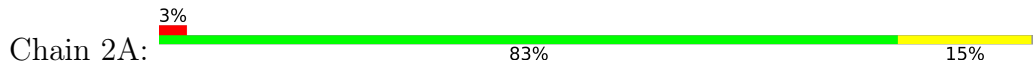
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

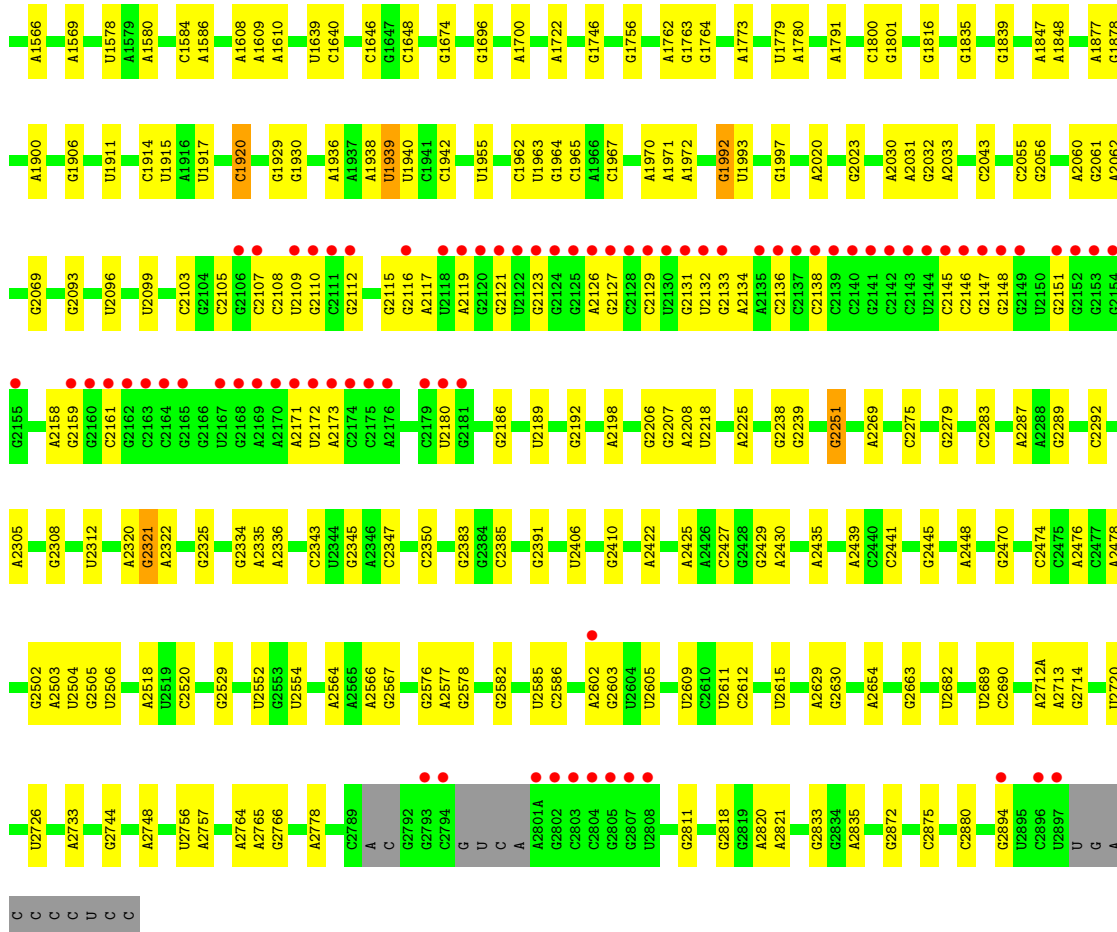
- Molecule 1: 23S Ribosomal RNA



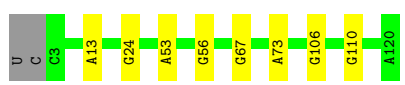
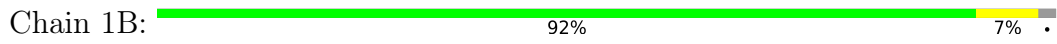


• Molecule 1: 23S Ribosomal RNA

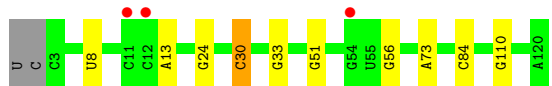
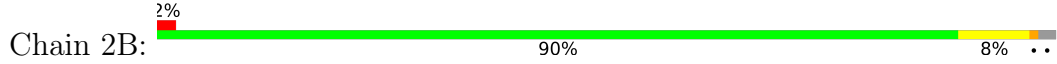




• Molecule 2: 5S Ribosomal RNA



• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2



• Molecule 3: 50S ribosomal protein L2

Chain 2D:  96%



- Molecule 4: 50S ribosomal protein L3

Chain 1E:  93%



- Molecule 4: 50S ribosomal protein L3

Chain 2E:  92%



- Molecule 5: 50S ribosomal protein L4

Chain 1F:  93%



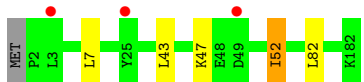
- Molecule 5: 50S ribosomal protein L4

Chain 2F:  94%



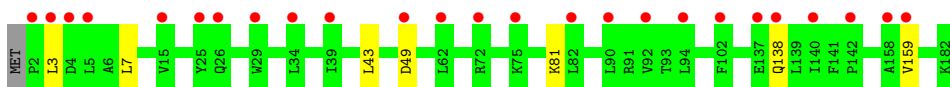
- Molecule 6: 50S ribosomal protein L5

Chain 1G:  97%



- Molecule 6: 50S ribosomal protein L5

Chain 2G:  96%

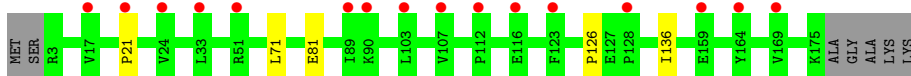


- Molecule 7: 50S ribosomal protein L6

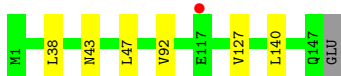




- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



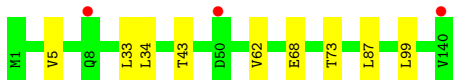
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



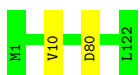
- Molecule 10: 50S ribosomal protein L14



There are no outlier residues recorded for this chain.

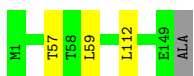
- Molecule 10: 50S ribosomal protein L14

Chain 2O:  98%



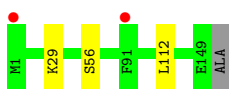
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  97%



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  97%



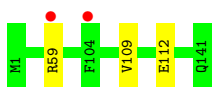
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  98%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q:  98%



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  93% 7%

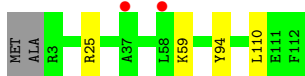


- Molecule 13: 50S ribosomal protein L17

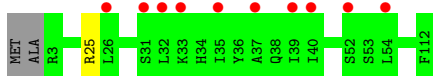
Chain 2R:  95% 5%



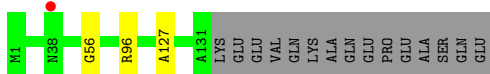
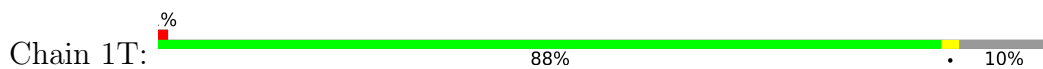
- Molecule 14: 50S ribosomal protein L18



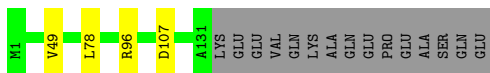
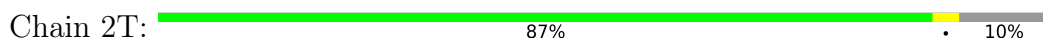
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



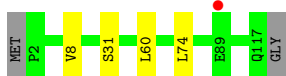
- Molecule 15: 50S ribosomal protein L19



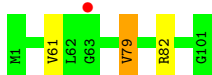
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



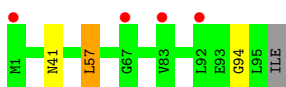
- Molecule 18: 50S ribosomal protein L22



- 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

Chain 1Z:  97%




- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  95%

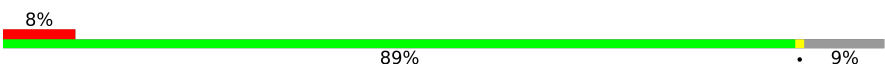


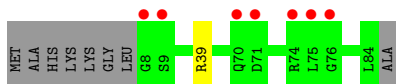
- Molecule 22: 50S ribosomal protein L27

Chain 10:  87%



- Molecule 22: 50S ribosomal protein L27

Chain 20:  89%



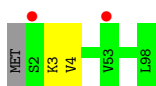
- Molecule 23: 50S ribosomal protein L28

Chain 11:  99%



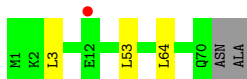
- Molecule 23: 50S ribosomal protein L28

Chain 21:  97%

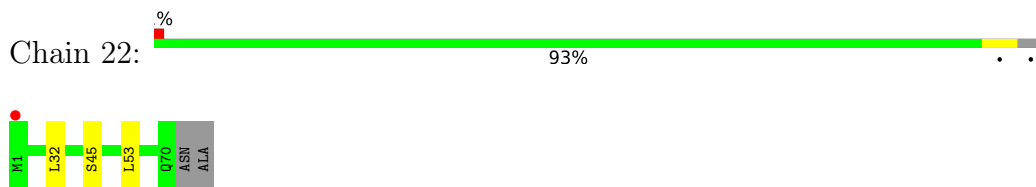


- Molecule 24: 50S ribosomal protein L29

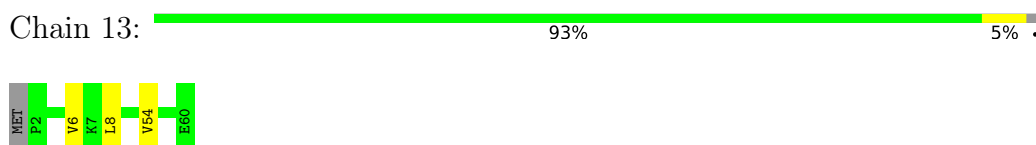
Chain 12:  93%



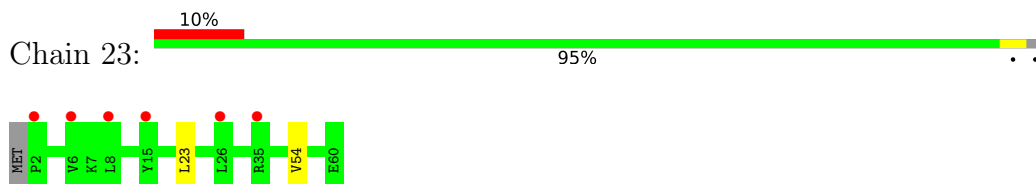
- Molecule 24: 50S ribosomal protein L29



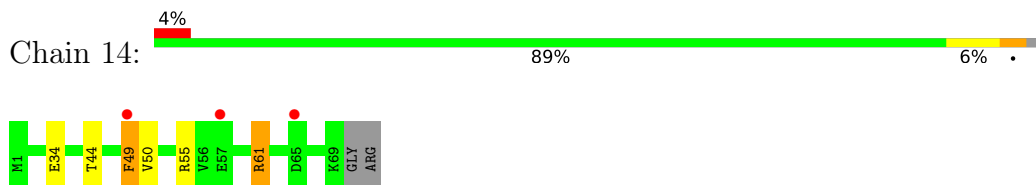
- Molecule 25: 50S ribosomal protein L30



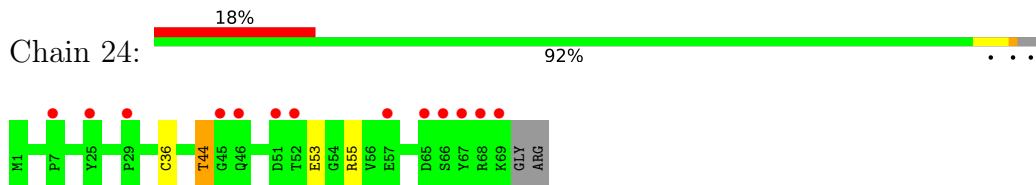
- Molecule 25: 50S ribosomal protein L30



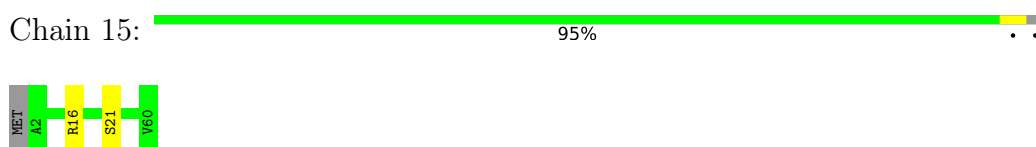
- Molecule 26: 50S ribosomal protein L31



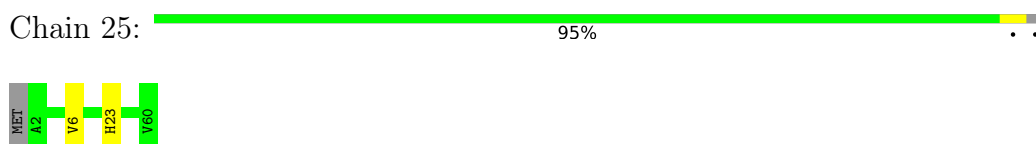
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  93% 6%

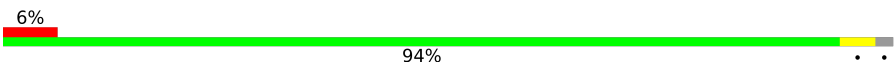


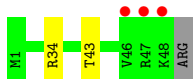
- Molecule 28: 50S ribosomal protein L33

Chain 26:  2% 94%



- Molecule 29: 50S ribosomal protein L34

Chain 17:  6% 94%



- Molecule 29: 50S ribosomal protein L34

Chain 27:  2% 96%



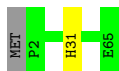
- Molecule 30: 50S ribosomal protein L35

Chain 18:  95%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  97%



- Molecule 31: 50S ribosomal protein L36

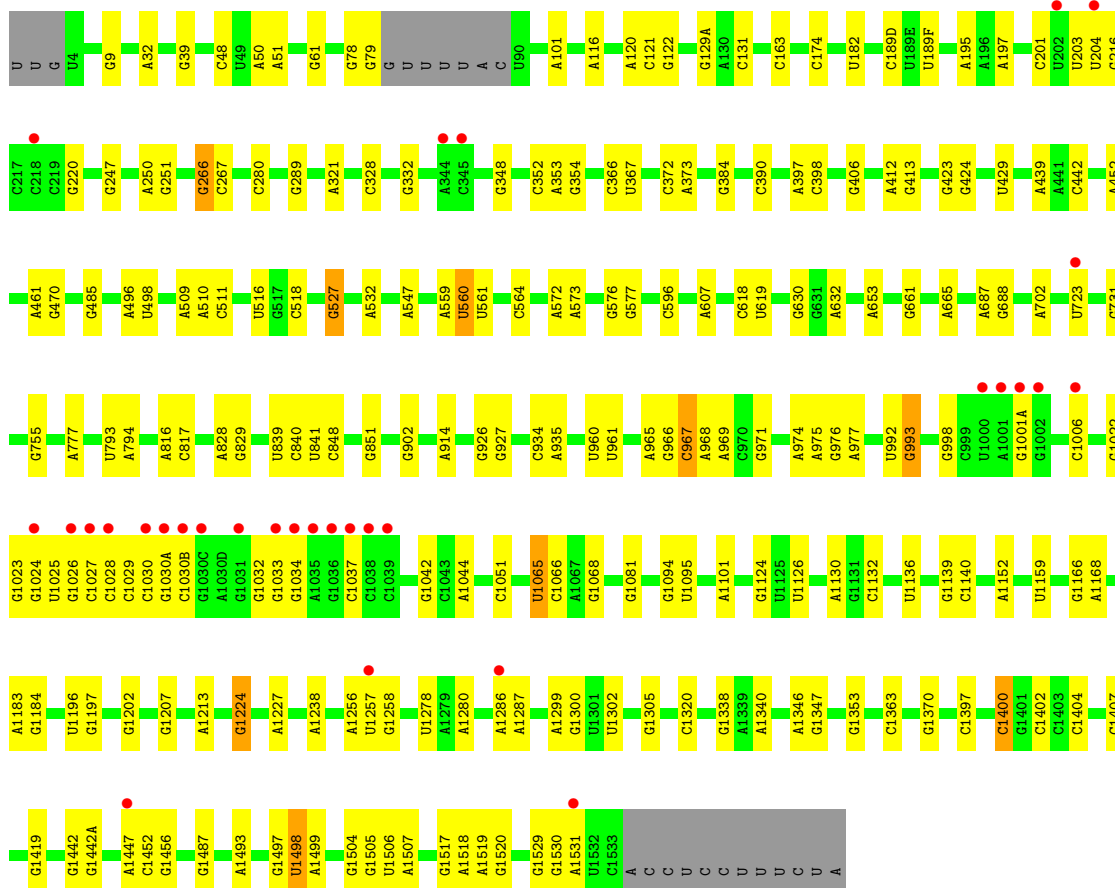
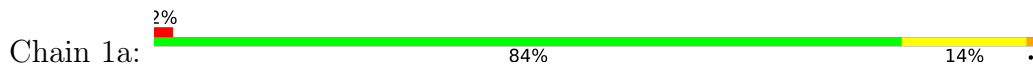
Chain 19:  100%

There are no outlier residues recorded for this chain.

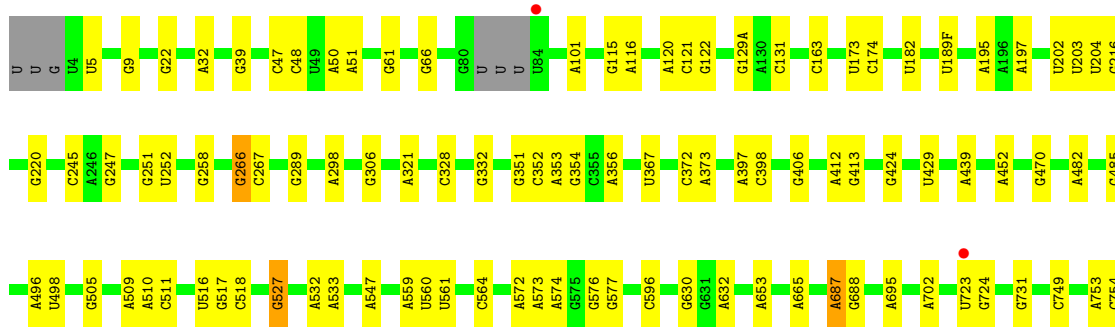
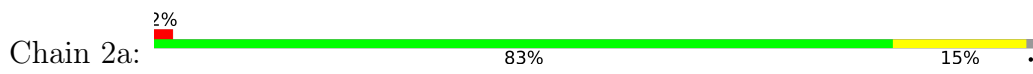
- Molecule 31: 50S ribosomal protein L36



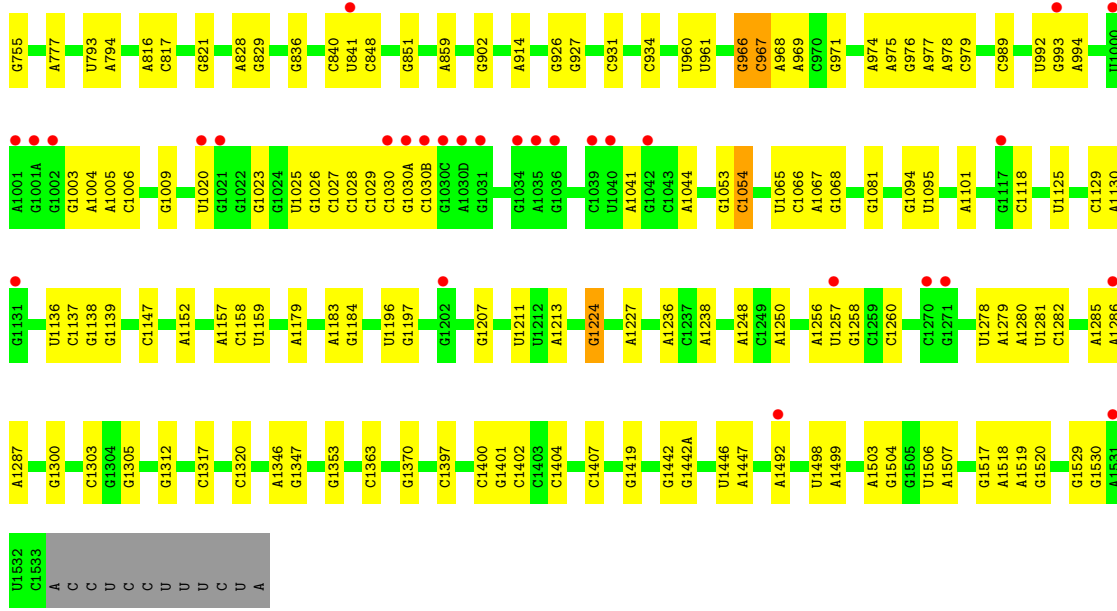
• Molecule 32: 16S Ribosomal RNA



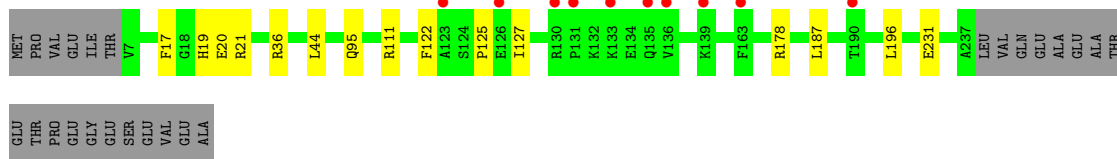
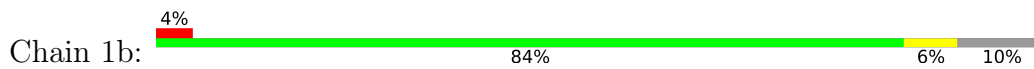
• Molecule 32: 16S Ribosomal RNA



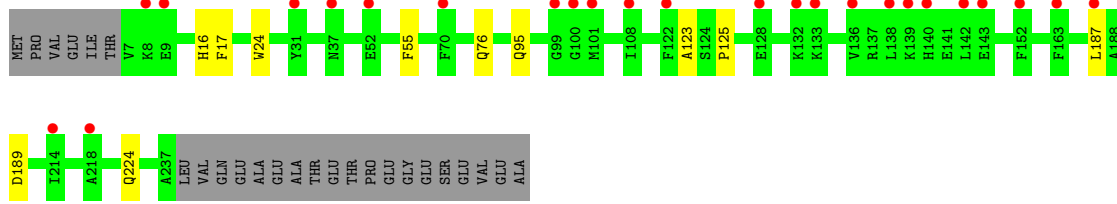
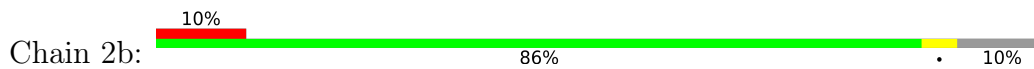




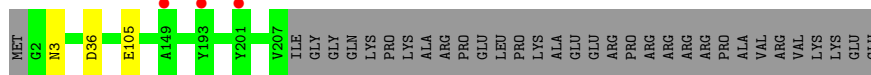
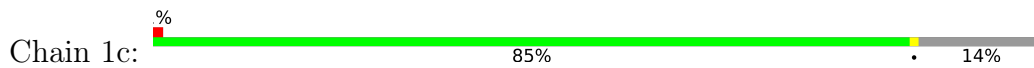
● Molecule 33: 30S ribosomal protein S2



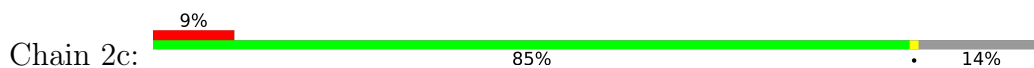
● Molecule 33: 30S ribosomal protein S2

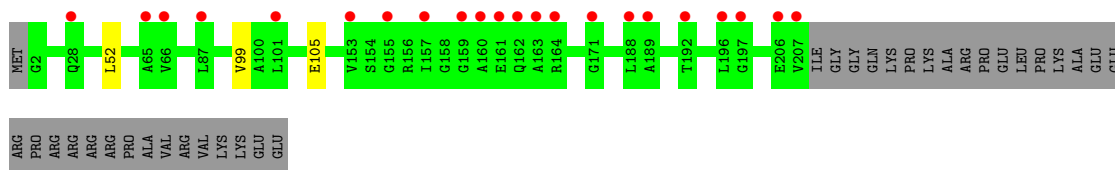


● Molecule 34: 30S ribosomal protein S3

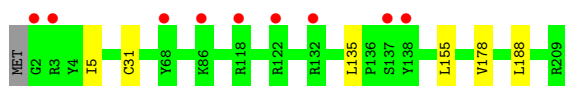


● Molecule 34: 30S ribosomal protein S3





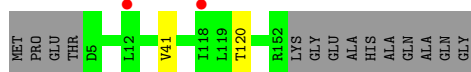
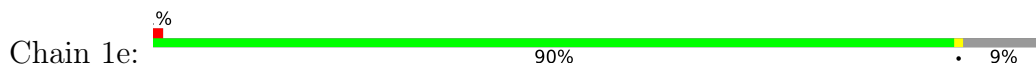
- Molecule 35: 30S ribosomal protein S4



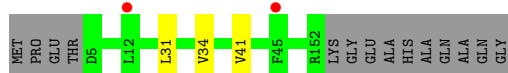
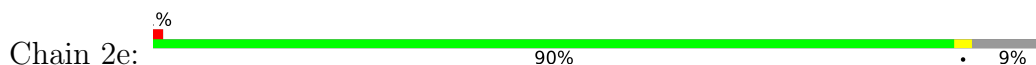
- Molecule 35: 30S ribosomal protein S4



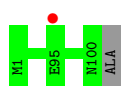
- Molecule 36: 30S ribosomal protein S5



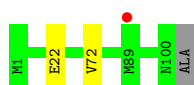
- Molecule 36: 30S ribosomal protein S5



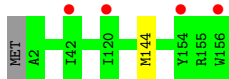
- Molecule 37: 30S ribosomal protein S6



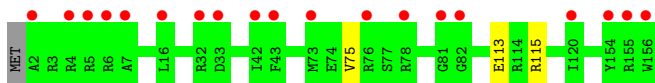
- Molecule 37: 30S ribosomal protein S6



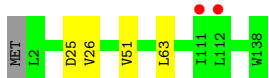
- Molecule 38: 30S ribosomal protein S7



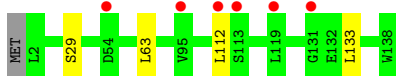
- Molecule 38: 30S ribosomal protein S7



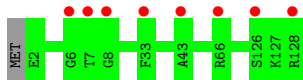
- Molecule 39: 30S ribosomal protein S8



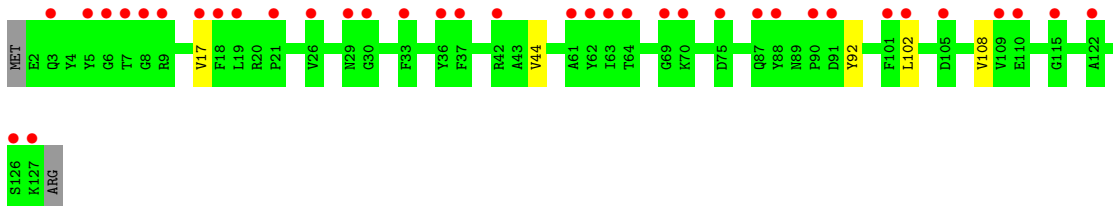
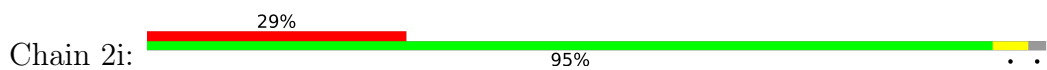
- Molecule 39: 30S ribosomal protein S8



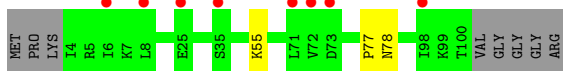
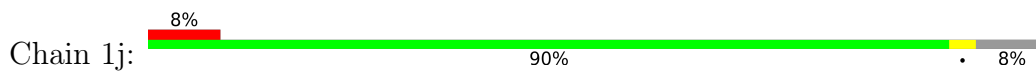
- Molecule 40: 30S ribosomal protein S9



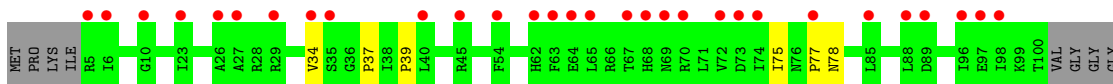
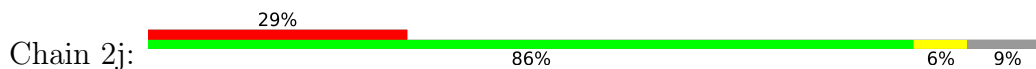
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

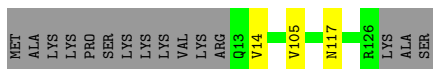
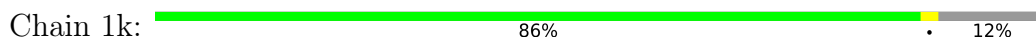


- Molecule 41: 30S ribosomal protein S10

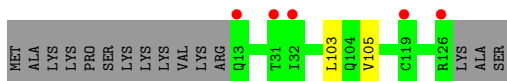
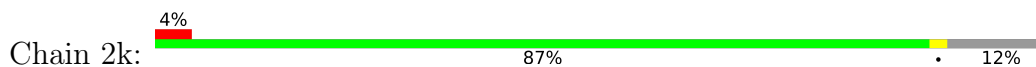


ARG

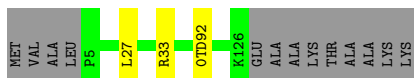
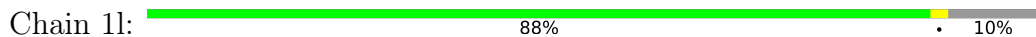
- Molecule 42: 30S ribosomal protein S11



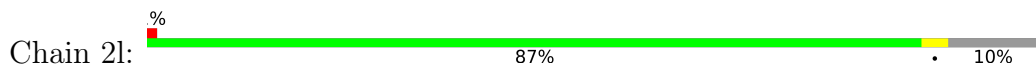
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

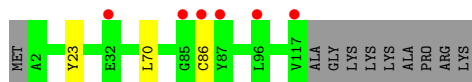


- Molecule 43: 30S ribosomal protein S12

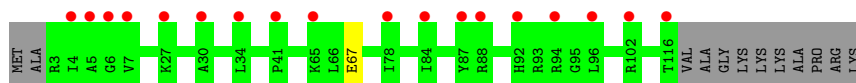
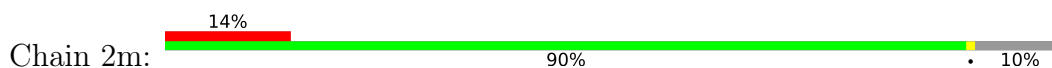


- Molecule 44: 30S ribosomal protein S13





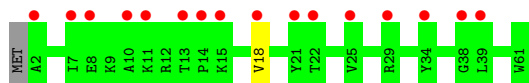
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



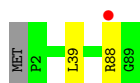
- Molecule 45: 30S ribosomal protein S14 type Z



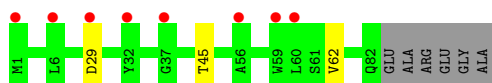
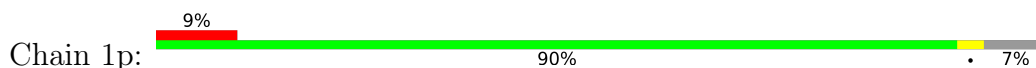
- Molecule 46: 30S ribosomal protein S15



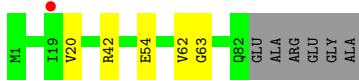
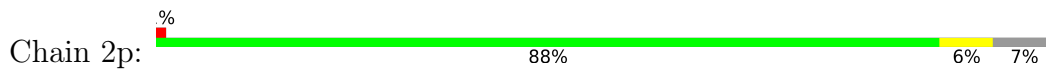
- Molecule 46: 30S ribosomal protein S15



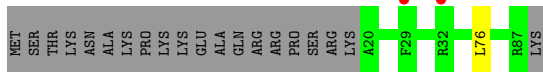
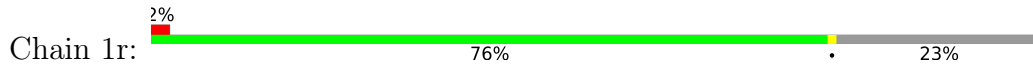
- Molecule 47: 30S ribosomal protein S16



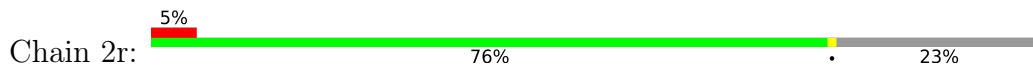
- Molecule 47: 30S ribosomal protein S16



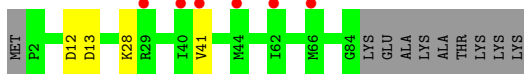
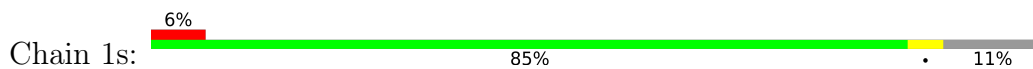
- Molecule 48: 30S ribosomal protein S18



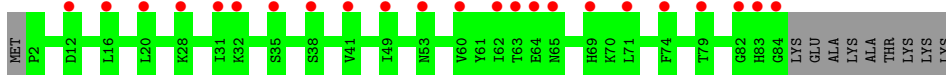
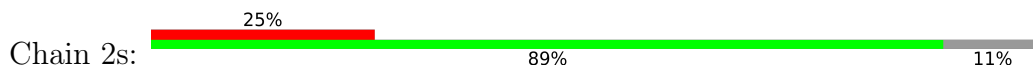
- Molecule 48: 30S ribosomal protein S18



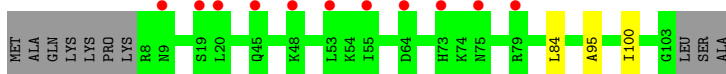
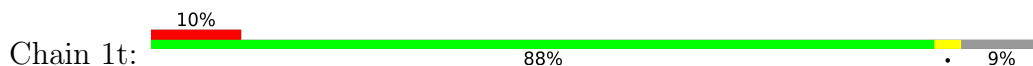
- Molecule 49: 30S ribosomal protein S19



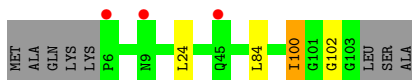
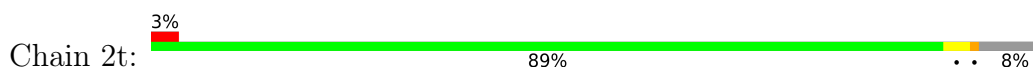
- Molecule 49: 30S ribosomal protein S19



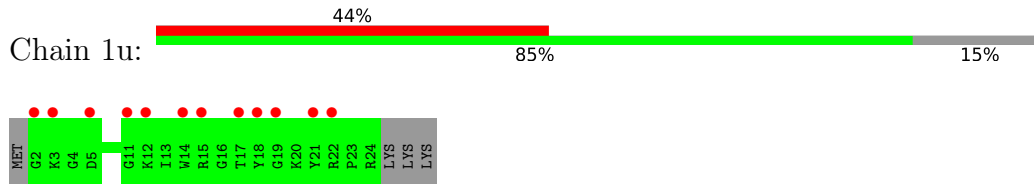
- Molecule 50: 30S ribosomal protein S20



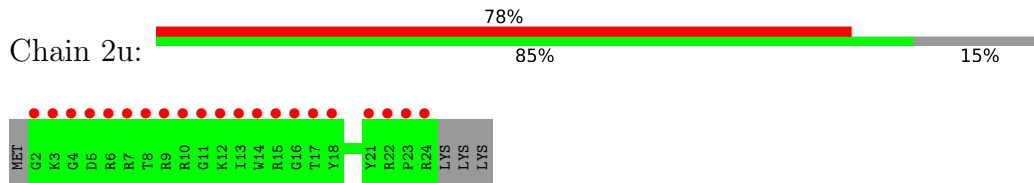
- Molecule 50: 30S ribosomal protein S20



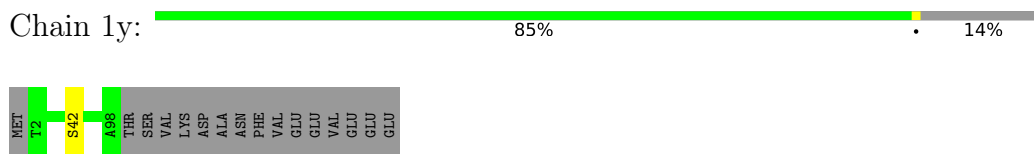
- Molecule 51: 30S ribosomal protein Thx



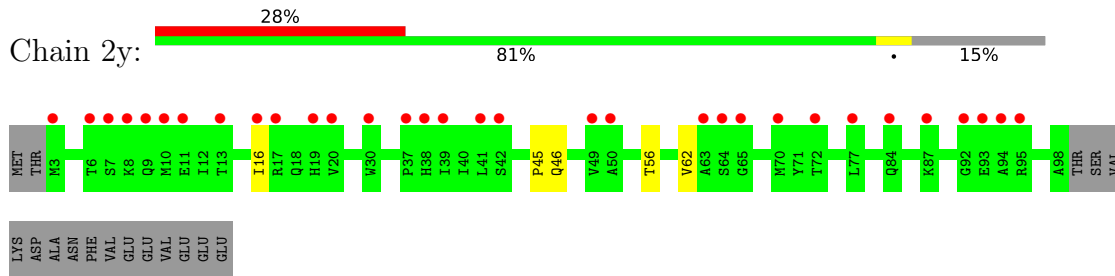
- Molecule 51: 30S ribosomal protein Thx



- Molecule 52: Ribosome-associated inhibitor A



- Molecule 52: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.81Å 450.83Å 621.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.25 49.93 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.93-3.25) 100.0 (49.93-3.25)	Depositor EDS
$R_{merge}$	0.47	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.25Å)	Xtrriage
Refinement program	PHENIX dev_2747	Depositor
R, $R_{free}$	0.226 , 0.270 0.226 , 0.270	Depositor DCC
$R_{free}$ test set	46129 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtrriage
Anisotropy	0.627	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	290709	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 5MC, MG, G7M, UR3, 5MU, OMG, M2G, MA6, SF4, 0TD, 2MG, 2MA, OMC, ZN, OMU, 4OC, MPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.30	0/68792	0.79	7/107386 (0.0%)
1	2A	0.25	0/68686	0.75	9/107216 (0.0%)
2	1B	0.29	0/2837	0.82	0/4426
2	2B	0.25	0/2837	0.81	1/4426 (0.0%)
3	1D	0.29	0/2181	0.49	0/2940
3	2D	0.27	0/2186	0.46	0/2944
4	1E	0.29	0/1592	0.46	0/2149
4	2E	0.26	0/1592	0.46	0/2149
5	1F	0.27	0/1621	0.45	0/2196
5	2F	0.25	0/1617	0.43	0/2191
6	1G	0.26	0/1452	0.45	0/1962
6	2G	0.25	0/1450	0.42	0/1958
7	1H	0.28	0/1356	0.44	0/1834
7	2H	0.25	0/1350	0.42	0/1826
8	1I	0.25	0/1110	0.44	0/1513
8	2I	0.24	0/1092	0.43	0/1491
9	1N	0.27	0/1148	0.45	0/1547
9	2N	0.25	0/1144	0.42	0/1543
10	1O	0.30	0/942	0.48	0/1268
10	2O	0.27	0/942	0.47	0/1268
11	1P	0.29	0/1152	0.47	0/1533
11	2P	0.27	0/1152	0.48	0/1533
12	1Q	0.28	0/1142	0.46	0/1525
12	2Q	0.27	0/1142	0.43	0/1525
13	1R	0.27	0/982	0.46	0/1312
13	2R	0.25	0/982	0.42	0/1312
14	1S	0.27	0/887	0.44	0/1180
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.27	0/1105	0.44	0/1476
15	2T	0.25	0/1097	0.42	0/1467
16	1U	0.29	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.25	0/977	0.38	0/1301
17	1V	0.29	0/786	0.49	0/1053
17	2V	0.25	0/782	0.46	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.26	0/897	0.42	0/1205
19	1X	0.29	0/764	0.48	0/1025
19	2X	0.26	0/764	0.47	1/1025 (0.1%)
20	1Y	0.28	0/823	0.45	0/1099
20	2Y	0.26	0/823	0.45	0/1100
21	1Z	0.26	0/1620	0.44	0/2200
21	2Z	0.25	0/1590	0.42	0/2162
22	10	0.27	0/614	0.49	0/818
22	20	0.26	0/614	0.43	0/818
23	11	0.27	0/763	0.45	0/1016
23	21	0.26	0/768	0.44	0/1021
24	12	0.27	0/590	0.41	0/781
24	22	0.24	0/594	0.35	0/785
25	13	0.26	0/474	0.44	0/635
25	23	0.23	0/469	0.41	0/630
26	14	0.25	0/559	0.48	0/754
26	24	0.25	0/549	0.46	0/741
27	15	0.27	0/474	0.49	0/640
27	25	0.25	0/470	0.42	0/636
28	16	0.27	0/460	0.46	0/613
28	26	0.26	0/456	0.42	0/608
29	17	0.27	0/426	0.42	0/561
29	27	0.25	0/426	0.41	0/561
30	18	0.29	0/525	0.46	0/691
30	28	0.26	0/525	0.45	0/691
31	19	0.28	0/310	0.46	0/407
31	29	0.25	0/310	0.43	0/407
32	1a	0.25	0/35799	0.80	12/55871 (0.0%)
32	2a	0.25	0/35894	0.83	20/56019 (0.0%)
33	1b	0.24	0/1876	0.39	0/2533
33	2b	0.24	0/1860	0.41	0/2518
34	1c	0.24	0/1582	0.42	0/2137
34	2c	0.24	0/1566	0.42	0/2119
35	1d	0.24	0/1695	0.40	0/2274
35	2d	0.25	0/1698	0.40	0/2277
36	1e	0.26	0/1149	0.45	0/1548
36	2e	0.25	0/1149	0.44	0/1548
37	1f	0.25	0/827	0.41	0/1120
37	2f	0.24	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.24	0/1254	0.37	0/1683
38	2g	0.24	0/1248	0.38	0/1676
39	1h	0.25	0/1118	0.44	0/1506
39	2h	0.25	0/1108	0.43	0/1494
40	1i	0.25	0/1005	0.42	0/1350
40	2i	0.25	0/985	0.40	0/1328
41	1j	0.24	0/732	0.43	0/993
41	2j	0.24	0/723	0.45	0/984
42	1k	0.25	0/849	0.45	0/1150
42	2k	0.25	0/848	0.44	0/1149
43	1l	0.26	0/937	0.46	0/1260
43	2l	0.25	0/937	0.49	0/1260
44	1m	0.23	0/924	0.44	0/1242
44	2m	0.23	0/905	0.41	0/1217
45	1n	0.25	0/501	0.41	0/664
45	2n	0.25	0/501	0.41	0/664
46	1o	0.24	0/739	0.38	0/985
46	2o	0.24	0/739	0.38	0/985
47	1p	0.24	0/697	0.42	0/939
47	2p	0.24	0/693	0.42	0/935
48	1r	0.25	0/560	0.44	0/746
48	2r	0.24	0/560	0.40	0/746
49	1s	0.23	0/663	0.43	0/895
49	2s	0.24	0/660	0.44	0/893
50	1t	0.24	0/733	0.37	0/968
50	2t	0.24	0/735	0.36	0/975
51	1u	0.23	0/203	0.41	0/266
51	2u	0.22	0/203	0.41	0/266
52	1y	0.25	0/776	0.41	0/1048
52	2y	0.23	0/761	0.40	0/1030
All	All	0.27	0/307745	0.71	50/460191 (0.0%)

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O3'-P-O5'	9.99	122.97	104.00
32	2a	754	C	C2-N1-C1'	7.50	127.05	118.80
32	2a	754	C	N1-C2-O2	7.10	123.16	118.90
1	1A	1313	U	C2-N1-C1'	6.41	125.40	117.70
32	1a	1224	G	N3-C4-N9	-6.24	122.26	126.00

There are no chirality outliers.

There are no planarity outliers.

## 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%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	62
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	15	47
5	1F	201/210 (96%)	193 (96%)	8 (4%)	0	100	100
5	2F	201/210 (96%)	189 (94%)	12 (6%)	0	100	100
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	14	46
6	2G	179/182 (98%)	162 (90%)	15 (8%)	2 (1%)	14	46
7	1H	172/180 (96%)	161 (94%)	7 (4%)	4 (2%)	6	29
7	2H	171/180 (95%)	156 (91%)	13 (8%)	2 (1%)	13	43
8	1I	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
8	2I	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	56
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	56

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	56
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	8	34
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	115 (89%)	12 (9%)	2 (2%)	9	37
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	47
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	7	33
18	1W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	6	31
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	46
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	29	62
21	2Z	199/206 (97%)	187 (94%)	11 (6%)	1 (0%)	29	62
22	10	75/85 (88%)	71 (95%)	3 (4%)	1 (1%)	12	41
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	46
24	12	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	10
26	24	67/71 (94%)	52 (78%)	13 (19%)	2 (3%)	4	24
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	199 (87%)	22 (10%)	8 (4%)	3	21
33	2b	229/256 (90%)	203 (89%)	22 (10%)	4 (2%)	9	36
34	1c	204/239 (85%)	190 (93%)	13 (6%)	1 (0%)	29	62
34	2c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	29	62
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	62
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	137 (94%)	9 (6%)	0	100	100
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	124/128 (97%)	111 (90%)	12 (10%)	1 (1%)	19	52
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	4	23
41	2j	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	2	12
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	50
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	50
43	1l	119/135 (88%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/135 (88%)	109 (92%)	10 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1m	114/126 (90%)	106 (93%)	7 (6%)	1 (1%)	17	50
44	2m	112/126 (89%)	106 (95%)	5 (4%)	1 (1%)	17	50
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	43
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	41
48	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
48	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	1s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	5	28
49	2s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	1t	94/106 (89%)	91 (97%)	2 (2%)	1 (1%)	14	46
50	2t	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	7	32
51	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
51	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
52	2y	94/113 (83%)	91 (97%)	2 (2%)	1 (1%)	14	46
All	All	11435/12150 (94%)	10717 (94%)	646 (6%)	72 (1%)	25	59

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	10	13	GLY
26	14	55	ARG
33	1b	125	PRO
41	1j	77	PRO
33	2b	17	PHE

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	200 (94%)	14 (6%)	17	46
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	54
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	40
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	40
5	1F	161/166 (97%)	154 (96%)	7 (4%)	29	59
5	2F	160/166 (96%)	154 (96%)	6 (4%)	33	62
6	1G	144/156 (92%)	140 (97%)	4 (3%)	43	69
6	2G	142/156 (91%)	137 (96%)	5 (4%)	36	64
7	1H	144/148 (97%)	142 (99%)	2 (1%)	67	81
7	2H	143/148 (97%)	140 (98%)	3 (2%)	53	75
8	1I	111/124 (90%)	105 (95%)	6 (5%)	22	53
8	2I	108/124 (87%)	105 (97%)	3 (3%)	43	69
9	1N	119/119 (100%)	111 (93%)	8 (7%)	16	45
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	39
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	98 (98%)	2 (2%)	55	76
11	1P	115/116 (99%)	112 (97%)	3 (3%)	46	71
11	2P	115/116 (99%)	113 (98%)	2 (2%)	60	78
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	70
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	77
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	37
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	50
14	1S	87/88 (99%)	85 (98%)	2 (2%)	50	73
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	83
15	1T	115/128 (90%)	114 (99%)	1 (1%)	78	87
15	2T	113/128 (88%)	109 (96%)	4 (4%)	36	64
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	46
16	2U	93/94 (99%)	89 (96%)	4 (4%)	29	59
17	1V	81/82 (99%)	78 (96%)	3 (4%)	34	62
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	62
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	84
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	82
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	71
20	1Y	86/91 (94%)	83 (96%)	3 (4%)	36	64
20	2Y	86/91 (94%)	85 (99%)	1 (1%)	71	83
21	1Z	169/179 (94%)	166 (98%)	3 (2%)	59	77
21	2Z	165/179 (92%)	161 (98%)	4 (2%)	49	72
22	10	61/67 (91%)	59 (97%)	2 (3%)	38	65
22	20	61/67 (91%)	60 (98%)	1 (2%)	62	79
23	11	79/83 (95%)	79 (100%)	0	100	100
23	21	81/83 (98%)	80 (99%)	1 (1%)	71	83
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	57
24	22	66/67 (98%)	63 (96%)	3 (4%)	27	58
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	50
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	61
26	14	58/63 (92%)	54 (93%)	4 (7%)	15	43
26	24	54/63 (86%)	51 (94%)	3 (6%)	21	52
27	15	51/52 (98%)	49 (96%)	2 (4%)	32	61
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	61
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	50
28	26	50/52 (96%)	48 (96%)	2 (4%)	31	61
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	55
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	72
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	62
30	28	54/55 (98%)	53 (98%)	1 (2%)	57	76
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	68
33	1b	191/220 (87%)	184 (96%)	7 (4%)	34	62
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34	62
34	1c	144/188 (77%)	142 (99%)	2 (1%)	67	81
34	2c	140/188 (74%)	138 (99%)	2 (1%)	67	81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	1d	171/181 (94%)	166 (97%)	5 (3%)	42	68
35	2d	172/181 (95%)	166 (96%)	6 (4%)	36	64
36	1e	114/123 (93%)	112 (98%)	2 (2%)	59	77
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	71
37	1f	85/90 (94%)	85 (100%)	0	100	100
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	72
38	1g	120/127 (94%)	119 (99%)	1 (1%)	81	89
38	2g	119/127 (94%)	116 (98%)	3 (2%)	47	71
39	1h	116/119 (98%)	112 (97%)	4 (3%)	37	64
39	2h	114/119 (96%)	110 (96%)	4 (4%)	36	64
40	1i	91/99 (92%)	91 (100%)	0	100	100
40	2i	88/99 (89%)	84 (96%)	4 (4%)	27	58
41	1j	68/92 (74%)	68 (100%)	0	100	100
41	2j	68/92 (74%)	67 (98%)	1 (2%)	65	80
42	1k	83/99 (84%)	81 (98%)	2 (2%)	49	72
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	83
43	1l	96/110 (87%)	94 (98%)	2 (2%)	53	75
43	2l	96/110 (87%)	93 (97%)	3 (3%)	40	67
44	1m	90/101 (89%)	88 (98%)	2 (2%)	52	74
44	2m	87/101 (86%)	87 (100%)	0	100	100
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	60
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	76
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	71
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	82
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	59
47	2p	68/74 (92%)	64 (94%)	4 (6%)	19	50
48	1r	59/77 (77%)	58 (98%)	1 (2%)	60	78
48	2r	59/77 (77%)	58 (98%)	1 (2%)	60	78
49	1s	68/80 (85%)	66 (97%)	2 (3%)	42	68
49	2s	67/80 (84%)	67 (100%)	0	100	100
50	1t	71/82 (87%)	69 (97%)	2 (3%)	43	69

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	2t	70/82 (85%)	67 (96%)	3 (4%)	29	59
51	1u	18/22 (82%)	18 (100%)	0	100	100
51	2u	18/22 (82%)	18 (100%)	0	100	100
52	1y	82/98 (84%)	81 (99%)	1 (1%)	71	83
52	2y	79/98 (81%)	75 (95%)	4 (5%)	24	54
All	All	9338/10072 (93%)	9038 (97%)	300 (3%)	39	66

5 of 300 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	2Z	150	LEU
45	2n	18	VAL
25	23	23	LEU
35	2d	12	CYS
25	13	8	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
49	1s	56	GLN
33	2b	78	GLN
34	2c	6	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2856/2894 (98%)	390 (13%)	17 (0%)
1	2A	2849/2894 (98%)	429 (15%)	25 (0%)
2	1B	117/120 (97%)	8 (6%)	0
2	2B	117/120 (97%)	10 (8%)	0
32	1a	1494/1522 (98%)	213 (14%)	0
32	2a	1498/1522 (98%)	223 (14%)	0
All	All	8931/9072 (98%)	1273 (14%)	42 (0%)

5 of 1273 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1067	A
1	2A	2126	A
1	2A	1073	A
1	2A	1491	G
1	2A	2172	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	1a	1498	32	19,22,23	1.76	5 (26%)	26,32,35	1.06	1 (3%)
32	MA6	1a	1518	32	19,26,27	1.43	4 (21%)	18,38,41	1.49	2 (11%)
1	5MU	2A	1915	1	19,22,23	1.97	7 (36%)	28,32,35	2.27	8 (28%)
32	2MG	1a	1207	32,54	18,26,27	1.80	4 (22%)	16,38,41	1.25	3 (18%)
1	2MA	2A	2503	54,1	17,25,26	1.03	2 (11%)	17,37,40	1.15	2 (11%)
32	5MC	1a	1404	32	18,22,23	1.93	5 (27%)	26,32,35	1.05	1 (3%)
32	MA6	1a	1519	32	19,26,27	1.42	4 (21%)	18,38,41	1.51	2 (11%)
32	4OC	1a	1402	32	20,23,24	1.62	4 (20%)	26,32,35	0.94	1 (3%)
32	MA6	2a	1518	32	19,26,27	1.51	4 (21%)	18,38,41	1.51	2 (11%)
1	PSU	2A	1917	1	18,21,22	1.99	7 (38%)	22,30,33	1.95	3 (13%)
32	M2G	1a	966	32	20,27,28	1.85	4 (20%)	22,40,43	1.28	3 (13%)
1	OMU	2A	2552	54,1	19,22,23	3.89	11 (57%)	26,31,34	1.81	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	UR3	2a	1498	32,54	19,22,23	1.71	5 (26%)	26,32,35	1.09	3 (11%)
1	5MU	1A	1939	54,1	19,22,23	2.07	8 (42%)	28,32,35	2.51	7 (25%)
1	5MC	2A	1962	1	18,22,23	1.95	5 (27%)	26,32,35	1.06	1 (3%)
32	PSU	1a	516	32	18,21,22	2.06	8 (44%)	22,30,33	1.97	4 (18%)
1	PSU	1A	2605	1	18,21,22	2.01	8 (44%)	22,30,33	1.94	4 (18%)
32	M2G	2a	966	32,54	20,27,28	1.83	3 (15%)	22,40,43	1.32	2 (9%)
32	PSU	2a	516	32,54	18,21,22	1.99	9 (50%)	22,30,33	1.99	5 (22%)
32	5MC	2a	1400	32	18,22,23	1.94	5 (27%)	26,32,35	1.10	1 (3%)
32	5MC	2a	1407	32	18,22,23	1.91	4 (22%)	26,32,35	1.21	2 (7%)
32	5MC	1a	1407	32	18,22,23	1.92	5 (27%)	26,32,35	1.17	2 (7%)
1	5MC	2A	1942	1	18,22,23	1.97	5 (27%)	26,32,35	1.17	1 (3%)
32	G7M	2a	527	32,54	20,26,27	1.56	4 (20%)	17,39,42	0.73	0
1	PSU	1A	1911	1	18,21,22	1.89	6 (33%)	22,30,33	1.56	4 (18%)
1	OMG	1A	2251	1	18,26,27	1.87	4 (22%)	19,38,41	1.38	3 (15%)
32	5MC	2a	967	32	18,22,23	1.90	5 (27%)	26,32,35	1.11	2 (7%)
32	5MC	1a	967	32	18,22,23	1.88	5 (27%)	26,32,35	1.30	2 (7%)
32	4OC	2a	1402	32	20,23,24	1.61	4 (20%)	26,32,35	0.92	1 (3%)
43	0TD	1l	92	43	7,9,10	1.39	0	6,11,13	1.47	1 (16%)
43	0TD	2l	92	43	7,9,10	1.42	0	6,11,13	2.29	2 (33%)
1	5MU	1A	1915	54,1	19,22,23	1.99	7 (36%)	28,32,35	2.33	10 (35%)
32	5MC	1a	1400	32	18,22,23	1.96	5 (27%)	26,32,35	1.12	2 (7%)
32	2MG	2a	1207	32	18,26,27	1.87	5 (27%)	16,38,41	1.38	3 (18%)
1	5MC	1A	1962	54,1	18,22,23	1.97	5 (27%)	26,32,35	1.13	1 (3%)
1	OMC	2A	1920	1	19,22,23	1.77	4 (21%)	26,31,34	0.95	1 (3%)
32	MA6	2a	1519	32	19,26,27	1.44	4 (21%)	18,38,41	1.53	2 (11%)
32	5MC	2a	1404	32	18,22,23	1.94	5 (27%)	26,32,35	1.07	2 (7%)
1	PSU	2A	1911	1	18,21,22	2.00	7 (38%)	22,30,33	1.67	4 (18%)
1	OMG	2A	2251	54,1	18,26,27	1.89	4 (22%)	19,38,41	1.28	4 (21%)
1	5MU	2A	1939	54,1	19,22,23	2.04	8 (42%)	28,32,35	2.24	6 (21%)
1	2MA	1A	2503	54,1	17,25,26	1.02	1 (5%)	17,37,40	1.24	2 (11%)
32	G7M	1a	527	32,54	20,26,27	1.52	3 (15%)	17,39,42	0.66	0
1	PSU	2A	2605	1	18,21,22	1.96	7 (38%)	22,30,33	1.93	4 (18%)
1	PSU	1A	1917	1	18,21,22	2.09	8 (44%)	22,30,33	2.06	4 (18%)
1	OMC	1A	1920	54,1	19,22,23	1.76	4 (21%)	26,31,34	1.09	4 (15%)
1	5MC	1A	1942	1	18,22,23	1.96	5 (27%)	26,32,35	1.13	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	1A	2552	54,1	19,22,23	3.94	11 (57%)	26,31,34	1.89	7 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	2/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32,54	-	3/5/27/28	0/3/3/3
1	2MA	2A	2503	54,1	-	1/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	OMU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32,54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	54,1	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	6/7/29/30	0/3/3/3
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,54	-	2/3/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1	-	1/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
43	0TD	2l	92	43	-	1/7/12/14	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1915	54,1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	4/9/27/28	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	54,1	-	3/5/27/28	0/3/3/3
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	0/3/25/26	0/3/3/3
32	G7M	1a	527	32,54	-	3/3/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	54,1	-	1/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2

The worst 5 of 247 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O4'-C4'	10.13	1.67	1.45
1	2A	2552	OMU	O4'-C4'	10.08	1.67	1.45
1	1A	2552	OMU	C3'-C4'	-9.67	1.28	1.53
1	2A	2552	OMU	C3'-C4'	-9.54	1.28	1.53
32	2a	966	M2G	C2-N2	5.84	1.46	1.35

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	C4-N3-C2	-6.31	119.18	127.35
1	1A	1939	5MU	C5-C4-N3	6.13	120.55	115.31
1	1A	1917	PSU	N1-C2-N3	5.95	121.87	115.13
1	1A	2605	PSU	N1-C2-N3	5.92	121.84	115.13
1	1A	1939	5MU	N3-C2-N1	5.82	122.62	114.89

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	1A	1939	5MU	C3'-C4'-C5'-O5'
1	1A	1939	5MU	O4'-C4'-C5'-O5'
1	1A	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2199 ligands modelled in this entry, 2188 are monoatomic - leaving 11 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
55	ARG	1F	303	-	10,11,11	0.72	1 (10%)	11,13,13	1.21	2 (18%)
55	ARG	1B	1001	-	10,11,11	0.72	1 (10%)	11,13,13	1.19	2 (18%)
57	SF4	1d	501	-	0,12,12	-	-	-	-	-
53	MPD	2A	3001	-	7,7,7	0.31	0	9,10,10	0.34	0
53	MPD	1a	1601	-	7,7,7	0.30	0	9,10,10	0.35	0
57	SF4	2d	501	-	0,12,12	-	-	-	-	-
53	MPD	1T	2001	-	7,7,7	0.28	0	9,10,10	0.28	0
53	MPD	2A	3002	-	7,7,7	0.28	0	9,10,10	0.17	0
53	MPD	1A	3001	-	7,7,7	0.28	0	9,10,10	0.21	0
53	MPD	2B	201	-	7,7,7	0.26	0	9,10,10	0.16	0
53	MPD	18	101	-	7,7,7	0.28	0	9,10,10	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	ARG	1F	303	-	-	2/11/11/11	-
55	ARG	1B	1001	-	-	1/11/11/11	-
57	SF4	1d	501	-	-	-	0/6/5/5
53	MPD	2A	3001	-	-	1/5/5/5	-
53	MPD	1a	1601	-	-	2/5/5/5	-
57	SF4	2d	501	-	-	-	0/6/5/5
53	MPD	1T	2001	-	-	0/5/5/5	-
53	MPD	2A	3002	-	-	4/5/5/5	-
53	MPD	1A	3001	-	-	0/5/5/5	-
53	MPD	2B	201	-	-	4/5/5/5	-
53	MPD	18	101	-	-	4/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1F	303	ARG	OXT-C	-2.10	1.23	1.30
55	1B	1001	ARG	OXT-C	-2.05	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1B	1001	ARG	OXT-C-O	-3.12	117.00	124.09
55	1F	303	ARG	OXT-C-O	-2.99	117.31	124.09
55	1F	303	ARG	OXT-C-CA	2.52	121.95	113.38
55	1B	1001	ARG	OXT-C-CA	2.34	121.34	113.38

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1B	1001	ARG	NE-CD-CG-CB
55	1F	303	ARG	O-C-CA-N
53	18	101	MPD	O2-C2-C3-C4
53	2A	3001	MPD	O2-C2-C3-C4
53	2A	3002	MPD	C2-C3-C4-C5

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 i

### 6.1 Protein, DNA and RNA chains i

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	2851/2894 (98%)	-0.25	87 (3%) 49 47	26, 52, 150, 184	0
1	2A	2847/2894 (98%)	-0.13	100 (3%) 44 40	46, 77, 156, 186	0
2	1B	118/120 (98%)	-0.52	0 100 100	45, 72, 90, 110	0
2	2B	118/120 (98%)	0.15	3 (2%) 57 53	86, 116, 133, 144	0
3	1D	275/276 (99%)	-0.36	1 (0%) 92 92	29, 47, 64, 93	0
3	2D	275/276 (99%)	-0.17	1 (0%) 92 92	43, 67, 83, 106	0
4	1E	204/206 (99%)	-0.19	0 100 100	29, 58, 79, 112	0
4	2E	204/206 (99%)	-0.00	1 (0%) 91 90	45, 73, 98, 109	0
5	1F	203/210 (96%)	-0.27	0 100 100	27, 55, 90, 120	0
5	2F	203/210 (96%)	-0.04	1 (0%) 91 90	44, 89, 109, 129	0
6	1G	181/182 (99%)	-0.16	3 (1%) 70 67	67, 91, 111, 134	0
6	2G	181/182 (99%)	0.77	25 (13%) 2 2	106, 127, 139, 147	0
7	1H	174/180 (96%)	-0.24	1 (0%) 89 89	45, 71, 91, 101	0
7	2H	173/180 (96%)	0.71	16 (9%) 9 10	81, 113, 130, 142	0
8	1I	147/148 (99%)	0.06	1 (0%) 87 88	61, 104, 121, 131	0
8	2I	146/148 (98%)	0.24	5 (3%) 45 42	70, 109, 126, 136	0
9	1N	140/140 (100%)	-0.22	1 (0%) 87 88	39, 52, 75, 100	0
9	2N	140/140 (100%)	0.30	3 (2%) 63 61	58, 90, 111, 122	0
10	1O	122/122 (100%)	-0.26	0 100 100	36, 57, 77, 86	0
10	2O	122/122 (100%)	-0.21	0 100 100	50, 68, 83, 92	0
11	1P	149/150 (99%)	-0.17	0 100 100	25, 63, 91, 116	0
11	2P	149/150 (99%)	0.24	2 (1%) 77 75	53, 91, 116, 128	0
12	1Q	141/141 (100%)	-0.30	0 100 100	39, 56, 70, 99	0
12	2Q	141/141 (100%)	0.04	2 (1%) 75 74	68, 87, 104, 115	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%)	-0.23	0 100 100	34, 50, 67, 83	0
13	2R	118/118 (100%)	-0.00	0 100 100	54, 68, 89, 99	0
14	1S	110/112 (98%)	-0.01	2 (1%) 68 65	52, 69, 84, 95	0
14	2S	110/112 (98%)	0.73	10 (9%) 9 10	95, 108, 118, 125	0
15	1T	131/146 (89%)	-0.17	1 (0%) 86 86	49, 63, 109, 117	0
15	2T	131/146 (89%)	-0.16	0 100 100	53, 74, 104, 123	0
16	1U	116/118 (98%)	-0.42	0 100 100	31, 45, 68, 83	0
16	2U	116/118 (98%)	-0.22	1 (0%) 84 84	59, 85, 101, 117	0
17	1V	101/101 (100%)	-0.09	1 (0%) 82 82	31, 58, 77, 87	0
17	2V	101/101 (100%)	0.12	3 (2%) 50 48	60, 100, 115, 129	0
18	1W	112/113 (99%)	-0.28	0 100 100	35, 48, 71, 91	0
18	2W	112/113 (99%)	-0.10	1 (0%) 84 84	48, 66, 96, 140	0
19	1X	95/96 (98%)	-0.13	0 100 100	39, 53, 74, 97	0
19	2X	95/96 (98%)	0.23	4 (4%) 36 33	58, 79, 106, 116	0
20	1Y	107/110 (97%)	-0.13	0 100 100	44, 66, 88, 103	0
20	2Y	107/110 (97%)	0.64	7 (6%) 18 18	75, 94, 111, 121	0
21	1Z	203/206 (98%)	-0.24	1 (0%) 91 90	57, 81, 105, 117	0
21	2Z	201/206 (97%)	0.55	18 (8%) 9 10	89, 111, 124, 141	0
22	10	77/85 (90%)	-0.10	0 100 100	40, 52, 66, 79	0
22	20	77/85 (90%)	0.66	7 (9%) 9 10	67, 86, 98, 117	0
23	11	97/98 (98%)	0.15	1 (1%) 82 82	36, 55, 88, 114	0
23	21	97/98 (98%)	0.23	2 (2%) 63 61	49, 75, 100, 112	0
24	12	70/72 (97%)	-0.12	1 (1%) 75 74	47, 66, 80, 108	0
24	22	70/72 (97%)	0.16	1 (1%) 75 74	80, 93, 103, 105	0
25	13	59/60 (98%)	0.19	0 100 100	38, 53, 87, 91	0
25	23	59/60 (98%)	0.88	6 (10%) 6 7	75, 90, 116, 126	0
26	14	69/71 (97%)	0.06	3 (4%) 35 33	83, 113, 141, 146	0
26	24	69/71 (97%)	1.02	13 (18%) 1 1	125, 144, 158, 160	0
27	15	59/60 (98%)	-0.51	0 100 100	34, 44, 79, 89	0
27	25	59/60 (98%)	-0.27	0 100 100	49, 74, 88, 100	0
28	16	53/54 (98%)	-0.31	0 100 100	45, 55, 71, 82	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%)	0.16	1 (1%) 66 64	71, 81, 93, 103	0
29	17	48/49 (97%)	0.33	3 (6%) 20 19	37, 46, 77, 81	0
29	27	48/49 (97%)	0.30	1 (2%) 63 61	53, 62, 83, 86	0
30	18	64/65 (98%)	-0.20	0 100 100	39, 49, 61, 83	0
30	28	64/65 (98%)	0.19	0 100 100	59, 73, 85, 90	0
31	19	37/37 (100%)	-0.02	0 100 100	40, 54, 64, 72	0
31	29	37/37 (100%)	0.54	1 (2%) 54 51	80, 89, 100, 105	0
32	1a	1488/1522 (97%)	-0.08	31 (2%) 63 61	50, 99, 152, 187	0
32	2a	1492/1522 (98%)	0.04	31 (2%) 63 61	63, 108, 154, 188	0
33	1b	231/256 (90%)	0.26	10 (4%) 35 33	100, 119, 139, 151	0
33	2b	231/256 (90%)	0.65	25 (10%) 5 6	111, 134, 146, 154	0
34	1c	206/239 (86%)	0.01	3 (1%) 73 71	86, 108, 129, 139	0
34	2c	206/239 (86%)	0.55	22 (10%) 6 6	104, 131, 139, 145	0
35	1d	208/209 (99%)	0.26	9 (4%) 35 33	84, 107, 124, 131	0
35	2d	208/209 (99%)	0.02	1 (0%) 91 90	76, 95, 107, 114	0
36	1e	148/162 (91%)	-0.07	2 (1%) 75 74	71, 91, 106, 126	0
36	2e	148/162 (91%)	0.17	2 (1%) 75 74	87, 104, 117, 144	0
37	1f	100/101 (99%)	-0.26	1 (1%) 82 82	65, 88, 107, 116	0
37	2f	100/101 (99%)	-0.09	1 (1%) 82 82	79, 99, 110, 114	0
38	1g	155/156 (99%)	0.20	4 (2%) 56 52	89, 106, 117, 133	0
38	2g	155/156 (99%)	0.75	19 (12%) 4 4	112, 122, 133, 150	0
39	1h	137/138 (99%)	0.24	2 (1%) 73 71	76, 94, 104, 107	0
39	2h	137/138 (99%)	0.52	6 (4%) 34 32	96, 109, 120, 128	0
40	1i	127/128 (99%)	0.44	8 (6%) 20 19	91, 117, 133, 142	0
40	2i	126/128 (98%)	1.48	37 (29%) 0 0	116, 137, 147, 153	0
41	1j	97/105 (92%)	0.64	8 (8%) 11 11	87, 121, 140, 149	0
41	2j	96/105 (91%)	1.55	30 (31%) 0 0	113, 137, 147, 164	0
42	1k	114/129 (88%)	0.03	0 100 100	60, 83, 101, 108	0
42	2k	114/129 (88%)	0.31	5 (4%) 34 32	84, 106, 122, 131	0
43	1l	121/135 (89%)	0.09	0 100 100	64, 80, 96, 114	0
43	2l	121/135 (89%)	0.15	2 (1%) 70 67	70, 87, 105, 122	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/126 (92%)	0.41	6 (5%) 27 25	90, 109, 119, 125	0
44	2m	114/126 (90%)	0.84	18 (15%) 2 2	111, 134, 141, 146	0
45	1n	60/61 (98%)	0.32	1 (1%) 70 67	95, 105, 115, 120	0
45	2n	60/61 (98%)	1.39	16 (26%) 0 0	116, 130, 138, 140	0
46	1o	88/89 (98%)	0.18	2 (2%) 60 58	67, 87, 107, 114	0
46	2o	88/89 (98%)	0.13	1 (1%) 80 80	78, 101, 120, 127	0
47	1p	82/88 (93%)	0.84	8 (9%) 7 7	83, 111, 127, 138	0
47	2p	82/88 (93%)	0.47	1 (1%) 79 77	77, 92, 110, 120	0
48	1r	68/88 (77%)	0.38	2 (2%) 51 50	69, 86, 111, 119	0
48	2r	68/88 (77%)	0.50	4 (5%) 22 21	90, 106, 120, 129	0
49	1s	83/93 (89%)	0.65	6 (7%) 15 15	89, 116, 132, 142	0
49	2s	83/93 (89%)	1.48	23 (27%) 0 0	116, 138, 146, 152	0
50	1t	96/106 (90%)	0.84	11 (11%) 4 4	95, 109, 124, 134	0
50	2t	98/106 (92%)	0.36	3 (3%) 49 47	78, 100, 117, 122	0
51	1u	23/27 (85%)	2.29	12 (52%) 0 0	101, 107, 112, 117	0
51	2u	23/27 (85%)	3.08	21 (91%) 0 0	120, 125, 130, 130	0
52	1y	97/113 (85%)	0.45	0 100 100	64, 85, 106, 116	0
52	2y	96/113 (84%)	1.54	32 (33%) 0 0	99, 115, 130, 140	0
All	All	20545/21222 (96%)	0.06	768 (3%) 41 38	25, 86, 140, 188	0

The worst 5 of 768 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	9.9
32	2a	1001(A)	G	7.7
1	1A	1091	G	7.6
26	24	68	ARG	7.6
32	2a	1001	A	7.1

## 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( $\text{\AA}^2$ )	Q<0.9
32	5MC	2a	967	21/22	0.79	0.25	112,121,129,135	0
32	M2G	2a	966	25/26	0.88	0.23	111,117,124,126	0
1	PSU	1A	1911	20/21	0.88	0.15	94,100,105,113	0
1	OMC	2A	1920	21/22	0.90	0.16	91,103,111,113	0
1	PSU	1A	1917	20/21	0.90	0.17	91,102,109,109	0
1	5MU	2A	1915	21/22	0.90	0.14	114,125,132,139	0
1	PSU	2A	1917	20/21	0.91	0.13	106,117,121,124	0
32	PSU	2a	516	20/21	0.92	0.13	97,104,116,117	0
43	0TD	1l	92	10/11	0.92	0.27	85,89,94,102	0
1	5MC	2A	1942	21/22	0.92	0.18	69,75,78,79	0
32	2MG	2a	1207	24/25	0.92	0.21	138,142,147,153	0
32	5MC	2a	1407	21/22	0.92	0.18	88,96,104,106	0
32	2MG	1a	1207	24/25	0.93	0.15	109,112,119,126	0
32	G7M	2a	527	24/25	0.93	0.19	84,91,98,100	0
43	0TD	2l	92	10/11	0.93	0.27	80,82,89,105	0
1	PSU	2A	1911	20/21	0.94	0.10	97,107,115,117	0
32	PSU	1a	516	20/21	0.94	0.12	80,90,97,98	0
32	5MC	2a	1400	21/22	0.94	0.22	97,105,110,111	0
32	4OC	2a	1402	22/23	0.94	0.19	81,94,100,103	0
32	5MC	2a	1404	21/22	0.94	0.17	88,94,102,105	0
1	5MU	1A	1915	21/22	0.94	0.17	100,108,116,117	0
32	MA6	2a	1518	24/25	0.94	0.22	78,87,92,95	0
32	MA6	2a	1519	24/25	0.94	0.23	78,89,96,98	0
1	OMC	1A	1920	21/22	0.94	0.18	74,83,97,101	0
32	5MC	1a	967	21/22	0.95	0.17	88,92,101,102	0
32	M2G	1a	966	25/26	0.95	0.16	83,88,97,99	0
32	5MC	1a	1407	21/22	0.95	0.17	71,77,85,86	0
32	MA6	1a	1518	24/25	0.96	0.17	61,66,70,74	0
32	MA6	1a	1519	24/25	0.96	0.18	57,67,73,75	0
32	4OC	1a	1402	22/23	0.96	0.17	61,68,71,73	0
32	5MC	1a	1404	21/22	0.96	0.16	60,65,71,72	0
1	5MU	1A	1939	21/22	0.96	0.19	34,46,54,57	0
1	OMG	1A	2251	24/25	0.97	0.15	31,36,42,46	0
1	OMU	1A	2552	21/22	0.97	0.18	43,48,52,59	0
32	UR3	1a	1498	21/22	0.97	0.15	60,68,72,84	0
1	5MC	1A	1962	21/22	0.97	0.17	50,56,61,63	0
1	5MU	2A	1939	21/22	0.97	0.17	53,57,61,62	0
32	5MC	1a	1400	21/22	0.97	0.16	64,71,76,84	0
1	5MC	2A	1962	21/22	0.97	0.14	54,59,69,74	0
1	OMG	2A	2251	24/25	0.97	0.17	52,60,65,67	0
32	UR3	2a	1498	21/22	0.97	0.16	83,86,91,94	0
1	2MA	2A	2503	23/24	0.97	0.20	44,50,59,61	0
1	PSU	2A	2605	20/21	0.97	0.16	53,63,70,75	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	G7M	1a	527	24/25	0.97	0.14	64,79,84,88	0
1	2MA	1A	2503	23/24	0.98	0.18	21,35,41,44	0
1	OMU	2A	2552	21/22	0.98	0.15	49,54,59,62	0
1	5MC	1A	1942	21/22	0.98	0.12	46,55,61,63	0
1	PSU	1A	2605	20/21	0.98	0.16	37,41,47,48	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
54	MG	1A	3834	1/1	0.07	0.60	90,90,90,90	0
54	MG	1A	3260	1/1	0.15	0.42	141,141,141,141	0
54	MG	2A	3565	1/1	0.20	0.59	155,155,155,155	0
54	MG	2A	3193	1/1	0.24	0.37	104,104,104,104	0
54	MG	1a	1839	1/1	0.25	0.90	95,95,95,95	0
54	MG	2A	3114	1/1	0.25	0.53	68,68,68,68	0
54	MG	2A	3087	1/1	0.26	0.53	99,99,99,99	0
54	MG	1a	1802	1/1	0.36	0.14	142,142,142,142	0
54	MG	2A	3463	1/1	0.38	0.18	90,90,90,90	0
54	MG	1A	3600	1/1	0.38	0.72	74,74,74,74	0
54	MG	2A	3597	1/1	0.38	0.15	101,101,101,101	0
54	MG	1a	1743	1/1	0.43	0.34	103,103,103,103	0
54	MG	2B	204	1/1	0.43	0.42	110,110,110,110	0
54	MG	2a	1690	1/1	0.43	0.61	94,94,94,94	0
54	MG	1A	3591	1/1	0.44	0.20	87,87,87,87	0
54	MG	2A	3488	1/1	0.45	0.41	97,97,97,97	0
54	MG	1A	3684	1/1	0.46	0.28	74,74,74,74	0
54	MG	1b	301	1/1	0.46	0.20	116,116,116,116	0
54	MG	1d	502	1/1	0.46	0.55	101,101,101,101	0
54	MG	1A	3629	1/1	0.47	0.34	73,73,73,73	0
54	MG	2B	203	1/1	0.50	0.26	74,74,74,74	0
54	MG	1A	3806	1/1	0.50	0.43	85,85,85,85	0

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3333	1/1	0.50	0.30	57,57,57,57	0
54	MG	2a	1664	1/1	0.52	0.49	94,94,94,94	0
54	MG	2a	1663	1/1	0.52	0.51	110,110,110,110	0
54	MG	2A	3301	1/1	0.53	0.47	103,103,103,103	0
54	MG	2B	211	1/1	0.54	0.57	89,89,89,89	0
54	MG	2a	1658	1/1	0.55	0.46	102,102,102,102	0
54	MG	1a	1850	1/1	0.55	0.31	129,129,129,129	0
54	MG	1B	1030	1/1	0.55	0.16	78,78,78,78	0
54	MG	1a	1760	1/1	0.55	0.22	128,128,128,128	0
54	MG	2A	3557	1/1	0.56	0.14	106,106,106,106	0
54	MG	2B	213	1/1	0.56	0.17	97,97,97,97	0
54	MG	2A	3637	1/1	0.56	0.22	64,64,64,64	0
54	MG	2a	1718	1/1	0.56	0.17	95,95,95,95	0
54	MG	2i	201	1/1	0.57	1.34	103,103,103,103	0
54	MG	2A	3036	1/1	0.58	0.28	64,64,64,64	0
54	MG	1a	1826	1/1	0.58	0.13	109,109,109,109	0
54	MG	2a	1655	1/1	0.58	1.18	114,114,114,114	0
54	MG	2B	214	1/1	0.59	0.10	101,101,101,101	0
54	MG	2A	3118	1/1	0.59	0.40	81,81,81,81	0
53	MPD	2B	201	8/8	0.59	0.67	101,115,117,121	0
54	MG	2A	3209	1/1	0.59	0.43	59,59,59,59	0
54	MG	2A	3615	1/1	0.60	0.46	75,75,75,75	0
54	MG	1a	1722	1/1	0.60	0.15	85,85,85,85	0
54	MG	1A	3703	1/1	0.60	0.25	41,41,41,41	0
54	MG	2A	3110	1/1	0.60	0.12	107,107,107,107	0
54	MG	2a	1668	1/1	0.60	0.19	90,90,90,90	0
54	MG	1a	1712	1/1	0.60	0.14	109,109,109,109	0
54	MG	2A	3302	1/1	0.60	0.20	59,59,59,59	0
54	MG	2A	3322	1/1	0.60	0.23	90,90,90,90	0
54	MG	2A	3392	1/1	0.61	0.21	81,81,81,81	0
54	MG	1a	1711	1/1	0.61	0.26	82,82,82,82	0
54	MG	1A	3577	1/1	0.61	0.15	72,72,72,72	0
54	MG	2A	3491	1/1	0.61	0.21	52,52,52,52	0
54	MG	2A	3543	1/1	0.61	0.20	89,89,89,89	0
54	MG	2A	3556	1/1	0.61	0.11	90,90,90,90	0
54	MG	1a	1768	1/1	0.61	0.15	81,81,81,81	0
54	MG	1A	3613	1/1	0.61	0.20	32,32,32,32	0
54	MG	1A	3356	1/1	0.62	0.18	88,88,88,88	0
54	MG	2A	3313	1/1	0.62	0.31	90,90,90,90	0
54	MG	1A	3818	1/1	0.63	0.25	59,59,59,59	0
54	MG	10	101	1/1	0.63	0.26	82,82,82,82	0
54	MG	1A	3748	1/1	0.63	0.12	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3058	1/1	0.63	0.51	70,70,70,70	0
54	MG	2A	3061	1/1	0.63	0.28	61,61,61,61	0
54	MG	2A	3083	1/1	0.64	0.23	87,87,87,87	0
54	MG	2a	1659	1/1	0.64	0.72	87,87,87,87	0
54	MG	1A	3111	1/1	0.64	0.10	69,69,69,69	0
54	MG	2B	205	1/1	0.64	0.48	70,70,70,70	0
54	MG	2A	3586	1/1	0.64	0.14	104,104,104,104	0
54	MG	2A	3197	1/1	0.64	0.22	78,78,78,78	0
54	MG	1a	1764	1/1	0.64	0.18	92,92,92,92	0
54	MG	1a	1843	1/1	0.64	0.50	81,81,81,81	0
54	MG	2A	3242	1/1	0.65	0.20	77,77,77,77	0
54	MG	2A	3022	1/1	0.65	0.51	80,80,80,80	0
54	MG	1e	203	1/1	0.65	0.47	89,89,89,89	0
54	MG	1A	3481	1/1	0.66	0.24	74,74,74,74	0
54	MG	1G	202	1/1	0.66	0.14	79,79,79,79	0
54	MG	2A	3482	1/1	0.66	0.20	106,106,106,106	0
54	MG	1a	1762	1/1	0.66	0.19	108,108,108,108	0
54	MG	2A	3051	1/1	0.66	0.25	78,78,78,78	0
54	MG	2a	1709	1/1	0.66	0.37	83,83,83,83	0
54	MG	2A	3356	1/1	0.66	0.29	91,91,91,91	0
54	MG	2a	1719	1/1	0.66	0.08	110,110,110,110	0
54	MG	2A	3373	1/1	0.66	0.27	87,87,87,87	0
54	MG	2A	3230	1/1	0.67	0.56	58,58,58,58	0
54	MG	1A	3855	1/1	0.67	0.22	54,54,54,54	0
54	MG	2A	3438	1/1	0.67	0.24	80,80,80,80	0
54	MG	2a	1693	1/1	0.67	0.23	84,84,84,84	0
54	MG	2A	3441	1/1	0.67	0.22	88,88,88,88	0
54	MG	1f	202	1/1	0.67	0.20	93,93,93,93	0
54	MG	2A	3561	1/1	0.67	0.10	97,97,97,97	0
54	MG	1B	1018	1/1	0.67	0.33	84,84,84,84	0
54	MG	2k	201	1/1	0.67	0.13	83,83,83,83	0
54	MG	2a	1681	1/1	0.68	0.07	94,94,94,94	0
54	MG	2a	1608	1/1	0.68	1.00	68,68,68,68	0
54	MG	1a	1761	1/1	0.68	0.24	114,114,114,114	0
54	MG	2A	3566	1/1	0.68	0.15	81,81,81,81	0
54	MG	2A	3334	1/1	0.68	0.24	49,49,49,49	0
54	MG	1A	3171	1/1	0.68	0.21	56,56,56,56	0
54	MG	2A	3187	1/1	0.68	0.59	70,70,70,70	0
54	MG	1A	3241	1/1	0.68	0.17	93,93,93,93	0
54	MG	2A	3244	1/1	0.69	0.27	72,72,72,72	0
54	MG	2a	1615	1/1	0.69	0.19	77,77,77,77	0
54	MG	1a	1665	1/1	0.69	0.43	86,86,86,86	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1a	1822	1/1	0.69	0.43	101,101,101,101	0
54	MG	1a	1852	1/1	0.69	0.13	106,106,106,106	0
54	MG	2A	3384	1/1	0.69	0.22	76,76,76,76	0
54	MG	2a	1737	1/1	0.69	0.26	131,131,131,131	0
54	MG	2A	3317	1/1	0.69	0.43	103,103,103,103	0
54	MG	1a	1858	1/1	0.69	0.39	90,90,90,90	0
54	MG	1A	3852	1/1	0.70	0.21	85,85,85,85	0
54	MG	2A	3086	1/1	0.70	0.41	94,94,94,94	0
54	MG	1A	3161	1/1	0.70	0.32	61,61,61,61	0
54	MG	2A	3630	1/1	0.70	0.43	58,58,58,58	0
54	MG	1a	1668	1/1	0.70	0.43	69,69,69,69	0
54	MG	1a	1694	1/1	0.70	0.43	73,73,73,73	0
54	MG	1A	3861	1/1	0.70	0.15	133,133,133,133	0
54	MG	1A	3880	1/1	0.70	0.20	50,50,50,50	0
54	MG	1B	1017	1/1	0.70	0.45	65,65,65,65	0
54	MG	1A	3815	1/1	0.70	0.32	61,61,61,61	0
54	MG	2A	3055	1/1	0.70	0.54	66,66,66,66	0
54	MG	2a	1607	1/1	0.70	0.22	94,94,94,94	0
54	MG	1A	3211	1/1	0.70	0.45	50,50,50,50	0
54	MG	1A	3757	1/1	0.70	0.12	44,44,44,44	0
54	MG	2a	1617	1/1	0.70	0.44	73,73,73,73	0
54	MG	1g	203	1/1	0.71	0.24	62,62,62,62	0
54	MG	1a	1769	1/1	0.71	0.23	90,90,90,90	0
54	MG	1a	1789	1/1	0.71	0.66	107,107,107,107	0
54	MG	2A	3045	1/1	0.71	0.44	74,74,74,74	0
54	MG	1Q	201	1/1	0.71	0.21	51,51,51,51	0
54	MG	2G	201	1/1	0.71	0.23	114,114,114,114	0
54	MG	2O	202	1/1	0.71	0.35	94,94,94,94	0
54	MG	2A	3183	1/1	0.71	0.44	84,84,84,84	0
54	MG	1A	3718	1/1	0.71	0.14	69,69,69,69	0
54	MG	1a	1603	1/1	0.71	0.13	118,118,118,118	0
54	MG	2a	1720	1/1	0.71	0.21	117,117,117,117	0
54	MG	2A	3325	1/1	0.71	0.08	96,96,96,96	0
54	MG	2a	1745	1/1	0.71	0.21	85,85,85,85	0
54	MG	1A	3418	1/1	0.71	0.25	39,39,39,39	0
54	MG	1A	3426	1/1	0.71	0.14	47,47,47,47	0
54	MG	1A	3472	1/1	0.72	0.28	43,43,43,43	0
54	MG	2T	201	1/1	0.72	0.14	61,61,61,61	0
54	MG	2I	104	1/1	0.72	0.23	95,95,95,95	0
54	MG	23	101	1/1	0.72	0.71	81,81,81,81	0
54	MG	2A	3410	1/1	0.72	0.33	75,75,75,75	0
54	MG	2A	3105	1/1	0.72	1.12	95,95,95,95	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3749	1/1	0.72	0.12	74,74,74,74	0
54	MG	2A	3452	1/1	0.72	0.41	70,70,70,70	0
54	MG	2A	3075	1/1	0.72	0.45	70,70,70,70	0
54	MG	1t	201	1/1	0.72	0.29	110,110,110,110	0
54	MG	2A	3377	1/1	0.72	0.37	57,57,57,57	0
54	MG	2a	1660	1/1	0.72	0.35	79,79,79,79	0
54	MG	1a	1823	1/1	0.72	0.20	99,99,99,99	0
54	MG	2a	1701	1/1	0.73	1.03	101,101,101,101	0
54	MG	1F	311	1/1	0.73	0.47	90,90,90,90	0
54	MG	1a	1779	1/1	0.73	0.28	81,81,81,81	0
54	MG	1a	1833	1/1	0.73	0.15	122,122,122,122	0
54	MG	2A	3403	1/1	0.73	0.13	74,74,74,74	0
54	MG	2a	1724	1/1	0.73	0.10	108,108,108,108	0
54	MG	2a	1731	1/1	0.73	0.16	86,86,86,86	0
54	MG	1a	1687	1/1	0.73	0.32	72,72,72,72	0
54	MG	2a	1742	1/1	0.73	0.12	96,96,96,96	0
54	MG	1e	202	1/1	0.73	0.50	78,78,78,78	0
54	MG	1A	3164	1/1	0.73	0.26	49,49,49,49	0
54	MG	1A	3737	1/1	0.73	0.10	74,74,74,74	0
54	MG	2A	3040	1/1	0.74	0.10	65,65,65,65	0
54	MG	2A	3569	1/1	0.74	0.14	87,87,87,87	0
54	MG	1A	3204	1/1	0.74	0.17	76,76,76,76	0
54	MG	1A	3227	1/1	0.74	0.40	88,88,88,88	0
54	MG	1a	1719	1/1	0.74	0.34	102,102,102,102	0
54	MG	2A	3537	1/1	0.74	0.20	97,97,97,97	0
54	MG	10	106	1/1	0.74	0.49	81,81,81,81	0
54	MG	1a	1735	1/1	0.74	0.19	83,83,83,83	0
54	MG	1A	3584	1/1	0.74	0.15	70,70,70,70	0
54	MG	2A	3447	1/1	0.74	0.17	69,69,69,69	0
54	MG	1a	1778	1/1	0.74	0.29	72,72,72,72	0
54	MG	1a	1792	1/1	0.75	0.31	111,111,111,111	0
54	MG	2A	3071	1/1	0.75	0.43	51,51,51,51	0
54	MG	1A	3678	1/1	0.75	0.31	115,115,115,115	0
54	MG	1a	1821	1/1	0.75	0.45	88,88,88,88	0
54	MG	1a	1602	1/1	0.75	0.28	63,63,63,63	0
54	MG	2A	3638	1/1	0.75	0.22	55,55,55,55	0
54	MG	2A	3455	1/1	0.75	0.33	68,68,68,68	0
54	MG	1A	3895	1/1	0.75	0.35	56,56,56,56	0
54	MG	2a	1683	1/1	0.75	0.17	83,83,83,83	0
54	MG	1A	3030	1/1	0.75	0.69	69,69,69,69	0
54	MG	2A	3005	1/1	0.75	0.31	68,68,68,68	0
54	MG	1A	3408	1/1	0.75	0.24	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3493	1/1	0.75	0.19	65,65,65,65	0
54	MG	2B	215	1/1	0.75	0.12	112,112,112,112	0
54	MG	1B	1019	1/1	0.75	0.09	75,75,75,75	0
54	MG	2A	3538	1/1	0.75	0.24	42,42,42,42	0
54	MG	2A	3151	1/1	0.75	0.47	72,72,72,72	0
54	MG	1A	3608	1/1	0.75	0.61	56,56,56,56	0
54	MG	1A	3720	1/1	0.75	0.70	64,64,64,64	0
53	MPD	1a	1601	8/8	0.75	0.33	97,116,129,130	0
54	MG	1A	3329	1/1	0.75	0.11	57,57,57,57	0
54	MG	2a	1752	1/1	0.75	0.13	103,103,103,103	0
54	MG	2a	1764	1/1	0.75	0.39	61,61,61,61	0
54	MG	2A	3207	1/1	0.75	0.41	61,61,61,61	0
54	MG	1A	3637	1/1	0.75	0.41	86,86,86,86	0
54	MG	2A	3215	1/1	0.76	0.18	65,65,65,65	0
54	MG	1a	1815	1/1	0.76	0.13	81,81,81,81	0
54	MG	2A	3408	1/1	0.76	0.20	81,81,81,81	0
54	MG	2A	3096	1/1	0.76	0.34	57,57,57,57	0
54	MG	2A	3102	1/1	0.76	0.17	95,95,95,95	0
54	MG	1A	3545	1/1	0.76	0.13	50,50,50,50	0
54	MG	2A	3572	1/1	0.76	0.11	57,57,57,57	0
54	MG	1A	3369	1/1	0.76	0.19	37,37,37,37	0
54	MG	1a	1663	1/1	0.76	0.66	68,68,68,68	0
54	MG	1B	1009	1/1	0.76	0.38	77,77,77,77	0
54	MG	1A	3086	1/1	0.76	0.32	68,68,68,68	0
54	MG	2A	3169	1/1	0.76	0.38	80,80,80,80	0
54	MG	1a	1683	1/1	0.76	0.15	73,73,73,73	0
54	MG	1n	103	1/1	0.76	0.40	100,100,100,100	0
54	MG	1a	1748	1/1	0.76	0.37	86,86,86,86	0
54	MG	2a	1762	1/1	0.76	0.33	105,105,105,105	0
54	MG	2A	3077	1/1	0.76	0.51	67,67,67,67	0
54	MG	1A	3828	1/1	0.76	0.22	64,64,64,64	0
54	MG	2j	201	1/1	0.76	0.37	112,112,112,112	0
54	MG	1A	3879	1/1	0.76	0.42	100,100,100,100	0
54	MG	1a	1681	1/1	0.77	0.20	113,113,113,113	0
54	MG	1A	3017	1/1	0.77	0.36	57,57,57,57	0
54	MG	1A	3887	1/1	0.77	0.17	40,40,40,40	0
54	MG	1A	3170	1/1	0.77	0.58	62,62,62,62	0
54	MG	1a	1770	1/1	0.77	0.20	99,99,99,99	0
54	MG	2A	3219	1/1	0.77	0.16	70,70,70,70	0
54	MG	1a	1695	1/1	0.77	0.14	94,94,94,94	0
54	MG	2A	3236	1/1	0.77	0.18	70,70,70,70	0
54	MG	1a	1709	1/1	0.77	0.83	99,99,99,99	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3028	1/1	0.77	0.44	47,47,47,47	0
54	MG	19	103	1/1	0.77	0.64	93,93,93,93	0
54	MG	1a	1799	1/1	0.77	0.15	96,96,96,96	0
54	MG	1g	202	1/1	0.77	0.36	85,85,85,85	0
54	MG	1A	3850	1/1	0.77	0.41	54,54,54,54	0
54	MG	2A	3522	1/1	0.77	0.28	96,96,96,96	0
54	MG	1a	1807	1/1	0.77	0.29	87,87,87,87	0
54	MG	1A	3373	1/1	0.77	0.10	67,67,67,67	0
54	MG	1y	204	1/1	0.77	0.46	99,99,99,99	0
54	MG	2a	1740	1/1	0.77	0.09	98,98,98,98	0
54	MG	2A	3545	1/1	0.77	0.16	110,110,110,110	0
54	MG	2A	3553	1/1	0.77	0.13	100,100,100,100	0
54	MG	1a	1634	1/1	0.77	0.22	62,62,62,62	0
54	MG	1A	3543	1/1	0.77	0.32	42,42,42,42	0
54	MG	1A	3715	1/1	0.77	0.14	71,71,71,71	0
53	MPD	2A	3002	8/8	0.77	0.41	89,92,94,95	0
54	MG	2a	1644	1/1	0.77	0.19	92,92,92,92	0
54	MG	1a	1670	1/1	0.77	0.34	91,91,91,91	0
54	MG	2A	3202	1/1	0.78	0.46	73,73,73,73	0
54	MG	1A	3743	1/1	0.78	0.31	47,47,47,47	0
54	MG	2a	1692	1/1	0.78	0.28	75,75,75,75	0
54	MG	1A	3243	1/1	0.78	0.18	45,45,45,45	0
54	MG	2A	3456	1/1	0.78	0.24	71,71,71,71	0
54	MG	1d	507	1/1	0.78	0.09	116,116,116,116	0
54	MG	2a	1715	1/1	0.78	0.11	88,88,88,88	0
54	MG	2A	3472	1/1	0.78	0.16	69,69,69,69	0
54	MG	2A	3575	1/1	0.78	0.20	52,52,52,52	0
54	MG	1a	1631	1/1	0.78	0.16	68,68,68,68	0
54	MG	1a	1679	1/1	0.78	0.25	57,57,57,57	0
54	MG	1A	3216	1/1	0.78	0.13	66,66,66,66	0
54	MG	1a	1636	1/1	0.78	0.23	77,77,77,77	0
54	MG	2A	3388	1/1	0.78	0.23	73,73,73,73	0
54	MG	2A	3533	1/1	0.78	0.20	61,61,61,61	0
54	MG	2A	3180	1/1	0.78	0.25	61,61,61,61	0
54	MG	1a	1857	1/1	0.78	0.14	92,92,92,92	0
54	MG	2A	3090	1/1	0.78	0.38	81,81,81,81	0
54	MG	2A	3304	1/1	0.78	0.19	65,65,65,65	0
54	MG	1P	205	1/1	0.78	0.42	117,117,117,117	0
54	MG	2a	1670	1/1	0.78	0.43	57,57,57,57	0
54	MG	2A	3097	1/1	0.78	0.29	71,71,71,71	0
54	MG	1A	3220	1/1	0.79	0.32	54,54,54,54	0
54	MG	2A	3576	1/1	0.79	0.19	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3582	1/1	0.79	0.30	91,91,91,91	0
54	MG	2A	3034	1/1	0.79	0.18	62,62,62,62	0
54	MG	1A	3619	1/1	0.79	0.33	55,55,55,55	0
54	MG	1A	3578	1/1	0.79	0.19	62,62,62,62	0
54	MG	1a	1650	1/1	0.79	0.82	74,74,74,74	0
54	MG	2a	1675	1/1	0.79	0.42	87,87,87,87	0
54	MG	2A	3481	1/1	0.79	0.37	92,92,92,92	0
54	MG	1A	3732	1/1	0.79	0.69	60,60,60,60	0
54	MG	1a	1808	1/1	0.79	0.26	63,63,63,63	0
54	MG	1d	506	1/1	0.79	0.10	98,98,98,98	0
54	MG	1a	1810	1/1	0.79	0.28	82,82,82,82	0
54	MG	2A	3519	1/1	0.79	0.13	64,64,64,64	0
54	MG	2A	3342	1/1	0.79	0.18	69,69,69,69	0
54	MG	1A	3353	1/1	0.79	0.14	38,38,38,38	0
54	MG	2A	3359	1/1	0.79	0.22	73,73,73,73	0
54	MG	2B	217	1/1	0.79	0.12	81,81,81,81	0
54	MG	1A	3354	1/1	0.79	0.22	38,38,38,38	0
54	MG	1A	3415	1/1	0.79	0.14	40,40,40,40	0
54	MG	2R	202	1/1	0.79	0.27	70,70,70,70	0
54	MG	2a	1733	1/1	0.79	0.20	86,86,86,86	0
54	MG	2A	3082	1/1	0.79	0.18	76,76,76,76	0
54	MG	1A	3694	1/1	0.79	0.22	61,61,61,61	0
54	MG	2A	3213	1/1	0.79	0.63	73,73,73,73	0
54	MG	1a	1773	1/1	0.79	0.22	77,77,77,77	0
54	MG	1a	1831	1/1	0.79	0.26	96,96,96,96	0
54	MG	2a	1754	1/1	0.79	0.18	121,121,121,121	0
54	MG	1a	1734	1/1	0.79	0.53	130,130,130,130	0
54	MG	1A	3303	1/1	0.79	0.13	60,60,60,60	0
54	MG	1a	1787	1/1	0.79	0.12	74,74,74,74	0
54	MG	2a	1645	1/1	0.79	0.22	120,120,120,120	0
54	MG	2A	3007	1/1	0.79	0.25	63,63,63,63	0
54	MG	1A	3641	1/1	0.80	0.27	33,33,33,33	0
54	MG	2A	3292	1/1	0.80	0.36	74,74,74,74	0
54	MG	1A	3735	1/1	0.80	0.20	58,58,58,58	0
54	MG	2A	3618	1/1	0.80	0.14	104,104,104,104	0
54	MG	1a	1782	1/1	0.80	0.36	86,86,86,86	0
54	MG	1A	3410	1/1	0.80	0.20	20,20,20,20	0
54	MG	2A	3307	1/1	0.80	0.19	75,75,75,75	0
54	MG	2A	3138	1/1	0.80	0.51	49,49,49,49	0
54	MG	1D	312	1/1	0.80	0.62	62,62,62,62	0
54	MG	2A	3165	1/1	0.80	0.25	72,72,72,72	0
54	MG	2B	206	1/1	0.80	0.36	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3498	1/1	0.80	0.23	67,67,67,67	0
54	MG	2a	1695	1/1	0.80	0.24	95,95,95,95	0
54	MG	1F	304	1/1	0.80	0.37	43,43,43,43	0
54	MG	2a	1708	1/1	0.80	0.15	72,72,72,72	0
54	MG	2A	3175	1/1	0.80	0.17	63,63,63,63	0
54	MG	2a	1711	1/1	0.80	0.10	80,80,80,80	0
54	MG	1A	3682	1/1	0.80	0.17	79,79,79,79	0
54	MG	1d	505	1/1	0.80	0.23	56,56,56,56	0
54	MG	2D	306	1/1	0.80	0.24	52,52,52,52	0
54	MG	1A	3683	1/1	0.80	0.17	34,34,34,34	0
54	MG	1A	3872	1/1	0.80	0.29	77,77,77,77	0
54	MG	2A	3194	1/1	0.80	0.14	60,60,60,60	0
54	MG	1a	1749	1/1	0.80	0.71	100,100,100,100	0
54	MG	2a	1734	1/1	0.80	0.13	62,62,62,62	0
54	MG	1a	1754	1/1	0.80	0.16	78,78,78,78	0
54	MG	1a	1675	1/1	0.80	0.32	68,68,68,68	0
54	MG	1A	3230	1/1	0.80	0.23	49,49,49,49	0
54	MG	1A	3617	1/1	0.80	0.26	100,100,100,100	0
54	MG	10	104	1/1	0.80	0.32	54,54,54,54	0
54	MG	1A	3618	1/1	0.80	0.39	68,68,68,68	0
54	MG	2A	3225	1/1	0.80	0.66	80,80,80,80	0
54	MG	1A	3384	1/1	0.80	0.30	74,74,74,74	0
54	MG	1A	3097	1/1	0.80	0.34	38,38,38,38	0
54	MG	2a	1657	1/1	0.80	0.37	89,89,89,89	0
54	MG	1A	3562	1/1	0.80	0.41	81,81,81,81	0
54	MG	2l	202	1/1	0.80	0.60	55,55,55,55	0
54	MG	1V	203	1/1	0.81	0.57	86,86,86,86	0
54	MG	2a	1680	1/1	0.81	0.42	121,121,121,121	0
54	MG	2A	3153	1/1	0.81	0.46	78,78,78,78	0
54	MG	1a	1714	1/1	0.81	0.30	83,83,83,83	0
54	MG	1h	201	1/1	0.81	0.34	64,64,64,64	0
54	MG	2A	3539	1/1	0.81	0.20	74,74,74,74	0
54	MG	2A	3171	1/1	0.81	0.15	84,84,84,84	0
54	MG	2A	3285	1/1	0.81	0.33	68,68,68,68	0
54	MG	2a	1697	1/1	0.81	0.17	75,75,75,75	0
54	MG	2A	3094	1/1	0.81	0.30	74,74,74,74	0
54	MG	2a	1707	1/1	0.81	0.24	84,84,84,84	0
54	MG	2A	3177	1/1	0.81	0.41	60,60,60,60	0
54	MG	1A	3143	1/1	0.81	0.34	70,70,70,70	0
54	MG	1a	1635	1/1	0.81	0.11	80,80,80,80	0
54	MG	2A	3305	1/1	0.81	0.24	58,58,58,58	0
54	MG	1A	3502	1/1	0.81	0.13	91,91,91,91	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3516	1/1	0.81	0.38	73,73,73,73	0
54	MG	2a	1605	1/1	0.81	0.17	91,91,91,91	0
54	MG	1A	3165	1/1	0.81	0.23	78,78,78,78	0
54	MG	2A	3574	1/1	0.81	0.23	56,56,56,56	0
54	MG	2a	1732	1/1	0.81	0.14	91,91,91,91	0
54	MG	2A	3462	1/1	0.81	0.17	74,74,74,74	0
54	MG	1A	3326	1/1	0.81	0.21	44,44,44,44	0
54	MG	2A	3464	1/1	0.81	0.54	69,69,69,69	0
54	MG	2a	1738	1/1	0.81	0.24	93,93,93,93	0
54	MG	1A	3037	1/1	0.81	0.48	56,56,56,56	0
54	MG	2A	3128	1/1	0.81	0.38	58,58,58,58	0
54	MG	2A	3610	1/1	0.81	0.16	61,61,61,61	0
54	MG	2a	1746	1/1	0.81	0.18	119,119,119,119	0
54	MG	2A	3130	1/1	0.81	0.36	62,62,62,62	0
54	MG	2A	3137	1/1	0.81	0.38	67,67,67,67	0
54	MG	2a	1759	1/1	0.81	0.54	80,80,80,80	0
54	MG	2A	3489	1/1	0.81	0.10	74,74,74,74	0
54	MG	2A	3346	1/1	0.81	0.17	89,89,89,89	0
54	MG	1a	1614	1/1	0.81	0.12	94,94,94,94	0
54	MG	2A	3149	1/1	0.81	0.25	78,78,78,78	0
54	MG	2A	3370	1/1	0.81	0.21	82,82,82,82	0
54	MG	2a	1673	1/1	0.81	0.36	69,69,69,69	0
56	ZN	14	101	1/1	0.81	0.06	135,135,135,135	0
54	MG	2A	3181	1/1	0.82	0.30	57,57,57,57	0
54	MG	1A	3506	1/1	0.82	0.19	65,65,65,65	0
54	MG	2A	3329	1/1	0.82	0.19	93,93,93,93	0
54	MG	1A	3236	1/1	0.82	0.45	52,52,52,52	0
54	MG	2A	3093	1/1	0.82	0.12	81,81,81,81	0
54	MG	1t	202	1/1	0.82	0.48	92,92,92,92	0
54	MG	2A	3501	1/1	0.82	0.26	60,60,60,60	0
54	MG	2A	3343	1/1	0.82	0.20	47,47,47,47	0
54	MG	1A	3530	1/1	0.82	0.33	103,103,103,103	0
54	MG	1A	3011	1/1	0.82	0.39	55,55,55,55	0
54	MG	1a	1784	1/1	0.82	0.73	82,82,82,82	0
54	MG	1A	3047	1/1	0.82	0.34	73,73,73,73	0
54	MG	1B	1007	1/1	0.82	0.28	67,67,67,67	0
54	MG	2A	3113	1/1	0.82	0.20	64,64,64,64	0
54	MG	1A	3560	1/1	0.82	0.11	48,48,48,48	0
54	MG	1B	1011	1/1	0.82	0.20	64,64,64,64	0
54	MG	1A	3063	1/1	0.82	0.44	41,41,41,41	0
54	MG	2A	3232	1/1	0.82	0.31	69,69,69,69	0
54	MG	2a	1604	1/1	0.82	0.18	91,91,91,91	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3404	1/1	0.82	0.20	81,81,81,81	0
54	MG	1A	3570	1/1	0.82	0.20	81,81,81,81	0
54	MG	1A	3724	1/1	0.82	0.63	91,91,91,91	0
54	MG	1A	3727	1/1	0.82	0.57	58,58,58,58	0
54	MG	1a	1811	1/1	0.82	0.61	118,118,118,118	0
54	MG	2a	1638	1/1	0.82	0.45	77,77,77,77	0
54	MG	1a	1705	1/1	0.82	0.07	93,93,93,93	0
54	MG	1a	1819	1/1	0.82	0.20	97,97,97,97	0
54	MG	2a	1647	1/1	0.82	0.33	67,67,67,67	0
54	MG	2a	1653	1/1	0.82	0.11	86,86,86,86	0
54	MG	1a	1820	1/1	0.82	0.22	124,124,124,124	0
54	MG	2A	3080	1/1	0.82	0.09	130,130,130,130	0
54	MG	2A	3081	1/1	0.82	0.35	52,52,52,52	0
54	MG	1A	3173	1/1	0.82	0.30	80,80,80,80	0
54	MG	2A	3601	1/1	0.82	0.15	75,75,75,75	0
54	MG	2A	3604	1/1	0.82	0.09	66,66,66,66	0
54	MG	1A	3179	1/1	0.82	0.34	49,49,49,49	0
54	MG	2A	3469	1/1	0.82	0.21	64,64,64,64	0
54	MG	1A	3191	1/1	0.82	0.25	64,64,64,64	0
55	ARG	1F	303	12/12	0.82	0.29	56,82,107,107	0
54	MG	2A	3320	1/1	0.82	0.12	72,72,72,72	0
54	MG	2a	1656	1/1	0.83	0.79	106,106,106,106	0
54	MG	2A	3399	1/1	0.83	0.11	68,68,68,68	0
54	MG	1A	3504	1/1	0.83	0.25	25,25,25,25	0
54	MG	1A	3837	1/1	0.83	0.30	56,56,56,56	0
54	MG	1A	3839	1/1	0.83	0.29	61,61,61,61	0
54	MG	1A	3848	1/1	0.83	0.18	55,55,55,55	0
54	MG	2A	3587	1/1	0.83	0.13	83,83,83,83	0
54	MG	1A	3185	1/1	0.83	0.14	61,61,61,61	0
54	MG	1A	3319	1/1	0.83	0.48	72,72,72,72	0
54	MG	2a	1671	1/1	0.83	0.23	79,79,79,79	0
54	MG	1a	1827	1/1	0.83	0.22	95,95,95,95	0
54	MG	2A	3031	1/1	0.83	0.15	75,75,75,75	0
54	MG	2A	3613	1/1	0.83	0.22	102,102,102,102	0
54	MG	2A	3453	1/1	0.83	0.12	43,43,43,43	0
54	MG	1R	203	1/1	0.83	0.45	52,52,52,52	0
54	MG	2a	1684	1/1	0.83	0.12	73,73,73,73	0
54	MG	2A	3251	1/1	0.83	0.16	76,76,76,76	0
54	MG	2A	3135	1/1	0.83	0.17	69,69,69,69	0
54	MG	1A	3106	1/1	0.83	0.33	48,48,48,48	0
54	MG	2B	202	1/1	0.83	0.25	99,99,99,99	0
54	MG	1A	3198	1/1	0.83	0.23	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1a	1842	1/1	0.83	0.14	73,73,73,73	0
54	MG	1A	3225	1/1	0.83	0.30	54,54,54,54	0
54	MG	1a	1700	1/1	0.83	0.33	77,77,77,77	0
54	MG	2A	3154	1/1	0.83	0.47	66,66,66,66	0
54	MG	2a	1710	1/1	0.83	0.24	98,98,98,98	0
54	MG	1A	3555	1/1	0.83	0.14	79,79,79,79	0
54	MG	1a	1856	1/1	0.83	0.20	83,83,83,83	0
54	MG	1A	3250	1/1	0.83	0.29	61,61,61,61	0
54	MG	1A	3435	1/1	0.83	0.20	51,51,51,51	0
54	MG	1A	3452	1/1	0.83	0.15	52,52,52,52	0
53	MPD	1T	2001	8/8	0.83	0.29	77,82,86,94	0
54	MG	2A	3517	1/1	0.83	0.16	57,57,57,57	0
54	MG	1A	3262	1/1	0.83	0.12	45,45,45,45	0
54	MG	1a	1801	1/1	0.83	0.17	107,107,107,107	0
54	MG	1A	3796	1/1	0.83	0.43	66,66,66,66	0
54	MG	2a	1735	1/1	0.83	0.18	76,76,76,76	0
54	MG	2a	1736	1/1	0.83	0.25	100,100,100,100	0
54	MG	2A	3188	1/1	0.83	0.36	67,67,67,67	0
54	MG	2A	3190	1/1	0.83	0.33	76,76,76,76	0
54	MG	1a	1803	1/1	0.83	0.09	93,93,93,93	0
54	MG	1A	3486	1/1	0.83	0.16	69,69,69,69	0
54	MG	2A	3365	1/1	0.83	0.38	70,70,70,70	0
54	MG	1A	3283	1/1	0.83	0.23	64,64,64,64	0
54	MG	2a	1616	1/1	0.83	0.19	80,80,80,80	0
54	MG	2A	3198	1/1	0.83	0.32	72,72,72,72	0
54	MG	2a	1758	1/1	0.83	0.10	102,102,102,102	0
54	MG	2a	1621	1/1	0.83	0.41	52,52,52,52	0
54	MG	2a	1636	1/1	0.83	0.14	99,99,99,99	0
54	MG	2A	3374	1/1	0.83	0.18	60,60,60,60	0
54	MG	2a	1643	1/1	0.83	0.39	51,51,51,51	0
54	MG	1a	1646	1/1	0.83	0.08	102,102,102,102	0
54	MG	1A	3700	1/1	0.83	0.31	58,58,58,58	0
54	MG	1A	3599	1/1	0.83	0.28	49,49,49,49	0
54	MG	2A	3210	1/1	0.83	0.30	61,61,61,61	0
54	MG	2A	3397	1/1	0.83	0.13	58,58,58,58	0
54	MG	1A	3446	1/1	0.84	0.12	60,60,60,60	0
54	MG	2A	3050	1/1	0.84	0.71	70,70,70,70	0
54	MG	2A	3627	1/1	0.84	0.10	55,55,55,55	0
54	MG	1a	1666	1/1	0.84	0.50	78,78,78,78	0
54	MG	1F	302	1/1	0.84	0.28	57,57,57,57	0
54	MG	1A	3355	1/1	0.84	0.17	20,20,20,20	0
54	MG	1a	1673	1/1	0.84	0.15	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3063	1/1	0.84	0.28	52,52,52,52	0
54	MG	2A	3487	1/1	0.84	0.12	75,75,75,75	0
54	MG	2a	1689	1/1	0.84	0.21	102,102,102,102	0
54	MG	1a	1776	1/1	0.84	0.18	91,91,91,91	0
54	MG	2A	3330	1/1	0.84	0.26	82,82,82,82	0
54	MG	2B	207	1/1	0.84	0.78	99,99,99,99	0
54	MG	1A	3317	1/1	0.84	0.29	76,76,76,76	0
54	MG	1A	3704	1/1	0.84	0.32	61,61,61,61	0
54	MG	2a	1698	1/1	0.84	0.18	95,95,95,95	0
54	MG	2A	3337	1/1	0.84	0.18	69,69,69,69	0
54	MG	1A	3548	1/1	0.84	0.20	63,63,63,63	0
54	MG	1A	3478	1/1	0.84	0.21	50,50,50,50	0
54	MG	1A	3479	1/1	0.84	0.15	70,70,70,70	0
54	MG	1T	2002	1/1	0.84	0.36	54,54,54,54	0
54	MG	1A	3413	1/1	0.84	0.18	42,42,42,42	0
54	MG	1A	3565	1/1	0.84	0.55	69,69,69,69	0
54	MG	2a	1716	1/1	0.84	0.10	89,89,89,89	0
54	MG	1A	3730	1/1	0.84	0.26	75,75,75,75	0
54	MG	1A	3332	1/1	0.84	0.24	36,36,36,36	0
54	MG	15	104	1/1	0.84	0.22	72,72,72,72	0
54	MG	1a	1806	1/1	0.84	0.36	85,85,85,85	0
54	MG	2A	3550	1/1	0.84	0.26	105,105,105,105	0
54	MG	1A	3009	1/1	0.84	0.27	59,59,59,59	0
54	MG	2A	3385	1/1	0.84	0.19	73,73,73,73	0
54	MG	1A	3662	1/1	0.84	0.18	43,43,43,43	0
54	MG	1A	3740	1/1	0.84	0.18	47,47,47,47	0
54	MG	1A	3672	1/1	0.84	0.30	78,78,78,78	0
54	MG	1a	1630	1/1	0.84	0.21	54,54,54,54	0
54	MG	2a	1633	1/1	0.84	0.14	92,92,92,92	0
54	MG	1A	3746	1/1	0.84	0.17	55,55,55,55	0
54	MG	2A	3117	1/1	0.84	0.27	45,45,45,45	0
54	MG	2a	1639	1/1	0.84	0.26	124,124,124,124	0
54	MG	1A	3674	1/1	0.84	0.11	57,57,57,57	0
54	MG	1A	3677	1/1	0.84	0.45	71,71,71,71	0
54	MG	2A	3424	1/1	0.84	0.16	88,88,88,88	0
54	MG	2A	3580	1/1	0.84	0.38	97,97,97,97	0
54	MG	1A	3308	1/1	0.84	0.18	40,40,40,40	0
54	MG	1A	3430	1/1	0.84	0.09	82,82,82,82	0
54	MG	1A	3389	1/1	0.84	0.18	56,56,56,56	0
54	MG	1a	1652	1/1	0.84	0.51	74,74,74,74	0
54	MG	2A	3143	1/1	0.84	0.27	61,61,61,61	0
54	MG	2A	3454	1/1	0.84	0.41	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2l	201	1/1	0.84	0.31	89,89,89,89	0
54	MG	2A	3609	1/1	0.84	0.20	80,80,80,80	0
54	MG	1A	3592	1/1	0.84	0.26	68,68,68,68	0
54	MG	2A	3042	1/1	0.84	0.23	65,65,65,65	0
54	MG	2A	3451	1/1	0.85	0.23	63,63,63,63	0
54	MG	1A	3781	1/1	0.85	0.16	55,55,55,55	0
54	MG	1A	3175	1/1	0.85	0.54	51,51,51,51	0
54	MG	2a	1667	1/1	0.85	0.54	79,79,79,79	0
54	MG	1A	3651	1/1	0.85	0.25	53,53,53,53	0
54	MG	1A	3423	1/1	0.85	0.47	81,81,81,81	0
54	MG	1A	3665	1/1	0.85	0.16	59,59,59,59	0
54	MG	1A	3666	1/1	0.85	0.26	43,43,43,43	0
54	MG	2A	3620	1/1	0.85	0.32	101,101,101,101	0
54	MG	2A	3044	1/1	0.85	0.20	71,71,71,71	0
54	MG	1A	3051	1/1	0.85	0.14	77,77,77,77	0
54	MG	1A	3605	1/1	0.85	0.38	71,71,71,71	0
54	MG	1A	3117	1/1	0.85	0.46	26,26,26,26	0
54	MG	2A	3473	1/1	0.85	0.06	104,104,104,104	0
54	MG	2A	3155	1/1	0.85	0.33	59,59,59,59	0
54	MG	1a	1684	1/1	0.85	0.34	56,56,56,56	0
54	MG	2A	3483	1/1	0.85	0.15	53,53,53,53	0
54	MG	2A	3486	1/1	0.85	0.25	96,96,96,96	0
54	MG	1a	1847	1/1	0.85	0.20	62,62,62,62	0
54	MG	2B	210	1/1	0.85	0.16	84,84,84,84	0
54	MG	1a	1685	1/1	0.85	0.10	74,74,74,74	0
54	MG	2A	3173	1/1	0.85	0.31	63,63,63,63	0
54	MG	1a	1619	1/1	0.85	0.19	102,102,102,102	0
54	MG	1a	1691	1/1	0.85	0.21	68,68,68,68	0
54	MG	2A	3073	1/1	0.85	0.20	60,60,60,60	0
54	MG	1a	1627	1/1	0.85	0.12	72,72,72,72	0
54	MG	2F	301	1/1	0.85	0.22	54,54,54,54	0
54	MG	2A	3076	1/1	0.85	0.31	76,76,76,76	0
54	MG	2A	3344	1/1	0.85	0.10	55,55,55,55	0
54	MG	1A	3612	1/1	0.85	0.15	45,45,45,45	0
54	MG	2A	3353	1/1	0.85	0.18	42,42,42,42	0
54	MG	2V	201	1/1	0.85	0.32	101,101,101,101	0
54	MG	2a	1725	1/1	0.85	0.20	73,73,73,73	0
54	MG	1a	1699	1/1	0.85	0.17	90,90,90,90	0
54	MG	1A	3169	1/1	0.85	0.51	56,56,56,56	0
54	MG	2A	3364	1/1	0.85	0.10	55,55,55,55	0
54	MG	2A	3542	1/1	0.85	0.15	90,90,90,90	0
54	MG	2a	1606	1/1	0.85	0.28	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1a	1703	1/1	0.85	0.09	54,54,54,54	0
54	MG	1a	1632	1/1	0.85	0.41	59,59,59,59	0
54	MG	2A	3196	1/1	0.85	0.47	58,58,58,58	0
54	MG	1a	1796	1/1	0.85	0.24	81,81,81,81	0
54	MG	1A	3124	1/1	0.85	0.15	67,67,67,67	0
54	MG	1a	1710	1/1	0.85	0.20	56,56,56,56	0
53	MPD	2A	3001	8/8	0.85	0.30	54,73,76,82	0
54	MG	1A	3860	1/1	0.85	0.26	65,65,65,65	0
54	MG	2a	1753	1/1	0.85	0.17	73,73,73,73	0
54	MG	1a	1713	1/1	0.85	0.09	92,92,92,92	0
54	MG	1a	1641	1/1	0.85	0.22	60,60,60,60	0
54	MG	1A	3690	1/1	0.85	0.60	51,51,51,51	0
54	MG	1A	3073	1/1	0.85	0.30	75,75,75,75	0
54	MG	1A	3476	1/1	0.85	0.76	65,65,65,65	0
54	MG	2A	3228	1/1	0.85	0.21	99,99,99,99	0
54	MG	2A	3577	1/1	0.85	0.10	54,54,54,54	0
54	MG	1a	1653	1/1	0.85	0.19	55,55,55,55	0
54	MG	1A	3242	1/1	0.85	0.10	90,90,90,90	0
54	MG	2A	3115	1/1	0.85	0.13	73,73,73,73	0
54	MG	1a	1745	1/1	0.85	0.24	78,78,78,78	0
54	MG	2A	3021	1/1	0.85	0.29	59,59,59,59	0
54	MG	1a	1763	1/1	0.86	0.21	96,96,96,96	0
54	MG	1A	3010	1/1	0.86	0.29	46,46,46,46	0
54	MG	2a	1646	1/1	0.86	0.13	69,69,69,69	0
54	MG	2A	3078	1/1	0.86	0.64	58,58,58,58	0
54	MG	1F	312	1/1	0.86	0.43	52,52,52,52	0
54	MG	2A	3570	1/1	0.86	0.22	69,69,69,69	0
54	MG	1A	3172	1/1	0.86	0.20	71,71,71,71	0
54	MG	1H	202	1/1	0.86	0.29	64,64,64,64	0
54	MG	1a	1771	1/1	0.86	0.36	89,89,89,89	0
54	MG	2A	3206	1/1	0.86	0.24	67,67,67,67	0
54	MG	2A	3395	1/1	0.86	0.21	97,97,97,97	0
54	MG	2A	3579	1/1	0.86	0.10	52,52,52,52	0
54	MG	1P	204	1/1	0.86	0.16	50,50,50,50	0
54	MG	1A	3821	1/1	0.86	0.24	51,51,51,51	0
54	MG	2A	3583	1/1	0.86	0.09	96,96,96,96	0
54	MG	1A	3822	1/1	0.86	0.09	65,65,65,65	0
54	MG	1A	3420	1/1	0.86	0.17	35,35,35,35	0
54	MG	1A	3422	1/1	0.86	0.11	45,45,45,45	0
54	MG	1A	3518	1/1	0.86	0.14	56,56,56,56	0
54	MG	1A	3713	1/1	0.86	0.26	60,60,60,60	0
54	MG	2A	3425	1/1	0.86	0.10	78,78,78,78	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3614	1/1	0.86	0.27	57,57,57,57	0
54	MG	1a	1791	1/1	0.86	0.14	70,70,70,70	0
54	MG	1A	3524	1/1	0.86	0.19	59,59,59,59	0
54	MG	2A	3450	1/1	0.86	0.30	49,49,49,49	0
54	MG	2A	3234	1/1	0.86	0.21	65,65,65,65	0
54	MG	2A	3111	1/1	0.86	0.14	57,57,57,57	0
54	MG	11	103	1/1	0.86	0.70	48,48,48,48	0
54	MG	1A	3286	1/1	0.86	0.18	32,32,32,32	0
54	MG	17	103	1/1	0.86	0.24	62,62,62,62	0
54	MG	2A	3258	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3264	1/1	0.86	0.14	98,98,98,98	0
54	MG	2A	3275	1/1	0.86	0.17	75,75,75,75	0
54	MG	2A	3279	1/1	0.86	0.13	74,74,74,74	0
54	MG	19	101	1/1	0.86	0.27	42,42,42,42	0
54	MG	1A	3537	1/1	0.86	0.27	39,39,39,39	0
54	MG	1A	3301	1/1	0.86	0.13	51,51,51,51	0
54	MG	2A	3480	1/1	0.86	0.12	61,61,61,61	0
54	MG	2A	3008	1/1	0.86	0.42	61,61,61,61	0
54	MG	1A	3118	1/1	0.86	0.29	59,59,59,59	0
54	MG	1a	1605	1/1	0.86	0.31	96,96,96,96	0
54	MG	2A	3029	1/1	0.86	0.19	48,48,48,48	0
54	MG	1A	3108	1/1	0.86	0.36	57,57,57,57	0
54	MG	2A	3032	1/1	0.86	0.21	61,61,61,61	0
54	MG	1A	3439	1/1	0.86	0.26	114,114,114,114	0
54	MG	1A	3445	1/1	0.86	0.31	43,43,43,43	0
54	MG	1A	3129	1/1	0.86	0.54	42,42,42,42	0
54	MG	1A	3374	1/1	0.86	0.14	73,73,73,73	0
54	MG	2A	3163	1/1	0.86	0.12	67,67,67,67	0
54	MG	2A	3508	1/1	0.86	0.23	64,64,64,64	0
54	MG	1A	3465	1/1	0.86	0.26	46,46,46,46	0
54	MG	2a	1603	1/1	0.86	0.41	58,58,58,58	0
54	MG	1A	3217	1/1	0.86	0.36	48,48,48,48	0
54	MG	1A	3324	1/1	0.86	0.14	57,57,57,57	0
54	MG	2A	3529	1/1	0.86	0.17	73,73,73,73	0
54	MG	1A	3396	1/1	0.86	0.26	25,25,25,25	0
54	MG	1A	3771	1/1	0.86	0.08	48,48,48,48	0
54	MG	1A	3780	1/1	0.86	0.12	57,57,57,57	0
54	MG	1A	3183	1/1	0.86	0.13	28,28,28,28	0
54	MG	2A	3351	1/1	0.86	0.17	74,74,74,74	0
54	MG	1A	3083	1/1	0.86	0.74	51,51,51,51	0
54	MG	2a	1625	1/1	0.86	0.39	94,94,94,94	0
54	MG	2e	201	1/1	0.86	0.18	85,85,85,85	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1629	1/1	0.86	0.42	110,110,110,110	0
54	MG	1A	3805	1/1	0.86	0.30	49,49,49,49	0
54	MG	2a	1635	1/1	0.86	0.16	78,78,78,78	0
54	MG	2A	3184	1/1	0.86	0.21	56,56,56,56	0
54	MG	2A	3363	1/1	0.86	0.48	76,76,76,76	0
54	MG	1A	3331	1/1	0.86	0.15	40,40,40,40	0
54	MG	1a	1664	1/1	0.86	0.30	80,80,80,80	0
54	MG	1a	1696	1/1	0.87	0.18	80,80,80,80	0
54	MG	2A	3328	1/1	0.87	0.19	78,78,78,78	0
54	MG	1a	1783	1/1	0.87	0.24	64,64,64,64	0
54	MG	1A	3549	1/1	0.87	0.29	59,59,59,59	0
54	MG	2A	3331	1/1	0.87	0.10	98,98,98,98	0
54	MG	1A	3036	1/1	0.87	0.14	56,56,56,56	0
54	MG	1A	3425	1/1	0.87	0.16	36,36,36,36	0
54	MG	1B	1028	1/1	0.87	0.21	75,75,75,75	0
54	MG	2A	3642	1/1	0.87	0.39	87,87,87,87	0
54	MG	1A	3707	1/1	0.87	0.38	91,91,91,91	0
54	MG	1a	1795	1/1	0.87	0.13	81,81,81,81	0
54	MG	2a	1679	1/1	0.87	0.12	68,68,68,68	0
54	MG	1D	309	1/1	0.87	0.33	71,71,71,71	0
54	MG	1A	3621	1/1	0.87	0.20	67,67,67,67	0
54	MG	1E	304	1/1	0.87	0.70	80,80,80,80	0
54	MG	1A	3714	1/1	0.87	0.19	44,44,44,44	0
54	MG	2B	208	1/1	0.87	0.49	79,79,79,79	0
54	MG	1A	3221	1/1	0.87	0.11	100,100,100,100	0
54	MG	1A	3103	1/1	0.87	0.18	25,25,25,25	0
54	MG	1A	3079	1/1	0.87	0.32	38,38,38,38	0
54	MG	1a	1731	1/1	0.87	0.09	73,73,73,73	0
54	MG	2A	3004	1/1	0.87	0.21	65,65,65,65	0
54	MG	2A	3104	1/1	0.87	0.21	67,67,67,67	0
54	MG	1A	3137	1/1	0.87	0.30	74,74,74,74	0
54	MG	1A	3024	1/1	0.87	0.12	71,71,71,71	0
54	MG	1A	3239	1/1	0.87	0.23	50,50,50,50	0
54	MG	2G	203	1/1	0.87	0.10	104,104,104,104	0
54	MG	2A	3010	1/1	0.87	0.44	62,62,62,62	0
54	MG	2A	3011	1/1	0.87	0.46	44,44,44,44	0
54	MG	2A	3017	1/1	0.87	0.48	76,76,76,76	0
54	MG	1A	3144	1/1	0.87	0.20	56,56,56,56	0
54	MG	1A	3038	1/1	0.87	0.09	53,53,53,53	0
54	MG	2A	3023	1/1	0.87	0.25	50,50,50,50	0
54	MG	1A	3851	1/1	0.87	0.31	75,75,75,75	0
54	MG	1A	3596	1/1	0.87	0.10	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
54	MG	1A	3532	1/1	0.87	0.39	46,46,46,46	0
54	MG	2A	3407	1/1	0.87	0.12	66,66,66,66	0
54	MG	1a	1671	1/1	0.87	0.65	71,71,71,71	0
54	MG	2A	3567	1/1	0.87	0.07	63,63,63,63	0
54	MG	1A	3471	1/1	0.87	0.15	62,62,62,62	0
54	MG	2A	3423	1/1	0.87	0.16	94,94,94,94	0
54	MG	1a	1828	1/1	0.87	0.21	116,116,116,116	0
54	MG	1A	3538	1/1	0.87	0.18	37,37,37,37	0
54	MG	2A	3288	1/1	0.87	0.16	39,39,39,39	0
54	MG	1A	3541	1/1	0.87	0.20	66,66,66,66	0
54	MG	2a	1632	1/1	0.87	0.21	63,63,63,63	0
54	MG	2a	1743	1/1	0.87	0.11	84,84,84,84	0
54	MG	2A	3445	1/1	0.87	0.25	68,68,68,68	0
54	MG	2A	3295	1/1	0.87	0.29	84,84,84,84	0
54	MG	2a	1748	1/1	0.87	0.15	100,100,100,100	0
54	MG	2A	3297	1/1	0.87	0.17	66,66,66,66	0
54	MG	1A	3357	1/1	0.87	0.17	26,26,26,26	0
54	MG	1A	3750	1/1	0.87	0.15	84,84,84,84	0
54	MG	2a	1640	1/1	0.87	0.32	100,100,100,100	0
54	MG	2a	1642	1/1	0.87	0.42	61,61,61,61	0
54	MG	1A	3687	1/1	0.87	0.08	66,66,66,66	0
54	MG	1A	3766	1/1	0.87	0.06	69,69,69,69	0
54	MG	2A	3588	1/1	0.87	0.08	93,93,93,93	0
54	MG	2A	3589	1/1	0.87	0.14	67,67,67,67	0
54	MG	1A	3360	1/1	0.87	0.11	30,30,30,30	0
54	MG	2a	1652	1/1	0.87	0.25	88,88,88,88	0
54	MG	1A	3776	1/1	0.87	0.14	40,40,40,40	0
54	MG	1A	3091	1/1	0.87	0.23	57,57,57,57	0
54	MG	2A	3067	1/1	0.87	0.44	46,46,46,46	0
54	MG	1B	1012	1/1	0.87	0.08	79,79,79,79	0
56	ZN	24	101	1/1	0.87	0.06	154,154,154,154	0
54	MG	1A	3587	1/1	0.88	0.09	64,64,64,64	0
54	MG	1a	1849	1/1	0.88	0.15	62,62,62,62	0
54	MG	2A	3263	1/1	0.88	0.16	85,85,85,85	0
54	MG	1A	3640	1/1	0.88	0.13	48,48,48,48	0
54	MG	2A	3420	1/1	0.88	0.18	51,51,51,51	0
54	MG	2A	3274	1/1	0.88	0.17	45,45,45,45	0
54	MG	1a	1781	1/1	0.88	0.12	83,83,83,83	0
54	MG	2A	3141	1/1	0.88	0.34	78,78,78,78	0
54	MG	2A	3049	1/1	0.88	0.15	65,65,65,65	0
54	MG	2A	3287	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3144	1/1	0.88	0.26	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1701	1/1	0.88	0.24	93,93,93,93	0
54	MG	1A	3759	1/1	0.88	0.21	51,51,51,51	0
54	MG	2A	3152	1/1	0.88	0.20	71,71,71,71	0
54	MG	2A	3592	1/1	0.88	0.10	63,63,63,63	0
54	MG	2A	3593	1/1	0.88	0.07	99,99,99,99	0
54	MG	1A	3075	1/1	0.88	0.63	48,48,48,48	0
54	MG	1A	3316	1/1	0.88	0.23	99,99,99,99	0
54	MG	1a	1637	1/1	0.88	1.17	79,79,79,79	0
54	MG	2A	3605	1/1	0.88	0.21	65,65,65,65	0
54	MG	1d	504	1/1	0.88	0.27	70,70,70,70	0
54	MG	1A	3864	1/1	0.88	0.16	50,50,50,50	0
54	MG	2A	3461	1/1	0.88	0.24	87,87,87,87	0
54	MG	1A	3544	1/1	0.88	0.19	69,69,69,69	0
54	MG	1A	3874	1/1	0.88	0.21	65,65,65,65	0
54	MG	1a	1651	1/1	0.88	0.11	54,54,54,54	0
54	MG	1A	3449	1/1	0.88	0.29	72,72,72,72	0
54	MG	2A	3471	1/1	0.88	0.26	58,58,58,58	0
54	MG	1A	3395	1/1	0.88	0.30	57,57,57,57	0
54	MG	2A	3178	1/1	0.88	0.50	44,44,44,44	0
54	MG	2A	3474	1/1	0.88	0.11	84,84,84,84	0
54	MG	2A	3478	1/1	0.88	0.15	85,85,85,85	0
54	MG	1V	201	1/1	0.88	0.31	56,56,56,56	0
54	MG	1A	3359	1/1	0.88	0.20	38,38,38,38	0
54	MG	1A	3554	1/1	0.88	0.18	70,70,70,70	0
54	MG	1a	1740	1/1	0.88	0.32	77,77,77,77	0
54	MG	2A	3186	1/1	0.88	0.26	65,65,65,65	0
54	MG	1A	3517	1/1	0.88	0.33	71,71,71,71	0
54	MG	1A	3007	1/1	0.88	0.26	35,35,35,35	0
54	MG	1A	3681	1/1	0.88	0.13	99,99,99,99	0
54	MG	2A	3490	1/1	0.88	0.14	64,64,64,64	0
54	MG	1A	3299	1/1	0.88	0.40	58,58,58,58	0
54	MG	2A	3492	1/1	0.88	0.17	51,51,51,51	0
54	MG	2A	3091	1/1	0.88	0.37	67,67,67,67	0
54	MG	2a	1722	1/1	0.88	0.06	109,109,109,109	0
54	MG	2A	3350	1/1	0.88	0.15	43,43,43,43	0
54	MG	1A	3526	1/1	0.88	0.23	83,83,83,83	0
54	MG	2a	1726	1/1	0.88	0.07	83,83,83,83	0
54	MG	2A	3006	1/1	0.88	0.28	64,64,64,64	0
54	MG	2A	3509	1/1	0.88	0.10	65,65,65,65	0
54	MG	1A	3823	1/1	0.88	0.12	82,82,82,82	0
54	MG	1A	3006	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3520	1/1	0.88	0.28	91,91,91,91	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3521	1/1	0.88	0.15	88,88,88,88	0
54	MG	2Y	201	1/1	0.88	0.10	66,66,66,66	0
54	MG	1B	1023	1/1	0.88	0.17	66,66,66,66	0
54	MG	2A	3524	1/1	0.88	0.21	47,47,47,47	0
54	MG	1A	3432	1/1	0.88	0.12	53,53,53,53	0
54	MG	2A	3531	1/1	0.88	0.48	74,74,74,74	0
54	MG	2a	1744	1/1	0.88	0.06	73,73,73,73	0
54	MG	1A	3836	1/1	0.88	0.15	35,35,35,35	0
54	MG	2A	3107	1/1	0.88	0.42	85,85,85,85	0
54	MG	2A	3109	1/1	0.88	0.61	57,57,57,57	0
54	MG	2a	1750	1/1	0.88	0.21	79,79,79,79	0
54	MG	1a	1613	1/1	0.88	0.12	69,69,69,69	0
54	MG	1A	3745	1/1	0.88	0.26	80,80,80,80	0
54	MG	2A	3383	1/1	0.88	0.07	81,81,81,81	0
54	MG	1A	3048	1/1	0.88	0.26	60,60,60,60	0
54	MG	1a	1832	1/1	0.88	0.13	90,90,90,90	0
54	MG	2A	3386	1/1	0.88	0.27	86,86,86,86	0
54	MG	2a	1627	1/1	0.88	0.20	69,69,69,69	0
54	MG	2A	3554	1/1	0.88	0.12	72,72,72,72	0
54	MG	1a	1623	1/1	0.88	0.26	62,62,62,62	0
54	MG	1A	3624	1/1	0.88	0.18	70,70,70,70	0
54	MG	1a	1774	1/1	0.88	0.17	103,103,103,103	0
54	MG	2A	3396	1/1	0.88	0.14	82,82,82,82	0
54	MG	2A	3120	1/1	0.88	0.32	82,82,82,82	0
54	MG	2A	3124	1/1	0.88	0.27	93,93,93,93	0
54	MG	2A	3568	1/1	0.88	0.09	78,78,78,78	0
54	MG	1A	3417	1/1	0.88	0.16	34,34,34,34	0
54	MG	1A	3534	1/1	0.89	0.39	57,57,57,57	0
54	MG	2a	1624	1/1	0.89	0.25	55,55,55,55	0
54	MG	2A	3339	1/1	0.89	0.12	68,68,68,68	0
54	MG	1A	3058	1/1	0.89	0.22	51,51,51,51	0
54	MG	2a	1628	1/1	0.89	0.24	94,94,94,94	0
54	MG	1A	3268	1/1	0.89	0.14	42,42,42,42	0
54	MG	2A	3536	1/1	0.89	0.53	71,71,71,71	0
54	MG	1A	3711	1/1	0.89	0.05	72,72,72,72	0
54	MG	2A	3157	1/1	0.89	0.20	56,56,56,56	0
54	MG	2A	3347	1/1	0.89	0.13	45,45,45,45	0
54	MG	1F	313	1/1	0.89	0.19	64,64,64,64	0
54	MG	1A	3270	1/1	0.89	0.48	59,59,59,59	0
54	MG	1A	3825	1/1	0.89	0.40	72,72,72,72	0
54	MG	2A	3354	1/1	0.89	0.34	92,92,92,92	0
54	MG	1N	203	1/1	0.89	0.45	88,88,88,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3341	1/1	0.89	0.19	30,30,30,30	0
54	MG	1A	3831	1/1	0.89	0.42	92,92,92,92	0
54	MG	1A	3350	1/1	0.89	0.14	55,55,55,55	0
54	MG	1A	3412	1/1	0.89	0.14	28,28,28,28	0
54	MG	2a	1649	1/1	0.89	0.14	40,40,40,40	0
54	MG	2a	1650	1/1	0.89	0.29	59,59,59,59	0
54	MG	1a	1693	1/1	0.89	0.31	68,68,68,68	0
54	MG	2A	3046	1/1	0.89	0.25	69,69,69,69	0
54	MG	1A	3474	1/1	0.89	0.15	56,56,56,56	0
54	MG	1T	2004	1/1	0.89	0.31	69,69,69,69	0
54	MG	1A	3098	1/1	0.89	0.36	44,44,44,44	0
54	MG	2A	3052	1/1	0.89	0.33	75,75,75,75	0
54	MG	1A	3012	1/1	0.89	0.21	58,58,58,58	0
54	MG	1W	203	1/1	0.89	0.21	45,45,45,45	0
54	MG	2A	3059	1/1	0.89	0.19	54,54,54,54	0
54	MG	2A	3060	1/1	0.89	0.18	66,66,66,66	0
54	MG	1A	3416	1/1	0.89	0.26	41,41,41,41	0
54	MG	1A	3231	1/1	0.89	0.22	55,55,55,55	0
54	MG	2A	3064	1/1	0.89	0.52	77,77,77,77	0
54	MG	1A	3482	1/1	0.89	0.17	52,52,52,52	0
54	MG	2A	3203	1/1	0.89	0.42	66,66,66,66	0
54	MG	2A	3069	1/1	0.89	0.16	60,60,60,60	0
54	MG	1a	1824	1/1	0.89	0.27	82,82,82,82	0
54	MG	1A	3126	1/1	0.89	0.23	42,42,42,42	0
54	MG	2A	3409	1/1	0.89	0.16	45,45,45,45	0
54	MG	13	102	1/1	0.89	0.26	55,55,55,55	0
54	MG	2A	3415	1/1	0.89	0.15	59,59,59,59	0
54	MG	2a	1685	1/1	0.89	0.59	71,71,71,71	0
54	MG	1A	3859	1/1	0.89	0.41	74,74,74,74	0
54	MG	2A	3598	1/1	0.89	0.20	64,64,64,64	0
54	MG	1A	3497	1/1	0.89	0.25	44,44,44,44	0
54	MG	1A	3573	1/1	0.89	0.18	30,30,30,30	0
54	MG	2A	3220	1/1	0.89	0.26	70,70,70,70	0
54	MG	1A	3113	1/1	0.89	0.22	54,54,54,54	0
54	MG	2A	3440	1/1	0.89	0.55	76,76,76,76	0
54	MG	1A	3177	1/1	0.89	0.27	49,49,49,49	0
54	MG	1A	3747	1/1	0.89	0.12	54,54,54,54	0
54	MG	1A	3676	1/1	0.89	0.38	77,77,77,77	0
54	MG	1a	1611	1/1	0.89	0.16	90,90,90,90	0
54	MG	1A	3130	1/1	0.89	0.32	39,39,39,39	0
54	MG	1A	3885	1/1	0.89	0.22	53,53,53,53	0
54	MG	1a	1616	1/1	0.89	0.20	106,106,106,106	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3218	1/1	0.89	0.16	50,50,50,50	0
54	MG	2A	3253	1/1	0.89	0.18	51,51,51,51	0
54	MG	1a	1746	1/1	0.89	0.29	91,91,91,91	0
54	MG	1a	1747	1/1	0.89	0.38	109,109,109,109	0
54	MG	2a	1721	1/1	0.89	0.11	86,86,86,86	0
54	MG	1A	3372	1/1	0.89	0.25	59,59,59,59	0
54	MG	1A	3896	1/1	0.89	0.48	51,51,51,51	0
54	MG	1d	503	1/1	0.89	0.28	85,85,85,85	0
54	MG	2A	3278	1/1	0.89	0.22	65,65,65,65	0
54	MG	1a	1751	1/1	0.89	0.19	80,80,80,80	0
54	MG	2A	3280	1/1	0.89	0.14	53,53,53,53	0
54	MG	2A	3281	1/1	0.89	0.16	65,65,65,65	0
54	MG	1a	1628	1/1	0.89	0.15	67,67,67,67	0
54	MG	1B	1004	1/1	0.89	0.13	60,60,60,60	0
54	MG	1A	3758	1/1	0.89	0.20	84,84,84,84	0
54	MG	2B	216	1/1	0.89	0.10	106,106,106,106	0
54	MG	1A	3244	1/1	0.89	0.23	87,87,87,87	0
54	MG	2a	1739	1/1	0.89	0.15	98,98,98,98	0
54	MG	1A	3520	1/1	0.89	0.14	51,51,51,51	0
54	MG	1A	3180	1/1	0.89	0.25	37,37,37,37	0
54	MG	1A	3382	1/1	0.89	0.16	63,63,63,63	0
54	MG	2G	202	1/1	0.89	0.15	108,108,108,108	0
54	MG	1A	3777	1/1	0.89	0.28	35,35,35,35	0
54	MG	2I	201	1/1	0.89	0.17	87,87,87,87	0
54	MG	1A	3602	1/1	0.89	0.68	54,54,54,54	0
54	MG	1a	1645	1/1	0.89	0.60	73,73,73,73	0
54	MG	1A	3131	1/1	0.89	0.18	39,39,39,39	0
54	MG	2T	202	1/1	0.89	0.32	65,65,65,65	0
54	MG	2A	3309	1/1	0.89	0.18	94,94,94,94	0
54	MG	1A	3782	1/1	0.89	0.13	35,35,35,35	0
54	MG	1y	202	1/1	0.89	0.29	98,98,98,98	0
54	MG	2A	3494	1/1	0.89	0.08	71,71,71,71	0
54	MG	2a	1763	1/1	0.89	0.13	96,96,96,96	0
54	MG	2A	3131	1/1	0.89	0.31	64,64,64,64	0
54	MG	1B	1029	1/1	0.89	0.17	80,80,80,80	0
54	MG	2f	201	1/1	0.89	0.15	79,79,79,79	0
54	MG	1A	3790	1/1	0.89	0.18	34,34,34,34	0
54	MG	1D	304	1/1	0.89	0.31	47,47,47,47	0
54	MG	1a	1780	1/1	0.89	0.35	83,83,83,83	0
54	MG	1D	307	1/1	0.89	0.26	36,36,36,36	0
54	MG	2a	1609	1/1	0.89	0.20	62,62,62,62	0
54	MG	1A	3699	1/1	0.89	0.15	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3386	1/1	0.89	0.17	67,67,67,67	0
54	MG	1A	3702	1/1	0.89	0.25	71,71,71,71	0
54	MG	2A	3391	1/1	0.90	0.19	65,65,65,65	0
54	MG	1A	3205	1/1	0.90	0.18	58,58,58,58	0
54	MG	2a	1634	1/1	0.90	0.29	101,101,101,101	0
54	MG	1A	3826	1/1	0.90	0.04	90,90,90,90	0
54	MG	1B	1022	1/1	0.90	0.13	59,59,59,59	0
54	MG	1f	201	1/1	0.90	0.21	68,68,68,68	0
54	MG	2A	3398	1/1	0.90	0.05	78,78,78,78	0
54	MG	1A	3604	1/1	0.90	0.78	55,55,55,55	0
54	MG	1a	1686	1/1	0.90	0.41	88,88,88,88	0
54	MG	1B	1026	1/1	0.90	0.21	94,94,94,94	0
54	MG	1a	1689	1/1	0.90	0.34	61,61,61,61	0
54	MG	1l	202	1/1	0.90	0.14	51,51,51,51	0
54	MG	1A	3089	1/1	0.90	0.42	45,45,45,45	0
54	MG	1A	3245	1/1	0.90	0.19	56,56,56,56	0
54	MG	1a	1788	1/1	0.90	0.17	106,106,106,106	0
54	MG	2A	3416	1/1	0.90	0.09	48,48,48,48	0
54	MG	2A	3578	1/1	0.90	0.15	52,52,52,52	0
54	MG	2A	3419	1/1	0.90	0.33	55,55,55,55	0
54	MG	1A	3229	1/1	0.90	0.43	38,38,38,38	0
54	MG	2A	3421	1/1	0.90	0.17	68,68,68,68	0
54	MG	1A	3556	1/1	0.90	0.15	53,53,53,53	0
54	MG	2A	3261	1/1	0.90	0.44	74,74,74,74	0
54	MG	1A	3558	1/1	0.90	0.48	81,81,81,81	0
54	MG	2A	3429	1/1	0.90	0.09	81,81,81,81	0
54	MG	1a	1793	1/1	0.90	0.17	89,89,89,89	0
54	MG	1a	1621	1/1	0.90	0.19	59,59,59,59	0
54	MG	2a	1665	1/1	0.90	0.19	37,37,37,37	0
54	MG	1A	3252	1/1	0.90	0.17	45,45,45,45	0
54	MG	2A	3443	1/1	0.90	0.14	111,111,111,111	0
54	MG	1a	1625	1/1	0.90	0.44	54,54,54,54	0
54	MG	2A	3122	1/1	0.90	0.25	74,74,74,74	0
54	MG	2A	3602	1/1	0.90	0.21	99,99,99,99	0
54	MG	2a	1674	1/1	0.90	0.28	66,66,66,66	0
54	MG	2A	3603	1/1	0.90	0.15	78,78,78,78	0
54	MG	1A	3450	1/1	0.90	0.17	61,61,61,61	0
54	MG	1A	3052	1/1	0.90	0.09	85,85,85,85	0
54	MG	2A	3012	1/1	0.90	0.23	73,73,73,73	0
54	MG	1a	1706	1/1	0.90	0.07	72,72,72,72	0
54	MG	1a	1629	1/1	0.90	0.47	68,68,68,68	0
54	MG	1A	3178	1/1	0.90	0.25	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2a	1687	1/1	0.90	0.16	70,70,70,70	0
54	MG	1A	3366	1/1	0.90	0.15	45,45,45,45	0
54	MG	2A	3457	1/1	0.90	0.12	79,79,79,79	0
54	MG	1a	1809	1/1	0.90	0.13	87,87,87,87	0
54	MG	1A	3626	1/1	0.90	0.25	58,58,58,58	0
54	MG	1A	3574	1/1	0.90	0.10	69,69,69,69	0
54	MG	2a	1696	1/1	0.90	0.10	82,82,82,82	0
54	MG	1A	3194	1/1	0.90	0.34	50,50,50,50	0
54	MG	2A	3150	1/1	0.90	0.12	135,135,135,135	0
54	MG	1a	1718	1/1	0.90	0.20	86,86,86,86	0
54	MG	1A	3102	1/1	0.90	0.21	42,42,42,42	0
54	MG	2A	3041	1/1	0.90	0.17	81,81,81,81	0
54	MG	2A	3314	1/1	0.90	0.08	81,81,81,81	0
54	MG	1A	3866	1/1	0.90	0.13	102,102,102,102	0
54	MG	1a	1727	1/1	0.90	0.15	67,67,67,67	0
54	MG	1A	3282	1/1	0.90	0.16	64,64,64,64	0
54	MG	2A	3161	1/1	0.90	0.32	59,59,59,59	0
54	MG	1a	1643	1/1	0.90	0.22	87,87,87,87	0
54	MG	2B	212	1/1	0.90	0.16	111,111,111,111	0
54	MG	2A	3484	1/1	0.90	0.15	64,64,64,64	0
54	MG	1A	3160	1/1	0.90	0.44	37,37,37,37	0
54	MG	1A	3654	1/1	0.90	0.07	59,59,59,59	0
54	MG	2A	3170	1/1	0.90	0.46	55,55,55,55	0
54	MG	1A	3789	1/1	0.90	0.07	58,58,58,58	0
54	MG	1A	3881	1/1	0.90	0.29	38,38,38,38	0
54	MG	2E	302	1/1	0.90	0.48	66,66,66,66	0
54	MG	1A	3659	1/1	0.90	0.47	62,62,62,62	0
54	MG	2A	3056	1/1	0.90	0.25	31,31,31,31	0
54	MG	1A	3224	1/1	0.90	0.27	45,45,45,45	0
54	MG	1a	1838	1/1	0.90	0.12	90,90,90,90	0
54	MG	1a	1659	1/1	0.90	0.12	70,70,70,70	0
54	MG	1a	1841	1/1	0.90	0.32	72,72,72,72	0
54	MG	2A	3507	1/1	0.90	0.10	50,50,50,50	0
54	MG	1a	1660	1/1	0.90	0.23	85,85,85,85	0
54	MG	1A	3888	1/1	0.90	0.47	80,80,80,80	0
54	MG	2A	3515	1/1	0.90	0.14	45,45,45,45	0
54	MG	2W	202	1/1	0.90	0.18	79,79,79,79	0
54	MG	1A	3664	1/1	0.90	0.16	32,32,32,32	0
54	MG	2A	3068	1/1	0.90	0.31	51,51,51,51	0
54	MG	1A	3292	1/1	0.90	0.08	45,45,45,45	0
54	MG	1A	3385	1/1	0.90	0.20	70,70,70,70	0
54	MG	1a	1851	1/1	0.90	0.24	76,76,76,76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1a	1667	1/1	0.90	0.24	85,85,85,85	0
54	MG	2A	3527	1/1	0.90	0.21	55,55,55,55	0
54	MG	1A	3817	1/1	0.90	0.09	32,32,32,32	0
54	MG	1A	3347	1/1	0.90	0.14	82,82,82,82	0
54	MG	2A	3199	1/1	0.90	0.34	64,64,64,64	0
54	MG	2a	1760	1/1	0.90	0.12	102,102,102,102	0
54	MG	2a	1761	1/1	0.90	0.20	90,90,90,90	0
54	MG	1A	3298	1/1	0.90	0.08	55,55,55,55	0
54	MG	1a	1672	1/1	0.90	0.26	85,85,85,85	0
54	MG	2A	3375	1/1	0.90	0.11	50,50,50,50	0
54	MG	2a	1618	1/1	0.90	0.18	97,97,97,97	0
54	MG	2a	1620	1/1	0.90	0.27	60,60,60,60	0
54	MG	1A	3734	1/1	0.90	0.11	82,82,82,82	0
54	MG	2a	1622	1/1	0.90	0.15	38,38,38,38	0
54	MG	2a	1623	1/1	0.90	0.20	60,60,60,60	0
54	MG	1B	1015	1/1	0.90	0.16	79,79,79,79	0
54	MG	1a	1676	1/1	0.90	0.35	85,85,85,85	0
54	MG	1A	3675	1/1	0.90	0.20	53,53,53,53	0
54	MG	2A	3212	1/1	0.90	0.21	58,58,58,58	0
54	MG	1a	1775	1/1	0.90	0.13	98,98,98,98	0
54	MG	2a	1614	1/1	0.91	0.14	82,82,82,82	0
54	MG	1A	3321	1/1	0.91	0.24	61,61,61,61	0
54	MG	1W	204	1/1	0.91	0.29	52,52,52,52	0
54	MG	2A	3332	1/1	0.91	0.19	82,82,82,82	0
54	MG	1Z	301	1/1	0.91	0.12	51,51,51,51	0
54	MG	1A	3424	1/1	0.91	0.19	38,38,38,38	0
54	MG	2A	3518	1/1	0.91	0.25	65,65,65,65	0
54	MG	2A	3336	1/1	0.91	0.23	92,92,92,92	0
54	MG	1A	3867	1/1	0.91	0.35	46,46,46,46	0
54	MG	1A	3581	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3341	1/1	0.91	0.20	83,83,83,83	0
54	MG	2A	3156	1/1	0.91	0.20	57,57,57,57	0
54	MG	1A	3322	1/1	0.91	0.25	58,58,58,58	0
54	MG	13	101	1/1	0.91	0.48	76,76,76,76	0
54	MG	1A	3114	1/1	0.91	0.17	40,40,40,40	0
54	MG	2A	3532	1/1	0.91	0.07	89,89,89,89	0
54	MG	2A	3035	1/1	0.91	0.11	68,68,68,68	0
54	MG	1A	3679	1/1	0.91	0.24	73,73,73,73	0
54	MG	1a	1698	1/1	0.91	0.30	48,48,48,48	0
54	MG	2a	1637	1/1	0.91	0.26	65,65,65,65	0
54	MG	1A	3056	1/1	0.91	0.28	42,42,42,42	0
54	MG	1A	3383	1/1	0.91	0.13	80,80,80,80	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3773	1/1	0.91	0.21	79,79,79,79	0
54	MG	1A	3433	1/1	0.91	0.11	66,66,66,66	0
54	MG	2A	3544	1/1	0.91	0.12	86,86,86,86	0
54	MG	1A	3057	1/1	0.91	0.21	56,56,56,56	0
54	MG	2A	3048	1/1	0.91	0.09	80,80,80,80	0
54	MG	1A	3150	1/1	0.91	0.25	41,41,41,41	0
54	MG	2A	3367	1/1	0.91	0.08	93,93,93,93	0
54	MG	2A	3369	1/1	0.91	0.22	53,53,53,53	0
54	MG	1a	1818	1/1	0.91	0.16	56,56,56,56	0
54	MG	1a	1606	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3563	1/1	0.91	0.15	67,67,67,67	0
54	MG	1A	3899	1/1	0.91	0.24	54,54,54,54	0
54	MG	1B	1002	1/1	0.91	0.12	57,57,57,57	0
54	MG	1A	3444	1/1	0.91	0.12	34,34,34,34	0
54	MG	2A	3057	1/1	0.91	0.16	55,55,55,55	0
54	MG	1A	3528	1/1	0.91	0.12	66,66,66,66	0
54	MG	1B	1008	1/1	0.91	0.20	64,64,64,64	0
54	MG	2a	1662	1/1	0.91	0.17	64,64,64,64	0
54	MG	1A	3785	1/1	0.91	0.23	63,63,63,63	0
54	MG	1B	1010	1/1	0.91	0.37	58,58,58,58	0
54	MG	1A	3695	1/1	0.91	0.10	57,57,57,57	0
54	MG	1a	1829	1/1	0.91	0.15	76,76,76,76	0
54	MG	2A	3066	1/1	0.91	0.18	50,50,50,50	0
54	MG	1a	1726	1/1	0.91	0.31	61,61,61,61	0
54	MG	1A	3026	1/1	0.91	0.18	48,48,48,48	0
54	MG	1A	3340	1/1	0.91	0.15	31,31,31,31	0
54	MG	1a	1837	1/1	0.91	0.07	64,64,64,64	0
54	MG	1a	1733	1/1	0.91	0.27	76,76,76,76	0
54	MG	2A	3585	1/1	0.91	0.16	81,81,81,81	0
54	MG	2A	3211	1/1	0.91	0.45	69,69,69,69	0
54	MG	2A	3074	1/1	0.91	0.07	80,80,80,80	0
54	MG	1A	3797	1/1	0.91	0.12	82,82,82,82	0
54	MG	1A	3799	1/1	0.91	0.44	53,53,53,53	0
54	MG	1A	3802	1/1	0.91	0.29	75,75,75,75	0
54	MG	1A	3803	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3224	1/1	0.91	0.19	51,51,51,51	0
54	MG	1A	3533	1/1	0.91	0.76	43,43,43,43	0
54	MG	2a	1691	1/1	0.91	0.13	91,91,91,91	0
54	MG	1B	1024	1/1	0.91	0.09	61,61,61,61	0
54	MG	1A	3289	1/1	0.91	0.09	47,47,47,47	0
54	MG	1A	3125	1/1	0.91	0.18	37,37,37,37	0
54	MG	1A	3451	1/1	0.91	0.32	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
54	MG	1A	3709	1/1	0.91	0.17	58,58,58,58	0
54	MG	1a	1752	1/1	0.91	0.21	61,61,61,61	0
54	MG	1A	3539	1/1	0.91	0.11	26,26,26,26	0
54	MG	2a	1704	1/1	0.91	0.19	84,84,84,84	0
54	MG	2A	3246	1/1	0.91	0.43	88,88,88,88	0
54	MG	2A	3248	1/1	0.91	0.31	48,48,48,48	0
54	MG	1a	1758	1/1	0.91	0.12	48,48,48,48	0
54	MG	1A	3402	1/1	0.91	0.24	58,58,58,58	0
54	MG	2A	3255	1/1	0.91	0.14	50,50,50,50	0
54	MG	2a	1713	1/1	0.91	0.11	85,85,85,85	0
54	MG	2A	3449	1/1	0.91	0.20	65,65,65,65	0
54	MG	2A	3257	1/1	0.91	0.10	89,89,89,89	0
54	MG	1A	3457	1/1	0.91	0.12	46,46,46,46	0
54	MG	2A	3641	1/1	0.91	0.83	88,88,88,88	0
54	MG	1A	3824	1/1	0.91	0.16	63,63,63,63	0
54	MG	2A	3101	1/1	0.91	0.27	56,56,56,56	0
54	MG	1A	3062	1/1	0.91	0.54	41,41,41,41	0
54	MG	1A	3469	1/1	0.91	0.14	73,73,73,73	0
54	MG	1a	1766	1/1	0.91	0.09	83,83,83,83	0
54	MG	2A	3277	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3458	1/1	0.91	0.33	59,59,59,59	0
54	MG	2A	3459	1/1	0.91	0.14	64,64,64,64	0
54	MG	2A	3460	1/1	0.91	0.08	73,73,73,73	0
54	MG	1e	201	1/1	0.91	0.17	66,66,66,66	0
54	MG	2A	3108	1/1	0.91	0.10	50,50,50,50	0
54	MG	1A	3127	1/1	0.91	0.22	44,44,44,44	0
54	MG	1A	3033	1/1	0.91	0.15	67,67,67,67	0
54	MG	2A	3284	1/1	0.91	0.10	43,43,43,43	0
54	MG	1A	3251	1/1	0.91	0.17	41,41,41,41	0
54	MG	1A	3728	1/1	0.91	0.28	60,60,60,60	0
54	MG	1a	1772	1/1	0.91	0.17	83,83,83,83	0
54	MG	1A	3305	1/1	0.91	0.22	23,23,23,23	0
54	MG	2A	3475	1/1	0.91	0.13	88,88,88,88	0
54	MG	2F	302	1/1	0.91	0.29	69,69,69,69	0
54	MG	1G	203	1/1	0.91	0.42	91,91,91,91	0
54	MG	1A	3069	1/1	0.91	0.23	39,39,39,39	0
54	MG	2A	3300	1/1	0.91	0.13	51,51,51,51	0
54	MG	1n	101	1/1	0.91	0.46	85,85,85,85	0
54	MG	1A	3311	1/1	0.91	0.17	74,74,74,74	0
54	MG	2P	202	1/1	0.91	0.20	90,90,90,90	0
54	MG	1A	3849	1/1	0.91	0.18	78,78,78,78	0
54	MG	1A	3658	1/1	0.91	0.11	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3258	1/1	0.91	0.17	81,81,81,81	0
54	MG	1A	3021	1/1	0.91	0.20	60,60,60,60	0
54	MG	2A	3133	1/1	0.91	0.26	66,66,66,66	0
54	MG	1A	3133	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3491	1/1	0.91	0.06	66,66,66,66	0
54	MG	1A	3492	1/1	0.91	0.20	70,70,70,70	0
54	MG	28	101	1/1	0.91	0.33	70,70,70,70	0
54	MG	2a	1601	1/1	0.91	0.15	74,74,74,74	0
54	MG	1a	1785	1/1	0.91	0.14	84,84,84,84	0
54	MG	1a	1786	1/1	0.91	0.09	82,82,82,82	0
54	MG	2A	3496	1/1	0.91	0.22	69,69,69,69	0
54	MG	1A	3495	1/1	0.91	0.25	65,65,65,65	0
54	MG	2A	3499	1/1	0.91	0.09	64,64,64,64	0
54	MG	1W	202	1/1	0.91	0.14	59,59,59,59	0
54	MG	2A	3503	1/1	0.91	0.14	69,69,69,69	0
54	MG	1A	3312	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3414	1/1	0.92	0.16	69,69,69,69	0
54	MG	1A	3901	1/1	0.92	0.27	64,64,64,64	0
54	MG	2A	3039	1/1	0.92	0.52	48,48,48,48	0
54	MG	2a	1610	1/1	0.92	0.39	106,106,106,106	0
54	MG	1A	3798	1/1	0.92	0.40	71,71,71,71	0
54	MG	1A	3135	1/1	0.92	0.10	72,72,72,72	0
54	MG	1B	1006	1/1	0.92	0.15	69,69,69,69	0
54	MG	2A	3516	1/1	0.92	0.41	85,85,85,85	0
54	MG	2A	3167	1/1	0.92	0.42	56,56,56,56	0
54	MG	2a	1619	1/1	0.92	0.09	81,81,81,81	0
54	MG	2A	3338	1/1	0.92	0.30	64,64,64,64	0
54	MG	1A	3215	1/1	0.92	0.14	29,29,29,29	0
54	MG	2A	3340	1/1	0.92	0.26	57,57,57,57	0
54	MG	1a	1708	1/1	0.92	0.32	64,64,64,64	0
54	MG	1A	3054	1/1	0.92	0.15	57,57,57,57	0
54	MG	1A	3320	1/1	0.92	0.13	52,52,52,52	0
54	MG	2a	1626	1/1	0.92	0.29	57,57,57,57	0
54	MG	2A	3525	1/1	0.92	0.23	61,61,61,61	0
54	MG	1A	3278	1/1	0.92	0.11	45,45,45,45	0
54	MG	2A	3345	1/1	0.92	0.26	70,70,70,70	0
54	MG	1A	3138	1/1	0.92	0.22	41,41,41,41	0
54	MG	1A	3182	1/1	0.92	0.50	44,44,44,44	0
54	MG	2A	3348	1/1	0.92	0.16	37,37,37,37	0
54	MG	1A	3723	1/1	0.92	0.38	59,59,59,59	0
54	MG	2A	3054	1/1	0.92	0.23	38,38,38,38	0
54	MG	1A	3219	1/1	0.92	0.20	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1617	1/1	0.92	0.21	79,79,79,79	0
54	MG	2A	3541	1/1	0.92	0.09	85,85,85,85	0
54	MG	1A	3328	1/1	0.92	0.10	35,35,35,35	0
54	MG	1a	1725	1/1	0.92	0.18	104,104,104,104	0
54	MG	1A	3381	1/1	0.92	0.26	58,58,58,58	0
54	MG	1A	3656	1/1	0.92	0.12	38,38,38,38	0
54	MG	1a	1830	1/1	0.92	0.29	62,62,62,62	0
54	MG	2A	3552	1/1	0.92	0.12	66,66,66,66	0
54	MG	1A	3139	1/1	0.92	0.33	42,42,42,42	0
54	MG	1A	3050	1/1	0.92	0.32	22,22,22,22	0
54	MG	1A	3249	1/1	0.92	0.25	45,45,45,45	0
54	MG	1B	1027	1/1	0.92	0.18	43,43,43,43	0
54	MG	1a	1737	1/1	0.92	0.11	94,94,94,94	0
54	MG	2A	3200	1/1	0.92	0.17	41,41,41,41	0
54	MG	1A	3575	1/1	0.92	0.09	41,41,41,41	0
54	MG	2A	3378	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3739	1/1	0.92	0.27	72,72,72,72	0
54	MG	2A	3204	1/1	0.92	0.18	51,51,51,51	0
54	MG	1A	3334	1/1	0.92	0.24	40,40,40,40	0
54	MG	1D	301	1/1	0.92	0.24	22,22,22,22	0
54	MG	1A	3338	1/1	0.92	0.20	18,18,18,18	0
54	MG	1A	3580	1/1	0.92	0.10	48,48,48,48	0
54	MG	1A	3840	1/1	0.92	0.18	62,62,62,62	0
54	MG	1a	1639	1/1	0.92	0.27	97,97,97,97	0
54	MG	1D	311	1/1	0.92	0.23	47,47,47,47	0
54	MG	1a	1855	1/1	0.92	0.10	74,74,74,74	0
54	MG	1A	3841	1/1	0.92	0.10	49,49,49,49	0
54	MG	1a	1756	1/1	0.92	0.30	78,78,78,78	0
54	MG	2A	3222	1/1	0.92	0.17	65,65,65,65	0
54	MG	1a	1757	1/1	0.92	0.16	62,62,62,62	0
54	MG	2A	3405	1/1	0.92	0.34	81,81,81,81	0
54	MG	1E	301	1/1	0.92	0.15	25,25,25,25	0
54	MG	1A	3843	1/1	0.92	0.39	54,54,54,54	0
54	MG	1a	1649	1/1	0.92	0.20	95,95,95,95	0
54	MG	1E	305	1/1	0.92	0.42	59,59,59,59	0
54	MG	2A	3411	1/1	0.92	0.07	78,78,78,78	0
54	MG	2A	3412	1/1	0.92	0.24	70,70,70,70	0
54	MG	2A	3595	1/1	0.92	0.24	68,68,68,68	0
54	MG	2A	3233	1/1	0.92	0.10	57,57,57,57	0
54	MG	1A	3442	1/1	0.92	0.20	35,35,35,35	0
53	MPD	1A	3001	8/8	0.92	0.24	58,65,67,67	0
54	MG	2A	3238	1/1	0.92	0.14	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3239	1/1	0.92	0.18	38,38,38,38	0
54	MG	1F	310	1/1	0.92	0.16	32,32,32,32	0
54	MG	2A	3098	1/1	0.92	0.22	58,58,58,58	0
54	MG	2A	3245	1/1	0.92	0.25	71,71,71,71	0
54	MG	2a	1700	1/1	0.92	0.08	106,106,106,106	0
54	MG	2A	3099	1/1	0.92	0.23	42,42,42,42	0
54	MG	2a	1702	1/1	0.92	0.14	83,83,83,83	0
54	MG	2a	1703	1/1	0.92	0.44	81,81,81,81	0
54	MG	2A	3436	1/1	0.92	0.18	73,73,73,73	0
54	MG	2A	3247	1/1	0.92	0.23	64,64,64,64	0
54	MG	2A	3439	1/1	0.92	0.12	65,65,65,65	0
54	MG	1A	3149	1/1	0.92	0.22	43,43,43,43	0
54	MG	2A	3621	1/1	0.92	0.23	73,73,73,73	0
54	MG	2A	3622	1/1	0.92	0.17	97,97,97,97	0
54	MG	1A	3588	1/1	0.92	0.09	82,82,82,82	0
54	MG	1A	3343	1/1	0.92	0.12	32,32,32,32	0
54	MG	2A	3633	1/1	0.92	0.23	46,46,46,46	0
54	MG	1A	3755	1/1	0.92	0.21	78,78,78,78	0
54	MG	1A	3856	1/1	0.92	0.25	53,53,53,53	0
54	MG	1A	3857	1/1	0.92	0.07	81,81,81,81	0
54	MG	1A	3525	1/1	0.92	0.12	62,62,62,62	0
54	MG	2A	3262	1/1	0.92	0.09	46,46,46,46	0
54	MG	1A	3593	1/1	0.92	0.24	84,84,84,84	0
54	MG	1l	201	1/1	0.92	0.06	65,65,65,65	0
54	MG	2A	3265	1/1	0.92	0.40	61,61,61,61	0
54	MG	2a	1730	1/1	0.92	0.26	97,97,97,97	0
54	MG	2A	3269	1/1	0.92	0.14	88,88,88,88	0
54	MG	2A	3273	1/1	0.92	0.07	73,73,73,73	0
54	MG	1A	3398	1/1	0.92	0.18	89,89,89,89	0
54	MG	1A	3399	1/1	0.92	0.08	78,78,78,78	0
54	MG	1R	201	1/1	0.92	0.29	46,46,46,46	0
54	MG	1o	101	1/1	0.92	0.15	42,42,42,42	0
54	MG	1A	3865	1/1	0.92	0.40	58,58,58,58	0
54	MG	2A	3119	1/1	0.92	0.55	76,76,76,76	0
54	MG	1A	3071	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3686	1/1	0.92	0.19	51,51,51,51	0
54	MG	1T	2006	1/1	0.92	0.21	83,83,83,83	0
54	MG	1U	202	1/1	0.92	0.15	37,37,37,37	0
54	MG	1A	3403	1/1	0.92	0.12	71,71,71,71	0
54	MG	1A	3603	1/1	0.92	0.12	51,51,51,51	0
54	MG	1A	3456	1/1	0.92	0.15	84,84,84,84	0
54	MG	2A	3134	1/1	0.92	0.46	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3298	1/1	0.92	0.25	82,82,82,82	0
54	MG	1A	3158	1/1	0.92	0.15	66,66,66,66	0
54	MG	1A	3259	1/1	0.92	0.33	79,79,79,79	0
54	MG	1a	1790	1/1	0.92	0.27	95,95,95,95	0
54	MG	2A	3139	1/1	0.92	0.44	74,74,74,74	0
54	MG	2R	201	1/1	0.92	0.25	58,58,58,58	0
54	MG	2A	3140	1/1	0.92	0.14	61,61,61,61	0
54	MG	2A	3485	1/1	0.92	0.14	66,66,66,66	0
54	MG	1X	102	1/1	0.92	0.09	62,62,62,62	0
54	MG	2T	203	1/1	0.92	0.29	73,73,73,73	0
54	MG	1A	3466	1/1	0.92	0.29	95,95,95,95	0
54	MG	2A	3312	1/1	0.92	0.10	62,62,62,62	0
54	MG	1a	1692	1/1	0.92	0.14	78,78,78,78	0
54	MG	20	101	1/1	0.92	0.29	80,80,80,80	0
54	MG	2A	3145	1/1	0.92	0.29	62,62,62,62	0
54	MG	1a	1794	1/1	0.92	0.16	78,78,78,78	0
54	MG	1A	3023	1/1	0.92	0.27	33,33,33,33	0
54	MG	1A	3470	1/1	0.92	0.17	45,45,45,45	0
54	MG	1A	3890	1/1	0.92	0.77	45,45,45,45	0
54	MG	2A	3326	1/1	0.92	0.15	75,75,75,75	0
54	MG	1A	3795	1/1	0.92	0.09	60,60,60,60	0
54	MG	1a	1661	1/1	0.93	0.40	86,86,86,86	0
54	MG	1A	3261	1/1	0.93	0.16	30,30,30,30	0
54	MG	2A	3286	1/1	0.93	0.18	53,53,53,53	0
54	MG	2A	3125	1/1	0.93	0.16	73,73,73,73	0
54	MG	2A	3127	1/1	0.93	0.13	49,49,49,49	0
54	MG	1A	3858	1/1	0.93	0.16	77,77,77,77	0
54	MG	1A	3760	1/1	0.93	0.08	71,71,71,71	0
54	MG	1A	3044	1/1	0.93	0.16	41,41,41,41	0
54	MG	1y	201	1/1	0.93	0.21	91,91,91,91	0
54	MG	1A	3392	1/1	0.93	0.15	80,80,80,80	0
54	MG	1A	3622	1/1	0.93	0.12	51,51,51,51	0
54	MG	2a	1602	1/1	0.93	0.18	62,62,62,62	0
54	MG	1A	3697	1/1	0.93	0.21	72,72,72,72	0
54	MG	1A	3623	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3779	1/1	0.93	0.10	68,68,68,68	0
54	MG	1A	3871	1/1	0.93	0.20	83,83,83,83	0
54	MG	2A	3308	1/1	0.93	0.33	52,52,52,52	0
54	MG	1a	1674	1/1	0.93	0.20	52,52,52,52	0
54	MG	2A	3311	1/1	0.93	0.27	66,66,66,66	0
54	MG	1A	3527	1/1	0.93	0.23	56,56,56,56	0
54	MG	2a	1611	1/1	0.93	0.11	76,76,76,76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3296	1/1	0.93	0.27	38,38,38,38	0
54	MG	1A	3628	1/1	0.93	0.30	47,47,47,47	0
54	MG	2A	3013	1/1	0.93	0.16	59,59,59,59	0
54	MG	2A	3016	1/1	0.93	0.20	71,71,71,71	0
54	MG	1A	3783	1/1	0.93	0.24	51,51,51,51	0
54	MG	2A	3323	1/1	0.93	0.13	65,65,65,65	0
54	MG	2A	3324	1/1	0.93	0.21	46,46,46,46	0
54	MG	2A	3506	1/1	0.93	0.18	64,64,64,64	0
54	MG	2A	3018	1/1	0.93	0.55	45,45,45,45	0
54	MG	1a	1682	1/1	0.93	0.10	69,69,69,69	0
54	MG	1A	3784	1/1	0.93	0.14	35,35,35,35	0
54	MG	2A	3511	1/1	0.93	0.13	89,89,89,89	0
54	MG	2A	3514	1/1	0.93	0.08	69,69,69,69	0
54	MG	1W	201	1/1	0.93	0.21	92,92,92,92	0
54	MG	2A	3024	1/1	0.93	0.39	68,68,68,68	0
54	MG	2A	3025	1/1	0.93	0.18	50,50,50,50	0
54	MG	2a	1630	1/1	0.93	0.36	55,55,55,55	0
54	MG	2a	1631	1/1	0.93	0.28	60,60,60,60	0
54	MG	2A	3158	1/1	0.93	0.10	68,68,68,68	0
54	MG	1A	3265	1/1	0.93	0.13	86,86,86,86	0
54	MG	2A	3030	1/1	0.93	0.21	64,64,64,64	0
54	MG	2A	3335	1/1	0.93	0.13	61,61,61,61	0
54	MG	2A	3164	1/1	0.93	0.25	62,62,62,62	0
54	MG	1A	3787	1/1	0.93	0.26	82,82,82,82	0
54	MG	1A	3705	1/1	0.93	0.16	46,46,46,46	0
54	MG	1X	101	1/1	0.93	0.16	66,66,66,66	0
54	MG	1a	1798	1/1	0.93	0.14	107,107,107,107	0
54	MG	1A	3484	1/1	0.93	0.25	64,64,64,64	0
54	MG	1a	1800	1/1	0.93	0.10	100,100,100,100	0
54	MG	1A	3892	1/1	0.93	0.29	35,35,35,35	0
54	MG	2A	3534	1/1	0.93	0.18	68,68,68,68	0
54	MG	2A	3176	1/1	0.93	0.27	54,54,54,54	0
54	MG	1A	3792	1/1	0.93	0.11	67,67,67,67	0
54	MG	10	103	1/1	0.93	0.31	56,56,56,56	0
54	MG	1A	3793	1/1	0.93	0.13	67,67,67,67	0
54	MG	2a	1651	1/1	0.93	0.24	68,68,68,68	0
54	MG	2A	3540	1/1	0.93	0.12	77,77,77,77	0
54	MG	1A	3267	1/1	0.93	0.18	58,58,58,58	0
54	MG	1A	3582	1/1	0.93	0.23	84,84,84,84	0
54	MG	1A	3650	1/1	0.93	0.22	61,61,61,61	0
54	MG	2A	3352	1/1	0.93	0.28	51,51,51,51	0
54	MG	1B	1003	1/1	0.93	0.23	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	15	103	1/1	0.93	0.15	67,67,67,67	0
54	MG	2A	3355	1/1	0.93	0.13	54,54,54,54	0
54	MG	1a	1812	1/1	0.93	0.16	90,90,90,90	0
54	MG	2A	3358	1/1	0.93	0.26	104,104,104,104	0
54	MG	1A	3583	1/1	0.93	0.23	60,60,60,60	0
54	MG	1A	3653	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3487	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3195	1/1	0.93	0.34	66,66,66,66	0
54	MG	2a	1669	1/1	0.93	0.22	61,61,61,61	0
54	MG	1a	1707	1/1	0.93	0.10	57,57,57,57	0
54	MG	1A	3535	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3489	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3490	1/1	0.93	0.17	60,60,60,60	0
54	MG	1a	1604	1/1	0.93	0.33	65,65,65,65	0
54	MG	2A	3201	1/1	0.93	0.29	51,51,51,51	0
54	MG	2A	3376	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3573	1/1	0.93	0.13	52,52,52,52	0
54	MG	2a	1682	1/1	0.93	0.21	71,71,71,71	0
54	MG	1A	3809	1/1	0.93	0.28	57,57,57,57	0
54	MG	1A	3811	1/1	0.93	0.51	58,58,58,58	0
54	MG	2A	3382	1/1	0.93	0.10	59,59,59,59	0
54	MG	2a	1686	1/1	0.93	0.05	67,67,67,67	0
54	MG	1A	3203	1/1	0.93	0.08	60,60,60,60	0
54	MG	2a	1688	1/1	0.93	0.20	64,64,64,64	0
54	MG	1a	1612	1/1	0.93	0.24	32,32,32,32	0
54	MG	1B	1016	1/1	0.93	0.17	55,55,55,55	0
54	MG	1A	3005	1/1	0.93	0.23	56,56,56,56	0
54	MG	1A	3729	1/1	0.93	0.20	46,46,46,46	0
54	MG	1A	3819	1/1	0.93	0.20	71,71,71,71	0
54	MG	2A	3584	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3072	1/1	0.93	0.14	51,51,51,51	0
54	MG	1a	1835	1/1	0.93	0.06	80,80,80,80	0
54	MG	2A	3214	1/1	0.93	0.34	48,48,48,48	0
54	MG	2a	1699	1/1	0.93	0.11	70,70,70,70	0
54	MG	1B	1020	1/1	0.93	0.12	50,50,50,50	0
54	MG	1a	1730	1/1	0.93	0.21	53,53,53,53	0
54	MG	1A	3594	1/1	0.93	0.30	31,31,31,31	0
54	MG	2A	3401	1/1	0.93	0.21	75,75,75,75	0
54	MG	2A	3221	1/1	0.93	0.21	65,65,65,65	0
54	MG	2a	1706	1/1	0.93	0.27	82,82,82,82	0
54	MG	1a	1622	1/1	0.93	0.16	106,106,106,106	0
54	MG	2A	3223	1/1	0.93	0.13	48,48,48,48	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3731	1/1	0.93	0.14	75,75,75,75	0
54	MG	1A	3595	1/1	0.93	0.22	50,50,50,50	0
54	MG	1a	1844	1/1	0.93	0.20	76,76,76,76	0
54	MG	1A	3668	1/1	0.93	0.18	41,41,41,41	0
54	MG	2A	3231	1/1	0.93	0.13	72,72,72,72	0
54	MG	2A	3606	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3607	1/1	0.93	0.26	52,52,52,52	0
54	MG	1a	1848	1/1	0.93	0.07	90,90,90,90	0
54	MG	2A	3413	1/1	0.93	0.20	77,77,77,77	0
54	MG	2A	3084	1/1	0.93	0.14	71,71,71,71	0
54	MG	1A	3376	1/1	0.93	0.22	30,30,30,30	0
54	MG	2a	1723	1/1	0.93	0.09	79,79,79,79	0
54	MG	2A	3418	1/1	0.93	0.16	71,71,71,71	0
54	MG	2A	3619	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3673	1/1	0.93	0.17	55,55,55,55	0
54	MG	2a	1728	1/1	0.93	0.05	87,87,87,87	0
54	MG	1A	3496	1/1	0.93	0.16	35,35,35,35	0
54	MG	1A	3406	1/1	0.93	0.13	67,67,67,67	0
54	MG	2A	3624	1/1	0.93	0.25	39,39,39,39	0
54	MG	2A	3241	1/1	0.93	0.07	86,86,86,86	0
54	MG	1A	3832	1/1	0.93	0.50	60,60,60,60	0
54	MG	2A	3243	1/1	0.93	0.07	67,67,67,67	0
54	MG	2A	3426	1/1	0.93	0.14	55,55,55,55	0
54	MG	2A	3428	1/1	0.93	0.08	61,61,61,61	0
54	MG	2A	3640	1/1	0.93	0.24	58,58,58,58	0
54	MG	1a	1633	1/1	0.93	0.09	85,85,85,85	0
54	MG	2A	3432	1/1	0.93	0.10	66,66,66,66	0
54	MG	2A	3433	1/1	0.93	0.09	43,43,43,43	0
54	MG	1A	3498	1/1	0.93	0.11	55,55,55,55	0
54	MG	1A	3744	1/1	0.93	0.19	55,55,55,55	0
54	MG	1D	308	1/1	0.93	0.14	55,55,55,55	0
54	MG	1a	1753	1/1	0.93	0.26	84,84,84,84	0
54	MG	2a	1747	1/1	0.93	0.42	129,129,129,129	0
54	MG	1A	3042	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3123	1/1	0.93	0.17	49,49,49,49	0
54	MG	2A	3444	1/1	0.93	0.13	68,68,68,68	0
54	MG	2A	3103	1/1	0.93	0.13	82,82,82,82	0
54	MG	1A	3411	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3680	1/1	0.93	0.10	64,64,64,64	0
54	MG	2A	3106	1/1	0.93	0.15	51,51,51,51	0
54	MG	1A	3309	1/1	0.93	0.26	59,59,59,59	0
54	MG	1A	3093	1/1	0.93	0.23	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3753	1/1	0.93	0.12	43,43,43,43	0
54	MG	1A	3754	1/1	0.93	0.13	29,29,29,29	0
54	MG	1A	3234	1/1	0.93	0.38	59,59,59,59	0
54	MG	2A	3272	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	3756	1/1	0.93	0.09	67,67,67,67	0
54	MG	1g	201	1/1	0.93	0.59	87,87,87,87	0
54	MG	1A	3475	1/1	0.93	0.22	44,44,44,44	0
54	MG	1a	1655	1/1	0.93	0.23	61,61,61,61	0
54	MG	1a	1657	1/1	0.93	0.17	95,95,95,95	0
54	MG	1A	3523	1/1	0.93	0.34	67,67,67,67	0
54	MG	2p	101	1/1	0.93	0.18	55,55,55,55	0
55	ARG	1B	1001	12/12	0.93	0.24	49,55,69,72	0
54	MG	1G	201	1/1	0.93	0.14	92,92,92,92	0
54	MG	2A	3121	1/1	0.93	0.23	82,82,82,82	0
54	MG	2A	3282	1/1	0.93	0.26	41,41,41,41	0
56	ZN	2n	101	1/1	0.93	0.09	120,120,120,120	0
54	MG	1A	3643	1/1	0.94	0.25	65,65,65,65	0
54	MG	1A	3725	1/1	0.94	0.12	76,76,76,76	0
54	MG	2A	3168	1/1	0.94	0.17	51,51,51,51	0
54	MG	1a	1697	1/1	0.94	0.25	63,63,63,63	0
54	MG	1A	3807	1/1	0.94	0.19	64,64,64,64	0
54	MG	15	101	1/1	0.94	0.26	44,44,44,44	0
54	MG	1A	3649	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3174	1/1	0.94	0.10	72,72,72,72	0
54	MG	1A	3200	1/1	0.94	0.28	40,40,40,40	0
54	MG	2A	3505	1/1	0.94	0.12	73,73,73,73	0
54	MG	2A	3047	1/1	0.94	0.17	61,61,61,61	0
54	MG	1A	3814	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3394	1/1	0.94	0.11	78,78,78,78	0
54	MG	1a	1816	1/1	0.94	0.10	79,79,79,79	0
54	MG	1a	1817	1/1	0.94	0.15	57,57,57,57	0
54	MG	1A	3027	1/1	0.94	0.23	49,49,49,49	0
54	MG	2A	3053	1/1	0.94	0.22	56,56,56,56	0
54	MG	1A	3348	1/1	0.94	0.13	37,37,37,37	0
54	MG	1A	3510	1/1	0.94	0.18	57,57,57,57	0
54	MG	1A	3657	1/1	0.94	0.09	64,64,64,64	0
54	MG	2A	3189	1/1	0.94	0.34	83,83,83,83	0
54	MG	1A	3514	1/1	0.94	0.29	58,58,58,58	0
54	MG	2A	3191	1/1	0.94	0.13	40,40,40,40	0
54	MG	1A	3397	1/1	0.94	0.23	67,67,67,67	0
54	MG	1a	1609	1/1	0.94	0.25	120,120,120,120	0
54	MG	1B	1021	1/1	0.94	0.09	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3738	1/1	0.94	0.13	43,43,43,43	0
54	MG	2A	3062	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3162	1/1	0.94	0.42	43,43,43,43	0
54	MG	1A	3663	1/1	0.94	0.15	51,51,51,51	0
54	MG	2A	3357	1/1	0.94	0.15	53,53,53,53	0
54	MG	1a	1720	1/1	0.94	0.27	94,94,94,94	0
54	MG	2A	3535	1/1	0.94	0.10	88,88,88,88	0
54	MG	1B	1025	1/1	0.94	0.15	70,70,70,70	0
54	MG	2A	3360	1/1	0.94	0.14	47,47,47,47	0
54	MG	2A	3361	1/1	0.94	0.16	53,53,53,53	0
54	MG	1a	1724	1/1	0.94	0.06	72,72,72,72	0
54	MG	1A	3742	1/1	0.94	0.13	59,59,59,59	0
54	MG	1A	3072	1/1	0.94	0.26	60,60,60,60	0
54	MG	1A	3401	1/1	0.94	0.05	53,53,53,53	0
54	MG	1a	1729	1/1	0.94	0.21	92,92,92,92	0
54	MG	1A	3585	1/1	0.94	0.13	62,62,62,62	0
54	MG	2A	3371	1/1	0.94	0.18	48,48,48,48	0
54	MG	2A	3549	1/1	0.94	0.39	60,60,60,60	0
54	MG	2A	3372	1/1	0.94	0.15	63,63,63,63	0
54	MG	1A	3835	1/1	0.94	0.33	50,50,50,50	0
54	MG	1A	3586	1/1	0.94	0.21	81,81,81,81	0
54	MG	1D	303	1/1	0.94	0.17	47,47,47,47	0
54	MG	2A	3555	1/1	0.94	0.11	71,71,71,71	0
54	MG	1A	3210	1/1	0.94	0.23	37,37,37,37	0
54	MG	2A	3079	1/1	0.94	0.32	67,67,67,67	0
54	MG	1a	1845	1/1	0.94	0.17	63,63,63,63	0
54	MG	2A	3562	1/1	0.94	0.12	64,64,64,64	0
54	MG	2A	3381	1/1	0.94	0.39	99,99,99,99	0
54	MG	1D	305	1/1	0.94	0.41	55,55,55,55	0
54	MG	1a	1739	1/1	0.94	0.55	81,81,81,81	0
54	MG	1A	3266	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3147	1/1	0.94	0.17	35,35,35,35	0
54	MG	1A	3212	1/1	0.94	0.17	43,43,43,43	0
54	MG	1A	3166	1/1	0.94	0.51	45,45,45,45	0
54	MG	2A	3389	1/1	0.94	0.16	69,69,69,69	0
54	MG	2A	3088	1/1	0.94	0.27	52,52,52,52	0
54	MG	2A	3089	1/1	0.94	0.13	61,61,61,61	0
54	MG	1A	3468	1/1	0.94	0.26	62,62,62,62	0
54	MG	1A	3274	1/1	0.94	0.22	22,22,22,22	0
54	MG	1A	3362	1/1	0.94	0.18	48,48,48,48	0
54	MG	1a	1750	1/1	0.94	0.22	89,89,89,89	0
54	MG	1A	3598	1/1	0.94	0.35	82,82,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1677	1/1	0.94	0.08	98,98,98,98	0
54	MG	1A	3363	1/1	0.94	0.10	52,52,52,52	0
54	MG	1A	3364	1/1	0.94	0.25	24,24,24,24	0
54	MG	1F	307	1/1	0.94	0.60	38,38,38,38	0
54	MG	1a	1755	1/1	0.94	0.15	57,57,57,57	0
54	MG	1A	3167	1/1	0.94	0.47	42,42,42,42	0
54	MG	1A	3280	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3148	1/1	0.94	0.13	54,54,54,54	0
54	MG	1a	1759	1/1	0.94	0.45	101,101,101,101	0
54	MG	1A	3136	1/1	0.94	0.10	43,43,43,43	0
54	MG	1A	3775	1/1	0.94	0.15	72,72,72,72	0
54	MG	1A	3607	1/1	0.94	0.17	50,50,50,50	0
54	MG	2A	3414	1/1	0.94	0.26	74,74,74,74	0
54	MG	1A	3691	1/1	0.94	0.41	61,61,61,61	0
54	MG	2A	3252	1/1	0.94	0.11	49,49,49,49	0
54	MG	1H	201	1/1	0.94	0.21	64,64,64,64	0
54	MG	2A	3254	1/1	0.94	0.15	69,69,69,69	0
54	MG	1a	1765	1/1	0.94	0.09	103,103,103,103	0
54	MG	2A	3256	1/1	0.94	0.17	54,54,54,54	0
54	MG	1A	3778	1/1	0.94	0.13	44,44,44,44	0
54	MG	1A	3327	1/1	0.94	0.11	26,26,26,26	0
54	MG	1A	3421	1/1	0.94	0.10	29,29,29,29	0
54	MG	2A	3608	1/1	0.94	0.34	86,86,86,86	0
54	MG	1A	3870	1/1	0.94	0.25	55,55,55,55	0
54	MG	1a	1662	1/1	0.94	0.20	69,69,69,69	0
54	MG	1A	3375	1/1	0.94	0.18	45,45,45,45	0
54	MG	2A	3614	1/1	0.94	0.32	64,64,64,64	0
54	MG	2A	3430	1/1	0.94	0.13	64,64,64,64	0
54	MG	2A	3431	1/1	0.94	0.27	46,46,46,46	0
54	MG	1Q	202	1/1	0.94	0.20	48,48,48,48	0
54	MG	2A	3266	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3435	1/1	0.94	0.19	81,81,81,81	0
54	MG	2A	3267	1/1	0.94	0.21	58,58,58,58	0
54	MG	2a	1714	1/1	0.94	0.08	84,84,84,84	0
54	MG	2A	3623	1/1	0.94	0.25	76,76,76,76	0
54	MG	2A	3437	1/1	0.94	0.22	48,48,48,48	0
54	MG	1A	3190	1/1	0.94	0.10	84,84,84,84	0
54	MG	2A	3629	1/1	0.94	0.13	67,67,67,67	0
54	MG	1A	3547	1/1	0.94	0.17	60,60,60,60	0
54	MG	2A	3632	1/1	0.94	0.09	75,75,75,75	0
54	MG	1A	3878	1/1	0.94	0.33	50,50,50,50	0
54	MG	1a	1777	1/1	0.94	0.07	99,99,99,99	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3442	1/1	0.94	0.36	74,74,74,74	0
54	MG	2A	3126	1/1	0.94	0.22	53,53,53,53	0
54	MG	2A	3003	1/1	0.94	0.37	49,49,49,49	0
54	MG	2a	1727	1/1	0.94	0.09	88,88,88,88	0
54	MG	1T	2003	1/1	0.94	0.35	83,83,83,83	0
54	MG	2A	3643	1/1	0.94	0.10	62,62,62,62	0
54	MG	1a	1669	1/1	0.94	0.17	110,110,110,110	0
54	MG	2A	3448	1/1	0.94	0.12	69,69,69,69	0
54	MG	1A	3080	1/1	0.94	0.43	59,59,59,59	0
54	MG	2A	3132	1/1	0.94	0.26	54,54,54,54	0
54	MG	1T	2005	1/1	0.94	0.29	53,53,53,53	0
54	MG	2A	3283	1/1	0.94	0.22	50,50,50,50	0
54	MG	1A	3291	1/1	0.94	0.14	57,57,57,57	0
54	MG	2A	3009	1/1	0.94	0.33	63,63,63,63	0
54	MG	2A	3136	1/1	0.94	0.29	62,62,62,62	0
54	MG	1A	3049	1/1	0.94	0.22	69,69,69,69	0
54	MG	1U	203	1/1	0.94	0.52	58,58,58,58	0
54	MG	1A	3428	1/1	0.94	0.20	67,67,67,67	0
54	MG	1A	3886	1/1	0.94	0.23	46,46,46,46	0
54	MG	2A	3014	1/1	0.94	0.26	66,66,66,66	0
54	MG	1a	1677	1/1	0.94	0.21	66,66,66,66	0
54	MG	2D	302	1/1	0.94	0.17	56,56,56,56	0
54	MG	2A	3299	1/1	0.94	0.13	53,53,53,53	0
54	MG	2a	1749	1/1	0.94	0.14	79,79,79,79	0
54	MG	1A	3222	1/1	0.94	0.20	52,52,52,52	0
54	MG	1A	3557	1/1	0.94	0.79	41,41,41,41	0
54	MG	2A	3146	1/1	0.94	0.14	70,70,70,70	0
54	MG	2A	3148	1/1	0.94	0.19	42,42,42,42	0
54	MG	2a	1757	1/1	0.94	0.23	92,92,92,92	0
54	MG	1A	3195	1/1	0.94	0.28	58,58,58,58	0
54	MG	2A	3306	1/1	0.94	0.15	34,34,34,34	0
54	MG	1A	3712	1/1	0.94	0.13	46,46,46,46	0
54	MG	2O	201	1/1	0.94	0.16	69,69,69,69	0
54	MG	1A	3493	1/1	0.94	0.15	68,68,68,68	0
54	MG	1A	3253	1/1	0.94	0.24	61,61,61,61	0
54	MG	2Q	201	1/1	0.94	0.27	83,83,83,83	0
54	MG	1A	3636	1/1	0.94	0.14	81,81,81,81	0
54	MG	2A	3027	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3104	1/1	0.94	0.30	33,33,33,33	0
54	MG	1A	3801	1/1	0.94	0.12	58,58,58,58	0
54	MG	1a	1690	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3569	1/1	0.94	0.28	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	2A	3321	1/1	0.94	0.14	77,77,77,77	0
54	MG	2X	101	1/1	0.94	0.12	84,84,84,84	0
54	MG	2A	3160	1/1	0.94	0.15	37,37,37,37	0
54	MG	10	105	1/1	0.94	0.10	57,57,57,57	0
54	MG	2I	101	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	3437	1/1	0.94	0.12	53,53,53,53	0
54	MG	1I	102	1/1	0.94	0.15	44,44,44,44	0
54	MG	1y	203	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3277	1/1	0.95	0.12	89,89,89,89	0
54	MG	1A	3646	1/1	0.95	0.18	71,71,71,71	0
54	MG	1A	3648	1/1	0.95	0.10	47,47,47,47	0
54	MG	2A	3259	1/1	0.95	0.28	59,59,59,59	0
54	MG	2A	3400	1/1	0.95	0.13	55,55,55,55	0
54	MG	1A	3741	1/1	0.95	0.46	51,51,51,51	0
54	MG	1G	204	1/1	0.95	0.10	73,73,73,73	0
54	MG	1A	3116	1/1	0.95	0.21	28,28,28,28	0
54	MG	1A	3564	1/1	0.95	0.63	65,65,65,65	0
54	MG	1A	3279	1/1	0.95	0.12	67,67,67,67	0
54	MG	1O	201	1/1	0.95	0.11	58,58,58,58	0
54	MG	1P	202	1/1	0.95	0.27	34,34,34,34	0
54	MG	2A	3268	1/1	0.95	0.17	58,58,58,58	0
54	MG	1P	203	1/1	0.95	0.12	52,52,52,52	0
54	MG	2A	3271	1/1	0.95	0.16	67,67,67,67	0
54	MG	1A	3566	1/1	0.95	0.31	69,69,69,69	0
54	MG	1A	3567	1/1	0.95	0.23	71,71,71,71	0
54	MG	1A	3568	1/1	0.95	0.25	51,51,51,51	0
54	MG	1A	3427	1/1	0.95	0.16	46,46,46,46	0
54	MG	1A	3159	1/1	0.95	0.46	46,46,46,46	0
54	MG	2a	1641	1/1	0.95	0.19	71,71,71,71	0
54	MG	2A	3020	1/1	0.95	0.09	60,60,60,60	0
54	MG	1R	202	1/1	0.95	0.45	41,41,41,41	0
54	MG	1A	3571	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3422	1/1	0.95	0.07	65,65,65,65	0
54	MG	1R	207	1/1	0.95	0.17	35,35,35,35	0
54	MG	1A	3213	1/1	0.95	0.23	60,60,60,60	0
54	MG	1A	3035	1/1	0.95	0.43	57,57,57,57	0
54	MG	2A	3026	1/1	0.95	0.27	42,42,42,42	0
54	MG	2A	3427	1/1	0.95	0.14	68,68,68,68	0
54	MG	1A	3134	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3434	1/1	0.95	0.07	67,67,67,67	0
54	MG	1A	3082	1/1	0.95	0.61	47,47,47,47	0
54	MG	1a	1797	1/1	0.95	0.17	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3436	1/1	0.95	0.12	68,68,68,68	0
54	MG	1A	3669	1/1	0.95	0.16	34,34,34,34	0
54	MG	1A	3337	1/1	0.95	0.06	70,70,70,70	0
54	MG	1A	3762	1/1	0.95	0.25	49,49,49,49	0
54	MG	1A	3876	1/1	0.95	0.10	29,29,29,29	0
54	MG	2A	3159	1/1	0.95	0.16	50,50,50,50	0
54	MG	1A	3764	1/1	0.95	0.33	62,62,62,62	0
54	MG	2A	3600	1/1	0.95	0.25	66,66,66,66	0
54	MG	1A	3119	1/1	0.95	0.50	44,44,44,44	0
54	MG	2A	3303	1/1	0.95	0.08	75,75,75,75	0
54	MG	2A	3162	1/1	0.95	0.10	101,101,101,101	0
54	MG	1A	3508	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3440	1/1	0.95	0.16	59,59,59,59	0
54	MG	1A	3391	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3515	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3120	1/1	0.95	0.34	39,39,39,39	0
54	MG	1A	3020	1/1	0.95	0.15	50,50,50,50	0
54	MG	1A	3589	1/1	0.95	0.17	43,43,43,43	0
54	MG	1A	3891	1/1	0.95	0.19	48,48,48,48	0
54	MG	2A	3172	1/1	0.95	0.36	80,80,80,80	0
54	MG	1A	3192	1/1	0.95	0.21	65,65,65,65	0
54	MG	2A	3318	1/1	0.95	0.16	38,38,38,38	0
54	MG	2A	3319	1/1	0.95	0.22	60,60,60,60	0
54	MG	1A	3447	1/1	0.95	0.52	70,70,70,70	0
54	MG	1A	3521	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3898	1/1	0.95	0.09	34,34,34,34	0
54	MG	1A	3344	1/1	0.95	0.13	45,45,45,45	0
54	MG	1A	3345	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3346	1/1	0.95	0.29	48,48,48,48	0
54	MG	2A	3628	1/1	0.95	0.24	60,60,60,60	0
54	MG	1A	3688	1/1	0.95	0.14	47,47,47,47	0
54	MG	2A	3327	1/1	0.95	0.10	77,77,77,77	0
54	MG	2a	1694	1/1	0.95	0.30	95,95,95,95	0
54	MG	1A	3689	1/1	0.95	0.12	99,99,99,99	0
54	MG	2A	3467	1/1	0.95	0.04	83,83,83,83	0
54	MG	2A	3636	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3597	1/1	0.95	0.34	57,57,57,57	0
54	MG	1A	3257	1/1	0.95	0.19	47,47,47,47	0
54	MG	1A	3454	1/1	0.95	0.15	67,67,67,67	0
54	MG	1a	1716	1/1	0.95	0.11	77,77,77,77	0
54	MG	1A	3794	1/1	0.95	0.45	67,67,67,67	0
54	MG	2A	3065	1/1	0.95	0.42	67,67,67,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1A	3455	1/1	0.95	0.11	38,38,38,38	0
54	MG	1A	3085	1/1	0.95	0.19	22,22,22,22	0
54	MG	1A	3531	1/1	0.95	0.12	45,45,45,45	0
54	MG	1a	1836	1/1	0.95	0.16	85,85,85,85	0
54	MG	1a	1608	1/1	0.95	0.12	78,78,78,78	0
54	MG	1A	3140	1/1	0.95	0.52	46,46,46,46	0
54	MG	1A	3463	1/1	0.95	0.16	54,54,54,54	0
54	MG	2B	209	1/1	0.95	0.22	64,64,64,64	0
54	MG	1A	3606	1/1	0.95	0.23	55,55,55,55	0
54	MG	1A	3304	1/1	0.95	0.12	30,30,30,30	0
54	MG	1A	3016	1/1	0.95	0.16	33,33,33,33	0
54	MG	1A	3804	1/1	0.95	0.15	81,81,81,81	0
54	MG	1A	3609	1/1	0.95	0.18	52,52,52,52	0
54	MG	1A	3536	1/1	0.95	0.09	42,42,42,42	0
54	MG	1a	1620	1/1	0.95	0.20	89,89,89,89	0
54	MG	2A	3349	1/1	0.95	0.19	54,54,54,54	0
54	MG	2D	301	1/1	0.95	0.56	63,63,63,63	0
54	MG	1A	3710	1/1	0.95	0.13	61,61,61,61	0
54	MG	1a	1738	1/1	0.95	0.36	78,78,78,78	0
54	MG	2A	3497	1/1	0.95	0.10	67,67,67,67	0
54	MG	1A	3808	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3306	1/1	0.95	0.20	57,57,57,57	0
54	MG	2a	1729	1/1	0.95	0.12	93,93,93,93	0
54	MG	2A	3500	1/1	0.95	0.11	89,89,89,89	0
54	MG	2A	3085	1/1	0.95	0.16	73,73,73,73	0
54	MG	2A	3502	1/1	0.95	0.13	57,57,57,57	0
54	MG	1a	1853	1/1	0.95	0.17	65,65,65,65	0
54	MG	2A	3504	1/1	0.95	0.16	71,71,71,71	0
54	MG	1a	1854	1/1	0.95	0.13	57,57,57,57	0
54	MG	2P	201	1/1	0.95	0.18	83,83,83,83	0
54	MG	1a	1742	1/1	0.95	0.33	95,95,95,95	0
54	MG	1a	1624	1/1	0.95	0.34	85,85,85,85	0
54	MG	1A	3810	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3199	1/1	0.95	0.34	58,58,58,58	0
54	MG	2a	1741	1/1	0.95	0.26	97,97,97,97	0
54	MG	2R	203	1/1	0.95	0.23	53,53,53,53	0
54	MG	1A	3615	1/1	0.95	0.18	57,57,57,57	0
54	MG	2A	3513	1/1	0.95	0.06	81,81,81,81	0
54	MG	2A	3362	1/1	0.95	0.23	75,75,75,75	0
54	MG	2T	204	1/1	0.95	0.35	71,71,71,71	0
54	MG	1A	3031	1/1	0.95	0.12	31,31,31,31	0
54	MG	1A	3540	1/1	0.95	0.23	36,36,36,36	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3716	1/1	0.95	0.13	50,50,50,50	0
54	MG	1A	3263	1/1	0.95	0.17	44,44,44,44	0
54	MG	1A	3039	1/1	0.95	0.24	38,38,38,38	0
54	MG	1A	3473	1/1	0.95	0.16	45,45,45,45	0
54	MG	2I	103	1/1	0.95	0.15	60,60,60,60	0
54	MG	2a	1755	1/1	0.95	0.17	79,79,79,79	0
54	MG	2a	1756	1/1	0.95	0.10	73,73,73,73	0
54	MG	1A	3361	1/1	0.95	0.14	49,49,49,49	0
54	MG	1A	3313	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3726	1/1	0.95	0.40	52,52,52,52	0
54	MG	1A	3128	1/1	0.95	0.49	44,44,44,44	0
54	MG	1A	3827	1/1	0.95	0.14	57,57,57,57	0
54	MG	2A	3528	1/1	0.95	0.09	60,60,60,60	0
54	MG	1A	3059	1/1	0.95	0.15	24,24,24,24	0
54	MG	1A	3365	1/1	0.95	0.16	22,22,22,22	0
54	MG	1A	3207	1/1	0.95	0.39	37,37,37,37	0
54	MG	2A	3380	1/1	0.95	0.15	48,48,48,48	0
54	MG	1a	1647	1/1	0.95	0.40	62,62,62,62	0
54	MG	1A	3269	1/1	0.95	0.23	30,30,30,30	0
54	MG	1A	3639	1/1	0.95	0.13	58,58,58,58	0
54	MG	1A	3733	1/1	0.95	0.17	35,35,35,35	0
54	MG	2a	1612	1/1	0.95	0.09	96,96,96,96	0
54	MG	1F	308	1/1	0.95	0.09	32,32,32,32	0
54	MG	2t	201	1/1	0.95	0.37	71,71,71,71	0
54	MG	1A	3238	1/1	0.95	0.19	31,31,31,31	0
54	MG	1A	3018	1/1	0.95	0.37	40,40,40,40	0
54	MG	1a	1656	1/1	0.95	0.23	73,73,73,73	0
54	MG	1A	3642	1/1	0.95	0.23	50,50,50,50	0
54	MG	1a	1658	1/1	0.95	0.26	55,55,55,55	0
54	MG	1A	3333	1/1	0.96	0.17	21,21,21,21	0
54	MG	2A	3260	1/1	0.96	0.14	48,48,48,48	0
54	MG	1A	3590	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3402	1/1	0.96	0.12	70,70,70,70	0
54	MG	1A	3390	1/1	0.96	0.11	65,65,65,65	0
54	MG	1A	3206	1/1	0.96	0.46	40,40,40,40	0
54	MG	1A	3335	1/1	0.96	0.23	38,38,38,38	0
54	MG	2A	3406	1/1	0.96	0.09	72,72,72,72	0
54	MG	1A	3854	1/1	0.96	0.19	34,34,34,34	0
54	MG	2A	3558	1/1	0.96	0.11	70,70,70,70	0
54	MG	1A	3336	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3285	1/1	0.96	0.20	67,67,67,67	0
54	MG	1A	3065	1/1	0.96	0.16	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
54	MG	1A	3761	1/1	0.96	0.17	38,38,38,38	0
54	MG	2A	3270	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3209	1/1	0.96	0.16	35,35,35,35	0
54	MG	1N	201	1/1	0.96	0.33	49,49,49,49	0
54	MG	1N	202	1/1	0.96	0.61	66,66,66,66	0
54	MG	1A	3290	1/1	0.96	0.13	37,37,37,37	0
54	MG	1A	3342	1/1	0.96	0.10	28,28,28,28	0
54	MG	1A	3767	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3769	1/1	0.96	0.05	69,69,69,69	0
54	MG	1A	3400	1/1	0.96	0.12	50,50,50,50	0
54	MG	1A	3459	1/1	0.96	0.17	58,58,58,58	0
54	MG	1A	3868	1/1	0.96	0.16	34,34,34,34	0
54	MG	2A	3147	1/1	0.96	0.51	69,69,69,69	0
54	MG	1A	3685	1/1	0.96	0.10	51,51,51,51	0
54	MG	1Q	203	1/1	0.96	0.18	51,51,51,51	0
54	MG	2A	3581	1/1	0.96	0.32	77,77,77,77	0
54	MG	2a	1648	1/1	0.96	0.35	64,64,64,64	0
54	MG	1A	3146	1/1	0.96	0.16	46,46,46,46	0
54	MG	1A	3246	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3873	1/1	0.96	0.15	56,56,56,56	0
54	MG	1R	204	1/1	0.96	0.27	53,53,53,53	0
54	MG	1A	3293	1/1	0.96	0.12	36,36,36,36	0
54	MG	2a	1654	1/1	0.96	0.24	100,100,100,100	0
54	MG	2A	3294	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3875	1/1	0.96	0.16	78,78,78,78	0
54	MG	2A	3296	1/1	0.96	0.17	47,47,47,47	0
54	MG	2A	3591	1/1	0.96	0.07	85,85,85,85	0
54	MG	1A	3467	1/1	0.96	0.14	67,67,67,67	0
54	MG	1A	3295	1/1	0.96	0.17	26,26,26,26	0
54	MG	1A	3109	1/1	0.96	0.41	46,46,46,46	0
54	MG	1A	3409	1/1	0.96	0.09	50,50,50,50	0
54	MG	1U	201	1/1	0.96	0.11	29,29,29,29	0
54	MG	1A	3611	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3884	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3542	1/1	0.96	0.12	49,49,49,49	0
54	MG	1V	202	1/1	0.96	0.28	67,67,67,67	0
54	MG	1a	1804	1/1	0.96	0.57	71,71,71,71	0
54	MG	1A	3110	1/1	0.96	0.08	64,64,64,64	0
54	MG	1a	1688	1/1	0.96	0.42	36,36,36,36	0
54	MG	1A	3022	1/1	0.96	0.23	43,43,43,43	0
54	MG	1A	3788	1/1	0.96	0.50	58,58,58,58	0
54	MG	1A	3889	1/1	0.96	0.28	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3352	1/1	0.96	0.14	62,62,62,62	0
54	MG	2A	3611	1/1	0.96	0.12	63,63,63,63	0
54	MG	1A	3616	1/1	0.96	0.13	61,61,61,61	0
54	MG	2A	3315	1/1	0.96	0.10	50,50,50,50	0
54	MG	1a	1813	1/1	0.96	0.19	76,76,76,76	0
54	MG	2A	3616	1/1	0.96	0.11	67,67,67,67	0
54	MG	2A	3617	1/1	0.96	0.14	66,66,66,66	0
54	MG	1a	1814	1/1	0.96	0.21	65,65,65,65	0
54	MG	1A	3112	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3893	1/1	0.96	0.29	44,44,44,44	0
54	MG	1A	3153	1/1	0.96	0.09	56,56,56,56	0
54	MG	2A	3179	1/1	0.96	0.35	70,70,70,70	0
54	MG	1A	3155	1/1	0.96	0.23	53,53,53,53	0
54	MG	1A	3708	1/1	0.96	0.51	49,49,49,49	0
54	MG	1A	3553	1/1	0.96	0.43	57,57,57,57	0
54	MG	1A	3900	1/1	0.96	0.19	54,54,54,54	0
54	MG	2A	3465	1/1	0.96	0.12	69,69,69,69	0
54	MG	2A	3466	1/1	0.96	0.10	70,70,70,70	0
54	MG	2A	3631	1/1	0.96	0.19	82,82,82,82	0
54	MG	1A	3156	1/1	0.96	0.29	39,39,39,39	0
54	MG	2A	3468	1/1	0.96	0.18	45,45,45,45	0
54	MG	1A	3157	1/1	0.96	0.18	42,42,42,42	0
54	MG	1l	104	1/1	0.96	0.41	61,61,61,61	0
54	MG	1a	1825	1/1	0.96	0.21	61,61,61,61	0
54	MG	1A	3307	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3419	1/1	0.96	0.14	64,64,64,64	0
54	MG	1A	3094	1/1	0.96	0.09	58,58,58,58	0
54	MG	2A	3476	1/1	0.96	0.21	78,78,78,78	0
54	MG	1A	3187	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3630	1/1	0.96	0.10	50,50,50,50	0
54	MG	17	101	1/1	0.96	0.96	44,44,44,44	0
54	MG	1A	3631	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3633	1/1	0.96	0.20	60,60,60,60	0
54	MG	1a	1834	1/1	0.96	0.18	74,74,74,74	0
54	MG	1A	3635	1/1	0.96	0.10	62,62,62,62	0
54	MG	1A	3002	1/1	0.96	0.15	46,46,46,46	0
54	MG	2a	1717	1/1	0.96	0.14	83,83,83,83	0
54	MG	1A	3563	1/1	0.96	0.24	66,66,66,66	0
53	MPD	18	101	8/8	0.96	0.28	47,49,54,59	0
54	MG	1A	3101	1/1	0.96	0.37	46,46,46,46	0
54	MG	2A	3205	1/1	0.96	0.16	53,53,53,53	0
54	MG	1A	3812	1/1	0.96	0.10	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	1a	1607	1/1	0.96	0.07	108,108,108,108	0
54	MG	1A	3226	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3055	1/1	0.96	0.21	40,40,40,40	0
54	MG	2A	3495	1/1	0.96	0.15	36,36,36,36	0
54	MG	1a	1610	1/1	0.96	0.15	85,85,85,85	0
54	MG	2D	305	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3228	1/1	0.96	0.18	62,62,62,62	0
54	MG	1A	3371	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3429	1/1	0.96	0.17	41,41,41,41	0
54	MG	1A	3163	1/1	0.96	0.14	50,50,50,50	0
54	MG	2A	3216	1/1	0.96	0.34	42,42,42,42	0
54	MG	1a	1615	1/1	0.96	0.17	39,39,39,39	0
54	MG	1A	3572	1/1	0.96	0.14	61,61,61,61	0
54	MG	1a	1736	1/1	0.96	0.04	76,76,76,76	0
54	MG	1A	3008	1/1	0.96	0.18	39,39,39,39	0
54	MG	1a	1618	1/1	0.96	0.22	81,81,81,81	0
54	MG	1A	3271	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3272	1/1	0.96	0.12	23,23,23,23	0
54	MG	1a	1741	1/1	0.96	0.55	89,89,89,89	0
54	MG	2A	3510	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3505	1/1	0.96	0.14	49,49,49,49	0
54	MG	1A	3325	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3087	1/1	0.96	0.16	32,32,32,32	0
54	MG	1D	302	1/1	0.96	0.16	55,55,55,55	0
54	MG	1A	3829	1/1	0.96	0.13	73,73,73,73	0
54	MG	2A	3235	1/1	0.96	0.08	84,84,84,84	0
54	MG	2T	205	1/1	0.96	0.15	43,43,43,43	0
54	MG	1A	3105	1/1	0.96	0.19	52,52,52,52	0
54	MG	2A	3237	1/1	0.96	0.17	71,71,71,71	0
54	MG	1A	3512	1/1	0.96	0.17	63,63,63,63	0
54	MG	1A	3438	1/1	0.96	0.16	27,27,27,27	0
54	MG	2A	3240	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3523	1/1	0.96	0.17	50,50,50,50	0
54	MG	1A	3201	1/1	0.96	0.57	49,49,49,49	0
54	MG	1A	3077	1/1	0.96	0.06	64,64,64,64	0
54	MG	2A	3526	1/1	0.96	0.18	77,77,77,77	0
54	MG	1A	3441	1/1	0.96	0.09	64,64,64,64	0
54	MG	1A	3667	1/1	0.96	0.11	32,32,32,32	0
54	MG	1A	3141	1/1	0.96	0.67	45,45,45,45	0
54	MG	2A	3530	1/1	0.96	0.21	62,62,62,62	0
54	MG	1E	303	1/1	0.96	0.23	31,31,31,31	0
54	MG	1A	3107	1/1	0.96	0.22	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3752	1/1	0.96	0.08	37,37,37,37	0
54	MG	2A	3249	1/1	0.96	0.19	74,74,74,74	0
54	MG	2A	3387	1/1	0.96	0.08	63,63,63,63	0
54	MG	1a	1638	1/1	0.96	0.25	42,42,42,42	0
54	MG	1A	3844	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1640	1/1	0.96	0.17	75,75,75,75	0
54	MG	1A	3845	1/1	0.96	0.23	50,50,50,50	0
54	MG	2a	1613	1/1	0.96	0.13	71,71,71,71	0
54	MG	2A	3393	1/1	0.96	0.13	77,77,77,77	0
54	MG	1a	1642	1/1	0.96	0.20	84,84,84,84	0
54	MG	1F	305	1/1	0.96	0.36	50,50,50,50	0
54	MG	2A	3123	1/1	0.96	0.28	47,47,47,47	0
54	MG	1A	3847	1/1	0.96	0.15	38,38,38,38	0
54	MG	2A	3310	1/1	0.97	0.17	55,55,55,55	0
54	MG	2A	3185	1/1	0.97	0.20	39,39,39,39	0
54	MG	1A	3378	1/1	0.97	0.13	71,71,71,71	0
54	MG	1a	1732	1/1	0.97	0.33	70,70,70,70	0
54	MG	1A	3099	1/1	0.97	0.48	51,51,51,51	0
54	MG	1a	1840	1/1	0.97	0.10	61,61,61,61	0
54	MG	2A	3316	1/1	0.97	0.13	58,58,58,58	0
54	MG	1A	3483	1/1	0.97	0.14	39,39,39,39	0
54	MG	1A	3151	1/1	0.97	0.16	46,46,46,46	0
54	MG	2A	3192	1/1	0.97	0.13	45,45,45,45	0
54	MG	2A	3590	1/1	0.97	0.08	52,52,52,52	0
54	MG	1F	301	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3765	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3853	1/1	0.97	0.10	33,33,33,33	0
54	MG	2A	3594	1/1	0.97	0.15	88,88,88,88	0
54	MG	1A	3431	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3596	1/1	0.97	0.08	52,52,52,52	0
54	MG	1F	306	1/1	0.97	0.38	41,41,41,41	0
54	MG	1A	3551	1/1	0.97	0.18	46,46,46,46	0
54	MG	1A	3768	1/1	0.97	0.12	51,51,51,51	0
54	MG	1A	3552	1/1	0.97	0.29	36,36,36,36	0
54	MG	1a	1744	1/1	0.97	0.09	63,63,63,63	0
54	MG	1A	3152	1/1	0.97	0.07	52,52,52,52	0
54	MG	1A	3772	1/1	0.97	0.08	57,57,57,57	0
54	MG	1A	3488	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3774	1/1	0.97	0.10	65,65,65,65	0
54	MG	1A	3294	1/1	0.97	0.18	31,31,31,31	0
54	MG	1A	3692	1/1	0.97	0.26	41,41,41,41	0
54	MG	1A	3693	1/1	0.97	0.42	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3003	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3620	1/1	0.97	0.17	47,47,47,47	0
54	MG	2a	1661	1/1	0.97	0.22	84,84,84,84	0
54	MG	2A	3612	1/1	0.97	0.39	72,72,72,72	0
54	MG	1a	1644	1/1	0.97	0.26	55,55,55,55	0
54	MG	2A	3470	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3869	1/1	0.97	0.38	58,58,58,58	0
54	MG	2a	1666	1/1	0.97	0.12	79,79,79,79	0
54	MG	1A	3084	1/1	0.97	0.16	40,40,40,40	0
54	MG	1A	3297	1/1	0.97	0.22	51,51,51,51	0
54	MG	1A	3004	1/1	0.97	0.43	48,48,48,48	0
54	MG	2A	3217	1/1	0.97	0.44	60,60,60,60	0
54	MG	2A	3218	1/1	0.97	0.19	73,73,73,73	0
54	MG	2a	1672	1/1	0.97	0.47	55,55,55,55	0
54	MG	2A	3477	1/1	0.97	0.12	83,83,83,83	0
54	MG	1A	3701	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3034	1/1	0.97	0.15	60,60,60,60	0
54	MG	2a	1676	1/1	0.97	0.15	93,93,93,93	0
54	MG	1A	3300	1/1	0.97	0.13	75,75,75,75	0
54	MG	2a	1678	1/1	0.97	0.20	53,53,53,53	0
54	MG	1A	3786	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3877	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3627	1/1	0.97	0.09	67,67,67,67	0
54	MG	1A	3232	1/1	0.97	0.15	68,68,68,68	0
54	MG	2A	3226	1/1	0.97	0.26	52,52,52,52	0
54	MG	1A	3706	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3229	1/1	0.97	0.21	56,56,56,56	0
54	MG	1A	3013	1/1	0.97	0.22	36,36,36,36	0
54	MG	1A	3882	1/1	0.97	0.29	42,42,42,42	0
54	MG	1A	3791	1/1	0.97	0.10	48,48,48,48	0
54	MG	2A	3639	1/1	0.97	0.26	67,67,67,67	0
54	MG	1R	205	1/1	0.97	0.16	49,49,49,49	0
54	MG	2A	3112	1/1	0.97	0.13	54,54,54,54	0
54	MG	1A	3500	1/1	0.97	0.13	73,73,73,73	0
54	MG	1A	3501	1/1	0.97	0.13	32,32,32,32	0
54	MG	1A	3632	1/1	0.97	0.14	57,57,57,57	0
54	MG	2A	3116	1/1	0.97	0.17	45,45,45,45	0
54	MG	1A	3235	1/1	0.97	0.20	53,53,53,53	0
54	MG	1A	3634	1/1	0.97	0.14	43,43,43,43	0
54	MG	1A	3503	1/1	0.97	0.06	66,66,66,66	0
54	MG	2A	3368	1/1	0.97	0.29	57,57,57,57	0
54	MG	1A	3443	1/1	0.97	0.13	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3121	1/1	0.97	0.47	43,43,43,43	0
54	MG	1A	3638	1/1	0.97	0.08	68,68,68,68	0
54	MG	1A	3894	1/1	0.97	0.16	46,46,46,46	0
54	MG	1A	3122	1/1	0.97	0.18	59,59,59,59	0
54	MG	2a	1705	1/1	0.97	0.21	93,93,93,93	0
54	MG	1A	3507	1/1	0.97	0.15	50,50,50,50	0
54	MG	1A	3897	1/1	0.97	0.34	48,48,48,48	0
54	MG	1A	3721	1/1	0.97	0.09	43,43,43,43	0
54	MG	2A	3250	1/1	0.97	0.10	60,60,60,60	0
54	MG	1A	3088	1/1	0.97	0.17	52,52,52,52	0
54	MG	1a	1678	1/1	0.97	0.20	57,57,57,57	0
54	MG	1A	3351	1/1	0.97	0.05	66,66,66,66	0
54	MG	1a	1680	1/1	0.97	0.19	105,105,105,105	0
54	MG	1A	3448	1/1	0.97	0.24	24,24,24,24	0
54	MG	2E	301	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3644	1/1	0.97	0.24	45,45,45,45	0
54	MG	1A	3043	1/1	0.97	0.12	50,50,50,50	0
54	MG	1A	3647	1/1	0.97	0.31	58,58,58,58	0
54	MG	1B	1005	1/1	0.97	0.13	71,71,71,71	0
54	MG	1A	3579	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3189	1/1	0.97	0.26	43,43,43,43	0
54	MG	2A	3390	1/1	0.97	0.08	71,71,71,71	0
54	MG	1A	3813	1/1	0.97	0.28	75,75,75,75	0
54	MG	11	101	1/1	0.97	0.34	66,66,66,66	0
54	MG	1A	3273	1/1	0.97	0.09	52,52,52,52	0
54	MG	2A	3394	1/1	0.97	0.35	48,48,48,48	0
54	MG	1A	3014	1/1	0.97	0.18	31,31,31,31	0
54	MG	2Q	202	1/1	0.97	0.14	70,70,70,70	0
54	MG	1A	3816	1/1	0.97	0.20	34,34,34,34	0
54	MG	1A	3275	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3315	1/1	0.97	0.17	48,48,48,48	0
54	MG	1A	3655	1/1	0.97	0.15	67,67,67,67	0
54	MG	1A	3276	1/1	0.97	0.13	46,46,46,46	0
54	MG	2A	3033	1/1	0.97	0.23	76,76,76,76	0
54	MG	1A	3092	1/1	0.97	0.12	29,29,29,29	0
54	MG	16	102	1/1	0.97	0.04	54,54,54,54	0
54	MG	1A	3458	1/1	0.97	0.08	41,41,41,41	0
54	MG	2W	201	1/1	0.97	0.46	65,65,65,65	0
54	MG	2A	3037	1/1	0.97	0.31	52,52,52,52	0
54	MG	2A	3038	1/1	0.97	0.17	71,71,71,71	0
54	MG	17	102	1/1	0.97	0.37	53,53,53,53	0
54	MG	1A	3145	1/1	0.97	0.38	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3193	1/1	0.97	0.59	61,61,61,61	0
54	MG	1a	1704	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3464	1/1	0.97	0.08	53,53,53,53	0
54	MG	1A	3248	1/1	0.97	0.15	42,42,42,42	0
54	MG	2A	3547	1/1	0.97	0.16	72,72,72,72	0
54	MG	1A	3529	1/1	0.97	0.23	52,52,52,52	0
54	MG	1A	3281	1/1	0.97	0.08	26,26,26,26	0
54	MG	2a	1751	1/1	0.97	0.16	60,60,60,60	0
54	MG	2A	3551	1/1	0.97	0.23	86,86,86,86	0
54	MG	1A	3830	1/1	0.97	0.21	59,59,59,59	0
54	MG	1A	3078	1/1	0.97	0.26	51,51,51,51	0
54	MG	2A	3166	1/1	0.97	0.32	52,52,52,52	0
54	MG	2A	3289	1/1	0.97	0.20	49,49,49,49	0
54	MG	2A	3291	1/1	0.97	0.20	64,64,64,64	0
54	MG	1A	3053	1/1	0.97	0.19	30,30,30,30	0
54	MG	2A	3293	1/1	0.97	0.09	44,44,44,44	0
54	MG	2A	3560	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3833	1/1	0.97	0.08	53,53,53,53	0
54	MG	1A	3367	1/1	0.97	0.13	46,46,46,46	0
54	MG	1A	3368	1/1	0.97	0.19	54,54,54,54	0
54	MG	2A	3564	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3284	1/1	0.97	0.22	60,60,60,60	0
54	MG	1A	3046	1/1	0.97	0.34	46,46,46,46	0
54	MG	1A	3223	1/1	0.97	0.17	55,55,55,55	0
54	MG	1A	3288	1/1	0.97	0.07	39,39,39,39	0
54	MG	1a	1721	1/1	0.97	0.08	53,53,53,53	0
54	MG	1D	306	1/1	0.97	0.14	53,53,53,53	0
54	MG	1A	3330	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3066	1/1	0.97	0.28	66,66,66,66	0
54	MG	2A	3434	1/1	0.97	0.16	47,47,47,47	0
54	MG	1A	3477	1/1	0.97	0.09	48,48,48,48	0
54	MG	1D	310	1/1	0.97	0.13	53,53,53,53	0
54	MG	1a	1728	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3254	1/1	0.97	0.50	62,62,62,62	0
54	MG	1A	3377	1/1	0.97	0.33	55,55,55,55	0
54	MG	1A	3323	1/1	0.98	0.12	67,67,67,67	0
54	MG	2A	3019	1/1	0.98	0.20	80,80,80,80	0
54	MG	1a	1723	1/1	0.98	0.21	75,75,75,75	0
54	MG	1A	3404	1/1	0.98	0.07	55,55,55,55	0
54	MG	1A	3405	1/1	0.98	0.21	54,54,54,54	0
54	MG	1A	3499	1/1	0.98	0.13	53,53,53,53	0
54	MG	1A	3076	1/1	0.98	0.16	46,46,46,46	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3407	1/1	0.98	0.21	41,41,41,41	0
54	MG	1R	206	1/1	0.98	0.12	33,33,33,33	0
54	MG	1A	3067	1/1	0.98	0.16	46,46,46,46	0
54	MG	2A	3028	1/1	0.98	0.31	44,44,44,44	0
54	MG	2A	3227	1/1	0.98	0.16	72,72,72,72	0
54	MG	1A	3041	1/1	0.98	0.12	32,32,32,32	0
54	MG	1A	3561	1/1	0.98	0.59	70,70,70,70	0
54	MG	1A	3453	1/1	0.98	0.20	39,39,39,39	0
54	MG	1A	3208	1/1	0.98	0.12	40,40,40,40	0
54	MG	1a	1648	1/1	0.98	0.30	56,56,56,56	0
54	MG	2D	303	1/1	0.98	0.17	52,52,52,52	0
54	MG	2D	304	1/1	0.98	0.42	51,51,51,51	0
54	MG	2A	3546	1/1	0.98	0.10	69,69,69,69	0
54	MG	1A	3233	1/1	0.98	0.17	66,66,66,66	0
54	MG	2A	3548	1/1	0.98	0.12	62,62,62,62	0
54	MG	1A	3264	1/1	0.98	0.09	47,47,47,47	0
54	MG	1A	3625	1/1	0.98	0.21	54,54,54,54	0
54	MG	1B	1013	1/1	0.98	0.11	49,49,49,49	0
54	MG	1B	1014	1/1	0.98	0.05	50,50,50,50	0
54	MG	1a	1654	1/1	0.98	0.23	80,80,80,80	0
54	MG	1A	3763	1/1	0.98	0.37	46,46,46,46	0
54	MG	2A	3446	1/1	0.98	0.16	53,53,53,53	0
54	MG	1A	3184	1/1	0.98	0.26	65,65,65,65	0
54	MG	1A	3509	1/1	0.98	0.14	52,52,52,52	0
54	MG	2A	3043	1/1	0.98	0.12	60,60,60,60	0
54	MG	2A	3559	1/1	0.98	0.21	50,50,50,50	0
54	MG	1A	3100	1/1	0.98	0.31	49,49,49,49	0
54	MG	1A	3511	1/1	0.98	0.09	52,52,52,52	0
54	MG	1A	3842	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3029	1/1	0.98	0.22	44,44,44,44	0
54	MG	1A	3696	1/1	0.98	0.10	30,30,30,30	0
54	MG	1A	3513	1/1	0.98	0.24	63,63,63,63	0
54	MG	1A	3846	1/1	0.98	0.08	43,43,43,43	0
54	MG	10	102	1/1	0.98	0.07	76,76,76,76	0
54	MG	1A	3698	1/1	0.98	0.13	69,69,69,69	0
54	MG	1A	3460	1/1	0.98	0.15	46,46,46,46	0
54	MG	1A	3462	1/1	0.98	0.14	33,33,33,33	0
54	MG	1A	3370	1/1	0.98	0.12	25,25,25,25	0
54	MG	1a	1846	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3237	1/1	0.98	0.13	61,61,61,61	0
54	MG	1A	3576	1/1	0.98	0.07	71,71,71,71	0
54	MG	1A	3188	1/1	0.98	0.11	38,38,38,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3519	1/1	0.98	0.22	39,39,39,39	0
54	MG	2a	1712	1/1	0.98	0.15	75,75,75,75	0
54	MG	2I	102	1/1	0.98	0.07	63,63,63,63	0
54	MG	1A	3064	1/1	0.98	0.21	43,43,43,43	0
54	MG	1A	3240	1/1	0.98	0.16	46,46,46,46	0
54	MG	1A	3522	1/1	0.98	0.14	59,59,59,59	0
54	MG	1A	3302	1/1	0.98	0.08	43,43,43,43	0
54	MG	2A	3366	1/1	0.98	0.24	47,47,47,47	0
54	MG	1A	3214	1/1	0.98	0.23	40,40,40,40	0
54	MG	1A	3339	1/1	0.98	0.22	34,34,34,34	0
54	MG	1A	3645	1/1	0.98	0.15	52,52,52,52	0
54	MG	1A	3168	1/1	0.98	0.19	58,58,58,58	0
54	MG	1A	3379	1/1	0.98	0.06	55,55,55,55	0
54	MG	2A	3070	1/1	0.98	0.16	59,59,59,59	0
54	MG	1A	3090	1/1	0.98	0.26	36,36,36,36	0
54	MG	2A	3479	1/1	0.98	0.16	52,52,52,52	0
54	MG	1A	3154	1/1	0.98	0.10	35,35,35,35	0
54	MG	1E	302	1/1	0.98	0.17	24,24,24,24	0
54	MG	1A	3717	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3115	1/1	0.98	0.24	42,42,42,42	0
54	MG	1A	3081	1/1	0.98	0.08	61,61,61,61	0
54	MG	2A	3379	1/1	0.98	0.24	73,73,73,73	0
54	MG	2A	3276	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3652	1/1	0.98	0.06	54,54,54,54	0
54	MG	1A	3247	1/1	0.98	0.23	27,27,27,27	0
54	MG	1A	3310	1/1	0.98	0.14	44,44,44,44	0
54	MG	1A	3142	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3197	1/1	0.98	0.16	49,49,49,49	0
54	MG	1A	3349	1/1	0.98	0.15	62,62,62,62	0
54	MG	2A	3182	1/1	0.98	0.15	53,53,53,53	0
54	MG	1A	3800	1/1	0.98	0.25	61,61,61,61	0
54	MG	1F	309	1/1	0.98	0.17	33,33,33,33	0
54	MG	1A	3174	1/1	0.98	0.25	53,53,53,53	0
54	MG	1A	3393	1/1	0.98	0.10	60,60,60,60	0
54	MG	1A	3660	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3661	1/1	0.98	0.06	32,32,32,32	0
54	MG	1A	3485	1/1	0.98	0.07	54,54,54,54	0
54	MG	1a	1702	1/1	0.98	0.11	47,47,47,47	0
54	MG	1A	3314	1/1	0.98	0.11	35,35,35,35	0
54	MG	2A	3092	1/1	0.98	0.10	53,53,53,53	0
54	MG	1A	3040	1/1	0.98	0.31	32,32,32,32	0
54	MG	1A	3176	1/1	0.98	0.18	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3095	1/1	0.98	0.16	58,58,58,58	0
54	MG	1A	3736	1/1	0.98	0.14	37,37,37,37	0
54	MG	1A	3074	1/1	0.98	0.22	47,47,47,47	0
54	MG	1A	3202	1/1	0.98	0.24	33,33,33,33	0
54	MG	1A	3060	1/1	0.98	0.18	34,34,34,34	0
54	MG	2A	3100	1/1	0.98	0.42	69,69,69,69	0
54	MG	2A	3512	1/1	0.98	0.09	67,67,67,67	0
54	MG	2A	3625	1/1	0.98	0.26	56,56,56,56	0
54	MG	2A	3626	1/1	0.98	0.17	44,44,44,44	0
54	MG	1a	1626	1/1	0.98	0.33	70,70,70,70	0
54	MG	1A	3546	1/1	0.98	0.11	43,43,43,43	0
54	MG	1A	3670	1/1	0.98	0.18	56,56,56,56	0
54	MG	1P	201	1/1	0.98	0.13	83,83,83,83	0
54	MG	1A	3671	1/1	0.98	0.18	39,39,39,39	0
54	MG	1a	1715	1/1	0.98	0.06	54,54,54,54	0
54	MG	1A	3287	1/1	0.98	0.21	47,47,47,47	0
54	MG	2A	3634	1/1	0.98	0.14	56,56,56,56	0
54	MG	2A	3208	1/1	0.98	0.17	68,68,68,68	0
54	MG	1a	1805	1/1	0.98	0.16	53,53,53,53	0
54	MG	1a	1717	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3358	1/1	0.98	0.05	54,54,54,54	0
54	MG	2A	3417	1/1	0.98	0.30	60,60,60,60	0
54	MG	1A	3494	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3015	1/1	0.98	0.13	53,53,53,53	0
56	ZN	1n	102	1/1	0.98	0.11	94,94,94,94	0
56	ZN	2Y	202	1/1	0.98	0.06	95,95,95,95	0
54	MG	1A	3610	1/1	0.98	0.08	42,42,42,42	0
56	ZN	25	101	1/1	0.98	0.07	83,83,83,83	0
56	ZN	26	101	1/1	0.98	0.12	72,72,72,72	0
56	ZN	29	101	1/1	0.98	0.07	101,101,101,101	0
54	MG	1A	3132	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3480	1/1	0.99	0.45	50,50,50,50	0
54	MG	2A	3129	1/1	0.99	0.18	37,37,37,37	0
54	MG	1A	3838	1/1	0.99	0.22	42,42,42,42	0
54	MG	1A	3019	1/1	0.99	0.17	45,45,45,45	0
54	MG	1A	3601	1/1	0.99	0.18	39,39,39,39	0
54	MG	1A	3559	1/1	0.99	0.20	61,61,61,61	0
54	MG	1A	3186	1/1	0.99	0.34	60,60,60,60	0
54	MG	1A	3070	1/1	0.99	0.16	47,47,47,47	0
54	MG	1A	3318	1/1	0.99	0.15	32,32,32,32	0
54	MG	1A	3095	1/1	0.99	0.24	41,41,41,41	0
54	MG	1A	3380	1/1	0.99	0.08	23,23,23,23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3015	1/1	0.99	0.28	36,36,36,36	0
54	MG	1A	3820	1/1	0.99	0.30	59,59,59,59	0
54	MG	1a	1767	1/1	0.99	0.05	46,46,46,46	0
54	MG	2A	3142	1/1	0.99	0.33	28,28,28,28	0
54	MG	1A	3719	1/1	0.99	0.08	51,51,51,51	0
54	MG	1A	3025	1/1	0.99	0.24	38,38,38,38	0
54	MG	1A	3770	1/1	0.99	0.06	37,37,37,37	0
54	MG	2A	3635	1/1	0.99	0.27	64,64,64,64	0
54	MG	1A	3032	1/1	0.99	0.09	45,45,45,45	0
54	MG	2A	3599	1/1	0.99	0.11	48,48,48,48	0
54	MG	1A	3883	1/1	0.99	0.45	51,51,51,51	0
54	MG	1A	3722	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3181	1/1	0.99	0.39	46,46,46,46	0
54	MG	1A	3045	1/1	0.99	0.13	41,41,41,41	0
54	MG	1A	3061	1/1	0.99	0.23	48,48,48,48	0
54	MG	1A	3550	1/1	0.99	0.07	46,46,46,46	0
54	MG	1A	3751	1/1	0.99	0.04	47,47,47,47	0
54	MG	2A	3290	1/1	0.99	0.11	57,57,57,57	0
54	MG	2A	3571	1/1	0.99	0.06	68,68,68,68	0
56	ZN	1Y	201	1/1	0.99	0.10	83,83,83,83	0
54	MG	1A	3387	1/1	0.99	0.12	33,33,33,33	0
56	ZN	15	102	1/1	0.99	0.07	53,53,53,53	0
56	ZN	19	102	1/1	0.99	0.11	50,50,50,50	0
54	MG	1A	3255	1/1	0.99	0.12	42,42,42,42	0
54	MG	1A	3256	1/1	0.99	0.09	48,48,48,48	0
54	MG	1A	3862	1/1	0.99	0.08	35,35,35,35	0
54	MG	1A	3863	1/1	0.99	0.09	50,50,50,50	0
54	MG	1A	3068	1/1	0.99	0.21	36,36,36,36	0
54	MG	1A	3196	1/1	0.99	0.12	37,37,37,37	0
54	MG	1A	3461	1/1	0.99	0.12	42,42,42,42	0
57	SF4	1d	501	8/8	0.99	0.17	77,92,105,112	0
57	SF4	2d	501	8/8	0.99	0.15	71,89,97,104	0
54	MG	1A	3388	1/1	1.00	0.11	23,23,23,23	0
56	ZN	16	101	1/1	1.00	0.10	52,52,52,52	0
54	MG	1A	3096	1/1	1.00	0.18	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.