



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:29 am BST

PDB ID : 6FKR  
Title : Crystal structure of the dolphin proline-rich antimicrobial peptide Tur1A bound to the Thermus thermophilus 70S ribosome  
Authors : Mardirossian, M.; Perebaskine, N.; Benincasa, M.; Gambato, S.; Hofmann, S.; Huter, P.; Muller, C.; Hilpert, K.; Innis, C.A.; Tossi, A.; Wilson, D.N.  
Deposited on : 2018-01-24  
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

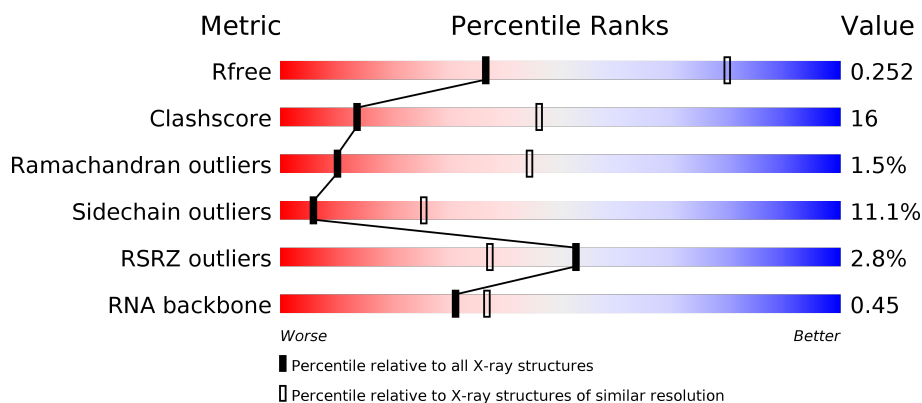
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.









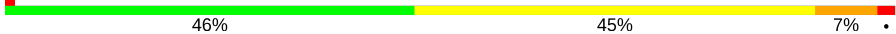
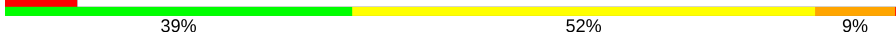



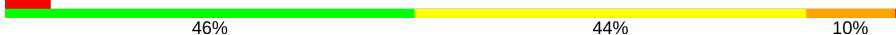













Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2901	 3% 17% 43% 32% 7%
1	2A	2901	 3% 20% 44% 29% 6%
2	1B	120	 21% 53% 23%
2	2B	120	 23% 47% 27%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	275	
3	2D	275	
4	1E	204	
4	2E	204	
5	1F	203	
5	2F	203	
6	1G	181	
6	2G	181	
7	1H	174	
7	2H	174	
8	1I	147	
8	2I	147	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	149	
11	2P	149	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	110	
14	2S	110	
15	1T	131	

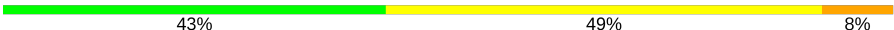











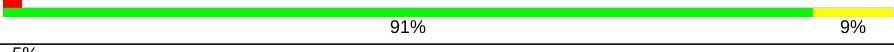
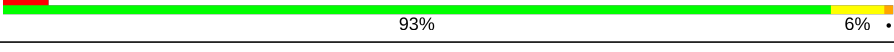


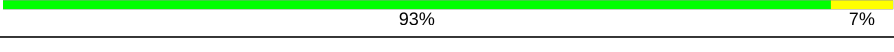
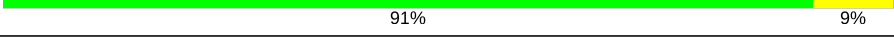
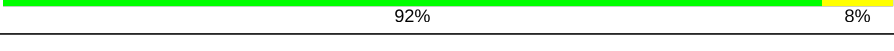
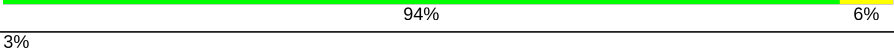
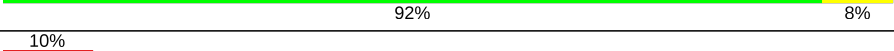
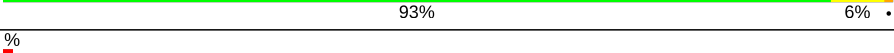
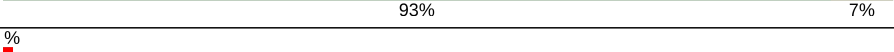
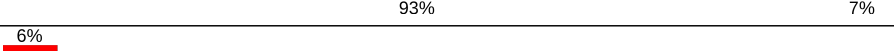
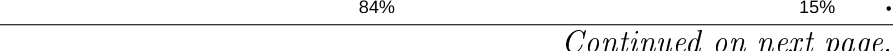
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	131	
16	1U	116	
16	2U	116	
17	1V	101	
17	2V	101	
18	1W	112	
18	2W	112	
19	1X	95	
19	2X	95	
20	1Y	107	
20	2Y	107	
21	1Z	203	
21	2Z	203	
22	10	77	
22	20	77	
23	11	97	
23	21	97	
24	12	70	
24	22	70	
25	13	59	
25	23	59	
26	14	69	
26	24	69	
27	15	59	
27	25	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	53	
28	26	53	
29	17	48	
29	27	48	
30	18	64	
30	28	64	
31	19	37	
31	29	37	
32	1a	1507	
32	2a	1507	
33	1b	231	
33	2b	231	
34	1c	206	
34	2c	206	
35	1d	208	
35	2d	208	
36	1e	148	
36	2e	148	
37	1f	100	
37	2f	100	
38	1g	155	
38	2g	155	
39	1h	137	
39	2h	137	
40	1i	127	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2i	127	
41	1j	97	
41	2j	97	
42	1k	114	
42	2k	114	
43	1l	122	
43	2l	122	
44	1m	116	
44	2m	116	
45	1n	60	
45	2n	60	
46	1o	88	
46	2o	88	
47	1p	82	
47	2p	82	
48	1q	99	
48	2q	99	
49	1r	68	
49	2r	68	
50	1s	83	
50	2s	83	
51	1t	96	
51	2t	96	
52	1u	23	
52	2u	23	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
53	1y	22	
54	1z	97	
54	2z	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1A	3032	-	-	-	X
55	MG	1A	3040	-	-	-	X
55	MG	1A	3048	-	-	-	X
55	MG	1A	3074	-	-	-	X
55	MG	1A	3081	-	-	-	X
55	MG	1A	3085	-	-	-	X
55	MG	1A	3122	-	-	-	X
55	MG	1A	3173	-	-	-	X
55	MG	1A	3184	-	-	-	X
55	MG	1A	3253	-	-	-	X
55	MG	1A	3480	-	-	-	X
55	MG	1A	3493	-	-	-	X
55	MG	1A	3528	-	-	-	X
55	MG	1A	3553	-	-	-	X
55	MG	1A	3562	-	-	-	X
55	MG	1A	3584	-	-	-	X
55	MG	1A	3602	-	-	-	X
55	MG	1A	3638	-	-	-	X
55	MG	1A	3650	-	-	-	X
55	MG	1A	3717	-	-	-	X
55	MG	1A	3780	-	-	-	X
55	MG	1A	3912	-	-	-	X
55	MG	1A	3946	-	-	-	X
55	MG	1A	3957	-	-	-	X
55	MG	1B	217	-	-	-	X
55	MG	1Q	203	-	-	-	X
55	MG	1X	102	-	-	-	X
55	MG	1a	1632	-	-	-	X
55	MG	1a	1640	-	-	-	X
55	MG	1a	1644	-	-	-	X
55	MG	1a	1661	-	-	-	X
55	MG	1a	1666	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1a	1669	-	-	-	X
55	MG	1a	1676	-	-	-	X
55	MG	1a	1680	-	-	-	X
55	MG	1a	1684	-	-	-	X
55	MG	1a	1770	-	-	-	X
55	MG	1a	1806	-	-	-	X
55	MG	1a	1835	-	-	-	X
55	MG	1d	303	-	-	-	X
55	MG	23	102	-	-	-	X
55	MG	29	101	-	-	-	X
55	MG	29	104	-	-	-	X
55	MG	2A	3022	-	-	-	X
55	MG	2A	3025	-	-	-	X
55	MG	2A	3051	-	-	-	X
55	MG	2A	3098	-	-	-	X
55	MG	2A	3109	-	-	-	X
55	MG	2A	3116	-	-	-	X
55	MG	2A	3152	-	-	-	X
55	MG	2A	3164	-	-	-	X
55	MG	2A	3176	-	-	-	X
55	MG	2A	3177	-	-	-	X
55	MG	2A	3187	-	-	-	X
55	MG	2A	3194	-	-	-	X
55	MG	2A	3199	-	-	-	X
55	MG	2A	3202	-	-	-	X
55	MG	2A	3230	-	-	-	X
55	MG	2A	3232	-	-	-	X
55	MG	2A	3250	-	-	-	X
55	MG	2A	3279	-	-	-	X
55	MG	2A	3404	-	-	-	X
55	MG	2A	3413	-	-	-	X
55	MG	2A	3419	-	-	-	X
55	MG	2A	3559	-	-	-	X
55	MG	2A	3591	-	-	-	X
55	MG	2A	3594	-	-	-	X
55	MG	2A	3599	-	-	-	X
55	MG	2A	3641	-	-	-	X
55	MG	2A	3644	-	-	-	X
55	MG	2A	3650	-	-	-	X
55	MG	2A	3694	-	-	-	X
55	MG	2A	3720	-	-	-	X
55	MG	2A	3727	-	-	-	X

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3751	-	-	-	X
55	MG	2A	3753	-	-	-	X
55	MG	2A	3764	-	-	-	X
55	MG	2A	3781	-	-	-	X
55	MG	2A	3782	-	-	-	X
55	MG	2A	3784	-	-	-	X
55	MG	2A	3795	-	-	-	X
55	MG	2A	3800	-	-	-	X
55	MG	2A	3819	-	-	-	X
55	MG	2A	3907	-	-	-	X
55	MG	2A	3911	-	-	-	X
55	MG	2A	3915	-	-	-	X
55	MG	2A	3929	-	-	-	X
55	MG	2A	3931	-	-	-	X
55	MG	2A	3939	-	-	-	X
55	MG	2A	3941	-	-	-	X
55	MG	2A	3944	-	-	-	X
55	MG	2A	3945	-	-	-	X
55	MG	2A	3969	-	-	-	X
55	MG	2B	3008	-	-	-	X
55	MG	2B	3009	-	-	-	X
55	MG	2B	3014	-	-	-	X
55	MG	2B	3016	-	-	-	X
55	MG	2B	3026	-	-	-	X
55	MG	2D	308	-	-	-	X
55	MG	2F	310	-	-	-	X
55	MG	2H	8001	-	-	-	X
55	MG	2Y	201	-	-	-	X
55	MG	2a	1617	-	-	-	X
55	MG	2a	1619	-	-	-	X
55	MG	2a	1624	-	-	-	X
55	MG	2a	1631	-	-	-	X
55	MG	2a	1635	-	-	-	X
55	MG	2a	1639	-	-	-	X
55	MG	2a	1640	-	-	-	X
55	MG	2a	1643	-	-	-	X
55	MG	2a	1651	-	-	-	X
55	MG	2a	1663	-	-	-	X
55	MG	2a	1665	-	-	-	X
55	MG	2a	1668	-	-	-	X
55	MG	2a	1672	-	-	-	X
55	MG	2a	1796	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2a	1827	-	-	-	X
55	MG	2a	1828	-	-	-	X
55	MG	2a	1834	-	-	-	X
55	MG	2d	504	-	-	-	X
55	MG	2i	3001	-	-	-	X
55	MG	2z	101	-	-	-	X

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 294294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61872	27540	11574	19886	2872			
1	2A	2872	Total	C	N	O	P	0	0	0
			61872	27540	11574	19886	2872			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	652R	G	C	conflict	GB 37223181
1A	1227	G	UNK	conflict	GB 37223181
2A	652R	G	C	conflict	GB 37223181
2A	1227	G	UNK	conflict	GB 37223181

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	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			

*Continued on next page...*

*Continued from previous page...*

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	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
			775	498	141	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	520	153	131	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	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

- 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			
26	24	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

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

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

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

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

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



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

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

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

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

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	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
			814	516	144	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
			1235	769	244	216	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	127	Total	C	N	O	0	0	0
			986	625	193	168			

- 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			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	2j	97	Total	C	N	O	0	0	0
			719	446	142	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			
42	2k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			

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

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

- Molecule 53 is a protein called Tur1A peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	1y	22	Total	C	N	O	0	0	0
			168	111	34	23			

- Molecule 54 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1z	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
54	2z	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2E	6	Total	Mg	0	0
			6	6		
55	17	2	Total	Mg	0	0
			2	2		
55	2d	3	Total	Mg	0	0
			3	3		
55	1T	2	Total	Mg	0	0
			2	2		
55	1N	4	Total	Mg	0	0
			4	4		
55	20	5	Total	Mg	0	0
			5	5		
55	18	3	Total	Mg	0	0
			3	3		
55	1o	2	Total	Mg	0	0
			2	2		
55	2W	3	Total	Mg	0	0
			3	3		
55	1Y	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	13	2	Total 2	Mg 2	0	0
55	1f	1	Total 1	Mg 1	0	0
55	2h	2	Total 2	Mg 2	0	0
55	1P	4	Total 4	Mg 4	0	0
55	2B	26	Total 26	Mg 26	0	0
55	2a	242	Total 242	Mg 242	0	0
55	1k	1	Total 1	Mg 1	0	0
55	1E	5	Total 5	Mg 5	0	0
55	2z	2	Total 2	Mg 2	0	0
55	1b	1	Total 1	Mg 1	0	0
55	2l	2	Total 2	Mg 2	0	0
55	2F	11	Total 11	Mg 11	0	0
55	28	2	Total 2	Mg 2	0	0
55	2e	1	Total 1	Mg 1	0	0
55	1W	3	Total 3	Mg 3	0	0
55	1A	957	Total 957	Mg 957	0	0
55	1t	1	Total 1	Mg 1	0	0
55	1n	1	Total 1	Mg 1	0	0
55	2P	2	Total 2	Mg 2	0	0
55	1X	2	Total 2	Mg 2	0	0
55	2i	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	25	4	Total 4	Mg 4	0	0
55	2b	1	Total 1	Mg 1	0	0
55	2T	3	Total 3	Mg 3	0	0
55	1D	17	Total 17	Mg 17	0	0
55	2N	3	Total 3	Mg 3	0	0
55	1e	1	Total 1	Mg 1	0	0
55	2G	3	Total 3	Mg 3	0	0
55	29	3	Total 3	Mg 3	0	0
55	2f	1	Total 1	Mg 1	0	0
55	1V	3	Total 3	Mg 3	0	0
55	2X	2	Total 2	Mg 2	0	0
55	1a	245	Total 245	Mg 245	0	0
55	2Q	4	Total 4	Mg 4	0	0
55	15	5	Total 5	Mg 5	0	0
55	1R	4	Total 4	Mg 4	0	0
55	2t	2	Total 2	Mg 2	0	0
55	2U	5	Total 5	Mg 5	0	0
55	1G	3	Total 3	Mg 3	0	0
55	11	4	Total 4	Mg 4	0	0
55	1d	5	Total 5	Mg 5	0	0
55	1H	2	Total 2	Mg 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	21	1	Total 1	Mg 1	0	0
55	2g	1	Total 1	Mg 1	0	0
55	1i	1	Total 1	Mg 1	0	0
55	2Y	1	Total 1	Mg 1	0	0
55	23	2	Total 2	Mg 2	0	0
55	2R	3	Total 3	Mg 3	0	0
55	2D	17	Total 17	Mg 17	0	0
55	1U	5	Total 5	Mg 5	0	0
55	27	2	Total 2	Mg 2	0	0
55	19	3	Total 3	Mg 3	0	0
55	1l	2	Total 2	Mg 2	0	0
55	2V	5	Total 5	Mg 5	0	0
55	1F	14	Total 14	Mg 14	0	0
55	2H	2	Total 2	Mg 2	0	0
55	10	7	Total 7	Mg 7	0	0
55	1g	1	Total 1	Mg 1	0	0
55	2o	2	Total 2	Mg 2	0	0
55	1Q	4	Total 4	Mg 4	0	0
55	2A	971	Total 971	Mg 971	0	0
55	1h	1	Total 1	Mg 1	0	0
55	1B	28	Total 28	Mg 28	0	0

*Continued on next page...*



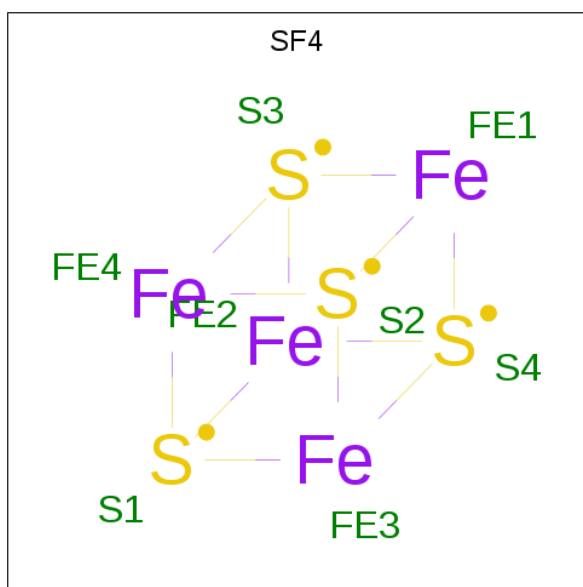
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2S	1	Total	Mg	0	0
			1	1		

- 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	1n	1	Total	Zn	0	0
			1	1		
56	15	1	Total	Zn	0	0
			1	1		
56	29	1	Total	Zn	0	0
			1	1		
56	19	1	Total	Zn	0	0
			1	1		
56	26	1	Total	Zn	0	0
			1	1		
56	25	1	Total	Zn	0	0
			1	1		
56	24	1	Total	Zn	0	0
			1	1		
56	2n	1	Total	Zn	0	0
			1	1		
56	2Y	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		

- 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	0	0
			8	4	4		
57	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1782	Total	O	0	0
			1782	1782		
58	1B	45	Total	O	0	0
			45	45		
58	1D	15	Total	O	0	0
			15	15		
58	1E	18	Total	O	0	0
			18	18		
58	1F	14	Total	O	0	0
			14	14		
58	1G	2	Total	O	0	0
			2	2		
58	1H	5	Total	O	0	0
			5	5		
58	1N	7	Total	O	0	0
			7	7		
58	1P	12	Total	O	0	0
			12	12		
58	1Q	6	Total	O	0	0
			6	6		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1R	6	Total 6	O 6	0	0
58	1T	5	Total 5	O 5	0	0
58	1U	7	Total 7	O 7	0	0
58	1V	3	Total 3	O 3	0	0
58	1W	1	Total 1	O 1	0	0
58	1X	6	Total 6	O 6	0	0
58	1Y	5	Total 5	O 5	0	0
58	10	6	Total 6	O 6	0	0
58	11	2	Total 2	O 2	0	0
58	13	2	Total 2	O 2	0	0
58	15	2	Total 2	O 2	0	0
58	16	2	Total 2	O 2	0	0
58	17	2	Total 2	O 2	0	0
58	18	9	Total 9	O 9	0	0
58	19	2	Total 2	O 2	0	0
58	1a	406	Total 406	O 406	0	0
58	1d	8	Total 8	O 8	0	0
58	1e	4	Total 4	O 4	0	0
58	1f	1	Total 1	O 1	0	0
58	1h	1	Total 1	O 1	0	0
58	1j	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1l	3	Total 3	O 3	0	0
58	1m	3	Total 3	O 3	0	0
58	1n	1	Total 1	O 1	0	0
58	1o	1	Total 1	O 1	0	0
58	1p	1	Total 1	O 1	0	0
58	1t	1	Total 1	O 1	0	0
58	1z	3	Total 3	O 3	0	0
58	2A	1771	Total 1771	O 1771	0	0
58	2B	46	Total 46	O 46	0	0
58	2D	14	Total 14	O 14	0	0
58	2E	20	Total 20	O 20	0	0
58	2F	12	Total 12	O 12	0	0
58	2G	2	Total 2	O 2	0	0
58	2H	4	Total 4	O 4	0	0
58	2N	7	Total 7	O 7	0	0
58	2P	11	Total 11	O 11	0	0
58	2Q	7	Total 7	O 7	0	0
58	2R	6	Total 6	O 6	0	0
58	2T	5	Total 5	O 5	0	0
58	2U	8	Total 8	O 8	0	0
58	2V	5	Total 5	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2W	2	Total	O	0	0
			2	2		
58	2X	7	Total	O	0	0
			7	7		
58	2Y	5	Total	O	0	0
			5	5		
58	20	8	Total	O	0	0
			8	8		
58	21	2	Total	O	0	0
			2	2		
58	23	2	Total	O	0	0
			2	2		
58	25	4	Total	O	0	0
			4	4		
58	26	2	Total	O	0	0
			2	2		
58	27	2	Total	O	0	0
			2	2		
58	28	11	Total	O	0	0
			11	11		
58	29	2	Total	O	0	0
			2	2		
58	2a	404	Total	O	0	0
			404	404		
58	2d	8	Total	O	0	0
			8	8		
58	2e	6	Total	O	0	0
			6	6		
58	2f	1	Total	O	0	0
			1	1		
58	2h	1	Total	O	0	0
			1	1		
58	2j	1	Total	O	0	0
			1	1		
58	2l	3	Total	O	0	0
			3	3		
58	2m	2	Total	O	0	0
			2	2		
58	2n	1	Total	O	0	0
			1	1		
58	2o	3	Total	O	0	0
			3	3		

*Continued on next page...*

*Continued from previous page...*

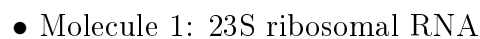
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2p	1	Total	O	0	0
			1	1		
58	2z	4	Total	O	0	0
			4	4		





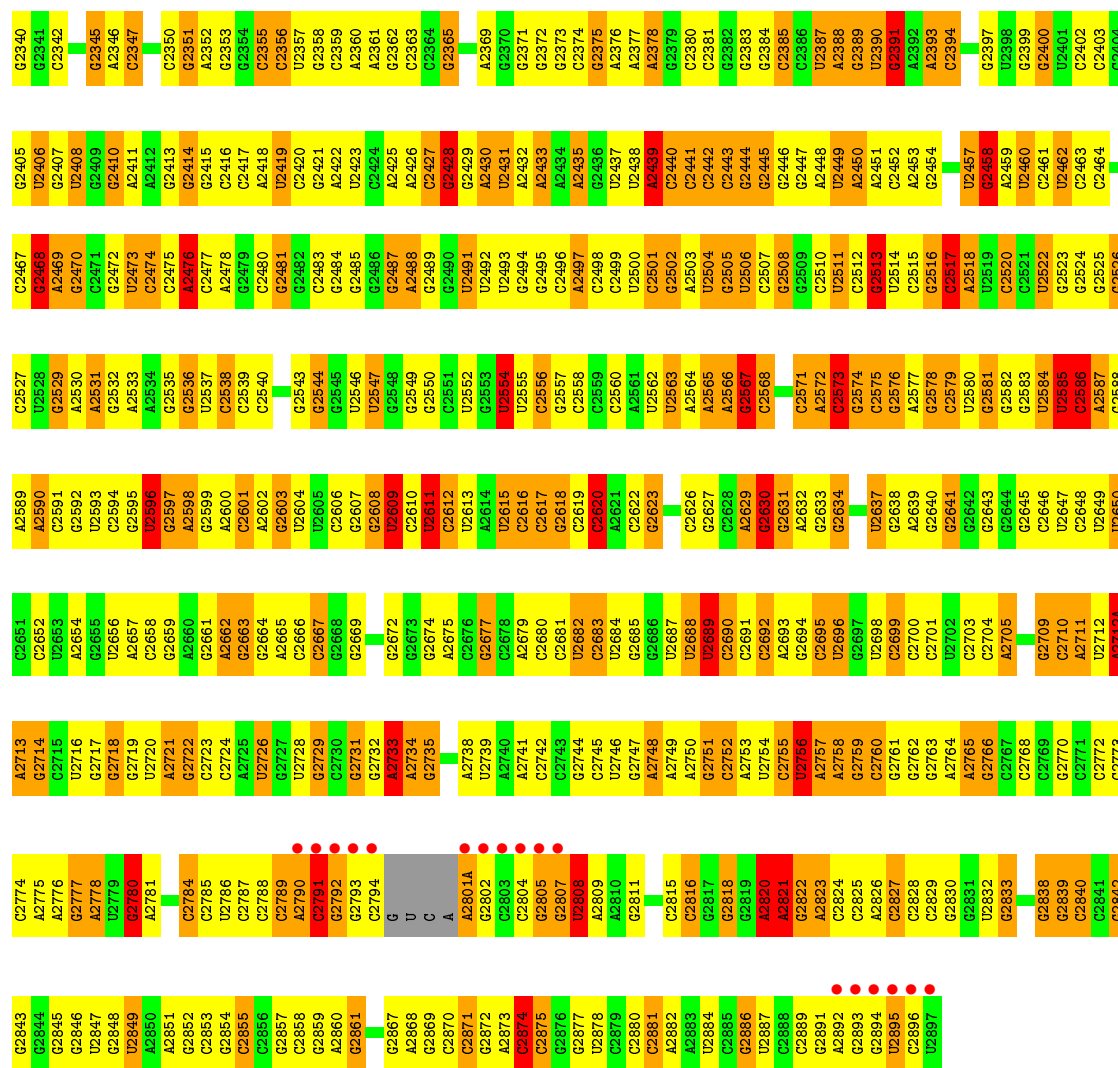


U2504	C2441	C2380	C2317	G2256	G2186	A2126	C2064	G2003	U1943	U1864	C1797	C1712	G1591
G2505	C2442	C2381	G2318	G2257	G2187	G2127	C2065	G2004	U1944	U1865	U1798	U1713	C1592
U2506	C2443	G2382	G2319	G2258	C2188	C2128	C2066	A2005	G1945	A1877	G1799		G1593
C2507	G2444	G2383	A2320	G2259	U2189	G2129	G2067	C2006	U1946	C1878	C1800	U1720	G1594
G2508	G2445	G2384	G2321	G2260	G2190	U2130	G2068	C2007	C1947	C1879	G1801	G1721	G1595
G2509	G2446	G2385	A2322	G2261	G2191	G2131	G2069	C2008	G1948	C1880	A1802	G1722	A1596
C2510	G2447	G2386	G2323	U2262	G2192	U2132	G2070	G2009	G1949		A1803	U1739	A1597
U2511	G2448	U2387	G2324	C2263	G2193	G2133	A2071	G2010	U1950	G1883	C1804	G1740	C1598
C2512	U2449	A2388	G2325	G2264	G2194	A2134	G2072	U2011	U1951	A1884		G1741	C1599
G2513	A2450	G2389	C2326	U2265	C2195	C2136	G2073	G2012	A1952	A1885		G1742	G1600
U2514	A2451	U2390	G2327	A2266	G2196	U2074	U2074	A2013	A1953	C1886	A1809	C1743	G1601
G2515	G2452	G2391	A2328	A2267	U2197	G2137	U2075	A2014	G1954	C1887	A1810		G1602
G2516	A2453	A2392	G2329	A2268	G2198	C2138	U2076	A2015	U1955	C1888	G1811	C1745A	U1603
C2517	G2454	A2393	G2330	G2269	G2199	C2139	A2077	U2016	U1956	A1889			A1604
A2518	G2455	C2394	G2331	G2270	C2200	G2140	G2078	A2019	C1957	A1890	G1812	G1750	G1605
U2519	G2456	C2395	U2332	G2271	C2201	G2141	U2079	A2020	C1958	A1891	G1814	G1751	G1606
G2520	C2457	G2396	A2333	U2272	C2202	C2142	G2080	A2021	G1959	C1892	A1815	G1752	A1607
C2521	G2458	G2397	G2334	A2273	U2203	G2143	C2081	C2021	G1960	C1893	G1816	G1753	A1608
U2522	A2459	U2398	A2335	A2274	C2205	U2144	A2082	U2022	C1961		G1817	C1754	A1609
G2523	U2460	G2399	A2336	G2275	G2206	C2145	G2083	G2023	C1962	G1896	A1818	G1755	A1610
G2524	C2461	G2400	G2337	G2276	G2207	G2146	G2084	G2024	U1963	A1897	A1819	G1756	G1611
G2525	U2462	U2401		G2277	A2208	G2147	C2085	C2025	G1964	U1898	U1820	U1757	G1612
G2526	C2463	C2402	G2340	A2278	U2218	G2148	U2086	C2026	C1965	U1899	A1821	G1758	G1613
G2527	C2464	C2403	G2341	G2279	G2219	G2149	G2087	G2027	A1966	A1900	G1822	A1759	A1614
U2528	C2465	A2404	C2342	G2280	G2220	U2150	G2088	U2028	C1967	A1901	G1823		C1615
G2529	C2466	G2405	C2343	G2281	G2221	G2151	U2089	G2029	G1968	C1902	G1824		A1616
A2530	G2467	U2406	U2344	G2282	G2222	G2152	G2090	A2030	A1969	G1903	A1825	G1763	C1617
G2531	G2468	C2407	G2345	G2283	G2223	G2153	U2091	G2031	A1970	G1904	G1826	G1764	A1618
	A2469		G2346	C2284	G2224	G2154	U2092	G2032	A1971	C1905		C1765	G1619
A2534	C2470	G2410	C2347	G2285	A2225	G2155	G2093	A2033	A1972	U1766	A1829	G1767	G1620
G2535	C2471	A2411	U2348	A2286	G2226	G2156	G2094	U2034	G1973	C1906	C1830	C1768	U1621
G2536	G2472	A2412	G2349	A2287	A2227	G2157		G2035	C1974		C1831	U1768	G1622
U2537	U2473	A2413	C2350	A2288	G2228	A2158	U2098	G2036	G1975	A1913	G1832	G1769	C1625
G2538	C2474	G2414	G2351	G2289	G2229	G2159	U2099	G2037	U1976	U1915	C1833	G1770	G1626
C2539	G2475	G2415	A2352	G2290	G2230	G2160	G2107	G2038	A1977	A1916	U1834	C1771	G1686
G2540	A2476	C2416	G2353	U2291	C2231	C2161	G2101	C2039	A1978	U1917		G1772	G1627
A2541	C2477	G2417	G2354	C2292	U2232	G2162	U2102	C2040	C1979	A1918	G1837	A1773	G1628
G2542	U2478	A2418	C2355	C2293	U2233	C2163	C2103	U2041	G1980	A1919	C1838	C1774	U1629
		U2419	G2356	G2294	G2234	C2164	A2104	A2042	A1981	C1920	G1839	U1775	G1630
G2543	C2483	C2420	U2357	G2295	G2235	G2165	C2105	C2043	C1982	G1921	U1841	G1776	C1631
G2544	G2484	G2421	G2358	U2296	G2236	G2166	G2106	C2044	G1983		G1842	U1777	A1631A
U2545	G2485	A2422	C2359	G2297	G2237	U2167	C2107	C2045	G1984	C1924	G1843	U1778	A1632
U2546	G2486	U2423	A2360	A2298	G2238	G2168	C2108	G2046	G1985	U1925	G1844	U1779	G1633
G2547	C2487	C2424	A2361	G2299	G2239	A2169	U2109	U2047	A1986	U1926	C1844	A1780	A1634
G2548		A2425	G2362	G2300	G2240	G2170	C2110	G2048	G1987	A1927	G1845	C1781	
G2549	A2488			C2301	A2441	A2171	C2111	G2049	G1988	A1928	G1846	C1782	G1696
G2550	G2489	A2426	G2363	G2302	G2242	U2172	C2112	C2050	G1989	G1929	A1847	A1783	A1697
C2551	G2490	G2427	G2364	G2303	U2243	A2173	U2113	A2051	C1990	G1930	A1848	A1784	A1698
U2552	U2491	G2428	G2365	G2304	U2244	G2174	A2114	G2052	U1991	U1931	G1849	A1785	U1699
G2553	U2492	G2429	A2366	A2305	U2245	C2175	G2115	G2053	G1992	A1932	G1850	A1786	C1640
U2554	U2493	A2430	A2369	G2306	G2246	A2176	G2116	A2054	U1993	G1933	U1851	A1787	A1641
U2555	G2494	U2431	G2370	G2307	A2247	C2177	A2117	C2055	U1994	C1934	C1852	G1788	G1642
C2556	G2495	A2432	G2371		A2248	C2178	U2118	C2056	U1995	A1935	A1853	G1789	G1643
G2557	C2496	A2433	G2372	A2310	U2249	C2179	A2119	A2057	U1996	A1936	A1854	C1790	C1644
C2558	A2497	A2434	G2373	A2311	G2250	U2180	G2120	A2058	G1997	A1937	G1855	A1791	G1705
	G2498	A2435	C2374	A2312	G2251	G2181	G2121	A2059	G1998	A1938	G1856	G1792	U1706
A2561	C2499	G2436	G2375	U2312	G2252	G2182	U2122	A2060	C1999	U1939	G1857	C1793	G1647
U2562	U2500	U2437	A2376	C2313	G2253	C2183	G2123	G2061	G2000	U1940	C1794	U1795	C1648
U2563	C2501	U2438	A2377	G2314	G2254	G2184	A2062	A2062	A2001	C1941	G1858	C1796	G1649
A2564	U2502	A2439	A2378	G2315	G2255	C2185	G2125	C2063	G2002	C1942		U1796	G1650
U2565	A2503	C2440	G2379	C2316	G2256	C2185	G2125				G1863		G1651



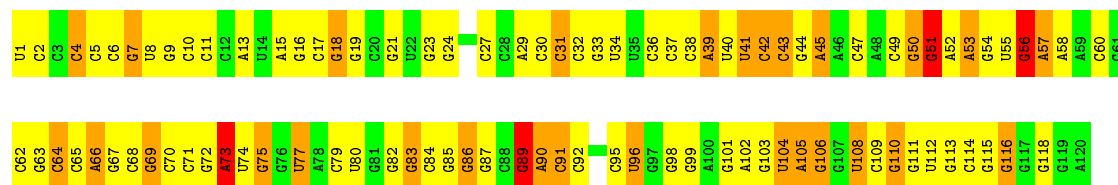
U1385	A1274	A1214	U1026	G966	A901	U839	U779	A718	U657	G615	U557	G494
A1386	A1275	G1215	A1027	G967	G902	C840	G790	C719	C688	G616	G558	G495
G1337	G1276	C1217	A1028	G968	C903	A841	A781	C720	C659	C618	G559	G496
G1338	G1277	C1216	A1029	U969	C904	G842	A782	C721	G660	G619	G560	G497
G1339	A1278	G1218	G1030	G970	U905	G843	A783	G722	G661	G620	G561	G498
U1340	G1279	A1155	G1031	G972	G906	C844	A784	G723	G662	A621	G562	U499
U1341	G1280	A1156	A1032	A873	U907	G845	G785	U724	G663	G622	G563	G500
A1342	U1281	A1220	U1033	G974	C908	C846	G786	G725	C664	G623	C564	A501
G1343	U1282	C1221A	U1034	C975	G909	U847	U787	G726	C665	G624	A502	A502
G1344	G1283	G1222	U1035	G975A	A910	G848	A788	A727	G666	G625	U566	G504
C1345	A1284	G1223	U1036	G976	A911	A849	A789	G728	G667	U626	A567	U504
G1346	G1285	G1224	G1037	G977	G912	C850	G790	G729	G668	A627	U568	A505
A1348	A1286	G1225	G1038	G978	U913	U851	C791	G730	G669	G628	U569	G506
A1349	U1287	A1226	G1039	G979	G914	G852	G782	C731	A670	G629	G570	A507
C1350	U1288	G1227	C1040	A980	C915	G853	A793	G732	G671	G630	A571	G508
C1351	G1289	G1228	A981	A981	G916	G854	G794	G733	C672	A631	G573	C509
U1352	G1290	U1039	G982	G982	A917	G855	C795	A734	G673	A632	G574	C510
A1353	C1291	G1230	A983	A983	A918	C856	C796	A735	G674	A633	G575	U511
A1354	U1292	G1231	G1044	A984	U922	C857	C797	G736	A675	C634	A576	G512
G1355	U1293	U1234	A1045	C985	U922	U858	G798	C737	A676	C635	U576	A513
A1359	G1294	G1235	A1046	C986	C923	G859	G799	G738	A677	G636	G577	A514
A1360	G1295	G1236	A1047	G987	C924	U860	A800	G739	C678	A637	U578	A515
G1361	G1296	A1237	C1049	A988	C925	A861	G801	U740	G679	G638	A579	C516
C1362	U1297	G1238	A1050	G989	A926	G862	A802	G741	G680	U639	C580	C517
G1363	G1298	G1239	G1051	A990	G927	A863	U803	G742	G681	C640	C581	G518
G1364	U1299	U1240	C1052	C991	G928	G864	A804	G743	G682	C641	G582	U519
A1365	U1300	G1241	G1053	C992	U930	C865	G805	A746	G683	G642	G583	G520
G1366	A1301	A1242	A1054	G993	G931	A866	C806	U747	G684	A643	C584	G521
G1367	A1302	G1243	G1055	C994	G932	U867	U807	G748	A685	A644	G585	G522
G1368	G1303	C1244	G1056	C995	U935	U868	G808	G749	G686	C645	A586	C523
G1369	G1304	G1245	A1057	A996	C935	G869	G809	C750	C587	A646	U524	U524
U1370	U1305	G1246	G1058	C997	C936	A870	U810	A750	U688	G647	U525	U525
A1372	G1306	A1246	G1059	C998	U937	U871	U811	A751	A689	G648	C527	A526
G1373	A1307	G1247	U1060	U999	G938	A872	C812	G752	G690	G649	A590	C527
G1374	G1308	G1248	U1061	A1000	C939	G873	U813	C753	C691	C650	A591	A528
G1375	G1309	U1249	G1062	A1001	G940	C874	C814	C754	C692	G592	G592	A529
G1376	G1310	G1250	G1063	G1002	A941	G875	C815	C755	C693	G593	G593	G530
G1377	G1311	G1251	C1064	G1003	G942	C876	C816	C756	U694	U594	C595	C531
A1378	U1312	G1252	C1065	C1004	U943	U877	C817	U757	G695	G652C	C596	A532
A1379	G1313	G1253	U1066	C1005	G944	A878	G818	C758	G696	G652D	G596	G533
G1380	U1314	A1254	A1067	C1006	A945	G879	A819	G759	C697	G652E	U597	U534
G1381	C1315	U1255	G1068	C1007	G946	G880	A820	G760	C698	G652F	G598	G535
G1382	G1316	G1256	A1069	G1008	G947	C881	A821	A761	A699	G	G599	A536
G1383	U1317	C1257	A1070	A1009	G948	G882	U822	U762	G600	C	G600	C537
A1384	C1318	G1258	G1071	A1010	C951	G883	G823	G763	G601	C	G601	G538
G1385	G1319	G1259	C1072	U1011	C951	C886	A824	A764	G602	G	G602	G539
C1386	C1320	G1260	A1073	U1012	G952	C887	C825	G765	A603	C	A603	C540
G1387	C1321	C1261	G1074	U1013	A953	A887	U826	C766	G604	A	G604	C541
G1388	A1322	U1262	C1075	U1014	G954	C888	U827	U767	C605	C	C605	C542
G1389	U1323	G1263	C1076	G1015	C955	C889	U828	G768	U606	C	U606	C543
U1390	G1324	U1264	A1077	G1016	G956	A890	A829	G769	U607	C	U607	G545
U1391	U1325	A1265	U1078	G1017	A957	G892	G830	G770	A608	G	A608	C
A1392	G1326	G1266	C1079	C1018	U958	C893	G831	G771	G610	G	G610	A
A1393	C1327	U1267	U1019	U1019	A959	C894	G832	C772	G711	G	G711	A548
U1394	G1328	C1207	U1020	U1020	A960	U895	U833	U773	G613	C652S	G613	G549
U1395	U1329	A1268	U1021	A1021	C961	A896	C834	A774	G713	C652T	G614	G551
U1396	C1330	G1269	U1022	G1022	G962	C897	A835	G775	G714	G652U	U614	U554
U1397	A1331	G1270	A1084	U1023	G963	C898	G836	A776	G715	G	U614B	U555
G1398	G1332	G1271	A1085	U1024	C964	A899	C837	A777	A716	A655	G614C	G556
C1399	C1333	U1212	A1086	G1025	C965	A900	C838	G778	G717	G656		
G1400	G1334	U1273	G1087	G1025								





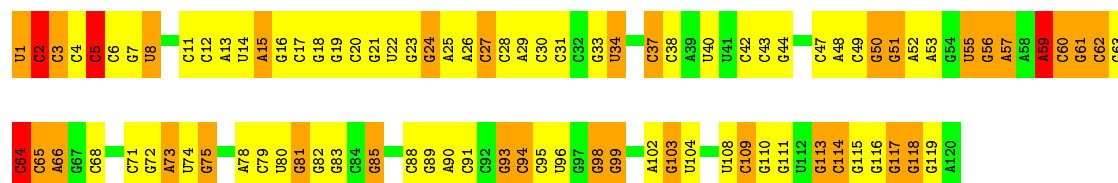
• Molecule 2: 5S ribosomal RNA

Chain 1B: 21% 53% 23%

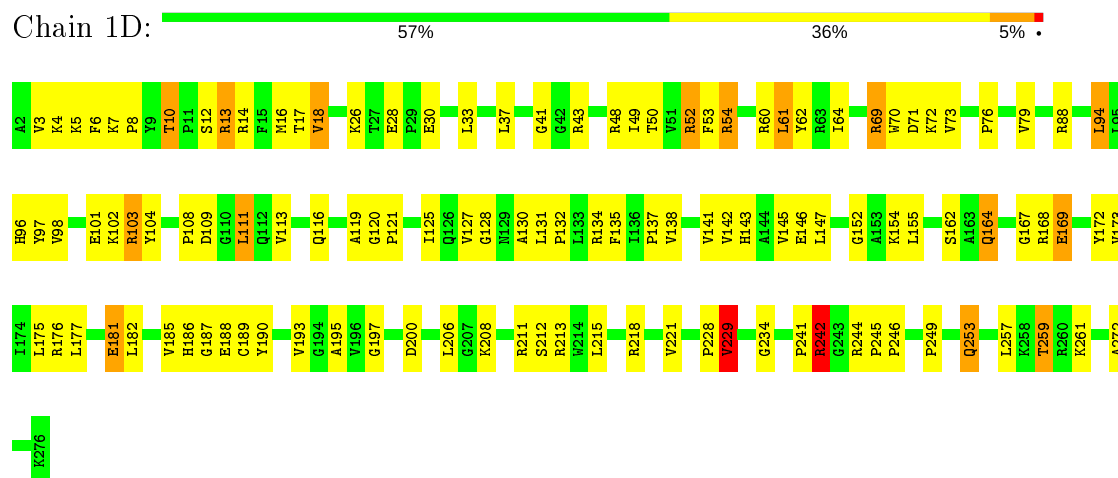


• Molecule 2: 5S ribosomal RNA

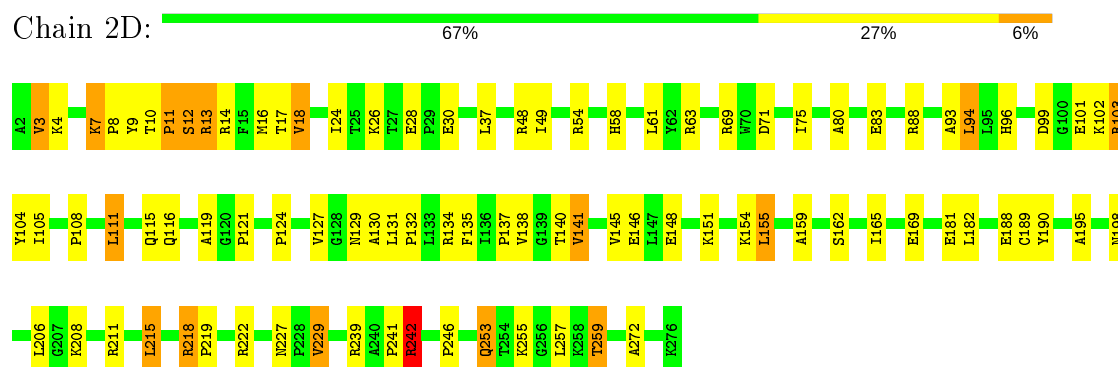
Chain 2B: 23% 47% 27%



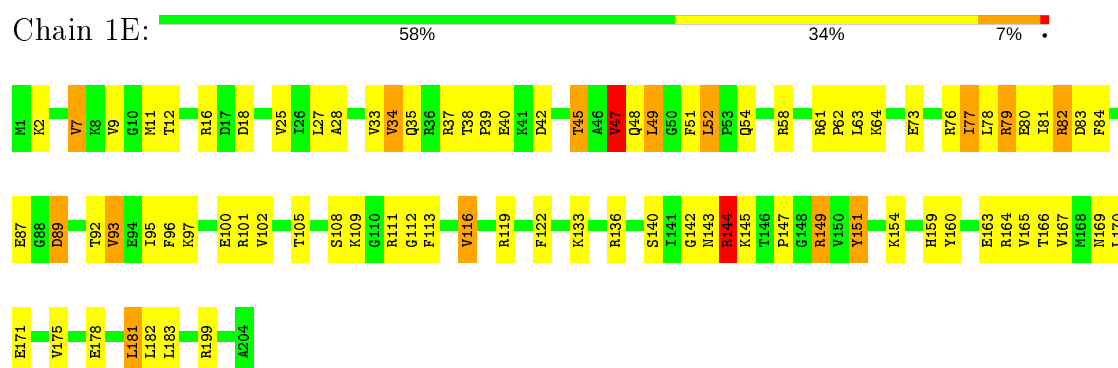
- Molecule 3: 50S ribosomal protein L2



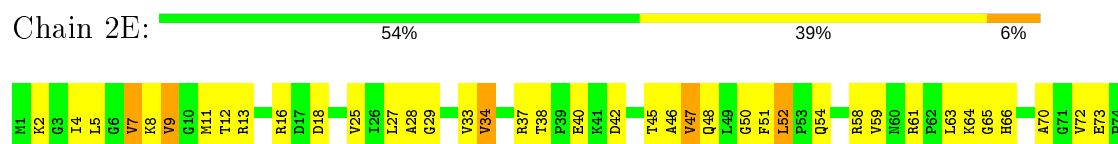
- Molecule 3: 50S ribosomal protein L2

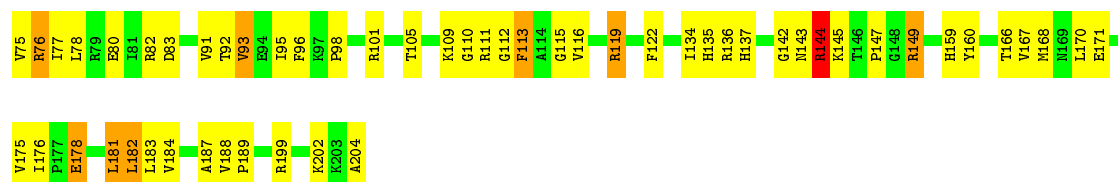


- Molecule 4: 50S ribosomal protein L3



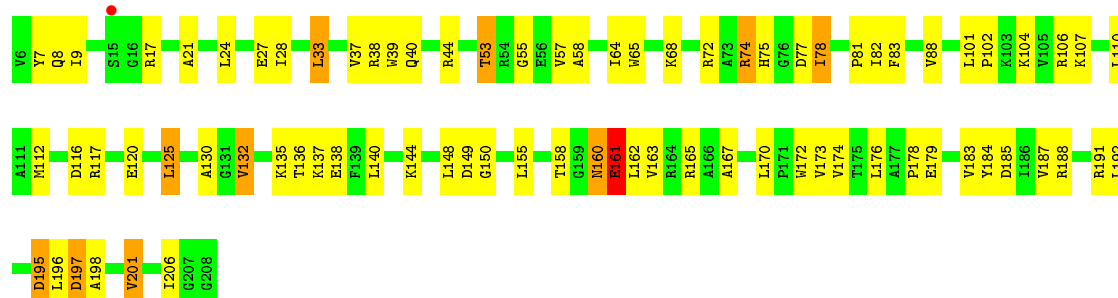
- Molecule 4: 50S ribosomal protein L3





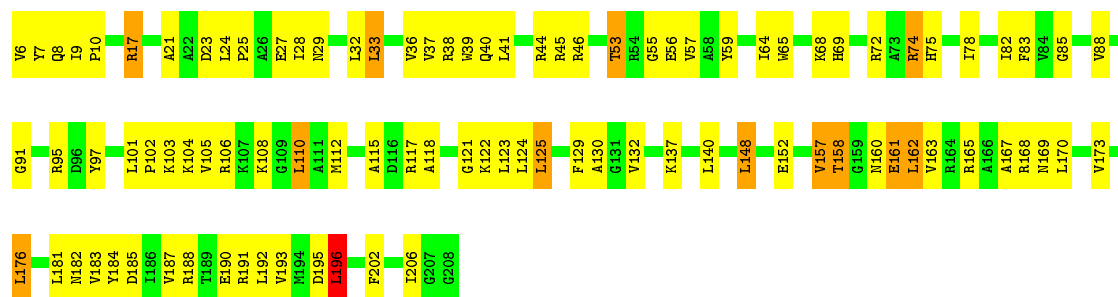
- Molecule 5: 50S ribosomal protein L4

Chain 1F: 61% 34% 5%



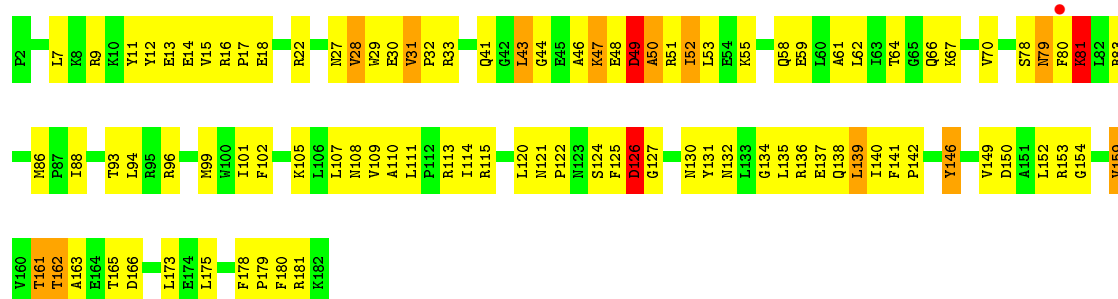
- Molecule 5: 50S ribosomal protein L4

Chain 2F: 53% 41% 6%



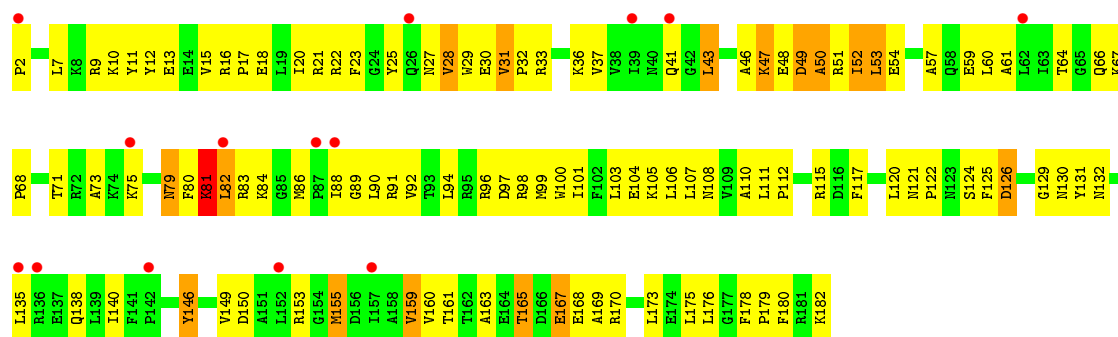
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 46% 45% 7%

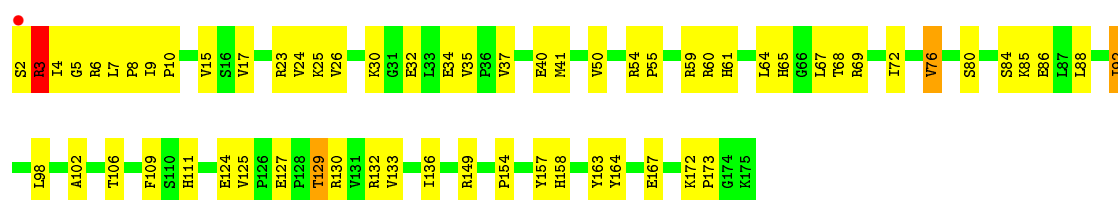


- Molecule 6: 50S ribosomal protein L5

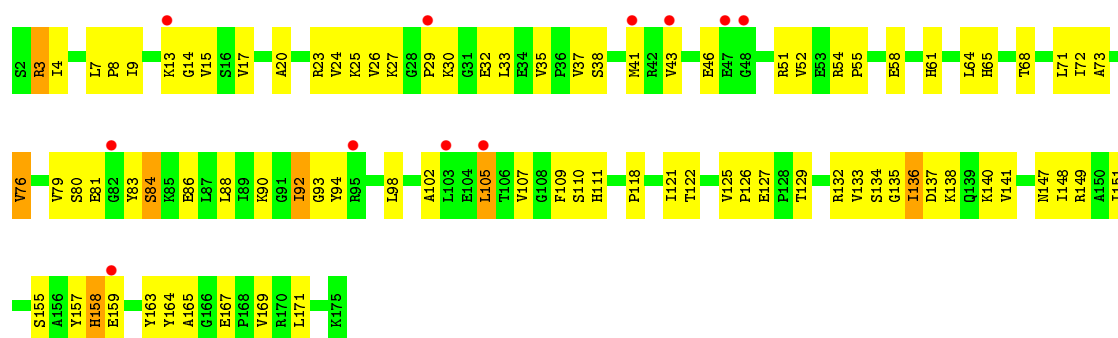
Chain 2G: 39% 52% 9%



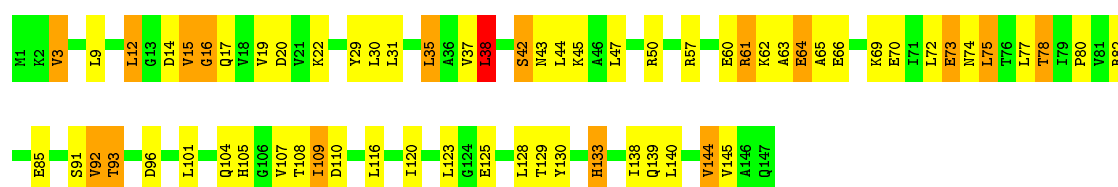
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6



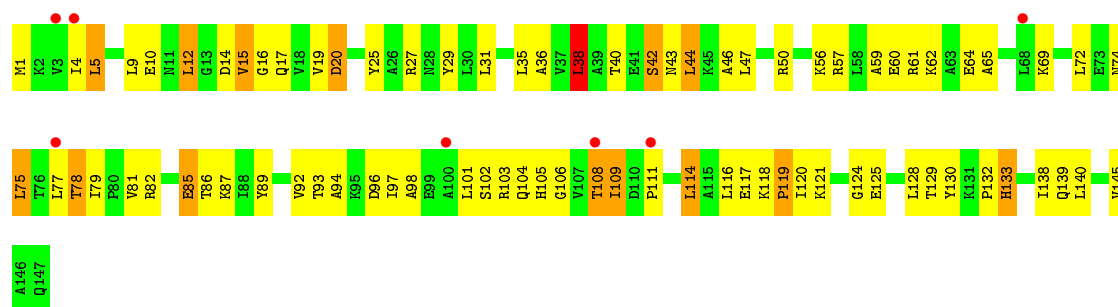
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

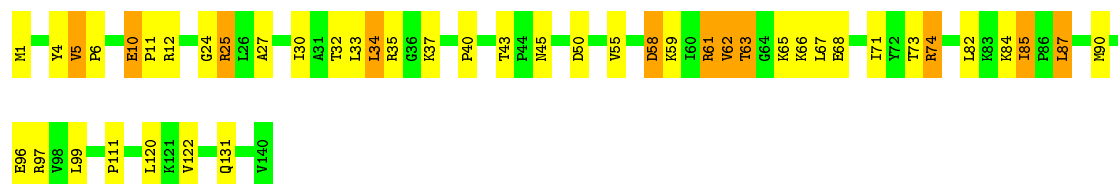






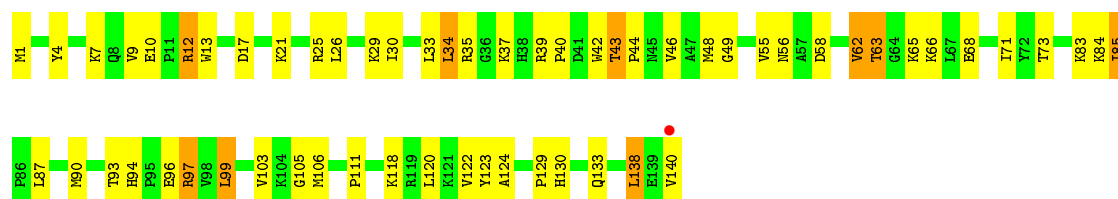
• Molecule 9: 50S ribosomal protein L13

Chain 1N: 68% 24% 8%



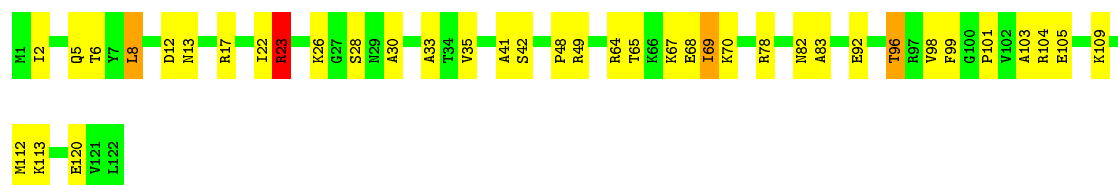
• Molecule 9: 50S ribosomal protein L13

Chain 2N: 58% 36% 6%



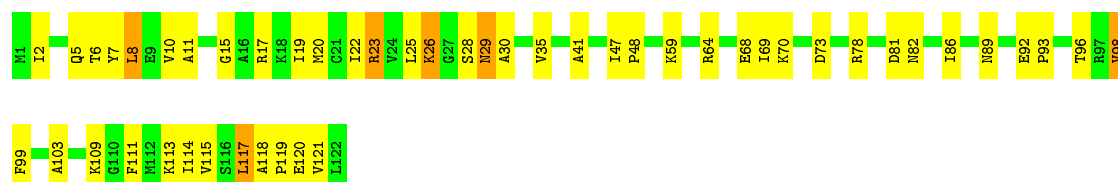
• Molecule 10: 50S ribosomal protein L14

Chain 1O: 68% 29% 3%

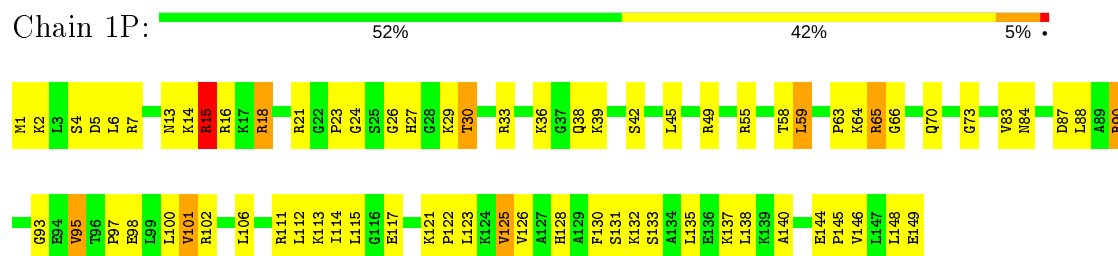


• Molecule 10: 50S ribosomal protein L14

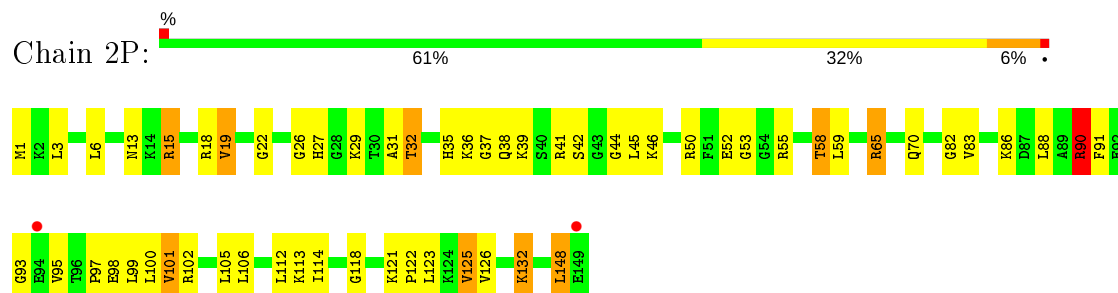
Chain 2O: 60% 35% 5%



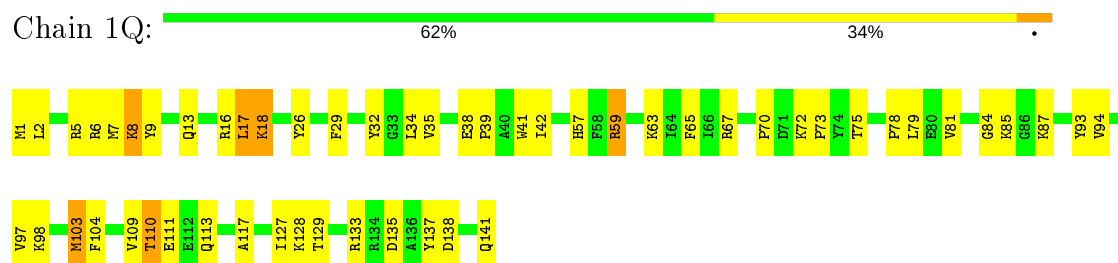
- Molecule 11: 50S ribosomal protein L15



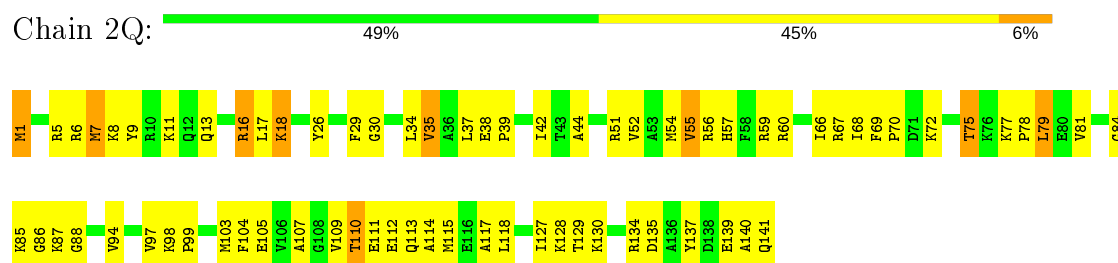
- Molecule 11: 50S ribosomal protein L15



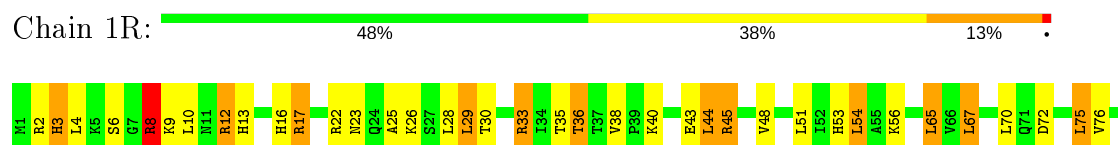
- Molecule 12: 50S ribosomal protein L16

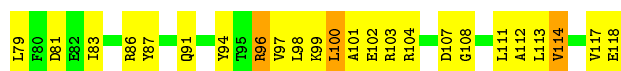


- Molecule 12: 50S ribosomal protein L16

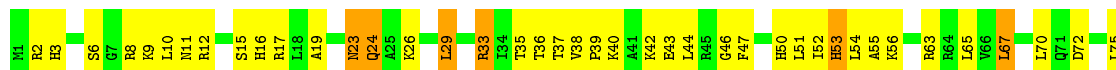


- Molecule 13: 50S ribosomal protein L17

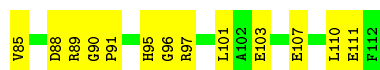




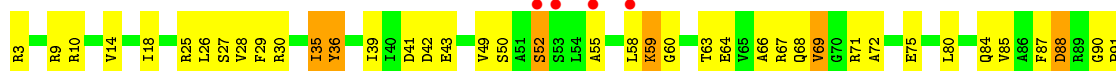
- Molecule 13: 50S ribosomal protein L17



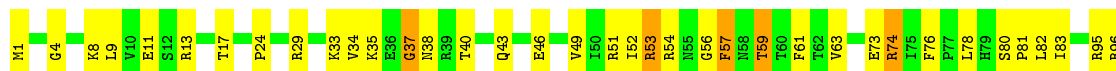
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

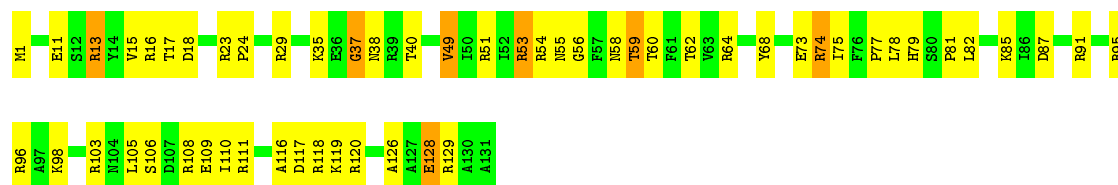


- Molecule 15: 50S ribosomal protein L19

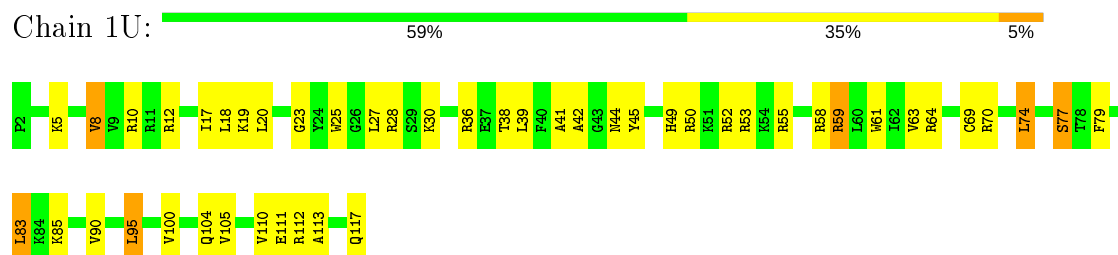


- Molecule 15: 50S ribosomal protein L19

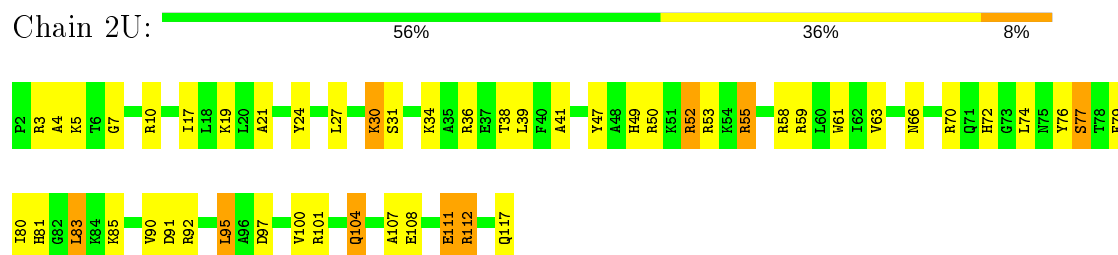




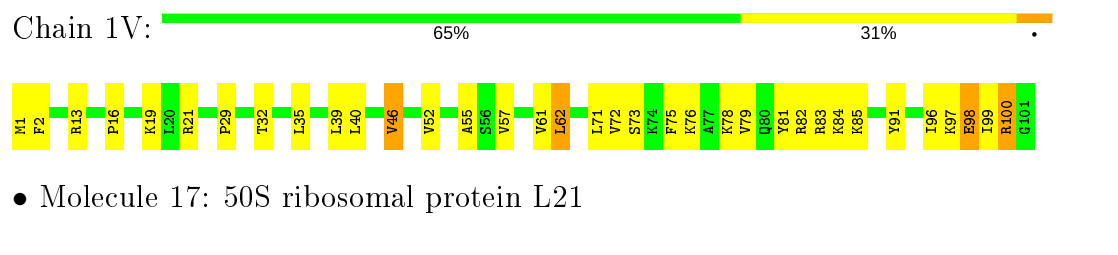
• Molecule 16: 50S ribosomal protein L20



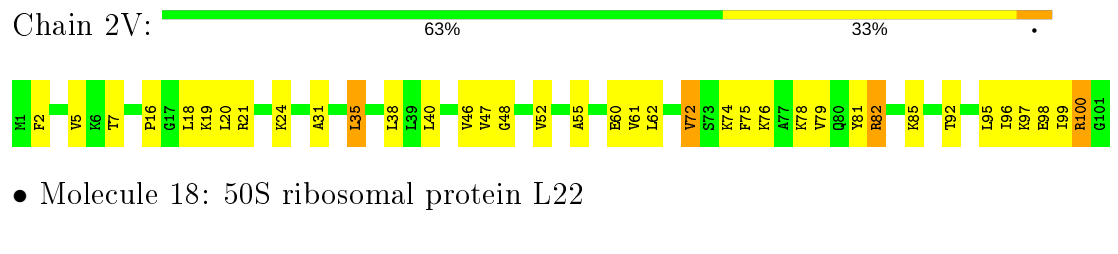
• Molecule 17: 50S ribosomal protein L21



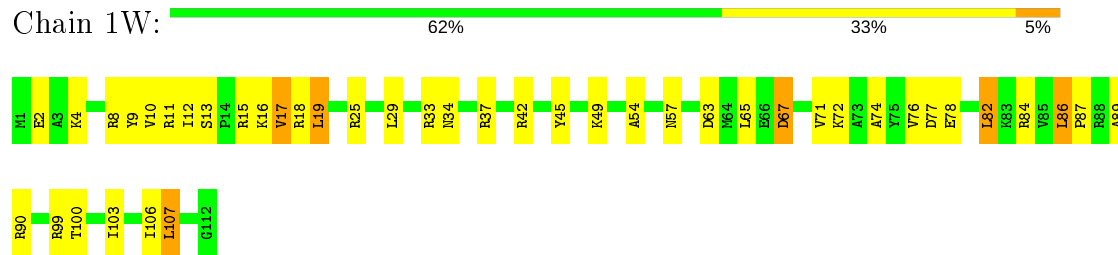
• Molecule 18: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L23

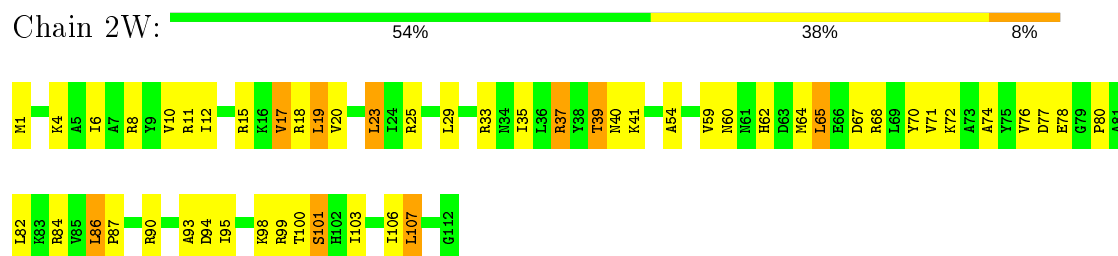


• Molecule 20: 50S ribosomal protein L24

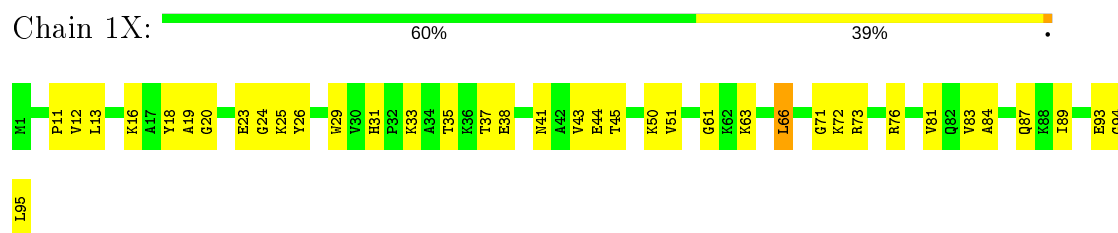


• Molecule 21: 50S ribosomal protein L25

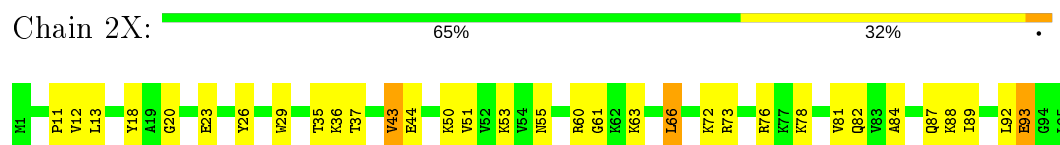
- Molecule 18: 50S ribosomal protein L22



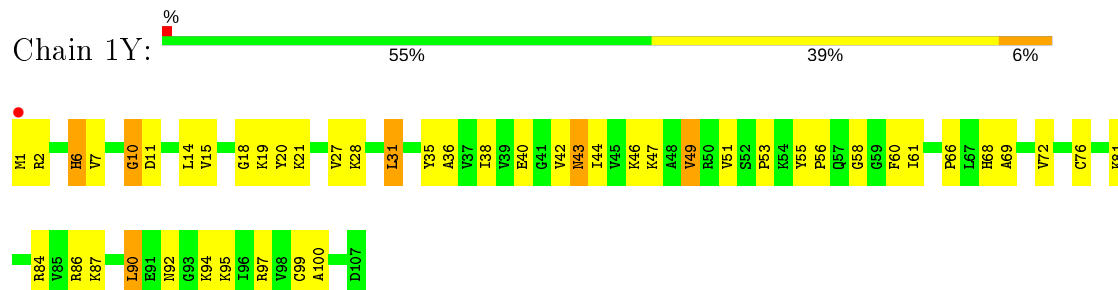
- Molecule 19: 50S ribosomal protein L23



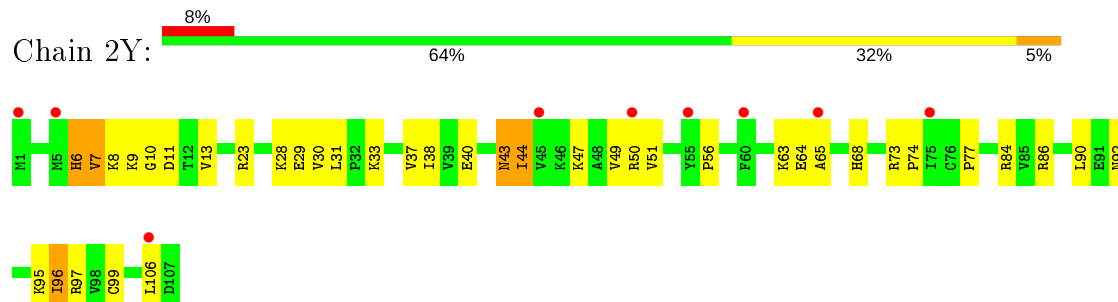
- Molecule 19: 50S ribosomal protein L23



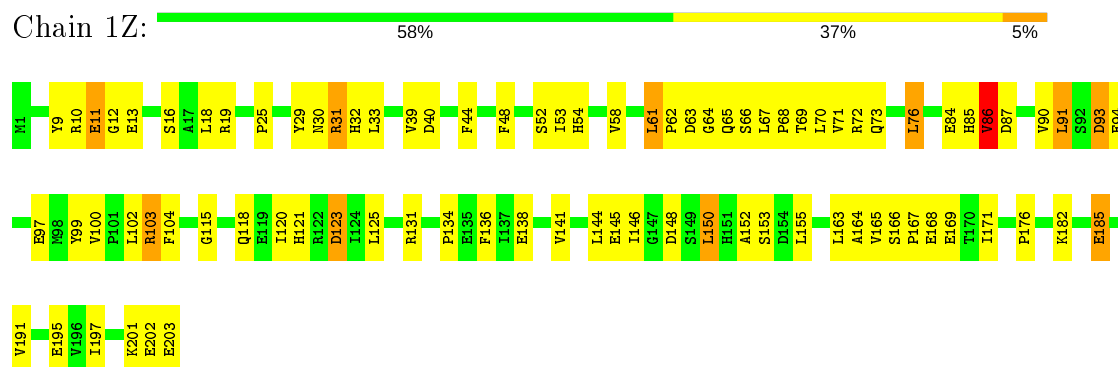
- Molecule 20: 50S ribosomal protein L24



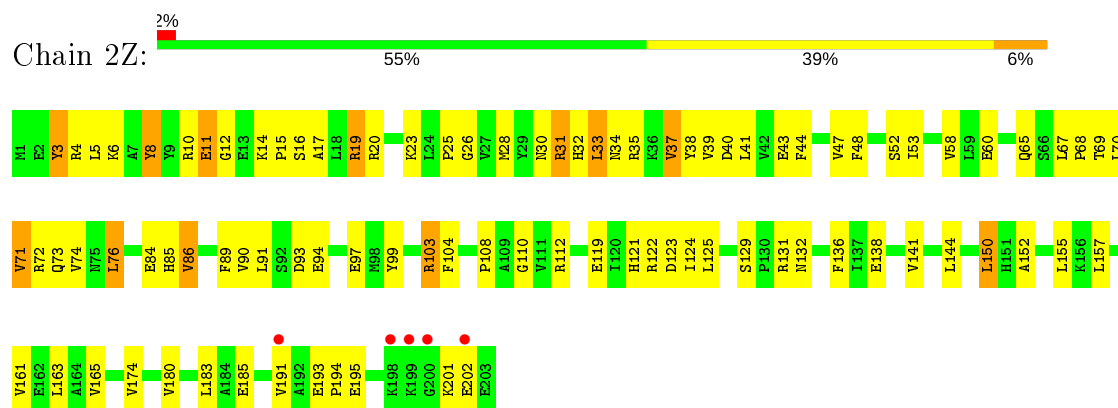
- Molecule 20: 50S ribosomal protein L24



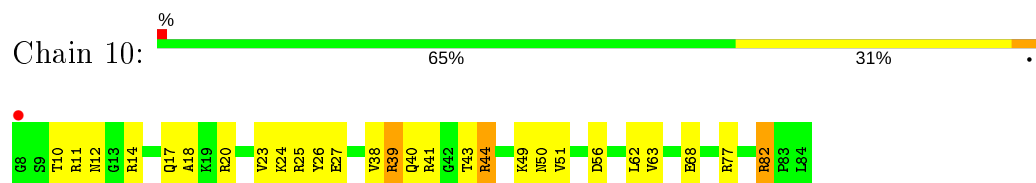
- Molecule 21: 50S ribosomal protein L25



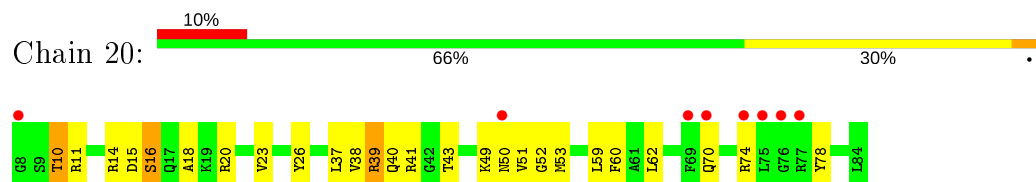
- Molecule 21: 50S ribosomal protein L25



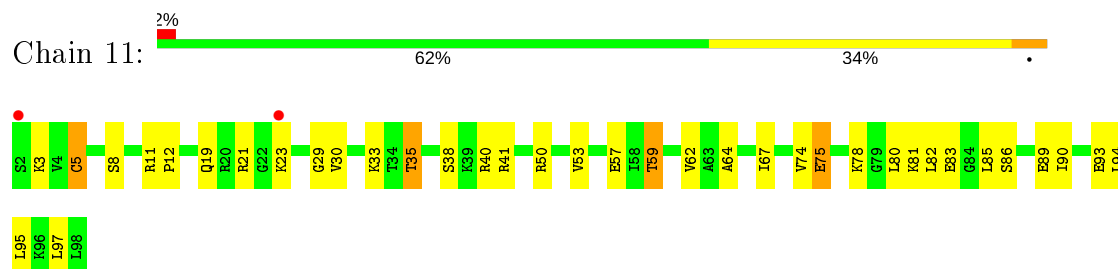
- Molecule 22: 50S ribosomal protein L27



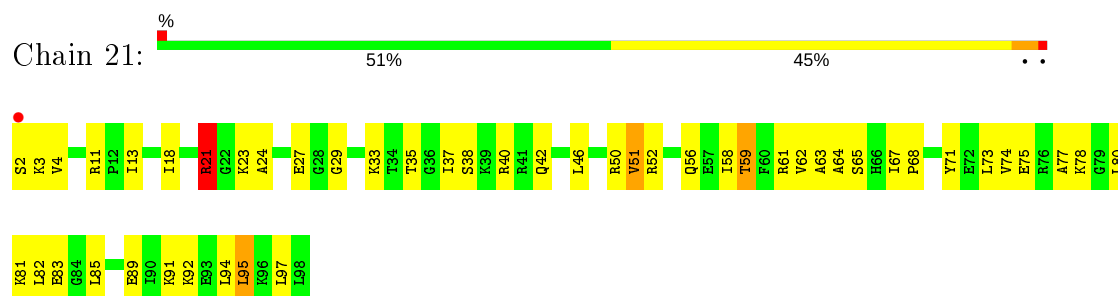
- Molecule 22: 50S ribosomal protein L27



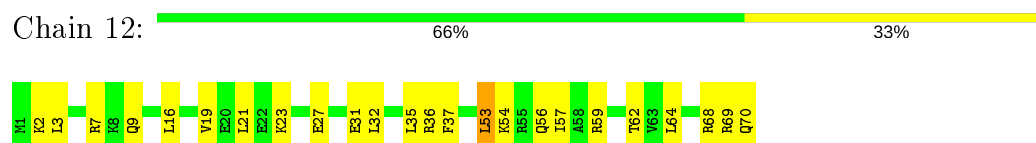
- Molecule 23: 50S ribosomal protein L28



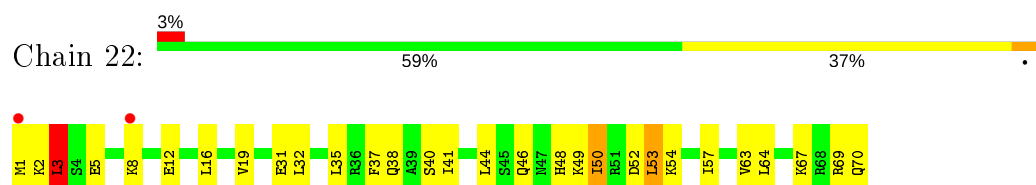
- Molecule 23: 50S ribosomal protein L28



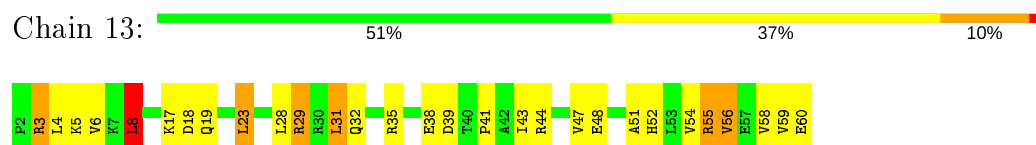
- Molecule 24: 50S ribosomal protein L29



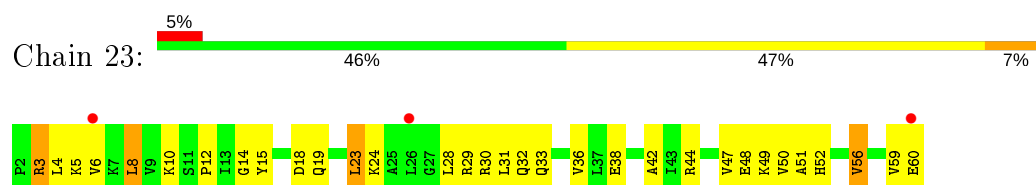
- Molecule 24: 50S ribosomal protein L29



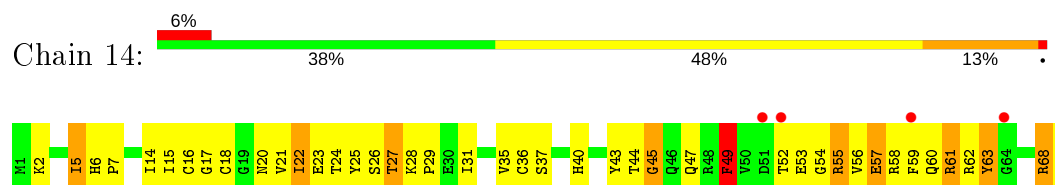
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31

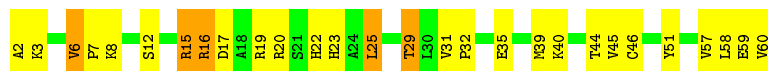


- Molecule 26: 50S ribosomal protein L31





- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



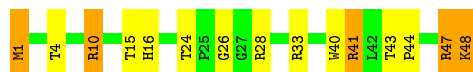
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



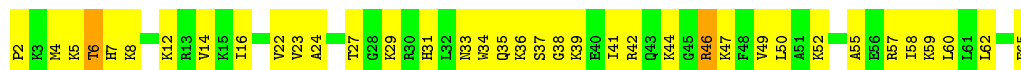
- Molecule 30: 50S ribosomal protein L35



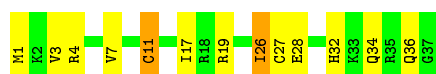




- Molecule 30: 50S ribosomal protein L35



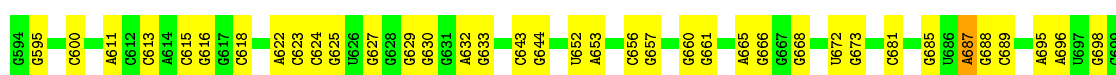
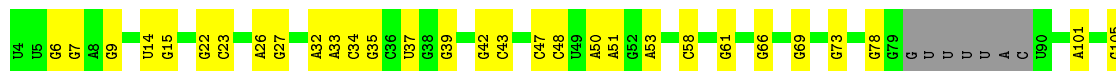
- Molecule 31: 50S ribosomal protein L36

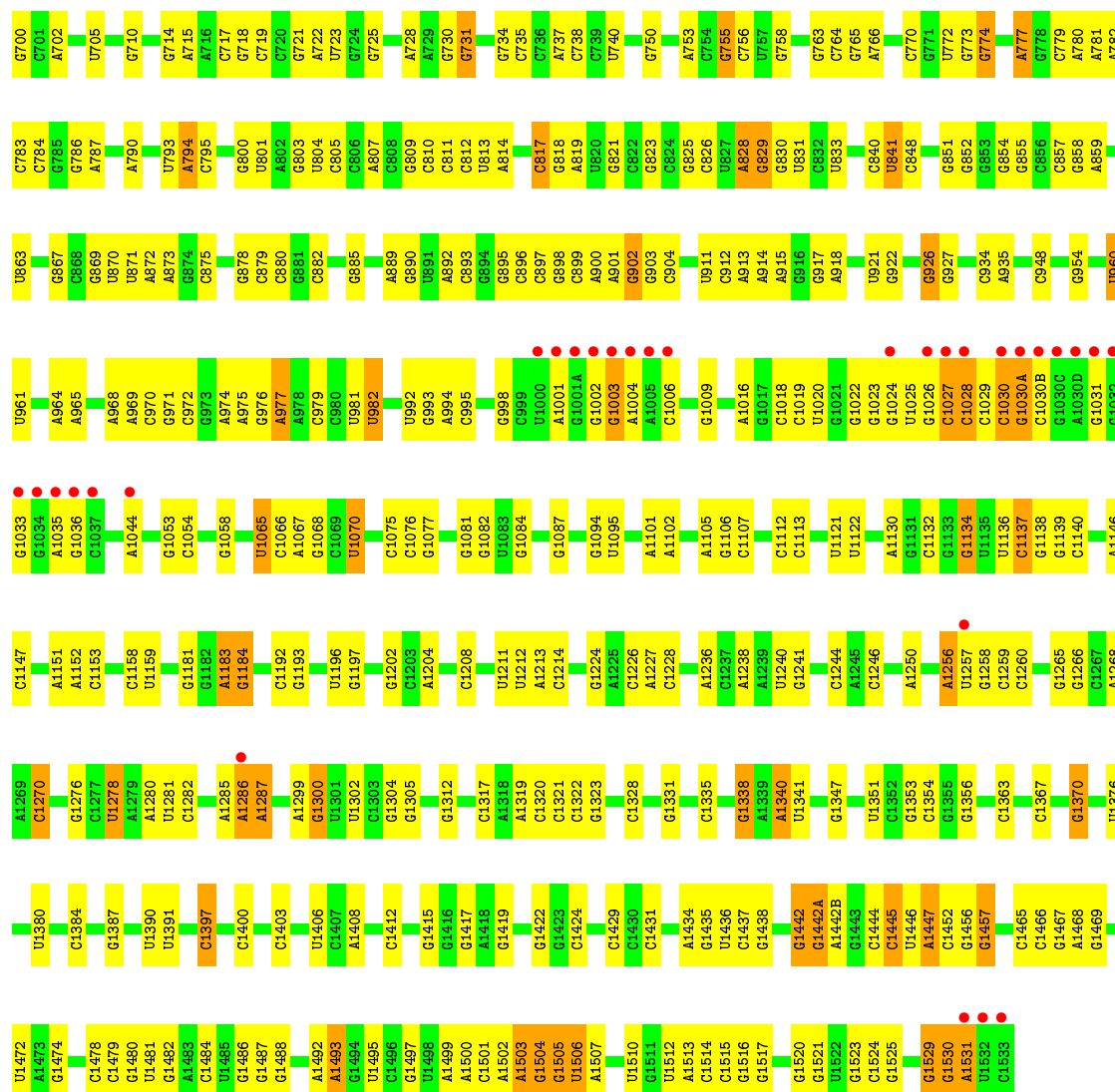


- Molecule 31: 50S ribosomal protein L36

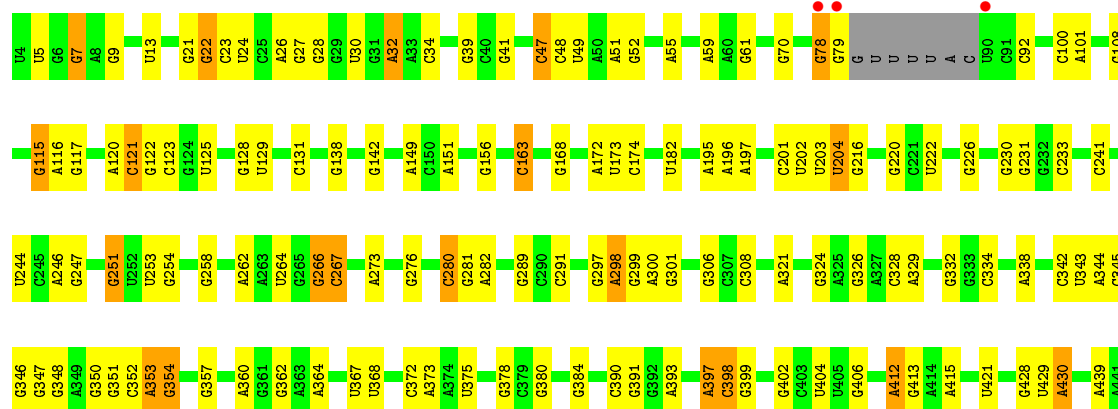


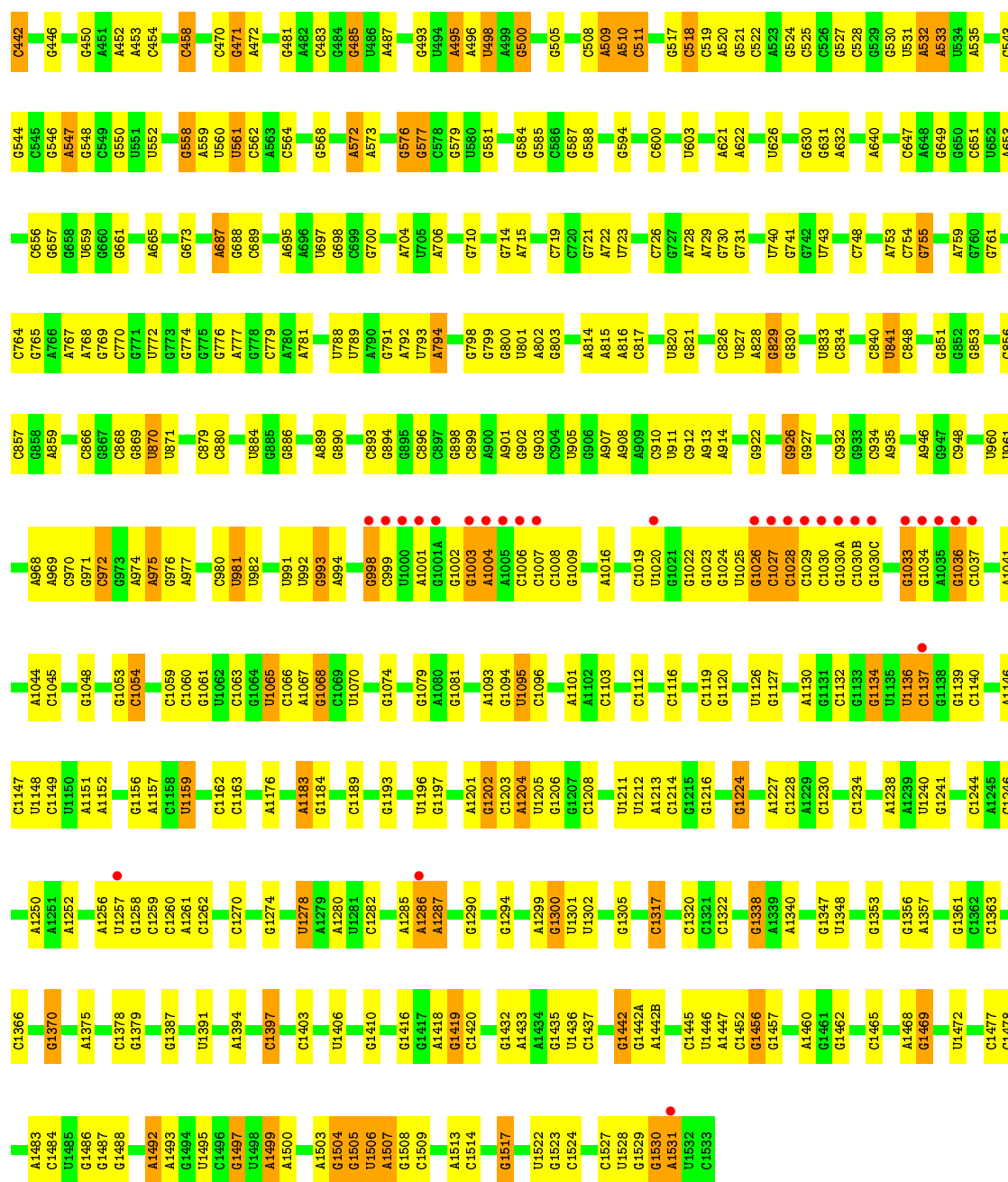
- Molecule 32: 16 ribosomal RNA

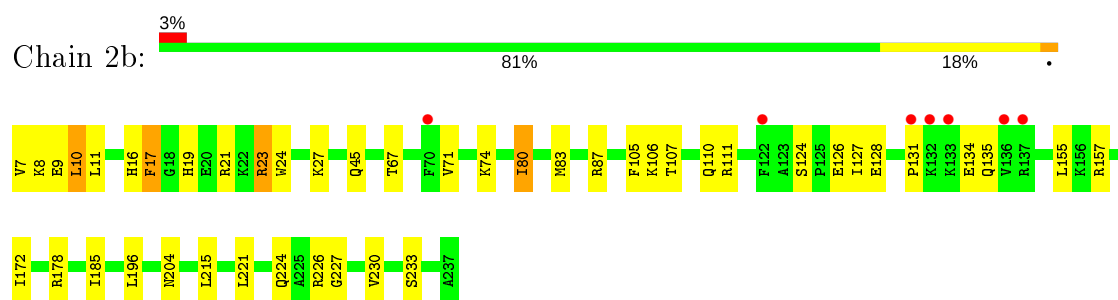




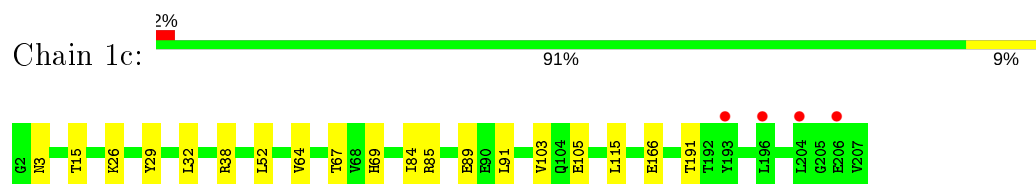
• Molecule 32: 16 ribosomal RNA



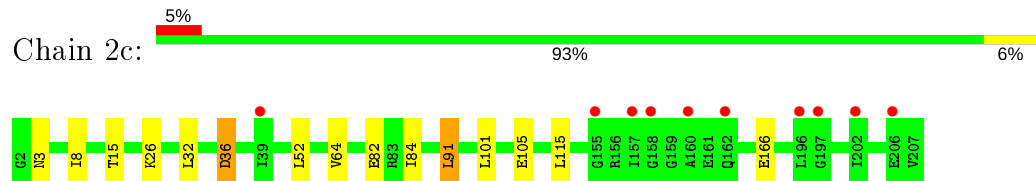




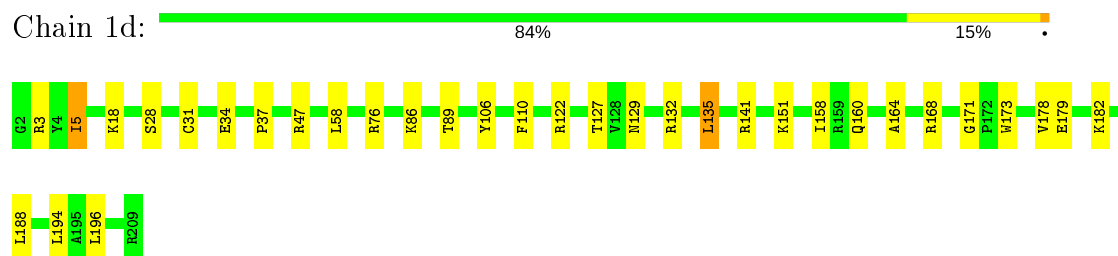
- Molecule 34: 30S ribosomal protein S3



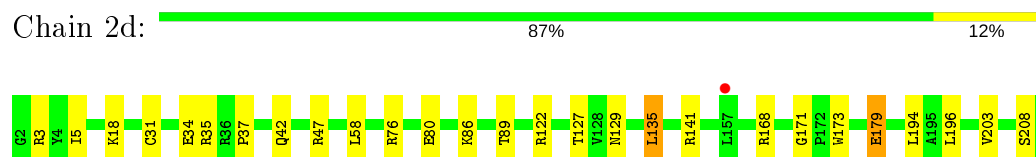
- Molecule 34: 30S ribosomal protein S3



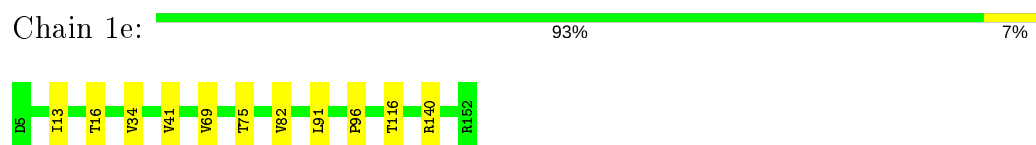
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

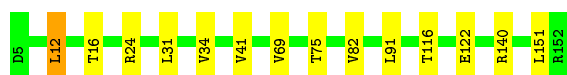


- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5

Chain 2e:  91% 9%



- Molecule 37: 30S ribosomal protein S6

Chain 1f:  92% 8%



- Molecule 37: 30S ribosomal protein S6

Chain 2f:  94% 6%

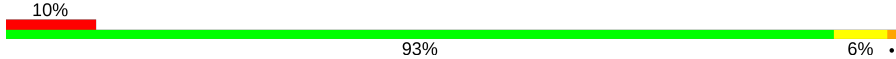


- Molecule 38: 30S ribosomal protein S7

Chain 1g:  3% 92% 8%



- Molecule 38: 30S ribosomal protein S7

Chain 2g:  10% 93% 6%



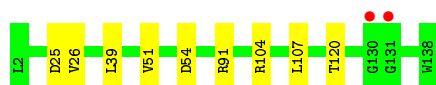
- Molecule 39: 30S ribosomal protein S8

Chain 1h:  0% 93% 7%

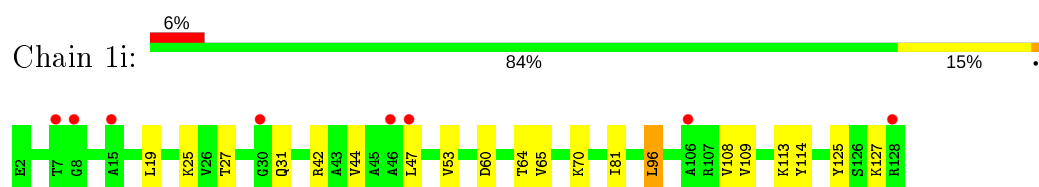


- Molecule 39: 30S ribosomal protein S8

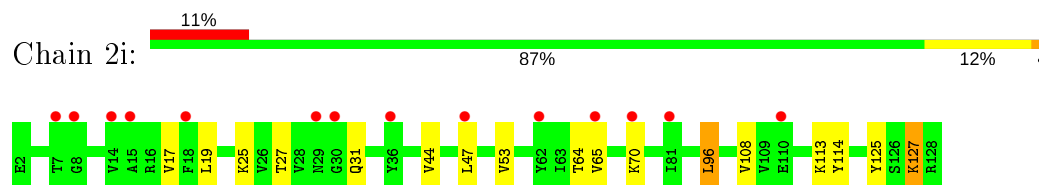
Chain 2h:  0% 93% 7%



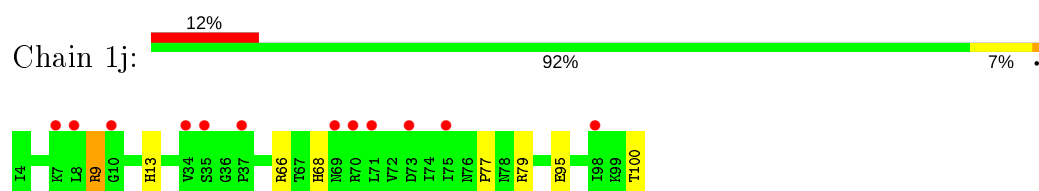
- Molecule 40: 30S ribosomal protein S9



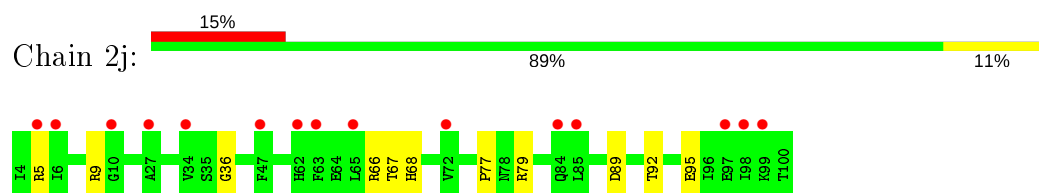
- Molecule 40: 30S ribosomal protein S9



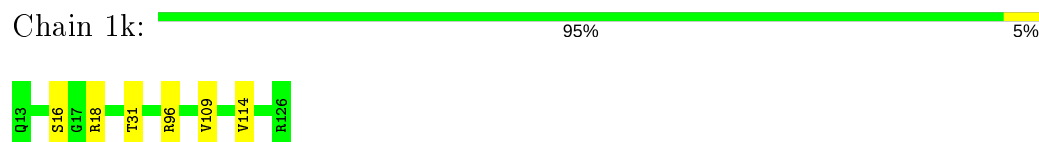
- Molecule 41: 30S ribosomal protein S10



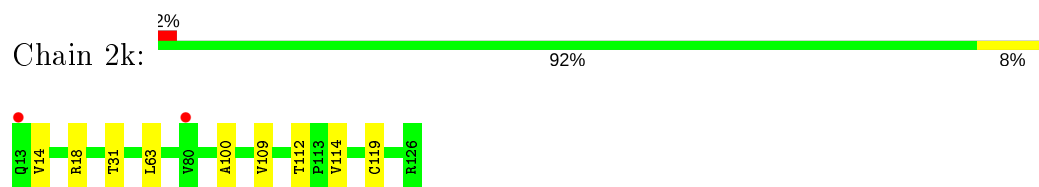
- Molecule 41: 30S ribosomal protein S10



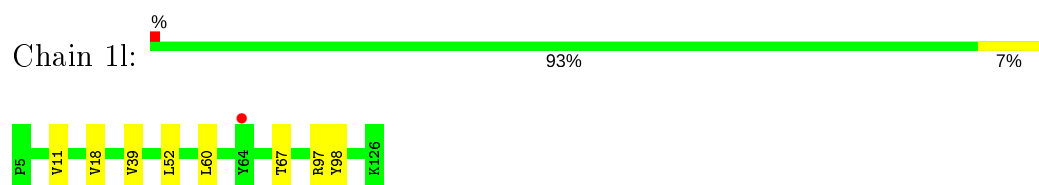
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

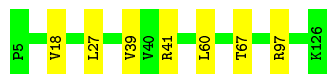


- Molecule 43: 30S ribosomal protein S12



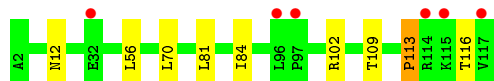
- Molecule 43: 30S ribosomal protein S12

Chain 2l:  94% 6%



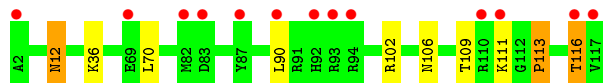
- Molecule 44: 30S ribosomal protein S13

Chain 1m:  5% 92% 7%




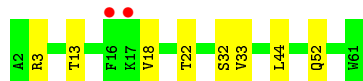
- Molecule 44: 30S ribosomal protein S13

Chain 2m:  11% 91% 6%

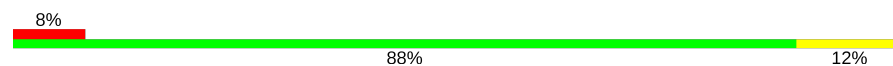


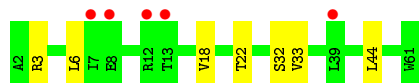
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:  3% 87% 13%



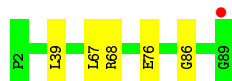
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:  8% 88% 12%



- Molecule 46: 30S ribosomal protein S15

Chain 1o:  % 94% 6%

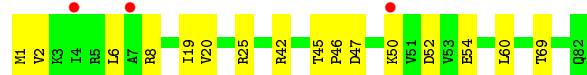
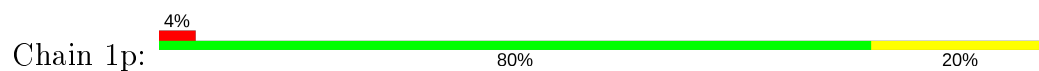


- Molecule 46: 30S ribosomal protein S15

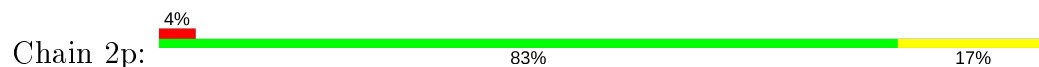
Chain 2o:  95% 5%



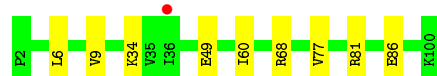
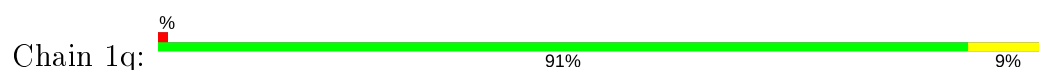
## • Molecule 47: 30S ribosomal protein S16



## • Molecule 47: 30S ribosomal protein S16



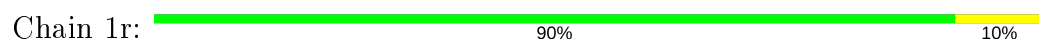
## • Molecule 48: 30S ribosomal protein S17



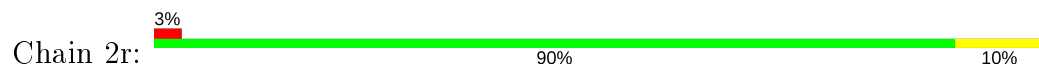
## • Molecule 48: 30S ribosomal protein S17



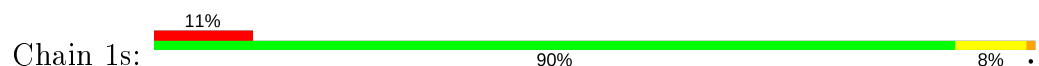
## • Molecule 49: 30S ribosomal protein S18



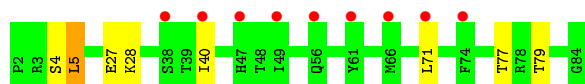
## • Molecule 49: 30S ribosomal protein S18



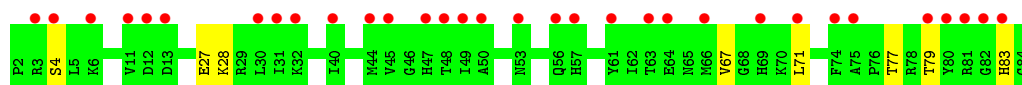
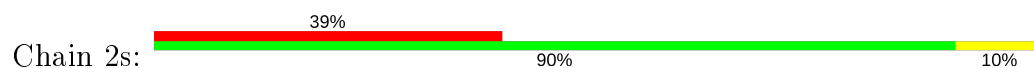
## • Molecule 50: 30S ribosomal protein S19



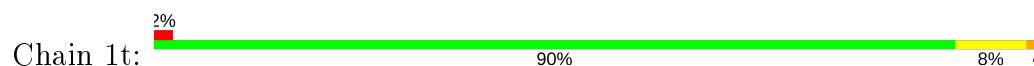




- Molecule 50: 30S ribosomal protein S19



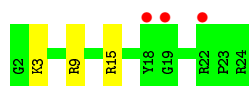
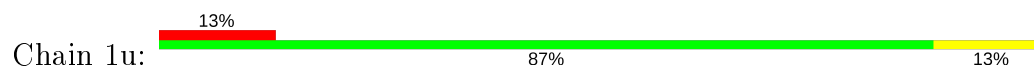
- Molecule 51: 30S ribosomal protein S20



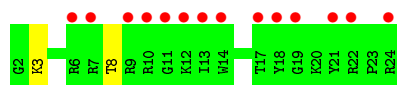
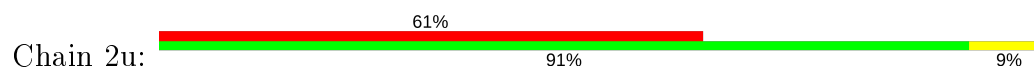
- Molecule 51: 30S ribosomal protein S20



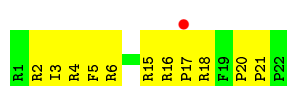
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



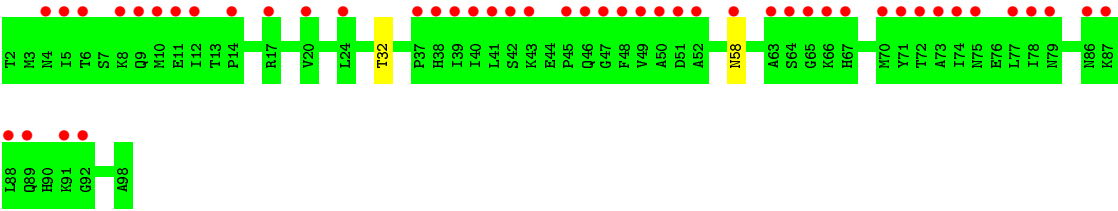
- Molecule 53: Tur1A peptide



- Molecule 54: Ribosome-associated inhibitor A



● Molecule 54: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.68Å 449.25Å 621.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 3.20 49.76 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.76-3.20) 98.6 (49.76-3.20)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.190 , 0.252 0.191 , 0.252	Depositor DCC
$R_{free}$ test set	47082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	294294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, OMG, MA6, SF4, 0TD, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1A	1.48	500/69032 (0.7%)	2.18	4548/107750 (4.2%)
1	2A	1.16	115/69032 (0.2%)	1.90	2782/107750 (2.6%)
2	1B	1.18	2/2879 (0.1%)	1.99	140/4490 (3.1%)
2	2B	1.12	4/2879 (0.1%)	1.83	98/4490 (2.2%)
3	1D	0.98	0/2181	1.14	8/2940 (0.3%)
3	2D	0.83	0/2181	1.05	7/2940 (0.2%)
4	1E	0.98	2/1592 (0.1%)	1.13	10/2149 (0.5%)
4	2E	0.82	0/1592	1.04	5/2149 (0.2%)
5	1F	0.96	0/1619	1.00	1/2193 (0.0%)
5	2F	0.71	0/1619	0.88	1/2193 (0.0%)
6	1G	0.61	0/1451	0.86	0/1961
6	2G	0.66	1/1451 (0.1%)	0.86	1/1961 (0.1%)
7	1H	0.84	0/1356	0.94	1/1834 (0.1%)
7	2H	0.72	0/1356	0.86	0/1834
8	1I	0.66	0/1109	0.90	1/1512 (0.1%)
8	2I	0.71	1/1109 (0.1%)	1.00	3/1512 (0.2%)
9	1N	0.93	0/1148	1.03	3/1547 (0.2%)
9	2N	0.71	0/1148	0.92	0/1547
10	1O	0.99	0/943	1.03	3/1269 (0.2%)
10	2O	0.84	0/943	1.00	1/1269 (0.1%)
11	1P	0.90	0/1152	1.07	2/1533 (0.1%)
11	2P	0.76	1/1152 (0.1%)	0.96	1/1533 (0.1%)
12	1Q	0.90	1/1143 (0.1%)	0.98	2/1527 (0.1%)
12	2Q	0.76	0/1143	0.96	2/1527 (0.1%)
13	1R	0.93	0/982	1.15	7/1312 (0.5%)
13	2R	0.75	0/982	1.00	2/1312 (0.2%)
14	1S	0.78	0/887	0.96	1/1180 (0.1%)
14	2S	0.73	0/887	0.97	1/1180 (0.1%)
15	1T	0.93	0/1105	1.06	2/1477 (0.1%)
15	2T	0.78	0/1105	0.99	2/1477 (0.1%)
16	1U	1.07	1/977 (0.1%)	1.09	4/1301 (0.3%)
16	2U	0.76	0/977	0.93	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.96	0/786	1.09	3/1053 (0.3%)
17	2V	0.75	0/786	0.92	0/1053
18	1W	1.05	0/897	1.11	3/1205 (0.2%)
18	2W	0.89	0/897	1.09	4/1205 (0.3%)
19	1X	1.01	0/764	1.00	0/1025
19	2X	0.85	0/764	0.98	0/1025
20	1Y	0.94	1/823 (0.1%)	1.01	1/1099 (0.1%)
20	2Y	0.77	0/823	1.00	2/1099 (0.2%)
21	1Z	0.74	0/1620	0.88	2/2200 (0.1%)
21	2Z	0.65	0/1620	0.90	1/2200 (0.0%)
22	10	0.93	0/616	1.08	3/821 (0.4%)
22	20	0.78	0/616	1.01	1/821 (0.1%)
23	11	0.99	0/761	0.99	1/1013 (0.1%)
23	21	0.82	0/761	0.96	1/1013 (0.1%)
24	12	0.82	0/590	0.96	1/781 (0.1%)
24	22	0.75	0/590	0.91	1/781 (0.1%)
25	13	0.98	0/474	1.07	3/635 (0.5%)
25	23	0.70	0/474	0.94	1/635 (0.2%)
26	14	0.64	0/559	0.86	0/754
26	24	0.70	0/559	0.86	0/754
27	15	1.02	1/473 (0.2%)	1.02	1/639 (0.2%)
27	25	0.82	1/473 (0.2%)	0.98	1/639 (0.2%)
28	16	0.87	0/460	0.93	0/613
28	26	0.72	0/460	0.92	0/613
29	17	1.06	0/426	1.01	2/561 (0.4%)
29	27	0.85	0/426	1.03	0/561
30	18	1.02	1/525 (0.2%)	0.99	1/691 (0.1%)
30	28	0.78	0/525	0.91	0/691
31	19	0.97	1/310 (0.3%)	0.98	0/407
31	29	0.74	0/310	0.95	0/407
32	1a	0.99	28/35795 (0.1%)	1.67	838/55864 (1.5%)
32	2a	0.96	18/35795 (0.1%)	1.63	747/55864 (1.3%)
33	1b	0.62	0/1876	0.86	0/2533
33	2b	0.61	0/1876	0.88	1/2533 (0.0%)
34	1c	0.53	0/1582	0.76	0/2137
34	2c	0.59	0/1582	0.81	2/2137 (0.1%)
35	1d	0.61	0/1695	0.81	1/2274 (0.0%)
35	2d	0.60	0/1695	0.88	1/2274 (0.0%)
36	1e	0.62	0/1149	0.86	0/1548
36	2e	0.64	1/1149 (0.1%)	0.87	2/1548 (0.1%)
37	1f	0.67	0/827	0.86	0/1120
37	2f	0.63	0/827	0.88	0/1120
38	1g	0.57	0/1254	0.76	0/1683

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.56	0/1254	0.80	1/1683 (0.1%)
39	1h	0.64	0/1118	0.83	0/1506
39	2h	0.57	0/1118	0.84	0/1506
40	1i	0.55	0/1005	0.79	0/1351
40	2i	0.58	0/1005	0.79	0/1351
41	1j	0.56	0/732	0.82	1/993 (0.1%)
41	2j	0.56	0/732	0.81	0/993
42	1k	0.65	0/849	0.81	0/1150
42	2k	0.67	1/849 (0.1%)	0.83	1/1150 (0.1%)
43	1l	0.68	0/937	0.87	0/1260
43	2l	0.67	0/937	0.87	0/1260
44	1m	0.53	0/924	0.78	0/1242
44	2m	0.64	0/924	0.84	1/1242 (0.1%)
45	1n	0.56	0/501	0.81	0/664
45	2n	0.60	0/501	0.75	0/664
46	1o	0.61	0/739	0.86	1/985 (0.1%)
46	2o	0.59	0/739	0.88	0/985
47	1p	0.56	0/697	0.85	0/939
47	2p	0.65	0/697	0.83	0/939
48	1q	0.68	0/836	0.90	0/1117
48	2q	0.66	0/836	0.87	0/1117
49	1r	0.63	0/560	0.87	0/746
49	2r	0.70	0/560	0.86	0/746
50	1s	0.53	0/663	0.80	1/895 (0.1%)
50	2s	0.65	0/663	0.76	0/895
51	1t	0.61	0/734	0.87	0/969
51	2t	0.56	0/734	0.82	0/969
52	1u	0.51	0/203	0.83	0/266
52	2u	0.56	0/203	0.83	0/266
53	1y	0.94	0/177	1.15	0/245
54	1z	0.64	0/776	0.84	0/1048
54	2z	0.71	0/776	0.82	0/1048
All	All	1.10	681/310361 (0.2%)	1.71	9271/463769 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	1E	0	1
4	2E	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
14	1S	0	1
14	2S	0	1
15	1T	0	1
15	2T	0	1
19	1X	0	1
19	2X	0	1
33	2b	0	1
44	1m	0	1
44	2m	0	1
53	1y	0	1
All	All	0	12

The worst 5 of 681 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	807	U	C2-N3	9.44	1.44	1.37
1	2A	2573	C	N3-C4	9.04	1.40	1.33
1	1A	783	A	C6-N1	-8.93	1.29	1.35
1	2A	687	C	N1-C6	-8.56	1.32	1.37
1	1A	2032	G	N7-C5	-8.51	1.34	1.39

The worst 5 of 9271 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2319	G	C6-C5-N7	-21.39	117.57	130.40
1	1A	2061	G	O5'-P-OP2	-19.75	87.00	110.70
1	1A	673	C	C5-C4-N4	-18.70	107.11	120.20
1	1A	673	C	N3-C4-C5	17.52	128.91	121.90
1	1A	2319	G	N1-C6-O6	17.08	130.15	119.90

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1E	11	MET	Peptide
14	1S	58	LEU	Peptide
15	1T	128	GLU	Peptide
19	1X	93	GLU	Peptide
44	1m	113	PRO	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61872	0	31187	1169	0
1	2A	61872	0	31190	1427	0
2	1B	2575	0	1304	59	0
2	2B	2575	0	1304	64	0
3	1D	2131	0	2207	99	0
3	2D	2131	0	2207	73	0
4	1E	1559	0	1618	64	0
4	2E	1559	0	1618	76	0
5	1F	1584	0	1625	55	0
5	2F	1584	0	1624	70	0
6	1G	1426	0	1445	79	0
6	2G	1426	0	1445	90	0
7	1H	1330	0	1407	48	0
7	2H	1330	0	1407	68	0
8	1I	1094	0	1127	47	1
8	2I	1094	0	1127	68	0
9	1N	1121	0	1195	33	0
9	2N	1121	0	1195	43	0
10	1O	933	0	996	26	0
10	2O	933	0	996	35	0
11	1P	1135	0	1212	65	0
11	2P	1135	0	1212	53	0
12	1Q	1122	0	1179	40	0
12	2Q	1122	0	1179	56	0
13	1R	968	0	1033	46	0
13	2R	968	0	1033	55	0
14	1S	877	0	938	44	0
14	2S	877	0	938	47	0
15	1T	1091	0	1151	38	0
15	2T	1091	0	1151	48	0
16	1U	959	0	1019	30	0
16	2U	959	0	1019	46	0
17	1V	775	0	841	23	0
17	2V	775	0	841	28	0
18	1W	886	0	940	31	0
18	2W	886	0	940	40	0
19	1X	750	0	814	32	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	23	0
20	1Y	810	0	892	29	0
20	2Y	810	0	892	26	0
21	1Z	1587	0	1598	57	0
21	2Z	1587	0	1598	68	0
22	10	608	0	622	25	0
22	20	608	0	622	26	0
23	11	754	0	823	26	0
23	21	754	0	823	41	0
24	12	588	0	643	18	0
24	22	588	0	643	21	0
25	13	469	0	518	24	0
25	23	469	0	517	28	0
26	14	546	0	522	37	0
26	24	546	0	522	33	0
27	15	459	0	476	23	0
27	25	459	0	476	25	0
28	16	453	0	473	20	0
28	26	453	0	473	21	0
29	17	418	0	467	12	0
29	27	418	0	467	24	0
30	18	517	0	582	28	0
30	28	517	0	582	31	0
31	19	307	0	335	7	0
31	29	307	0	335	14	0
32	1a	32246	0	16296	0	0
32	2a	32246	0	16294	0	1
33	1b	1842	0	1862	0	0
33	2b	1842	0	1862	0	0
34	1c	1558	0	1557	0	0
34	2c	1558	0	1557	0	0
35	1d	1665	0	1687	0	0
35	2d	1665	0	1687	0	0
36	1e	1133	0	1190	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	814	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1235	0	1249	0	0
39	1h	1098	0	1143	0	0
39	2h	1098	0	1143	0	0
40	1i	986	0	990	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	986	0	990	0	0
41	1j	719	0	672	0	0
41	2j	719	0	672	0	0
42	1k	834	0	838	0	0
42	2k	834	0	838	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	914	0	954	0	0
44	2m	914	0	954	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	681	0	697	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	648	0	658	0	0
50	2s	648	0	658	0	0
51	1t	732	0	809	0	0
51	2t	732	0	809	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1y	168	0	163	0	0
54	1z	764	0	786	0	0
54	2z	764	0	786	0	0
55	10	7	0	0	0	0
55	11	4	0	0	0	0
55	13	2	0	0	0	0
55	15	5	0	0	0	0
55	17	2	0	0	0	0
55	18	3	0	0	0	0
55	19	3	0	0	0	0
55	1A	957	0	0	0	0
55	1B	28	0	0	0	0
55	1D	17	0	0	0	0
55	1E	5	0	0	0	0
55	1F	14	0	0	0	0
55	1G	3	0	0	0	0
55	1H	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1N	4	0	0	0	0
55	1P	4	0	0	0	0
55	1Q	4	0	0	0	0
55	1R	4	0	0	0	0
55	1T	2	0	0	0	0
55	1U	5	0	0	0	0
55	1V	3	0	0	0	0
55	1W	3	0	0	0	0
55	1X	2	0	0	0	0
55	1Y	1	0	0	0	0
55	1a	245	0	0	0	0
55	1b	1	0	0	0	0
55	1d	5	0	0	0	0
55	1e	1	0	0	0	0
55	1f	1	0	0	0	0
55	1g	1	0	0	0	0
55	1h	1	0	0	0	0
55	1i	1	0	0	0	0
55	1k	1	0	0	0	0
55	1l	2	0	0	0	0
55	1n	1	0	0	0	0
55	1o	2	0	0	0	0
55	1t	1	0	0	0	0
55	20	5	0	0	0	0
55	21	1	0	0	0	0
55	23	2	0	0	0	0
55	25	4	0	0	0	0
55	27	2	0	0	0	0
55	28	2	0	0	0	0
55	29	3	0	0	0	0
55	2A	971	0	0	0	0
55	2B	26	0	0	0	0
55	2D	17	0	0	0	0
55	2E	6	0	0	0	0
55	2F	11	0	0	0	0
55	2G	3	0	0	0	0
55	2H	2	0	0	0	0
55	2N	3	0	0	0	0
55	2P	2	0	0	0	0
55	2Q	4	0	0	0	0
55	2R	3	0	0	0	0
55	2S	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	2T	3	0	0	0	0
55	2U	5	0	0	0	0
55	2V	5	0	0	0	0
55	2W	3	0	0	0	0
55	2X	2	0	0	0	0
55	2Y	1	0	0	0	0
55	2a	242	0	0	0	0
55	2b	1	0	0	0	0
55	2d	3	0	0	0	0
55	2e	1	0	0	0	0
55	2f	1	0	0	0	0
55	2g	1	0	0	0	0
55	2h	2	0	0	0	0
55	2i	1	0	0	0	0
55	2l	2	0	0	0	0
55	2o	2	0	0	0	0
55	2t	2	0	0	0	0
55	2z	2	0	0	0	0
56	14	1	0	0	0	0
56	15	1	0	0	0	0
56	16	1	0	0	0	0
56	19	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1n	1	0	0	0	0
56	24	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	29	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2n	1	0	0	0	0
57	1d	8	0	0	0	0
57	2d	8	0	0	0	0
58	10	6	0	0	1	0
58	11	2	0	0	0	0
58	13	2	0	0	0	0
58	15	2	0	0	0	0
58	16	2	0	0	0	0
58	17	2	0	0	0	0
58	18	9	0	0	0	0
58	19	2	0	0	0	0
58	1A	1782	0	0	11	0
58	1B	45	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1D	15	0	0	1	0
58	1E	18	0	0	0	0
58	1F	14	0	0	0	0
58	1G	2	0	0	0	0
58	1H	5	0	0	0	0
58	1N	7	0	0	0	0
58	1P	12	0	0	0	0
58	1Q	6	0	0	1	0
58	1R	6	0	0	1	0
58	1T	5	0	0	0	0
58	1U	7	0	0	0	0
58	1V	3	0	0	0	0
58	1W	1	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	5	0	0	0	0
58	1a	406	0	0	0	0
58	1d	8	0	0	0	0
58	1e	4	0	0	0	0
58	1f	1	0	0	0	0
58	1h	1	0	0	0	0
58	1j	1	0	0	0	0
58	1l	3	0	0	0	0
58	1m	3	0	0	0	0
58	1n	1	0	0	0	0
58	1o	1	0	0	0	0
58	1p	1	0	0	0	0
58	1t	1	0	0	0	0
58	1z	3	0	0	0	0
58	20	8	0	0	1	0
58	21	2	0	0	0	0
58	23	2	0	0	0	0
58	25	4	0	0	0	0
58	26	2	0	0	0	0
58	27	2	0	0	1	0
58	28	11	0	0	0	0
58	29	2	0	0	0	0
58	2A	1771	0	0	22	0
58	2B	46	0	0	0	0
58	2D	14	0	0	1	0
58	2E	20	0	0	0	0
58	2F	12	0	0	0	0
58	2G	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2H	4	0	0	0	0
58	2N	7	0	0	0	0
58	2P	11	0	0	1	0
58	2Q	7	0	0	0	0
58	2R	6	0	0	1	0
58	2T	5	0	0	0	0
58	2U	8	0	0	1	0
58	2V	5	0	0	0	0
58	2W	2	0	0	0	0
58	2X	7	0	0	0	0
58	2Y	5	0	0	0	0
58	2a	404	0	0	0	0
58	2d	8	0	0	0	0
58	2e	6	0	0	0	0
58	2f	1	0	0	0	0
58	2h	1	0	0	0	0
58	2j	1	0	0	0	0
58	2l	3	0	0	0	0
58	2m	2	0	0	0	0
58	2n	1	0	0	0	0
58	2o	3	0	0	0	0
58	2p	1	0	0	0	0
58	2z	4	0	0	0	0
All	All	294294	0	194907	4524	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 4524 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2552:2MU:C4	1:1A:2552:2MU:C5	1.75	1.59
1:2A:2552:2MU:C4	1:2A:2552:2MU:C5	1.76	1.57
1:2A:307:G:H21	1:2A:330:A:N6	1.23	1.37
1:1A:1359:A:N6	1:1A:1372:U:H3	1.37	1.22
1:2A:307:G:N2	1:2A:330:A:N6	1.99	1.09

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:91:SER:OG	32:2a:368:U:OP1[3_654]	2.16	0.04

## 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	273/275 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/275 (99%)	257 (94%)	14 (5%)	2 (1%)	22	61
4	1E	202/204 (99%)	189 (94%)	12 (6%)	1 (0%)	29	67
4	2E	202/204 (99%)	189 (94%)	12 (6%)	1 (0%)	29	67
5	1F	201/203 (99%)	187 (93%)	11 (6%)	3 (2%)	10	44
5	2F	201/203 (99%)	186 (92%)	13 (6%)	2 (1%)	15	54
6	1G	179/181 (99%)	155 (87%)	16 (9%)	8 (4%)	2	18
6	2G	179/181 (99%)	152 (85%)	20 (11%)	7 (4%)	3	22
7	1H	172/174 (99%)	156 (91%)	15 (9%)	1 (1%)	25	64
7	2H	172/174 (99%)	153 (89%)	17 (10%)	2 (1%)	13	49
8	1I	145/147 (99%)	118 (81%)	24 (17%)	3 (2%)	7	37
8	2I	145/147 (99%)	116 (80%)	25 (17%)	4 (3%)	5	29
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19	58
10	2O	120/122 (98%)	113 (94%)	4 (3%)	3 (2%)	5	32
11	1P	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22	61
11	2P	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	11	46
12	1Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	11	46
13	1R	116/118 (98%)	98 (84%)	16 (14%)	2 (2%)	9	42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	98 (84%)	17 (15%)	1 (1%)	17	56
14	1S	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
14	2S	108/110 (98%)	94 (87%)	14 (13%)	0	100	100
15	1T	129/131 (98%)	122 (95%)	6 (5%)	1 (1%)	19	58
15	2T	129/131 (98%)	120 (93%)	8 (6%)	1 (1%)	19	58
16	1U	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
16	2U	114/116 (98%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	54
18	1W	110/112 (98%)	100 (91%)	10 (9%)	0	100	100
18	2W	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	2 (2%)	1 (1%)	14	51
19	2X	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/107 (98%)	93 (89%)	11 (10%)	1 (1%)	15	54
20	2Y	105/107 (98%)	93 (89%)	11 (10%)	1 (1%)	15	54
21	1Z	201/203 (99%)	170 (85%)	30 (15%)	1 (0%)	29	67
21	2Z	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	29	67
22	10	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
22	20	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
23	11	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
23	21	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
24	12	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
24	22	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
25	13	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	8	41
25	23	57/59 (97%)	51 (90%)	6 (10%)	0	100	100
26	14	67/69 (97%)	52 (78%)	11 (16%)	4 (6%)	1	12
26	24	67/69 (97%)	51 (76%)	12 (18%)	4 (6%)	1	12
27	15	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
27	25	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
28	16	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
28	26	51/53 (96%)	48 (94%)	3 (6%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	17	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
29	27	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
30	18	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	28	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/231 (99%)	174 (76%)	39 (17%)	16 (7%)	1	8
33	2b	229/231 (99%)	174 (76%)	40 (18%)	15 (7%)	1	9
34	1c	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	44
34	2c	204/206 (99%)	173 (85%)	27 (13%)	4 (2%)	7	38
35	1d	206/208 (99%)	176 (85%)	24 (12%)	6 (3%)	4	28
35	2d	206/208 (99%)	172 (84%)	29 (14%)	5 (2%)	6	34
36	1e	146/148 (99%)	124 (85%)	20 (14%)	2 (1%)	11	46
36	2e	146/148 (99%)	125 (86%)	20 (14%)	1 (1%)	22	61
37	1f	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	54
37	2f	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	15	54
38	1g	153/155 (99%)	133 (87%)	18 (12%)	2 (1%)	12	47
38	2g	153/155 (99%)	132 (86%)	18 (12%)	3 (2%)	7	38
39	1h	135/137 (98%)	122 (90%)	13 (10%)	0	100	100
39	2h	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/127 (98%)	105 (84%)	16 (13%)	4 (3%)	4	26
40	2i	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	3	21
41	1j	95/97 (98%)	76 (80%)	17 (18%)	2 (2%)	7	37
41	2j	95/97 (98%)	72 (76%)	20 (21%)	3 (3%)	4	26
42	1k	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
42	2k	112/114 (98%)	97 (87%)	14 (12%)	1 (1%)	17	56
43	1l	119/122 (98%)	100 (84%)	19 (16%)	0	100	100
43	2l	119/122 (98%)	104 (87%)	15 (13%)	0	100	100
44	1m	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	8	41
44	2m	114/116 (98%)	101 (89%)	10 (9%)	3 (3%)	5	31
45	1n	58/60 (97%)	52 (90%)	5 (9%)	1 (2%)	9	42

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/88 (98%)	76 (88%)	9 (10%)	1 (1%)	13	49
46	2o	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	49
47	1p	80/82 (98%)	59 (74%)	19 (24%)	2 (2%)	5	32
47	2p	80/82 (98%)	60 (75%)	19 (24%)	1 (1%)	12	47
48	1q	97/99 (98%)	87 (90%)	7 (7%)	3 (3%)	4	26
48	2q	97/99 (98%)	85 (88%)	9 (9%)	3 (3%)	4	26
49	1r	66/68 (97%)	55 (83%)	9 (14%)	2 (3%)	4	28
49	2r	66/68 (97%)	56 (85%)	8 (12%)	2 (3%)	4	28
50	1s	81/83 (98%)	74 (91%)	6 (7%)	1 (1%)	13	49
50	2s	81/83 (98%)	71 (88%)	9 (11%)	1 (1%)	13	49
51	1t	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	20
51	2t	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	20
52	1u	21/23 (91%)	15 (71%)	5 (24%)	1 (5%)	2	17
52	2u	21/23 (91%)	17 (81%)	3 (14%)	1 (5%)	2	17
53	1y	20/22 (91%)	12 (60%)	4 (20%)	4 (20%)	0	0
54	1z	95/97 (98%)	89 (94%)	5 (5%)	1 (1%)	14	51
54	2z	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
All	All	11656/11860 (98%)	10281 (88%)	1200 (10%)	175 (2%)	10	44

5 of 175 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
6	1G	126	ASP
20	1Y	92	ASN
21	1Z	31	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/217 (99%)	188 (88%)	26 (12%)	5	22
3	2D	214/217 (99%)	191 (89%)	23 (11%)	6	27
4	1E	164/165 (99%)	143 (87%)	21 (13%)	4	20
4	2E	164/165 (99%)	146 (89%)	18 (11%)	6	26
5	1F	160/161 (99%)	132 (82%)	28 (18%)	2	9
5	2F	160/161 (99%)	139 (87%)	21 (13%)	4	19
6	1G	144/155 (93%)	127 (88%)	17 (12%)	5	23
6	2G	144/155 (93%)	132 (92%)	12 (8%)	11	40
7	1H	144/145 (99%)	134 (93%)	10 (7%)	15	49
7	2H	144/145 (99%)	134 (93%)	10 (7%)	15	49
8	1I	111/123 (90%)	87 (78%)	24 (22%)	1	5
8	2I	111/123 (90%)	91 (82%)	20 (18%)	1	9
9	1N	119/119 (100%)	103 (87%)	16 (13%)	4	18
9	2N	119/119 (100%)	102 (86%)	17 (14%)	3	15
10	1O	100/100 (100%)	90 (90%)	10 (10%)	7	30
10	2O	100/100 (100%)	93 (93%)	7 (7%)	15	48
11	1P	115/116 (99%)	102 (89%)	13 (11%)	6	25
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	28
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	8	30
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	8	30
13	1R	101/101 (100%)	84 (83%)	17 (17%)	2	10
13	2R	101/101 (100%)	88 (87%)	13 (13%)	4	19
14	1S	87/87 (100%)	74 (85%)	13 (15%)	3	14
14	2S	87/87 (100%)	77 (88%)	10 (12%)	5	24
15	1T	115/115 (100%)	104 (90%)	11 (10%)	8	32
15	2T	115/115 (100%)	107 (93%)	8 (7%)	15	48
16	1U	93/93 (100%)	80 (86%)	13 (14%)	3	16
16	2U	93/93 (100%)	81 (87%)	12 (13%)	4	19
17	1V	81/82 (99%)	69 (85%)	12 (15%)	3	14
17	2V	81/82 (99%)	74 (91%)	7 (9%)	10	38
18	1W	90/91 (99%)	79 (88%)	11 (12%)	5	22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	2W	90/91 (99%)	77 (86%)	13 (14%)	3	15
19	1X	77/77 (100%)	74 (96%)	3 (4%)	32	67
19	2X	77/77 (100%)	72 (94%)	5 (6%)	17	51
20	1Y	86/88 (98%)	75 (87%)	11 (13%)	4	20
20	2Y	86/88 (98%)	76 (88%)	10 (12%)	5	24
21	1Z	169/176 (96%)	147 (87%)	22 (13%)	4	19
21	2Z	169/176 (96%)	147 (87%)	22 (13%)	4	19
22	10	61/62 (98%)	60 (98%)	1 (2%)	62	84
22	20	61/62 (98%)	58 (95%)	3 (5%)	25	61
23	11	79/82 (96%)	72 (91%)	7 (9%)	9	35
23	21	79/82 (96%)	74 (94%)	5 (6%)	18	52
24	12	65/66 (98%)	59 (91%)	6 (9%)	9	33
24	22	65/66 (98%)	60 (92%)	5 (8%)	13	44
25	13	51/51 (100%)	41 (80%)	10 (20%)	1	7
25	23	51/51 (100%)	44 (86%)	7 (14%)	3	17
26	14	58/62 (94%)	48 (83%)	10 (17%)	2	10
26	24	58/62 (94%)	49 (84%)	9 (16%)	2	12
27	15	51/51 (100%)	45 (88%)	6 (12%)	5	23
27	25	51/51 (100%)	46 (90%)	5 (10%)	8	31
28	16	51/51 (100%)	43 (84%)	8 (16%)	2	12
28	26	51/51 (100%)	46 (90%)	5 (10%)	8	31
29	17	41/41 (100%)	34 (83%)	7 (17%)	2	10
29	27	41/41 (100%)	34 (83%)	7 (17%)	2	10
30	18	54/54 (100%)	49 (91%)	5 (9%)	9	33
30	28	54/54 (100%)	49 (91%)	5 (9%)	9	33
31	19	34/34 (100%)	30 (88%)	4 (12%)	5	23
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	23
33	1b	191/199 (96%)	163 (85%)	28 (15%)	3	14
33	2b	191/199 (96%)	159 (83%)	32 (17%)	2	10
34	1c	144/160 (90%)	128 (89%)	16 (11%)	6	25
34	2c	144/160 (90%)	133 (92%)	11 (8%)	13	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	1d	171/180 (95%)	143 (84%)	28 (16%)	2	11
35	2d	171/180 (95%)	148 (86%)	23 (14%)	4	18
36	1e	114/114 (100%)	105 (92%)	9 (8%)	12	43
36	2e	114/114 (100%)	103 (90%)	11 (10%)	8	32
37	1f	85/90 (94%)	78 (92%)	7 (8%)	11	41
37	2f	85/90 (94%)	80 (94%)	5 (6%)	19	54
38	1g	120/126 (95%)	110 (92%)	10 (8%)	11	40
38	2g	120/126 (95%)	112 (93%)	8 (7%)	16	50
39	1h	116/118 (98%)	106 (91%)	10 (9%)	10	38
39	2h	116/118 (98%)	107 (92%)	9 (8%)	12	43
40	1i	91/98 (93%)	74 (81%)	17 (19%)	1	8
40	2i	91/98 (93%)	77 (85%)	14 (15%)	2	13
41	1j	68/87 (78%)	62 (91%)	6 (9%)	10	36
41	2j	68/87 (78%)	60 (88%)	8 (12%)	5	23
42	1k	83/86 (96%)	77 (93%)	6 (7%)	14	47
42	2k	83/86 (96%)	77 (93%)	6 (7%)	14	47
43	1l	96/102 (94%)	88 (92%)	8 (8%)	11	40
43	2l	96/102 (94%)	89 (93%)	7 (7%)	14	46
44	1m	90/94 (96%)	83 (92%)	7 (8%)	12	43
44	2m	90/94 (96%)	82 (91%)	8 (9%)	9	35
45	1n	49/49 (100%)	42 (86%)	7 (14%)	3	15
45	2n	49/49 (100%)	42 (86%)	7 (14%)	3	15
46	1o	78/79 (99%)	75 (96%)	3 (4%)	33	67
46	2o	78/79 (99%)	75 (96%)	3 (4%)	33	67
47	1p	69/71 (97%)	55 (80%)	14 (20%)	1	6
47	2p	69/71 (97%)	56 (81%)	13 (19%)	1	8
48	1q	94/94 (100%)	88 (94%)	6 (6%)	17	52
48	2q	94/94 (100%)	89 (95%)	5 (5%)	22	58
49	1r	59/59 (100%)	54 (92%)	5 (8%)	10	38
49	2r	59/59 (100%)	54 (92%)	5 (8%)	10	38
50	1s	68/72 (94%)	61 (90%)	7 (10%)	7	29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	2s	68/72 (94%)	61 (90%)	7 (10%)	7	29
51	1t	71/74 (96%)	63 (89%)	8 (11%)	6	25
51	2t	71/74 (96%)	64 (90%)	7 (10%)	8	30
52	1u	18/18 (100%)	16 (89%)	2 (11%)	6	25
52	2u	18/18 (100%)	17 (94%)	1 (6%)	21	57
53	1y	16/21 (76%)	10 (62%)	6 (38%)	0	0
54	1z	82/83 (99%)	80 (98%)	2 (2%)	49	77
54	2z	82/83 (99%)	80 (98%)	2 (2%)	49	77
All	All	9582/9879 (97%)	8519 (89%)	1063 (11%)	6	25

5 of 1063 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	1j	66	ARG
4	2E	76	ARG
40	2i	125	TYR
43	1l	60	LEU
49	1r	76	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
45	1n	52	GLN
8	2l	105	HIS
42	2k	93	GLN
48	1q	16	GLN
4	2E	48	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2901 (98%)	614 (21%)	46 (1%)
1	2A	2862/2901 (98%)	613 (21%)	51 (1%)
2	1B	119/120 (99%)	15 (12%)	0
2	2B	119/120 (99%)	19 (15%)	1 (0%)
32	1a	1494/1507 (99%)	245 (16%)	0
32	2a	1494/1507 (99%)	242 (16%)	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8951/9056 (98%)	1748 (19%)	98 (1%)

5 of 1748 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	14	A
1	1A	23	G
1	1A	34	C

5 of 98 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2756	U
1	2A	645	C
1	2A	2581	G
1	1A	2873	A
1	2A	266	G

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

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
1	5MU	1A	1939	1	15,22,23	1.81	3 (20%)	16,32,35	2.34	2 (12%)
1	4OC	1A	1920	1	15,22,24	2.25	6 (40%)	17,31,35	1.59	3 (17%)
1	PSU	1A	1911	1	17,21,22	2.05	4 (23%)	20,30,33	4.26	7 (35%)
1	OMG	2A	2251	1	18,26,27	2.54	6 (33%)	20,38,41	2.40	6 (30%)
1	OMG	1A	2251	1	18,26,27	2.35	7 (38%)	20,38,41	2.46	6 (30%)
1	5MC	2A	1962	1,55	15,22,23	1.41	2 (13%)	19,32,35	0.90	1 (5%)
1	5MU	1A	1915	1	15,22,23	1.17	2 (13%)	16,32,35	2.68	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	1A	1962	1	15,22,23	0.96	1 (6%)	19,32,35	1.48	3 (15%)
32	MA6	2a	1518	32	19,26,27	1.17	3 (15%)	18,38,41	4.33	4 (22%)
32	M2G	2a	966	32	20,27,28	3.02	7 (35%)	22,40,43	1.47	4 (18%)
1	2MU	1A	2552	1,55	14,22,24	7.76	7 (50%)	14,31,36	1.28	2 (14%)
1	2MA	2A	2503	1,55	17,25,26	2.27	4 (23%)	19,37,40	2.62	4 (21%)
1	PSU	2A	2605	1	17,21,22	2.05	6 (35%)	20,30,33	4.56	7 (35%)
43	0TD	2l	92	43	4,9,10	2.10	1 (25%)	3,11,13	3.32	2 (66%)
1	PSU	1A	1917	1	17,21,22	2.03	3 (17%)	20,30,33	4.42	6 (30%)
32	MA6	1a	1518	32	19,26,27	1.07	1 (5%)	18,38,41	5.51	3 (16%)
1	4OC	2A	1920	1	15,22,24	2.46	6 (40%)	17,31,35	1.53	2 (11%)
32	M2G	1a	966	32	20,27,28	2.83	7 (35%)	22,40,43	1.59	5 (22%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	4.44	3 (16%)
43	0TD	1l	92	43	4,9,10	2.12	2 (50%)	3,11,13	4.14	2 (66%)
32	5MC	1a	1400	32	15,22,23	1.32	2 (13%)	19,32,35	1.53	4 (21%)
32	2MG	2a	1207	55,32	19,26,27	3.31	6 (31%)	21,38,41	2.82	9 (42%)
32	UR3	2a	1498	32	14,22,23	1.89	2 (14%)	15,32,35	0.80	0
1	2MU	2A	2552	1,55	14,22,24	7.90	8 (57%)	14,31,36	0.98	1 (7%)
32	PSU	2a	516	55,32	17,21,22	2.76	6 (35%)	20,30,33	4.44	8 (40%)
1	PSU	2A	1917	1	17,21,22	1.84	4 (23%)	20,30,33	4.18	6 (30%)
32	5MC	2a	1407	32	15,22,23	0.74	0	19,32,35	0.98	1 (5%)
1	5MU	2A	1915	1	15,22,23	1.73	4 (26%)	16,32,35	2.51	1 (6%)
32	7MG	1a	527	55,32	22,26,27	2.79	6 (27%)	28,39,42	1.74	8 (28%)
32	5MC	2a	1404	32	15,22,23	1.06	1 (6%)	19,32,35	0.97	2 (10%)
32	PSU	1a	516	55,32	17,21,22	1.47	3 (17%)	20,30,33	4.35	8 (40%)
32	UR3	1a	1498	32	14,22,23	1.86	3 (21%)	15,32,35	0.82	0
32	5MC	1a	967	32	15,22,23	0.73	0	19,32,35	1.02	2 (10%)
1	PSU	2A	1911	1	17,21,22	2.23	4 (23%)	20,30,33	4.70	8 (40%)
32	2MG	1a	1207	55,32	19,26,27	3.49	6 (31%)	21,38,41	2.72	7 (33%)
32	4OC	2a	1402	32	16,23,24	2.26	7 (43%)	17,32,35	1.70	2 (11%)
32	5MC	1a	1404	32	15,22,23	1.22	1 (6%)	19,32,35	1.08	3 (15%)
32	7MG	2a	527	55,32	22,26,27	3.11	6 (27%)	28,39,42	1.65	7 (25%)
1	PSU	1A	2605	1	17,21,22	2.77	7 (41%)	20,30,33	5.05	8 (40%)
1	5MC	1A	1942	1	15,22,23	1.54	2 (13%)	19,32,35	0.95	1 (5%)
1	5MU	2A	1939	1	15,22,23	2.20	5 (33%)	16,32,35	2.33	2 (12%)
32	4OC	1a	1402	32	16,23,24	2.44	7 (43%)	17,32,35	1.32	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MA	1A	2503	1,55	17,25,26	2.37	6 (35%)	19,37,40	2.52	4 (21%)
32	5MC	2a	967	32	15,22,23	0.67	0	19,32,35	1.08	2 (10%)
1	5MC	2A	1942	1	15,22,23	1.32	2 (13%)	19,32,35	1.04	2 (10%)
32	5MC	2a	1400	32	15,22,23	1.03	1 (6%)	19,32,35	1.29	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.10	1 (6%)	19,32,35	1.04	1 (5%)
32	MA6	1a	1519	32	19,26,27	1.06	2 (10%)	18,38,41	5.04	3 (16%)

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
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1	-	1/5/27/28	0/3/3/3
1	OMG	1A	2251	1	-	1/5/27/28	0/3/3/3
1	5MC	2A	1962	1,55	-	2/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1962	1	-	3/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	2/7/29/30	0/3/3/3
1	2MU	1A	2552	1,55	-	0/7/27/28	0/2/2/2
1	2MA	2A	2503	1,55	-	2/3/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
1	PSU	1A	1917	1	-	3/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
43	0TD	1l	92	43	-	2/3/12/14	-
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	2MG	2a	1207	55,32	-	0/5/27/28	0/3/3/3
32	UR3	2a	1498	32	-	2/5/25/26	0/2/2/2
1	2MU	2A	2552	1,55	-	0/7/27/28	0/2/2/2
32	PSU	2a	516	55,32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	1/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	55,32	-	2/7/37/38	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	55,32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	1/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	55,32	-	0/5/27/28	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	2/5/25/26	0/2/2/2
32	7MG	2a	527	55,32	-	2/7/37/38	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	2/5/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	2MA	1A	2503	1,55	-	1/3/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3

The worst 5 of 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	2MU	C6-N1	17.06	1.56	1.35
1	1A	2552	2MU	C6-N1	16.80	1.56	1.35
1	2A	2552	2MU	C6-C5	-12.49	1.10	1.38
1	1A	2552	2MU	C4-N3	-12.25	1.11	1.33
1	2A	2552	2MU	C4-N3	-12.24	1.11	1.33

The worst 5 of 177 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	N1-C6-N6	-20.86	95.10	117.06
32	1a	1519	MA6	N1-C6-N6	-20.17	95.83	117.06
32	2a	1519	MA6	N1-C6-N6	-17.80	98.32	117.06
1	1A	2605	PSU	N1-C2-N3	-17.16	114.79	128.43
32	2a	1518	MA6	N1-C6-N6	-16.69	99.49	117.06

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1920	4OC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	2251	OMG	C1'-C2'-O2'-CM2
1	1A	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	5MU	2	0
1	1A	1920	4OC	1	0
1	2A	2251	OMG	2	0
1	1A	1915	5MU	2	0
1	1A	1962	5MC	1	0
1	1A	2552	2MU	3	0
1	2A	2503	2MA	3	0
1	1A	1917	PSU	1	0
1	2A	1920	4OC	2	0
1	2A	2552	2MU	2	0
1	2A	1915	5MU	1	0
1	2A	1911	PSU	1	0
1	1A	2605	PSU	1	0
1	2A	1939	5MU	2	0
1	1A	2503	2MA	2	0
1	2A	1942	5MC	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2708 ligands modelled in this entry, 2706 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	SF4	2d	501	35	0,12,12	0.00	-	-		
57	SF4	1d	302	35	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	2d	501	35	-	-	0/6/5/5
57	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data 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	2861/2901 (98%)	-0.21	86 (3%)	50	34	9, 28, 117, 139	0
1	2A	2861/2901 (98%)	-0.19	100 (3%)	44	28	23, 45, 119, 140	0
2	1B	120/120 (100%)	-0.53	0	100	100	20, 48, 70, 100	0
2	2B	120/120 (100%)	-0.42	0	100	100	47, 69, 82, 106	0
3	1D	275/275 (100%)	-0.51	0	100	100	12, 26, 43, 74	0
3	2D	275/275 (100%)	-0.40	0	100	100	21, 38, 51, 72	0
4	1E	204/204 (100%)	-0.46	0	100	100	10, 29, 55, 71	0
4	2E	204/204 (100%)	-0.28	0	100	100	22, 44, 63, 82	0
5	1F	203/203 (100%)	-0.39	1 (0%)	91	86	8, 31, 65, 93	0
5	2F	203/203 (100%)	-0.36	0	100	100	23, 52, 77, 96	0
6	1G	181/181 (100%)	-0.32	1 (0%)	89	83	43, 68, 90, 101	0
6	2G	181/181 (100%)	0.32	14 (7%)	13	7	66, 84, 98, 106	0
7	1H	174/174 (100%)	-0.47	1 (0%)	89	83	26, 43, 62, 76	0
7	2H	174/174 (100%)	0.40	11 (6%)	20	11	52, 72, 82, 93	0
8	1I	147/147 (100%)	-0.16	0	100	100	37, 73, 88, 93	0
8	2I	147/147 (100%)	0.22	7 (4%)	30	18	47, 85, 97, 102	0
9	1N	140/140 (100%)	-0.45	0	100	100	17, 28, 59, 66	0
9	2N	140/140 (100%)	-0.16	1 (0%)	87	81	33, 49, 70, 79	0
10	1O	122/122 (100%)	-0.43	0	100	100	16, 29, 48, 57	0
10	2O	122/122 (100%)	-0.41	0	100	100	29, 41, 59, 66	0
11	1P	149/149 (100%)	-0.33	0	100	100	8, 37, 57, 83	0
11	2P	149/149 (100%)	-0.04	2 (1%)	77	65	28, 55, 78, 86	0
12	1Q	141/141 (100%)	-0.38	0	100	100	20, 32, 46, 72	0
12	2Q	141/141 (100%)	-0.35	0	100	100	35, 50, 64, 81	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%)	-0.51	0 100 100	14, 23, 39, 58	0
13	2R	118/118 (100%)	-0.26	0 100 100	27, 38, 53, 66	0
14	1S	110/110 (100%)	-0.34	0 100 100	29, 45, 60, 69	0
14	2S	110/110 (100%)	0.14	4 (3%) 42 27	50, 64, 79, 82	0
15	1T	131/131 (100%)	-0.47	0 100 100	23, 35, 71, 88	0
15	2T	131/131 (100%)	-0.39	0 100 100	33, 47, 80, 92	0
16	1U	116/116 (100%)	-0.60	0 100 100	10, 19, 39, 60	0
16	2U	116/116 (100%)	-0.36	0 100 100	27, 44, 60, 66	0
17	1V	101/101 (100%)	-0.38	0 100 100	11, 29, 50, 65	0
17	2V	101/101 (100%)	-0.31	0 100 100	24, 54, 70, 75	0
18	1W	112/112 (100%)	-0.50	0 100 100	10, 19, 42, 99	0
18	2W	112/112 (100%)	-0.42	0 100 100	23, 34, 57, 97	0
19	1X	95/95 (100%)	-0.37	0 100 100	17, 27, 51, 68	0
19	2X	95/95 (100%)	-0.08	0 100 100	35, 46, 66, 76	0
20	1Y	107/107 (100%)	-0.27	1 (0%) 84 75	23, 41, 68, 78	0
20	2Y	107/107 (100%)	0.59	9 (8%) 11 6	43, 61, 78, 87	0
21	1Z	203/203 (100%)	-0.38	0 100 100	32, 57, 79, 96	0
21	2Z	203/203 (100%)	0.03	5 (2%) 57 43	53, 71, 89, 104	0
22	10	77/77 (100%)	-0.25	1 (1%) 77 65	20, 30, 52, 63	0
22	20	77/77 (100%)	0.33	8 (10%) 6 4	37, 48, 62, 70	0
23	11	97/97 (100%)	0.07	2 (2%) 63 49	17, 36, 68, 83	0
23	21	97/97 (100%)	-0.18	1 (1%) 82 72	30, 46, 74, 85	0
24	12	70/70 (100%)	-0.40	0 100 100	26, 41, 57, 87	0
24	22	70/70 (100%)	0.07	2 (2%) 51 36	47, 61, 74, 84	0
25	13	59/59 (100%)	-0.22	0 100 100	16, 26, 60, 79	0
25	23	59/59 (100%)	0.62	3 (5%) 28 16	36, 48, 71, 93	0
26	14	69/69 (100%)	-0.09	4 (5%) 23 13	62, 92, 109, 110	0
26	24	69/69 (100%)	0.38	7 (10%) 7 4	76, 100, 113, 119	0
27	15	59/59 (100%)	-0.61	0 100 100	10, 24, 45, 62	0
27	25	59/59 (100%)	-0.47	0 100 100	26, 40, 59, 82	0
28	16	53/53 (100%)	-0.44	0 100 100	28, 37, 50, 57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/53 (100%)	-0.11	0 100 100	41, 52, 62, 70	0
29	17	48/48 (100%)	-0.32	0 100 100	12, 17, 50, 59	0
29	27	48/48 (100%)	-0.23	1 (2%) 63 49	24, 31, 56, 72	0
30	18	64/64 (100%)	-0.41	0 100 100	15, 22, 35, 42	0
30	28	64/64 (100%)	-0.10	0 100 100	32, 39, 51, 57	0
31	19	37/37 (100%)	0.05	0 100 100	28, 36, 59, 63	0
31	29	37/37 (100%)	0.41	3 (8%) 12 6	47, 54, 70, 73	0
32	1a	1488/1507 (98%)	-0.15	33 (2%) 62 48	27, 76, 115, 143	0
32	2a	1488/1507 (98%)	-0.11	31 (2%) 63 49	33, 79, 116, 143	0
33	1b	231/231 (100%)	-0.12	7 (3%) 50 34	70, 88, 100, 113	0
33	2b	231/231 (100%)	0.03	7 (3%) 50 34	75, 91, 104, 113	0
34	1c	206/206 (100%)	-0.00	4 (1%) 66 53	72, 89, 100, 105	0
34	2c	206/206 (100%)	0.15	10 (4%) 29 17	82, 93, 104, 109	0
35	1d	208/208 (100%)	-0.18	0 100 100	57, 80, 93, 98	0
35	2d	208/208 (100%)	-0.09	1 (0%) 91 86	61, 81, 94, 103	0
36	1e	148/148 (100%)	-0.19	0 100 100	45, 69, 83, 94	0
36	2e	148/148 (100%)	-0.14	0 100 100	50, 72, 85, 100	0
37	1f	100/100 (100%)	-0.33	0 100 100	52, 71, 81, 86	0
37	2f	100/100 (100%)	-0.36	0 100 100	54, 71, 84, 88	0
38	1g	155/155 (100%)	0.09	4 (2%) 56 40	72, 84, 95, 105	0
38	2g	155/155 (100%)	0.37	15 (9%) 7 4	78, 88, 98, 106	0
39	1h	137/137 (100%)	-0.03	2 (1%) 73 61	50, 69, 79, 87	0
39	2h	137/137 (100%)	-0.07	2 (1%) 73 61	56, 73, 82, 94	0
40	1i	127/127 (100%)	0.37	8 (6%) 20 11	68, 96, 105, 108	0
40	2i	127/127 (100%)	0.79	14 (11%) 5 3	77, 99, 108, 112	0
41	1j	97/97 (100%)	0.76	12 (12%) 4 2	75, 97, 107, 113	0
41	2j	97/97 (100%)	0.88	15 (15%) 2 1	81, 100, 109, 112	0
42	1k	114/114 (100%)	-0.24	0 100 100	39, 64, 81, 90	0
42	2k	114/114 (100%)	0.03	2 (1%) 68 55	52, 71, 85, 98	0
43	1l	121/122 (99%)	-0.10	1 (0%) 86 78	42, 61, 77, 87	0
43	2l	121/122 (99%)	-0.14	0 100 100	50, 66, 79, 88	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	116/116 (100%)	0.24	6 (5%) 27 15	71, 89, 97, 99	0
44	2m	116/116 (100%)	0.46	13 (11%) 5 3	79, 97, 104, 109	0
45	1n	60/60 (100%)	0.32	2 (3%) 46 30	70, 86, 94, 100	0
45	2n	60/60 (100%)	0.76	5 (8%) 11 6	82, 92, 100, 102	0
46	1o	88/88 (100%)	-0.07	1 (1%) 80 69	46, 66, 83, 91	0
46	2o	88/88 (100%)	-0.14	0 100 100	52, 68, 88, 93	0
47	1p	82/82 (100%)	0.37	3 (3%) 41 26	64, 78, 92, 100	0
47	2p	82/82 (100%)	0.42	3 (3%) 41 26	65, 75, 91, 101	0
48	1q	99/99 (100%)	-0.13	1 (1%) 82 72	52, 68, 79, 84	0
48	2q	99/99 (100%)	0.09	0 100 100	53, 69, 81, 86	0
49	1r	68/68 (100%)	0.16	0 100 100	53, 66, 81, 91	0
49	2r	68/68 (100%)	0.16	2 (2%) 51 36	54, 69, 86, 94	0
50	1s	83/83 (100%)	0.67	9 (10%) 5 3	78, 94, 102, 108	0
50	2s	83/83 (100%)	1.66	32 (38%) 0 0	84, 101, 111, 116	0
51	1t	96/96 (100%)	0.10	2 (2%) 63 49	65, 76, 90, 95	0
51	2t	96/96 (100%)	-0.17	1 (1%) 82 72	60, 75, 90, 93	0
52	1u	23/23 (100%)	1.21	3 (13%) 3 2	78, 84, 90, 94	0
52	2u	23/23 (100%)	1.91	14 (60%) 0 0	82, 90, 97, 99	0
53	1y	22/22 (100%)	-0.20	1 (4%) 33 21	16, 39, 78, 90	0
54	1z	97/97 (100%)	0.29	1 (1%) 82 72	52, 63, 79, 84	0
54	2z	97/97 (100%)	2.03	48 (49%) 0 0	63, 75, 85, 93	0
All	All	20796/20916 (99%)	-0.12	590 (2%) 53 37	8, 58, 104, 143	0

The worst 5 of 590 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1087	G	13.6
32	2a	1036	G	10.7
1	1A	1089	G	10.2
1	1A	1081	U	9.6
1	1A	1079	C	9.0



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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	5MU	1A	1915	21/22	0.93	0.25	81,89,96,98	0
32	M2G	2a	966	25/26	0.93	0.18	65,73,81,86	0
1	PSU	1A	1917	20/21	0.93	0.16	61,75,81,85	0
32	PSU	2a	516	20/21	0.93	0.19	72,81,90,91	0
32	PSU	1a	516	20/21	0.93	0.17	69,78,82,84	0
32	7MG	2a	527	24/25	0.93	0.23	61,66,74,77	0
1	PSU	2A	1917	20/21	0.94	0.13	76,81,94,98	0
1	PSU	2A	1911	20/21	0.94	0.10	65,72,79,80	0
1	5MU	2A	1915	21/22	0.94	0.18	86,95,109,116	0
32	5MC	1a	1407	21/22	0.94	0.18	38,55,60,63	0
1	4OC	2A	1920	21/23	0.95	0.15	55,67,70,73	0
32	2MG	1a	1207	24/25	0.95	0.16	82,91,97,98	0
32	4OC	2a	1402	22/23	0.95	0.17	56,59,64,70	0
32	2MG	2a	1207	24/25	0.95	0.22	91,98,105,108	0
32	4OC	1a	1402	22/23	0.95	0.20	51,55,61,63	0
32	5MC	2a	967	21/22	0.95	0.15	65,74,83,89	0
1	PSU	1A	1911	20/21	0.95	0.13	64,69,74,74	0
32	MA6	2a	1518	24/25	0.96	0.18	43,53,58,61	0
32	5MC	2a	1407	21/22	0.96	0.14	50,59,65,66	0
32	UR3	2a	1498	21/22	0.96	0.17	47,52,58,61	0
32	7MG	1a	527	24/25	0.96	0.19	52,56,64,67	0
32	5MC	2a	1404	21/22	0.96	0.15	47,54,61,64	0
32	M2G	1a	966	25/26	0.96	0.16	56,64,75,80	0
1	5MC	2A	1942	21/22	0.96	0.19	37,44,48,50	0
32	5MC	2a	1400	21/22	0.96	0.21	64,68,73,77	0
32	5MC	1a	967	21/22	0.96	0.18	61,69,81,82	0
32	UR3	1a	1498	21/22	0.97	0.19	39,50,58,61	0
32	5MC	1a	1400	21/22	0.97	0.17	51,55,58,60	0
1	OMG	2A	2251	24/25	0.97	0.17	29,34,37,43	0
1	2MA	2A	2503	23/24	0.97	0.18	19,23,26,34	0
1	PSU	2A	2605	20/21	0.97	0.17	21,28,33,36	0
32	5MC	1a	1404	21/22	0.97	0.13	42,50,53,57	0
43	0TD	2l	92	10/11	0.97	0.20	64,71,79,83	0
1	PSU	1A	2605	20/21	0.97	0.18	11,17,22,26	0
1	5MU	2A	1939	21/22	0.97	0.18	26,31,36,40	0
1	5MU	1A	1939	21/22	0.97	0.19	14,22,25,27	0
1	4OC	1A	1920	21/23	0.97	0.17	47,60,68,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	5MC	2A	1962	21/22	0.97	0.12	32,41,48,55	0
32	MA6	2a	1519	24/25	0.97	0.24	44,51,54,55	0
43	0TD	1l	92	10/11	0.97	0.23	64,66,69,72	0
1	5MC	1A	1962	21/22	0.98	0.15	25,29,32,41	0
1	2MA	1A	2503	23/24	0.98	0.18	7,11,12,12	0
32	MA6	1a	1518	24/25	0.98	0.18	36,42,45,48	0
1	OMG	1A	2251	24/25	0.98	0.16	17,21,27,28	0
1	5MC	1A	1942	21/22	0.98	0.17	19,27,30,36	0
1	2MU	2A	2552	21/23	0.98	0.17	24,29,32,34	0
32	MA6	1a	1519	24/25	0.98	0.19	34,40,44,49	0
1	2MU	1A	2552	21/23	0.99	0.20	15,19,22,25	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2B	3016	1/1	-0.10	0.96	85,85,85,85	0
55	MG	2H	8001	1/1	-0.01	0.75	93,93,93,93	0
55	MG	2A	3911	1/1	0.09	0.87	53,53,53,53	0
55	MG	2A	3764	1/1	0.17	0.83	70,70,70,70	0
55	MG	2a	1613	1/1	0.27	0.28	72,72,72,72	0
55	MG	2A	3260	1/1	0.29	0.19	94,94,94,94	0
55	MG	2a	1754	1/1	0.30	0.27	104,104,104,104	0
55	MG	2a	1672	1/1	0.36	0.60	64,64,64,64	0
55	MG	2B	3014	1/1	0.37	0.56	76,76,76,76	0
55	MG	2i	3001	1/1	0.37	0.45	73,73,73,73	0
55	MG	1A	3256	1/1	0.38	0.29	68,68,68,68	0
55	MG	1A	3170	1/1	0.39	0.37	62,62,62,62	0
55	MG	2a	1838	1/1	0.40	0.19	111,111,111,111	0
55	MG	1a	1676	1/1	0.41	0.43	46,46,46,46	0
55	MG	2G	3001	1/1	0.43	0.30	92,92,92,92	0
55	MG	1a	1835	1/1	0.43	0.75	81,81,81,81	0
55	MG	2a	1779	1/1	0.45	0.31	92,92,92,92	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3048	1/1	0.45	0.66	43,43,43,43	0
55	MG	2A	3279	1/1	0.45	0.64	83,83,83,83	0
55	MG	2g	3001	1/1	0.46	0.32	64,64,64,64	0
55	MG	1A	3085	1/1	0.46	0.65	32,32,32,32	0
55	MG	2A	3694	1/1	0.48	1.05	75,75,75,75	0
55	MG	2A	3591	1/1	0.49	0.54	50,50,50,50	0
55	MG	2B	3006	1/1	0.51	0.21	64,64,64,64	0
55	MG	2A	3800	1/1	0.51	0.44	73,73,73,73	0
55	MG	1a	1659	1/1	0.51	0.23	70,70,70,70	0
55	MG	2A	3419	1/1	0.52	0.63	60,60,60,60	0
55	MG	2A	3051	1/1	0.52	0.57	51,51,51,51	0
55	MG	2a	1724	1/1	0.52	0.28	96,96,96,96	0
55	MG	1B	217	1/1	0.53	0.55	57,57,57,57	0
55	MG	2B	3026	1/1	0.55	0.94	83,83,83,83	0
55	MG	2A	3784	1/1	0.55	0.79	86,86,86,86	0
55	MG	2a	1643	1/1	0.55	0.70	86,86,86,86	0
55	MG	2A	3187	1/1	0.55	0.51	63,63,63,63	0
55	MG	1A	3553	1/1	0.56	1.03	37,37,37,37	0
55	MG	1a	1661	1/1	0.56	0.81	67,67,67,67	0
55	MG	1a	1753	1/1	0.57	0.20	81,81,81,81	0
55	MG	2a	1830	1/1	0.57	0.30	119,119,119,119	0
55	MG	1a	1644	1/1	0.58	0.42	70,70,70,70	0
55	MG	2A	3623	1/1	0.58	0.27	54,54,54,54	0
55	MG	2a	1834	1/1	0.59	0.59	76,76,76,76	0
55	MG	1A	3528	1/1	0.59	1.34	31,31,31,31	0
55	MG	2a	1671	1/1	0.59	0.35	49,49,49,49	0
55	MG	1a	1763	1/1	0.60	0.14	91,91,91,91	0
55	MG	2A	3939	1/1	0.60	1.17	53,53,53,53	0
55	MG	2a	1783	1/1	0.62	0.12	90,90,90,90	0
55	MG	2B	3008	1/1	0.62	0.60	69,69,69,69	0
55	MG	2A	3781	1/1	0.62	0.50	53,53,53,53	0
55	MG	1a	1770	1/1	0.62	0.49	53,53,53,53	0
55	MG	2A	3644	1/1	0.62	0.62	48,48,48,48	0
55	MG	1a	1680	1/1	0.62	0.41	65,65,65,65	0
55	MG	2a	1663	1/1	0.62	0.53	86,86,86,86	0
55	MG	2a	1665	1/1	0.62	0.68	48,48,48,48	0
55	MG	2a	1678	1/1	0.63	0.25	60,60,60,60	0
55	MG	2A	3116	1/1	0.64	1.08	45,45,45,45	0
55	MG	2A	3326	1/1	0.64	0.26	54,54,54,54	0
55	MG	2A	3176	1/1	0.64	0.54	81,81,81,81	0
55	MG	2a	1619	1/1	0.64	0.66	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
55	MG	2A	3888	1/1	0.65	0.36	63,63,63,63	0
55	MG	2B	3023	1/1	0.65	0.33	92,92,92,92	0
55	MG	1A	3253	1/1	0.65	1.00	59,59,59,59	0
55	MG	2A	3753	1/1	0.65	0.83	41,41,41,41	0
55	MG	2a	1748	1/1	0.65	0.28	71,71,71,71	0
55	MG	1X	102	1/1	0.65	0.58	49,49,49,49	0
55	MG	2A	3109	1/1	0.65	0.46	43,43,43,43	0
55	MG	2A	3046	1/1	0.66	0.29	50,50,50,50	0
55	MG	2D	315	1/1	0.66	0.16	60,60,60,60	0
55	MG	2D	308	1/1	0.66	0.51	64,64,64,64	0
55	MG	2B	3025	1/1	0.66	0.38	63,63,63,63	0
55	MG	1A	3061	1/1	0.66	0.18	34,34,34,34	0
55	MG	1a	1614	1/1	0.66	0.36	75,75,75,75	0
55	MG	2D	314	1/1	0.66	0.36	50,50,50,50	0
55	MG	20	104	1/1	0.66	0.32	62,62,62,62	0
55	MG	20	102	1/1	0.66	0.20	66,66,66,66	0
55	MG	2A	3559	1/1	0.67	0.98	63,63,63,63	0
55	MG	2A	3915	1/1	0.67	0.78	70,70,70,70	0
55	MG	2A	3727	1/1	0.67	0.43	67,67,67,67	0
55	MG	2a	1624	1/1	0.67	0.46	62,62,62,62	0
55	MG	1A	3650	1/1	0.68	0.52	76,76,76,76	0
55	MG	2A	3945	1/1	0.68	0.61	81,81,81,81	0
55	MG	2a	1796	1/1	0.68	0.80	95,95,95,95	0
55	MG	2a	1828	1/1	0.68	0.44	90,90,90,90	0
55	MG	2A	3164	1/1	0.68	0.46	44,44,44,44	0
55	MG	1A	3255	1/1	0.68	0.15	57,57,57,57	0
55	MG	1a	1828	1/1	0.68	0.39	74,74,74,74	0
55	MG	2A	3073	1/1	0.68	0.27	41,41,41,41	0
55	MG	1a	1666	1/1	0.69	0.85	42,42,42,42	0
55	MG	2Y	201	1/1	0.69	1.18	61,61,61,61	0
55	MG	2B	3009	1/1	0.69	1.03	72,72,72,72	0
55	MG	1d	301	1/1	0.69	0.11	110,110,110,110	0
55	MG	2a	1820	1/1	0.69	0.27	51,51,51,51	0
55	MG	1A	3717	1/1	0.69	0.60	29,29,29,29	0
56	ZN	24	501	1/1	0.69	0.08	150,150,150,150	0
55	MG	2z	101	1/1	0.69	1.02	111,111,111,111	0
55	MG	2A	3923	1/1	0.69	0.36	83,83,83,83	0
55	MG	1a	1684	1/1	0.69	0.72	44,44,44,44	0
55	MG	2A	3521	1/1	0.69	0.34	48,48,48,48	0
55	MG	1n	502	1/1	0.70	0.24	74,74,74,74	0
55	MG	2a	1651	1/1	0.70	0.45	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
55	MG	2A	3720	1/1	0.70	0.46	60,60,60,60	0
55	MG	1a	1771	1/1	0.70	0.15	92,92,92,92	0
55	MG	2A	3885	1/1	0.70	0.17	67,67,67,67	0
55	MG	1a	1759	1/1	0.70	0.16	94,94,94,94	0
55	MG	2A	3735	1/1	0.70	0.10	103,103,103,103	0
55	MG	2a	1747	1/1	0.70	0.23	106,106,106,106	0
55	MG	2A	3580	1/1	0.70	0.31	60,60,60,60	0
55	MG	2A	3194	1/1	0.70	0.65	40,40,40,40	0
55	MG	2A	3917	1/1	0.71	0.33	71,71,71,71	0
55	MG	1A	3480	1/1	0.71	0.49	45,45,45,45	0
55	MG	2a	1666	1/1	0.71	0.32	68,68,68,68	0
55	MG	1A	3685	1/1	0.71	0.26	43,43,43,43	0
55	MG	2B	3017	1/1	0.71	0.34	68,68,68,68	0
55	MG	1A	3957	1/1	0.71	0.41	78,78,78,78	0
55	MG	2A	3202	1/1	0.71	0.67	61,61,61,61	0
55	MG	2d	502	1/1	0.71	0.29	48,48,48,48	0
55	MG	2A	3641	1/1	0.72	0.53	57,57,57,57	0
55	MG	1a	1672	1/1	0.72	0.37	70,70,70,70	0
55	MG	2a	1615	1/1	0.72	0.38	80,80,80,80	0
55	MG	1A	3912	1/1	0.72	0.45	35,35,35,35	0
55	MG	1a	1653	1/1	0.73	0.36	43,43,43,43	0
55	MG	2A	3744	1/1	0.73	0.17	58,58,58,58	0
55	MG	2A	3819	1/1	0.73	0.80	55,55,55,55	0
55	MG	2a	1655	1/1	0.73	0.36	62,62,62,62	0
55	MG	2B	3010	1/1	0.73	0.19	70,70,70,70	0
55	MG	2a	1635	1/1	0.73	0.41	63,63,63,63	0
55	MG	2A	3599	1/1	0.73	0.40	52,52,52,52	0
55	MG	1A	3081	1/1	0.73	0.70	41,41,41,41	0
55	MG	2A	3542	1/1	0.73	0.27	66,66,66,66	0
55	MG	2A	3944	1/1	0.73	0.58	57,57,57,57	0
55	MG	1A	3320	1/1	0.73	0.13	44,44,44,44	0
55	MG	2A	3726	1/1	0.73	0.37	73,73,73,73	0
55	MG	2A	3690	1/1	0.73	0.24	43,43,43,43	0
55	MG	2A	3025	1/1	0.74	1.08	42,42,42,42	0
55	MG	2A	3199	1/1	0.74	0.74	32,32,32,32	0
55	MG	1A	3602	1/1	0.74	0.54	46,46,46,46	0
55	MG	1a	1626	1/1	0.74	0.30	47,47,47,47	0
55	MG	2a	1668	1/1	0.74	1.39	60,60,60,60	0
55	MG	1Q	203	1/1	0.74	0.40	40,40,40,40	0
55	MG	1a	1669	1/1	0.74	0.42	61,61,61,61	0
55	MG	2A	3931	1/1	0.74	0.98	63,63,63,63	0
55	MG	1A	3589	1/1	0.74	0.16	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
55	MG	2A	3259	1/1	0.74	0.15	82,82,82,82	0
55	MG	2A	3586	1/1	0.74	0.26	35,35,35,35	0
55	MG	1A	3493	1/1	0.74	0.48	44,44,44,44	0
55	MG	2a	1650	1/1	0.74	0.20	51,51,51,51	0
55	MG	2d	504	1/1	0.75	0.44	66,66,66,66	0
55	MG	1A	3780	1/1	0.75	0.41	39,39,39,39	0
55	MG	2A	3626	1/1	0.75	0.37	64,64,64,64	0
55	MG	2A	3595	1/1	0.75	0.28	79,79,79,79	0
55	MG	2A	3152	1/1	0.75	0.58	36,36,36,36	0
55	MG	1A	3718	1/1	0.75	0.34	58,58,58,58	0
55	MG	2S	201	1/1	0.75	0.27	46,46,46,46	0
55	MG	1d	303	1/1	0.75	0.42	59,59,59,59	0
55	MG	1A	3699	1/1	0.75	0.33	47,47,47,47	0
55	MG	1A	3032	1/1	0.75	0.77	30,30,30,30	0
55	MG	1A	3946	1/1	0.75	0.48	40,40,40,40	0
55	MG	2A	3828	1/1	0.75	0.20	88,88,88,88	0
55	MG	1a	1837	1/1	0.75	0.24	93,93,93,93	0
55	MG	2a	1617	1/1	0.76	0.94	83,83,83,83	0
55	MG	1A	3122	1/1	0.76	0.53	39,39,39,39	0
55	MG	1A	3219	1/1	0.76	0.30	30,30,30,30	0
55	MG	2A	3008	1/1	0.76	0.29	40,40,40,40	0
55	MG	1B	227	1/1	0.76	0.38	29,29,29,29	0
55	MG	1A	3274	1/1	0.76	0.37	79,79,79,79	0
55	MG	29	104	1/1	0.76	0.99	75,75,75,75	0
55	MG	1A	3621	1/1	0.76	0.35	58,58,58,58	0
55	MG	2a	1827	1/1	0.76	0.56	77,77,77,77	0
55	MG	2a	1719	1/1	0.76	0.14	76,76,76,76	0
55	MG	1a	1643	1/1	0.76	0.28	61,61,61,61	0
55	MG	2A	3098	1/1	0.76	0.65	50,50,50,50	0
55	MG	2A	3033	1/1	0.76	0.40	44,44,44,44	0
55	MG	2A	3250	1/1	0.76	0.72	54,54,54,54	0
55	MG	2a	1832	1/1	0.76	0.39	83,83,83,83	0
55	MG	1A	3638	1/1	0.76	0.43	49,49,49,49	0
55	MG	2A	3022	1/1	0.77	0.42	49,49,49,49	0
55	MG	23	102	1/1	0.77	1.09	59,59,59,59	0
55	MG	2A	3031	1/1	0.77	0.37	45,45,45,45	0
55	MG	1a	1832	1/1	0.77	0.10	104,104,104,104	0
55	MG	1a	1602	1/1	0.77	0.08	78,78,78,78	0
55	MG	1A	3046	1/1	0.77	0.38	40,40,40,40	0
55	MG	2G	3002	1/1	0.77	0.09	71,71,71,71	0
55	MG	2B	3015	1/1	0.77	0.22	62,62,62,62	0
55	MG	2t	201	1/1	0.77	0.21	75,75,75,75	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1640	1/1	0.77	0.77	60,60,60,60	0
55	MG	2B	3011	1/1	0.77	0.22	89,89,89,89	0
55	MG	1F	304	1/1	0.77	0.18	31,31,31,31	0
55	MG	1A	3783	1/1	0.77	0.39	67,67,67,67	0
55	MG	2A	3596	1/1	0.77	0.11	68,68,68,68	0
55	MG	2A	3907	1/1	0.77	0.67	56,56,56,56	0
55	MG	1A	3550	1/1	0.77	0.31	36,36,36,36	0
55	MG	2A	3751	1/1	0.77	0.60	77,77,77,77	0
55	MG	2A	3850	1/1	0.77	0.13	81,81,81,81	0
55	MG	2A	3961	1/1	0.77	0.39	52,52,52,52	0
55	MG	29	101	1/1	0.77	0.41	46,46,46,46	0
55	MG	2A	3515	1/1	0.77	0.35	68,68,68,68	0
55	MG	1A	3074	1/1	0.77	0.64	31,31,31,31	0
55	MG	2a	1646	1/1	0.78	0.09	76,76,76,76	0
55	MG	2A	3795	1/1	0.78	0.83	42,42,42,42	0
55	MG	2A	3532	1/1	0.78	0.14	56,56,56,56	0
55	MG	2a	1639	1/1	0.78	0.58	63,63,63,63	0
55	MG	1A	3040	1/1	0.78	0.44	39,39,39,39	0
55	MG	2A	3230	1/1	0.78	0.59	49,49,49,49	0
55	MG	1A	3729	1/1	0.78	0.18	95,95,95,95	0
55	MG	2A	3969	1/1	0.78	1.10	53,53,53,53	0
55	MG	2A	3178	1/1	0.78	0.34	37,37,37,37	0
55	MG	2a	1755	1/1	0.78	0.26	99,99,99,99	0
55	MG	2A	3413	1/1	0.78	0.49	36,36,36,36	0
55	MG	2A	3378	1/1	0.78	0.16	72,72,72,72	0
55	MG	2A	3941	1/1	0.78	0.59	104,104,104,104	0
55	MG	2A	3710	1/1	0.78	0.19	40,40,40,40	0
55	MG	1A	3481	1/1	0.78	0.20	56,56,56,56	0
55	MG	1A	3119	1/1	0.78	0.28	35,35,35,35	0
55	MG	1A	3846	1/1	0.78	0.19	29,29,29,29	0
55	MG	2A	3594	1/1	0.78	0.73	43,43,43,43	0
55	MG	1a	1668	1/1	0.78	0.33	60,60,60,60	0
55	MG	2B	3005	1/1	0.78	0.37	74,74,74,74	0
55	MG	2A	3929	1/1	0.78	0.75	58,58,58,58	0
55	MG	1a	1806	1/1	0.78	0.40	74,74,74,74	0
55	MG	1A	3918	1/1	0.78	0.30	35,35,35,35	0
55	MG	2B	3003	1/1	0.79	0.17	67,67,67,67	0
55	MG	1A	3914	1/1	0.79	0.20	40,40,40,40	0
55	MG	2A	3232	1/1	0.79	0.44	44,44,44,44	0
55	MG	2A	3394	1/1	0.79	0.13	72,72,72,72	0
55	MG	2a	1736	1/1	0.79	0.31	46,46,46,46	0
55	MG	1a	1640	1/1	0.79	0.61	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1779	1/1	0.79	0.15	81,81,81,81	0
55	MG	1A	3584	1/1	0.79	0.83	32,32,32,32	0
55	MG	2A	3487	1/1	0.79	0.33	52,52,52,52	0
55	MG	2A	3123	1/1	0.79	0.30	49,49,49,49	0
55	MG	2a	1631	1/1	0.79	1.53	56,56,56,56	0
55	MG	2F	310	1/1	0.79	0.44	40,40,40,40	0
55	MG	2A	3567	1/1	0.79	0.35	53,53,53,53	0
55	MG	2A	3650	1/1	0.79	0.45	71,71,71,71	0
55	MG	2a	1684	1/1	0.79	0.34	53,53,53,53	0
55	MG	1A	3562	1/1	0.79	0.41	63,63,63,63	0
55	MG	1A	3184	1/1	0.79	0.57	33,33,33,33	0
55	MG	2A	3930	1/1	0.79	0.26	61,61,61,61	0
55	MG	1A	3173	1/1	0.79	0.45	49,49,49,49	0
55	MG	2A	3417	1/1	0.79	0.19	46,46,46,46	0
55	MG	1a	1750	1/1	0.79	0.25	68,68,68,68	0
55	MG	2A	3262	1/1	0.79	0.39	51,51,51,51	0
55	MG	2A	3404	1/1	0.79	0.46	78,78,78,78	0
55	MG	1i	3001	1/1	0.79	0.26	74,74,74,74	0
55	MG	1A	3812	1/1	0.79	0.24	96,96,96,96	0
55	MG	2A	3302	1/1	0.80	0.22	51,51,51,51	0
55	MG	1A	3660	1/1	0.80	0.45	55,55,55,55	0
55	MG	1A	3264	1/1	0.80	0.35	58,58,58,58	0
55	MG	1a	1632	1/1	0.80	1.21	57,57,57,57	0
55	MG	2t	202	1/1	0.80	0.38	72,72,72,72	0
55	MG	2A	3508	1/1	0.80	0.40	59,59,59,59	0
55	MG	2A	3891	1/1	0.80	0.14	72,72,72,72	0
55	MG	17	101	1/1	0.80	0.77	34,34,34,34	0
55	MG	1a	1748	1/1	0.80	0.13	86,86,86,86	0
55	MG	2A	3628	1/1	0.80	0.39	79,79,79,79	0
55	MG	2a	1676	1/1	0.80	0.26	102,102,102,102	0
55	MG	2A	3130	1/1	0.80	0.21	41,41,41,41	0
55	MG	2A	3782	1/1	0.80	0.47	58,58,58,58	0
55	MG	2D	316	1/1	0.80	0.74	58,58,58,58	0
55	MG	1a	1778	1/1	0.80	0.18	92,92,92,92	0
55	MG	2A	3868	1/1	0.80	0.38	106,106,106,106	0
55	MG	2A	3874	1/1	0.80	0.39	67,67,67,67	0
55	MG	2A	3938	1/1	0.80	0.28	46,46,46,46	0
55	MG	2A	3347	1/1	0.80	0.15	44,44,44,44	0
55	MG	1a	1740	1/1	0.80	0.26	81,81,81,81	0
55	MG	2A	3615	1/1	0.80	0.20	70,70,70,70	0
55	MG	1A	3138	1/1	0.80	0.10	52,52,52,52	0
55	MG	1B	211	1/1	0.80	0.42	58,58,58,58	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1647	1/1	0.80	0.11	65,65,65,65	0
55	MG	1a	1628	1/1	0.80	0.20	38,38,38,38	0
55	MG	2A	3177	1/1	0.80	0.40	42,42,42,42	0
55	MG	1a	1810	1/1	0.80	0.18	81,81,81,81	0
55	MG	2A	3452	1/1	0.80	0.15	82,82,82,82	0
55	MG	1a	1807	1/1	0.80	0.11	98,98,98,98	0
55	MG	19	101	1/1	0.80	0.35	24,24,24,24	0
55	MG	2A	3068	1/1	0.80	0.90	39,39,39,39	0
55	MG	2a	1625	1/1	0.80	0.36	59,59,59,59	0
55	MG	1l	3001	1/1	0.80	0.13	59,59,59,59	0
55	MG	2a	1686	1/1	0.81	0.10	78,78,78,78	0
55	MG	1A	3411	1/1	0.81	0.19	51,51,51,51	0
55	MG	2a	1636	1/1	0.81	1.08	63,63,63,63	0
55	MG	1a	1704	1/1	0.81	0.25	67,67,67,67	0
55	MG	2a	1721	1/1	0.81	0.43	84,84,84,84	0
55	MG	1A	3297	1/1	0.81	0.64	34,34,34,34	0
55	MG	1a	1841	1/1	0.81	0.25	52,52,52,52	0
55	MG	1a	1608	1/1	0.81	0.40	74,74,74,74	0
55	MG	1a	1765	1/1	0.81	0.35	81,81,81,81	0
55	MG	2A	3679	1/1	0.81	0.23	60,60,60,60	0
55	MG	1A	3325	1/1	0.81	0.28	29,29,29,29	0
55	MG	2A	3742	1/1	0.81	0.19	52,52,52,52	0
55	MG	2a	1661	1/1	0.81	0.35	60,60,60,60	0
55	MG	1A	3269	1/1	0.81	0.48	49,49,49,49	0
55	MG	2A	3765	1/1	0.81	0.32	67,67,67,67	0
55	MG	1a	1791	1/1	0.81	0.36	64,64,64,64	0
55	MG	2A	3235	1/1	0.81	0.28	63,63,63,63	0
55	MG	1B	204	1/1	0.81	0.14	63,63,63,63	0
55	MG	2A	3040	1/1	0.81	0.42	51,51,51,51	0
55	MG	2a	1809	1/1	0.81	0.15	68,68,68,68	0
55	MG	2A	3857	1/1	0.81	0.68	47,47,47,47	0
55	MG	2A	3779	1/1	0.81	0.15	60,60,60,60	0
55	MG	2a	1627	1/1	0.81	0.27	25,25,25,25	0
55	MG	2A	3884	1/1	0.81	0.08	65,65,65,65	0
55	MG	1a	1789	1/1	0.81	0.15	117,117,117,117	0
55	MG	1A	3494	1/1	0.81	0.13	28,28,28,28	0
55	MG	1A	3623	1/1	0.81	0.15	59,59,59,59	0
55	MG	2A	3473	1/1	0.81	0.19	66,66,66,66	0
55	MG	1A	3231	1/1	0.81	0.39	40,40,40,40	0
55	MG	2a	1660	1/1	0.81	0.48	42,42,42,42	0
55	MG	2A	3511	1/1	0.81	0.30	64,64,64,64	0
55	MG	2a	1658	1/1	0.81	0.21	83,83,83,83	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1764	1/1	0.81	0.30	67,67,67,67	0
55	MG	1a	1845	1/1	0.81	0.99	107,107,107,107	0
55	MG	2A	3007	1/1	0.81	0.28	59,59,59,59	0
55	MG	1a	1838	1/1	0.81	0.49	27,27,27,27	0
55	MG	1A	3224	1/1	0.81	0.41	32,32,32,32	0
55	MG	20	101	1/1	0.81	0.54	48,48,48,48	0
55	MG	1a	1756	1/1	0.81	0.23	75,75,75,75	0
55	MG	2E	305	1/1	0.81	0.29	53,53,53,53	0
55	MG	2A	3502	1/1	0.81	0.09	69,69,69,69	0
55	MG	2A	3006	1/1	0.81	0.40	42,42,42,42	0
55	MG	2A	3689	1/1	0.81	0.20	37,37,37,37	0
55	MG	2A	3146	1/1	0.81	0.32	68,68,68,68	0
55	MG	2a	1751	1/1	0.81	0.20	93,93,93,93	0
55	MG	2o	101	1/1	0.81	0.29	66,66,66,66	0
55	MG	20	105	1/1	0.81	0.99	62,62,62,62	0
55	MG	2A	3619	1/1	0.81	0.31	74,74,74,74	0
55	MG	2a	1605	1/1	0.82	0.30	82,82,82,82	0
55	MG	2A	3640	1/1	0.82	0.11	72,72,72,72	0
55	MG	2A	3299	1/1	0.82	0.27	44,44,44,44	0
55	MG	1a	1751	1/1	0.82	0.18	98,98,98,98	0
55	MG	2A	3618	1/1	0.82	0.16	83,83,83,83	0
55	MG	1a	1679	1/1	0.82	0.19	46,46,46,46	0
55	MG	2A	3677	1/1	0.82	0.35	48,48,48,48	0
55	MG	2a	1697	1/1	0.82	0.13	66,66,66,66	0
55	MG	2A	3459	1/1	0.82	0.09	53,53,53,53	0
55	MG	2a	1677	1/1	0.82	0.20	68,68,68,68	0
55	MG	2A	3350	1/1	0.82	0.13	40,40,40,40	0
55	MG	2A	3667	1/1	0.82	0.22	89,89,89,89	0
55	MG	1a	1788	1/1	0.82	0.06	70,70,70,70	0
55	MG	1a	1809	1/1	0.82	0.11	85,85,85,85	0
55	MG	2A	3605	1/1	0.82	0.17	55,55,55,55	0
55	MG	2a	1702	1/1	0.82	0.22	52,52,52,52	0
55	MG	2a	1806	1/1	0.82	0.23	84,84,84,84	0
55	MG	1A	3724	1/1	0.82	0.77	47,47,47,47	0
55	MG	1A	3778	1/1	0.82	0.51	46,46,46,46	0
55	MG	2A	3513	1/1	0.82	0.30	66,66,66,66	0
55	MG	1A	3786	1/1	0.82	0.08	65,65,65,65	0
55	MG	2A	3004	1/1	0.82	0.27	54,54,54,54	0
55	MG	1a	1744	1/1	0.82	0.55	64,64,64,64	0
55	MG	2A	3754	1/1	0.82	0.37	39,39,39,39	0
55	MG	1a	1833	1/1	0.82	0.21	98,98,98,98	0
55	MG	1a	1641	1/1	0.82	0.40	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3495	1/1	0.82	0.09	42,42,42,42	0
55	MG	1A	3265	1/1	0.82	0.51	43,43,43,43	0
55	MG	2A	3608	1/1	0.82	0.30	48,48,48,48	0
55	MG	1A	3174	1/1	0.82	0.15	40,40,40,40	0
55	MG	1D	311	1/1	0.82	0.16	43,43,43,43	0
55	MG	2A	3524	1/1	0.82	0.52	74,74,74,74	0
55	MG	1a	1754	1/1	0.82	0.19	66,66,66,66	0
55	MG	2A	3421	1/1	0.82	0.09	54,54,54,54	0
55	MG	2A	3233	1/1	0.82	0.28	56,56,56,56	0
55	MG	2A	3916	1/1	0.82	1.27	48,48,48,48	0
55	MG	1A	3940	1/1	0.82	0.64	51,51,51,51	0
55	MG	2A	3845	1/1	0.82	0.92	42,42,42,42	0
55	MG	1A	3762	1/1	0.82	0.23	50,50,50,50	0
55	MG	2a	1670	1/1	0.82	0.22	56,56,56,56	0
55	MG	2A	3038	1/1	0.82	0.39	46,46,46,46	0
55	MG	1B	215	1/1	0.82	0.45	50,50,50,50	0
55	MG	1A	3239	1/1	0.82	0.21	46,46,46,46	0
55	MG	2A	3971	1/1	0.82	0.31	73,73,73,73	0
55	MG	2A	3311	1/1	0.82	0.11	66,66,66,66	0
55	MG	2a	1607	1/1	0.82	0.23	49,49,49,49	0
55	MG	2A	3245	1/1	0.82	0.38	54,54,54,54	0
55	MG	2h	3002	1/1	0.83	0.59	73,73,73,73	0
55	MG	2A	3179	1/1	0.83	0.59	39,39,39,39	0
55	MG	2A	3950	1/1	0.83	0.19	55,55,55,55	0
55	MG	1A	3645	1/1	0.83	0.47	45,45,45,45	0
55	MG	2W	3003	1/1	0.83	0.46	43,43,43,43	0
55	MG	2A	3009	1/1	0.83	0.32	31,31,31,31	0
55	MG	2A	3783	1/1	0.83	0.35	42,42,42,42	0
55	MG	1A	3744	1/1	0.83	0.19	29,29,29,29	0
55	MG	2P	202	1/1	0.83	0.24	84,84,84,84	0
55	MG	1A	3080	1/1	0.83	0.43	22,22,22,22	0
55	MG	1A	3313	1/1	0.83	0.31	41,41,41,41	0
55	MG	2A	3226	1/1	0.83	0.42	41,41,41,41	0
55	MG	2A	3434	1/1	0.83	0.13	39,39,39,39	0
55	MG	1A	3271	1/1	0.83	0.91	29,29,29,29	0
55	MG	2A	3492	1/1	0.83	1.07	41,41,41,41	0
55	MG	2a	1722	1/1	0.83	0.20	52,52,52,52	0
55	MG	1A	3290	1/1	0.83	0.27	21,21,21,21	0
55	MG	2A	3155	1/1	0.83	0.34	45,45,45,45	0
55	MG	1A	3372	1/1	0.83	0.19	68,68,68,68	0
55	MG	2X	101	1/1	0.83	0.79	64,64,64,64	0
55	MG	2a	1621	1/1	0.83	0.24	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
55	MG	1B	208	1/1	0.83	0.14	41,41,41,41	0
55	MG	2N	202	1/1	0.83	0.43	64,64,64,64	0
55	MG	2A	3734	1/1	0.83	0.20	81,81,81,81	0
55	MG	1a	1681	1/1	0.83	0.40	59,59,59,59	0
55	MG	2A	3658	1/1	0.83	0.45	45,45,45,45	0
55	MG	2B	3018	1/1	0.83	0.13	70,70,70,70	0
55	MG	2A	3439	1/1	0.83	0.10	50,50,50,50	0
55	MG	1A	3878	1/1	0.83	0.42	49,49,49,49	0
55	MG	2A	3701	1/1	0.83	0.49	60,60,60,60	0
55	MG	1a	1615	1/1	0.83	0.18	72,72,72,72	0
55	MG	2a	1842	1/1	0.83	0.52	71,71,71,71	0
55	MG	1A	3574	1/1	0.83	0.21	49,49,49,49	0
55	MG	1d	304	1/1	0.83	0.26	68,68,68,68	0
55	MG	2A	3557	1/1	0.83	0.28	77,77,77,77	0
55	MG	2a	1784	1/1	0.83	0.12	125,125,125,125	0
55	MG	2A	3721	1/1	0.83	0.32	47,47,47,47	0
55	MG	2a	1669	1/1	0.83	0.17	56,56,56,56	0
55	MG	2A	3631	1/1	0.84	0.11	75,75,75,75	0
55	MG	2A	3655	1/1	0.84	0.54	53,53,53,53	0
55	MG	2A	3556	1/1	0.84	0.28	65,65,65,65	0
55	MG	1A	3782	1/1	0.84	0.35	60,60,60,60	0
55	MG	1A	3899	1/1	0.84	0.17	68,68,68,68	0
55	MG	1B	203	1/1	0.84	0.23	46,46,46,46	0
55	MG	2A	3271	1/1	0.84	0.23	34,34,34,34	0
55	MG	2A	3708	1/1	0.84	0.14	63,63,63,63	0
55	MG	1A	3199	1/1	0.84	0.24	44,44,44,44	0
55	MG	2A	3380	1/1	0.84	0.06	35,35,35,35	0
55	MG	2A	3461	1/1	0.84	0.23	88,88,88,88	0
55	MG	1A	3152	1/1	0.84	0.22	37,37,37,37	0
55	MG	2A	3169	1/1	0.84	0.58	54,54,54,54	0
55	MG	2E	306	1/1	0.84	0.16	35,35,35,35	0
55	MG	2A	3624	1/1	0.84	0.75	56,56,56,56	0
55	MG	1A	3455	1/1	0.84	0.20	89,89,89,89	0
55	MG	2A	3106	1/1	0.84	0.34	43,43,43,43	0
55	MG	2A	3872	1/1	0.84	0.20	71,71,71,71	0
55	MG	2A	3630	1/1	0.84	0.13	73,73,73,73	0
55	MG	2h	3001	1/1	0.84	0.34	43,43,43,43	0
55	MG	2A	3680	1/1	0.84	0.16	53,53,53,53	0
55	MG	2A	3335	1/1	0.84	0.13	77,77,77,77	0
55	MG	2D	312	1/1	0.84	0.30	48,48,48,48	0
55	MG	2A	3207	1/1	0.84	0.66	58,58,58,58	0
55	MG	2a	1664	1/1	0.84	0.71	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3033	1/1	0.84	0.20	49,49,49,49	0
55	MG	1a	1799	1/1	0.84	0.06	73,73,73,73	0
55	MG	1U	201	1/1	0.84	0.29	26,26,26,26	0
55	MG	1A	3723	1/1	0.84	0.33	63,63,63,63	0
55	MG	2A	3332	1/1	0.84	0.13	61,61,61,61	0
55	MG	2A	3159	1/1	0.84	0.31	45,45,45,45	0
55	MG	1A	3096	1/1	0.84	0.26	48,48,48,48	0
55	MG	1a	1635	1/1	0.84	0.20	46,46,46,46	0
55	MG	2a	1752	1/1	0.84	0.14	77,77,77,77	0
55	MG	2A	3881	1/1	0.84	0.48	49,49,49,49	0
55	MG	2A	3776	1/1	0.84	1.21	69,69,69,69	0
55	MG	2A	3206	1/1	0.84	0.25	54,54,54,54	0
55	MG	1A	3654	1/1	0.84	0.22	35,35,35,35	0
55	MG	1A	3646	1/1	0.84	0.32	38,38,38,38	0
55	MG	1A	3916	1/1	0.84	0.07	116,116,116,116	0
55	MG	2A	3248	1/1	0.84	0.28	44,44,44,44	0
55	MG	2A	3490	1/1	0.84	0.20	68,68,68,68	0
55	MG	2A	3142	1/1	0.84	0.14	78,78,78,78	0
55	MG	2A	3174	1/1	0.84	0.41	36,36,36,36	0
55	MG	2A	3027	1/1	0.84	0.13	42,42,42,42	0
55	MG	2A	3553	1/1	0.84	0.11	51,51,51,51	0
55	MG	1F	308	1/1	0.84	0.61	39,39,39,39	0
55	MG	2A	3568	1/1	0.84	0.70	53,53,53,53	0
55	MG	2A	3049	1/1	0.84	0.48	44,44,44,44	0
55	MG	1A	3133	1/1	0.84	0.55	47,47,47,47	0
55	MG	1A	3649	1/1	0.84	0.23	40,40,40,40	0
55	MG	1A	3009	1/1	0.84	0.31	19,19,19,19	0
55	MG	1A	3603	1/1	0.84	0.13	48,48,48,48	0
55	MG	1A	3518	1/1	0.85	0.12	50,50,50,50	0
55	MG	2A	3010	1/1	0.85	0.56	49,49,49,49	0
55	MG	2a	1767	1/1	0.85	0.35	74,74,74,74	0
55	MG	2A	3673	1/1	0.85	0.19	58,58,58,58	0
55	MG	2a	1620	1/1	0.85	0.29	58,58,58,58	0
55	MG	2a	1735	1/1	0.85	0.16	87,87,87,87	0
55	MG	2a	1616	1/1	0.85	0.20	69,69,69,69	0
55	MG	2A	3875	1/1	0.85	0.66	102,102,102,102	0
55	MG	1a	1741	1/1	0.85	0.38	42,42,42,42	0
55	MG	2a	1612	1/1	0.85	0.27	42,42,42,42	0
55	MG	1a	1758	1/1	0.85	0.16	99,99,99,99	0
55	MG	2A	3648	1/1	0.85	0.12	49,49,49,49	0
55	MG	2B	3007	1/1	0.85	0.12	52,52,52,52	0
55	MG	1A	3873	1/1	0.85	0.34	20,20,20,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3833	1/1	0.85	0.20	44,44,44,44	0
55	MG	1A	3127	1/1	0.85	0.18	34,34,34,34	0
55	MG	1A	3161	1/1	0.85	0.66	26,26,26,26	0
55	MG	2A	3676	1/1	0.85	0.22	62,62,62,62	0
55	MG	2A	3555	1/1	0.85	0.28	54,54,54,54	0
55	MG	2A	3777	1/1	0.85	0.48	63,63,63,63	0
55	MG	1A	3673	1/1	0.85	0.86	40,40,40,40	0
55	MG	2a	1749	1/1	0.85	0.23	75,75,75,75	0
55	MG	2A	3029	1/1	0.85	0.24	39,39,39,39	0
55	MG	2A	3001	1/1	0.85	0.13	47,47,47,47	0
55	MG	2e	201	1/1	0.85	0.21	57,57,57,57	0
55	MG	1a	1609	1/1	0.85	0.27	80,80,80,80	0
55	MG	1A	3809	1/1	0.85	0.11	63,63,63,63	0
55	MG	2A	3543	1/1	0.85	0.28	57,57,57,57	0
55	MG	2A	3200	1/1	0.85	0.51	41,41,41,41	0
55	MG	2a	1717	1/1	0.85	0.29	90,90,90,90	0
55	MG	1A	3722	1/1	0.85	0.20	49,49,49,49	0
55	MG	2A	3951	1/1	0.85	0.71	38,38,38,38	0
55	MG	2A	3231	1/1	0.85	0.13	59,59,59,59	0
55	MG	2A	3603	1/1	0.85	0.23	59,59,59,59	0
55	MG	1A	3175	1/1	0.85	0.15	50,50,50,50	0
55	MG	1A	3466	1/1	0.85	0.24	36,36,36,36	0
55	MG	2A	3842	1/1	0.85	0.23	65,65,65,65	0
55	MG	2A	3675	1/1	0.85	0.49	63,63,63,63	0
55	MG	2A	3100	1/1	0.85	0.24	56,56,56,56	0
55	MG	2A	3330	1/1	0.85	0.10	78,78,78,78	0
55	MG	2A	3456	1/1	0.85	0.14	62,62,62,62	0
55	MG	1a	1670	1/1	0.86	0.19	55,55,55,55	0
55	MG	2A	3504	1/1	0.86	0.73	71,71,71,71	0
55	MG	2A	3919	1/1	0.86	0.21	122,122,122,122	0
55	MG	25	103	1/1	0.86	0.71	49,49,49,49	0
55	MG	2A	3030	1/1	0.86	0.37	23,23,23,23	0
55	MG	1a	1785	1/1	0.86	0.17	96,96,96,96	0
55	MG	1A	3616	1/1	0.86	0.11	38,38,38,38	0
55	MG	2A	3112	1/1	0.86	1.11	32,32,32,32	0
55	MG	2A	3469	1/1	0.86	0.32	58,58,58,58	0
55	MG	1A	3804	1/1	0.86	0.48	26,26,26,26	0
55	MG	2A	3670	1/1	0.86	0.26	57,57,57,57	0
55	MG	1A	3789	1/1	0.86	0.09	42,42,42,42	0
55	MG	2A	3554	1/1	0.86	0.17	67,67,67,67	0
55	MG	1A	3566	1/1	0.86	0.11	52,52,52,52	0
55	MG	2A	3061	1/1	0.86	0.19	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3849	1/1	0.86	0.27	64,64,64,64	0
55	MG	1A	3864	1/1	0.86	0.56	51,51,51,51	0
55	MG	1A	3198	1/1	0.86	0.14	67,67,67,67	0
55	MG	1A	3073	1/1	0.86	0.22	36,36,36,36	0
55	MG	2A	3672	1/1	0.86	0.19	65,65,65,65	0
55	MG	1A	3258	1/1	0.86	0.21	38,38,38,38	0
55	MG	1a	1775	1/1	0.86	0.21	68,68,68,68	0
55	MG	1A	3580	1/1	0.86	0.32	26,26,26,26	0
55	MG	2a	1759	1/1	0.86	0.25	84,84,84,84	0
55	MG	2l	3002	1/1	0.86	0.19	70,70,70,70	0
55	MG	2A	3132	1/1	0.86	0.24	36,36,36,36	0
55	MG	1a	1674	1/1	0.86	0.26	68,68,68,68	0
55	MG	1A	3613	1/1	0.86	0.11	53,53,53,53	0
55	MG	2a	1694	1/1	0.86	0.20	53,53,53,53	0
55	MG	1A	3233	1/1	0.86	0.40	33,33,33,33	0
55	MG	2V	204	1/1	0.86	0.54	53,53,53,53	0
55	MG	2A	3510	1/1	0.86	0.12	43,43,43,43	0
55	MG	1a	1673	1/1	0.86	0.27	35,35,35,35	0
55	MG	2a	1673	1/1	0.86	0.20	61,61,61,61	0
55	MG	1a	1772	1/1	0.86	0.20	71,71,71,71	0
55	MG	2A	3519	1/1	0.86	0.15	51,51,51,51	0
55	MG	1A	3882	1/1	0.86	0.11	56,56,56,56	0
55	MG	2A	3861	1/1	0.86	0.16	50,50,50,50	0
55	MG	1A	3146	1/1	0.86	0.45	22,22,22,22	0
55	MG	1f	8001	1/1	0.86	0.36	68,68,68,68	0
55	MG	1A	3532	1/1	0.86	0.24	68,68,68,68	0
55	MG	2a	1808	1/1	0.86	0.29	76,76,76,76	0
55	MG	1A	3691	1/1	0.86	0.12	39,39,39,39	0
55	MG	1a	1677	1/1	0.86	0.36	102,102,102,102	0
55	MG	2A	3620	1/1	0.86	0.98	65,65,65,65	0
55	MG	2A	3083	1/1	0.86	1.06	35,35,35,35	0
55	MG	1A	3763	1/1	0.86	0.13	40,40,40,40	0
55	MG	2A	3320	1/1	0.86	0.10	72,72,72,72	0
55	MG	1A	3879	1/1	0.86	0.44	33,33,33,33	0
55	MG	1a	1629	1/1	0.86	0.58	51,51,51,51	0
55	MG	1A	3172	1/1	0.86	0.32	52,52,52,52	0
55	MG	1A	3634	1/1	0.86	0.14	34,34,34,34	0
55	MG	2A	3218	1/1	0.86	0.53	45,45,45,45	0
55	MG	1A	3733	1/1	0.86	0.11	37,37,37,37	0
55	MG	1a	1777	1/1	0.86	0.08	72,72,72,72	0
55	MG	2A	3251	1/1	0.86	0.28	60,60,60,60	0
55	MG	18	3301	1/1	0.86	0.54	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
55	MG	1A	3163	1/1	0.86	0.67	32,32,32,32	0
55	MG	1A	3148	1/1	0.86	0.38	38,38,38,38	0
55	MG	1D	315	1/1	0.86	0.18	68,68,68,68	0
55	MG	2A	3151	1/1	0.86	0.36	37,37,37,37	0
55	MG	2A	3097	1/1	0.87	0.68	69,69,69,69	0
55	MG	1A	3672	1/1	0.87	0.11	44,44,44,44	0
55	MG	1A	3132	1/1	0.87	0.24	22,22,22,22	0
55	MG	1a	1746	1/1	0.87	0.12	55,55,55,55	0
55	MG	1k	3001	1/1	0.87	0.13	53,53,53,53	0
55	MG	2a	1709	1/1	0.87	0.29	102,102,102,102	0
55	MG	2A	3011	1/1	0.87	0.28	54,54,54,54	0
55	MG	2A	3462	1/1	0.87	0.56	59,59,59,59	0
55	MG	2a	1681	1/1	0.87	0.18	54,54,54,54	0
55	MG	2A	3261	1/1	0.87	0.19	39,39,39,39	0
55	MG	1A	3182	1/1	0.87	0.28	24,24,24,24	0
55	MG	1U	204	1/1	0.87	0.59	22,22,22,22	0
55	MG	1A	3866	1/1	0.87	0.09	79,79,79,79	0
55	MG	2A	3441	1/1	0.87	0.10	87,87,87,87	0
55	MG	1A	3538	1/1	0.87	0.22	48,48,48,48	0
55	MG	2A	3032	1/1	0.87	1.01	51,51,51,51	0
55	MG	2A	3110	1/1	0.87	0.71	58,58,58,58	0
55	MG	1a	1671	1/1	0.87	0.21	49,49,49,49	0
55	MG	2A	3137	1/1	0.87	0.29	36,36,36,36	0
55	MG	2A	3201	1/1	0.87	0.20	71,71,71,71	0
55	MG	2z	102	1/1	0.87	0.28	78,78,78,78	0
55	MG	1A	3669	1/1	0.87	0.12	47,47,47,47	0
55	MG	1A	3467	1/1	0.87	0.11	23,23,23,23	0
55	MG	1a	1601	1/1	0.87	0.16	45,45,45,45	0
55	MG	2a	1606	1/1	0.87	0.11	53,53,53,53	0
55	MG	2A	3867	1/1	0.87	0.15	58,58,58,58	0
55	MG	2a	1634	1/1	0.87	0.30	59,59,59,59	0
55	MG	1A	3715	1/1	0.87	0.17	16,16,16,16	0
55	MG	1A	3636	1/1	0.87	0.54	40,40,40,40	0
55	MG	2A	3811	1/1	0.87	0.20	65,65,65,65	0
55	MG	1o	102	1/1	0.87	0.26	29,29,29,29	0
55	MG	1a	1675	1/1	0.87	0.27	25,25,25,25	0
55	MG	2A	3585	1/1	0.87	0.26	65,65,65,65	0
55	MG	2a	1810	1/1	0.87	0.10	105,105,105,105	0
55	MG	10	102	1/1	0.87	0.41	36,36,36,36	0
55	MG	2A	3548	1/1	0.87	0.24	69,69,69,69	0
55	MG	2A	3541	1/1	0.87	0.21	41,41,41,41	0
55	MG	1a	1630	1/1	0.87	0.30	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
55	MG	1A	3900	1/1	0.87	0.15	32,32,32,32	0
55	MG	1A	3010	1/1	0.87	0.58	32,32,32,32	0
55	MG	1A	3514	1/1	0.87	0.24	38,38,38,38	0
55	MG	1a	1715	1/1	0.87	0.14	58,58,58,58	0
55	MG	1A	3486	1/1	0.87	0.12	35,35,35,35	0
55	MG	1A	3501	1/1	0.87	0.26	31,31,31,31	0
55	MG	1A	3002	1/1	0.87	0.44	49,49,49,49	0
55	MG	2A	3212	1/1	0.87	0.51	51,51,51,51	0
55	MG	2A	3120	1/1	0.87	0.07	54,54,54,54	0
55	MG	1d	306	1/1	0.87	0.06	98,98,98,98	0
55	MG	1A	3166	1/1	0.87	0.22	33,33,33,33	0
55	MG	2A	3055	1/1	0.87	0.25	51,51,51,51	0
55	MG	1A	3651	1/1	0.87	0.10	37,37,37,37	0
55	MG	2A	3763	1/1	0.87	0.44	61,61,61,61	0
55	MG	1A	3041	1/1	0.87	0.14	26,26,26,26	0
55	MG	1A	3781	1/1	0.87	0.27	28,28,28,28	0
55	MG	2D	303	1/1	0.87	0.27	41,41,41,41	0
55	MG	1A	3144	1/1	0.87	0.31	29,29,29,29	0
55	MG	1A	3054	1/1	0.87	0.23	34,34,34,34	0
55	MG	1a	1826	1/1	0.87	0.22	53,53,53,53	0
55	MG	1A	3151	1/1	0.87	0.16	20,20,20,20	0
55	MG	1A	3938	1/1	0.87	0.89	21,21,21,21	0
55	MG	1A	3012	1/1	0.87	0.48	15,15,15,15	0
55	MG	1A	3027	1/1	0.87	0.23	46,46,46,46	0
55	MG	2A	3359	1/1	0.87	0.10	34,34,34,34	0
55	MG	1P	204	1/1	0.87	0.16	68,68,68,68	0
55	MG	2A	3257	1/1	0.87	0.20	47,47,47,47	0
55	MG	2A	3182	1/1	0.87	0.47	49,49,49,49	0
55	MG	2A	3370	1/1	0.87	0.24	76,76,76,76	0
55	MG	1A	3855	1/1	0.87	0.29	37,37,37,37	0
55	MG	2A	3817	1/1	0.88	0.08	66,66,66,66	0
55	MG	1A	3018	1/1	0.88	0.65	20,20,20,20	0
55	MG	2A	3566	1/1	0.88	0.27	26,26,26,26	0
55	MG	2a	1654	1/1	0.88	0.18	42,42,42,42	0
55	MG	2A	3184	1/1	0.88	0.64	42,42,42,42	0
55	MG	1A	3209	1/1	0.88	0.46	54,54,54,54	0
55	MG	1a	1656	1/1	0.88	0.21	71,71,71,71	0
55	MG	1A	3847	1/1	0.88	0.13	41,41,41,41	0
55	MG	1a	1801	1/1	0.88	0.19	69,69,69,69	0
55	MG	1A	3635	1/1	0.88	0.13	65,65,65,65	0
55	MG	1A	3497	1/1	0.88	0.36	37,37,37,37	0
55	MG	2A	3948	1/1	0.88	0.56	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
55	MG	1A	3145	1/1	0.88	1.16	24,24,24,24	0
55	MG	1A	3657	1/1	0.88	0.52	32,32,32,32	0
55	MG	1A	3230	1/1	0.88	0.61	36,36,36,36	0
55	MG	2A	3294	1/1	0.88	0.08	77,77,77,77	0
55	MG	1A	3556	1/1	0.88	0.89	34,34,34,34	0
55	MG	2R	201	1/1	0.88	0.95	48,48,48,48	0
55	MG	13	102	1/1	0.88	1.24	32,32,32,32	0
55	MG	2A	3560	1/1	0.88	0.39	85,85,85,85	0
55	MG	1a	1766	1/1	0.88	0.10	62,62,62,62	0
55	MG	1A	3599	1/1	0.88	0.16	34,34,34,34	0
55	MG	1A	3871	1/1	0.88	0.40	48,48,48,48	0
55	MG	1a	1611	1/1	0.88	0.25	48,48,48,48	0
55	MG	2A	3829	1/1	0.88	0.26	77,77,77,77	0
55	MG	1A	3515	1/1	0.88	0.36	49,49,49,49	0
55	MG	2A	3709	1/1	0.88	0.23	78,78,78,78	0
55	MG	1A	3743	1/1	0.88	0.62	19,19,19,19	0
55	MG	1A	3677	1/1	0.88	0.12	57,57,57,57	0
55	MG	2A	3531	1/1	0.88	0.07	51,51,51,51	0
55	MG	1A	3094	1/1	0.88	0.84	23,23,23,23	0
55	MG	2a	1782	1/1	0.88	0.16	79,79,79,79	0
55	MG	2a	1738	1/1	0.88	0.29	83,83,83,83	0
55	MG	2A	3635	1/1	0.88	0.06	54,54,54,54	0
55	MG	2A	3317	1/1	0.88	0.09	45,45,45,45	0
55	MG	2A	3126	1/1	0.88	0.26	71,71,71,71	0
55	MG	2a	1803	1/1	0.88	0.22	81,81,81,81	0
55	MG	1A	3534	1/1	0.88	0.14	14,14,14,14	0
55	MG	1A	3631	1/1	0.88	0.23	70,70,70,70	0
55	MG	2a	1785	1/1	0.88	0.09	77,77,77,77	0
55	MG	2a	1825	1/1	0.88	0.08	97,97,97,97	0
55	MG	1A	3668	1/1	0.88	0.09	43,43,43,43	0
55	MG	1A	3177	1/1	0.88	0.47	46,46,46,46	0
55	MG	2A	3535	1/1	0.88	0.16	50,50,50,50	0
55	MG	2a	1629	1/1	0.88	0.24	44,44,44,44	0
55	MG	1A	3727	1/1	0.88	0.18	39,39,39,39	0
55	MG	2A	3954	1/1	0.88	1.10	36,36,36,36	0
55	MG	2A	3195	1/1	0.88	0.51	42,42,42,42	0
55	MG	2A	3791	1/1	0.88	0.08	63,63,63,63	0
55	MG	2G	3003	1/1	0.88	0.11	66,66,66,66	0
55	MG	2U	205	1/1	0.88	0.55	49,49,49,49	0
55	MG	2a	1757	1/1	0.88	0.16	69,69,69,69	0
55	MG	2a	1778	1/1	0.88	0.20	63,63,63,63	0
55	MG	2A	3252	1/1	0.88	0.44	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	ZN	14	501	1/1	0.88	0.03	138,138,138,138	0
55	MG	2a	1662	1/1	0.88	0.73	90,90,90,90	0
55	MG	1A	3883	1/1	0.88	0.23	39,39,39,39	0
55	MG	2A	3539	1/1	0.88	0.12	20,20,20,20	0
55	MG	2F	311	1/1	0.88	0.41	72,72,72,72	0
55	MG	2A	3036	1/1	0.88	0.23	49,49,49,49	0
55	MG	1A	3570	1/1	0.88	0.29	24,24,24,24	0
55	MG	2a	1793	1/1	0.88	0.58	66,66,66,66	0
55	MG	1A	3609	1/1	0.88	0.35	63,63,63,63	0
55	MG	1A	3593	1/1	0.88	0.28	48,48,48,48	0
55	MG	1D	316	1/1	0.88	0.26	53,53,53,53	0
55	MG	2A	3168	1/1	0.88	0.79	38,38,38,38	0
55	MG	2A	3319	1/1	0.88	0.23	81,81,81,81	0
55	MG	1d	305	1/1	0.88	0.31	59,59,59,59	0
55	MG	1A	3800	1/1	0.88	0.11	48,48,48,48	0
55	MG	1A	3109	1/1	0.88	0.09	19,19,19,19	0
55	MG	1a	1618	1/1	0.88	0.51	89,89,89,89	0
55	MG	2A	3466	1/1	0.88	0.09	37,37,37,37	0
55	MG	2A	3501	1/1	0.88	0.24	41,41,41,41	0
55	MG	2A	3331	1/1	0.88	0.22	46,46,46,46	0
55	MG	2A	3563	1/1	0.88	1.03	46,46,46,46	0
55	MG	1A	3784	1/1	0.88	0.37	54,54,54,54	0
55	MG	2a	1713	1/1	0.88	0.12	78,78,78,78	0
55	MG	1A	3213	1/1	0.88	0.54	29,29,29,29	0
55	MG	2A	3304	1/1	0.88	0.21	51,51,51,51	0
55	MG	2a	1690	1/1	0.88	0.32	53,53,53,53	0
55	MG	1G	3001	1/1	0.89	0.12	96,96,96,96	0
55	MG	2A	3932	1/1	0.89	0.41	56,56,56,56	0
55	MG	2A	3958	1/1	0.89	0.21	59,59,59,59	0
55	MG	10	107	1/1	0.89	0.80	40,40,40,40	0
55	MG	1A	3126	1/1	0.89	0.49	47,47,47,47	0
55	MG	1A	3904	1/1	0.89	0.21	36,36,36,36	0
55	MG	2A	3714	1/1	0.89	0.23	50,50,50,50	0
55	MG	2a	1766	1/1	0.89	0.09	94,94,94,94	0
55	MG	2A	3156	1/1	0.89	1.00	47,47,47,47	0
55	MG	1A	3893	1/1	0.89	0.16	53,53,53,53	0
55	MG	1a	1757	1/1	0.89	0.14	83,83,83,83	0
55	MG	1A	3509	1/1	0.89	0.14	45,45,45,45	0
55	MG	1A	3190	1/1	0.89	0.53	36,36,36,36	0
55	MG	1A	3038	1/1	0.89	0.79	47,47,47,47	0
55	MG	2A	3527	1/1	0.89	0.29	28,28,28,28	0
55	MG	1a	1689	1/1	0.89	0.32	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
55	MG	1I	102	1/1	0.89	0.30	36,36,36,36	0
55	MG	2a	1836	1/1	0.89	0.31	46,46,46,46	0
55	MG	2A	3922	1/1	0.89	0.18	17,17,17,17	0
55	MG	1B	205	1/1	0.89	0.16	49,49,49,49	0
55	MG	2A	3967	1/1	0.89	0.76	48,48,48,48	0
55	MG	2W	3002	1/1	0.89	0.31	41,41,41,41	0
55	MG	1A	3575	1/1	0.89	0.18	43,43,43,43	0
55	MG	1A	3453	1/1	0.89	0.08	36,36,36,36	0
55	MG	2A	3806	1/1	0.89	1.59	54,54,54,54	0
55	MG	1A	3648	1/1	0.89	0.13	66,66,66,66	0
55	MG	2A	3457	1/1	0.89	0.28	55,55,55,55	0
55	MG	2A	3070	1/1	0.89	0.23	37,37,37,37	0
55	MG	1A	3579	1/1	0.89	0.12	49,49,49,49	0
55	MG	1A	3687	1/1	0.89	0.13	46,46,46,46	0
55	MG	2A	3336	1/1	0.89	0.39	57,57,57,57	0
55	MG	1A	3197	1/1	0.89	0.24	21,21,21,21	0
55	MG	2A	3856	1/1	0.89	0.45	47,47,47,47	0
55	MG	2a	1628	1/1	0.89	0.88	52,52,52,52	0
55	MG	2A	3669	1/1	0.89	0.47	31,31,31,31	0
55	MG	2A	3703	1/1	0.89	0.20	56,56,56,56	0
55	MG	2a	1765	1/1	0.89	0.38	35,35,35,35	0
55	MG	2A	3270	1/1	0.89	0.43	45,45,45,45	0
55	MG	1a	1690	1/1	0.89	0.23	65,65,65,65	0
55	MG	1A	3322	1/1	0.89	0.25	30,30,30,30	0
55	MG	1A	3104	1/1	0.89	0.79	26,26,26,26	0
55	MG	1D	303	1/1	0.89	0.73	27,27,27,27	0
55	MG	1A	3656	1/1	0.89	0.96	36,36,36,36	0
55	MG	2A	3860	1/1	0.89	0.19	58,58,58,58	0
55	MG	2a	1741	1/1	0.89	0.35	66,66,66,66	0
55	MG	2a	1801	1/1	0.89	0.16	86,86,86,86	0
55	MG	2A	3482	1/1	0.89	0.40	50,50,50,50	0
55	MG	1a	1682	1/1	0.89	0.20	56,56,56,56	0
55	MG	2A	3086	1/1	0.89	0.10	61,61,61,61	0
55	MG	1A	3860	1/1	0.89	0.07	54,54,54,54	0
55	MG	2A	3699	1/1	0.89	0.10	56,56,56,56	0
55	MG	2A	3970	1/1	0.89	0.49	54,54,54,54	0
55	MG	2A	3814	1/1	0.89	0.13	92,92,92,92	0
55	MG	2R	202	1/1	0.89	0.26	43,43,43,43	0
55	MG	1A	3140	1/1	0.89	0.93	32,32,32,32	0
55	MG	1A	3195	1/1	0.89	0.19	34,34,34,34	0
55	MG	1A	3242	1/1	0.89	0.23	40,40,40,40	0
55	MG	2A	3892	1/1	0.89	0.30	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
55	MG	2A	3743	1/1	0.89	0.27	55,55,55,55	0
55	MG	1A	3754	1/1	0.89	0.33	16,16,16,16	0
55	MG	2D	317	1/1	0.89	0.68	61,61,61,61	0
55	MG	1A	3934	1/1	0.89	0.27	67,67,67,67	0
55	MG	1B	228	1/1	0.89	0.16	53,53,53,53	0
55	MG	1A	3752	1/1	0.89	0.30	29,29,29,29	0
55	MG	2A	3069	1/1	0.89	0.61	36,36,36,36	0
55	MG	2A	3372	1/1	0.89	0.40	56,56,56,56	0
55	MG	1A	3586	1/1	0.89	0.64	9,9,9,9	0
55	MG	2A	3124	1/1	0.89	0.75	48,48,48,48	0
55	MG	19	104	1/1	0.89	0.17	58,58,58,58	0
55	MG	2A	3683	1/1	0.89	0.14	57,57,57,57	0
55	MG	1a	1755	1/1	0.89	0.23	76,76,76,76	0
55	MG	1a	1844	1/1	0.89	0.09	70,70,70,70	0
55	MG	1a	1708	1/1	0.89	0.23	63,63,63,63	0
55	MG	1A	3732	1/1	0.89	0.04	91,91,91,91	0
55	MG	1a	1648	1/1	0.89	0.14	44,44,44,44	0
55	MG	1A	3950	1/1	0.89	0.60	10,10,10,10	0
55	MG	2a	1787	1/1	0.89	0.39	66,66,66,66	0
55	MG	1A	3077	1/1	0.89	0.24	51,51,51,51	0
55	MG	1a	1650	1/1	0.89	0.27	59,59,59,59	0
55	MG	1a	1686	1/1	0.89	0.24	33,33,33,33	0
55	MG	2A	3081	1/1	0.89	0.25	40,40,40,40	0
55	MG	1a	1663	1/1	0.89	0.38	86,86,86,86	0
55	MG	2A	3258	1/1	0.89	0.73	63,63,63,63	0
55	MG	1A	3229	1/1	0.89	0.14	42,42,42,42	0
55	MG	1A	3488	1/1	0.89	0.23	54,54,54,54	0
55	MG	2A	3395	1/1	0.89	0.11	22,22,22,22	0
55	MG	2a	1626	1/1	0.89	0.10	53,53,53,53	0
55	MG	1A	3266	1/1	0.89	0.47	29,29,29,29	0
55	MG	2A	3564	1/1	0.89	0.83	42,42,42,42	0
55	MG	1A	3034	1/1	0.89	0.26	18,18,18,18	0
55	MG	2a	1675	1/1	0.89	0.20	44,44,44,44	0
55	MG	2A	3316	1/1	0.89	0.22	32,32,32,32	0
55	MG	1a	1642	1/1	0.89	0.20	89,89,89,89	0
55	MG	2a	1732	1/1	0.89	0.62	78,78,78,78	0
55	MG	2a	1611	1/1	0.89	0.76	48,48,48,48	0
55	MG	2A	3621	1/1	0.89	0.22	62,62,62,62	0
55	MG	1A	3544	1/1	0.89	0.17	51,51,51,51	0
55	MG	1A	3731	1/1	0.90	0.10	60,60,60,60	0
55	MG	1A	3149	1/1	0.90	0.41	15,15,15,15	0
55	MG	2D	304	1/1	0.90	0.28	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3120	1/1	0.90	0.26	26,26,26,26	0
55	MG	1A	3196	1/1	0.90	0.54	23,23,23,23	0
55	MG	2A	3093	1/1	0.90	0.19	37,37,37,37	0
55	MG	1A	3564	1/1	0.90	0.35	25,25,25,25	0
55	MG	2A	3533	1/1	0.90	0.13	65,65,65,65	0
55	MG	2U	201	1/1	0.90	0.72	55,55,55,55	0
55	MG	2A	3528	1/1	0.90	0.13	62,62,62,62	0
55	MG	2a	1788	1/1	0.90	0.18	86,86,86,86	0
55	MG	1a	1794	1/1	0.90	0.27	45,45,45,45	0
55	MG	1A	3330	1/1	0.90	0.41	57,57,57,57	0
55	MG	1A	3456	1/1	0.90	0.13	55,55,55,55	0
55	MG	1A	3506	1/1	0.90	0.19	44,44,44,44	0
55	MG	1a	1813	1/1	0.90	0.14	76,76,76,76	0
55	MG	1l	3002	1/1	0.90	0.25	62,62,62,62	0
55	MG	2A	3402	1/1	0.90	0.16	47,47,47,47	0
55	MG	1a	1658	1/1	0.90	1.30	41,41,41,41	0
55	MG	1a	1795	1/1	0.90	0.17	66,66,66,66	0
55	MG	2A	3534	1/1	0.90	0.78	43,43,43,43	0
55	MG	2a	1813	1/1	0.90	0.07	72,72,72,72	0
55	MG	1A	3071	1/1	0.90	0.29	26,26,26,26	0
55	MG	2A	3732	1/1	0.90	0.24	95,95,95,95	0
55	MG	1a	1685	1/1	0.90	0.62	55,55,55,55	0
55	MG	2a	1637	1/1	0.90	0.13	47,47,47,47	0
55	MG	2A	3682	1/1	0.90	0.10	49,49,49,49	0
55	MG	1a	1731	1/1	0.90	0.16	59,59,59,59	0
55	MG	2a	1641	1/1	0.90	0.29	95,95,95,95	0
55	MG	2A	3656	1/1	0.90	0.08	62,62,62,62	0
55	MG	2A	3108	1/1	0.90	0.85	50,50,50,50	0
55	MG	1A	3639	1/1	0.90	0.30	33,33,33,33	0
55	MG	1D	317	1/1	0.90	0.34	38,38,38,38	0
55	MG	1A	3031	1/1	0.90	0.30	22,22,22,22	0
55	MG	1a	1734	1/1	0.90	0.19	61,61,61,61	0
55	MG	2A	3741	1/1	0.90	0.26	45,45,45,45	0
55	MG	2A	3019	1/1	0.90	0.57	40,40,40,40	0
55	MG	2a	1799	1/1	0.90	0.15	46,46,46,46	0
55	MG	1a	1662	1/1	0.90	0.24	72,72,72,72	0
55	MG	2a	1804	1/1	0.90	0.07	88,88,88,88	0
55	MG	1A	3214	1/1	0.90	0.56	22,22,22,22	0
55	MG	2A	3705	1/1	0.90	0.26	54,54,54,54	0
55	MG	2A	3397	1/1	0.90	0.49	49,49,49,49	0
55	MG	2A	3747	1/1	0.90	0.31	43,43,43,43	0
55	MG	2A	3447	1/1	0.90	0.13	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3592	1/1	0.90	0.41	23,23,23,23	0
55	MG	2A	3827	1/1	0.90	0.11	48,48,48,48	0
55	MG	1A	3774	1/1	0.90	0.57	54,54,54,54	0
55	MG	2A	3750	1/1	0.90	0.19	75,75,75,75	0
55	MG	2A	3837	1/1	0.90	0.13	42,42,42,42	0
55	MG	2A	3636	1/1	0.90	0.34	67,67,67,67	0
55	MG	1A	3374	1/1	0.90	0.09	21,21,21,21	0
55	MG	1A	3051	1/1	0.90	0.36	18,18,18,18	0
55	MG	2A	3924	1/1	0.90	0.78	43,43,43,43	0
55	MG	2A	3834	1/1	0.90	0.28	26,26,26,26	0
55	MG	2A	3012	1/1	0.90	0.53	34,34,34,34	0
55	MG	1A	3504	1/1	0.90	0.10	32,32,32,32	0
55	MG	1V	201	1/1	0.90	0.27	16,16,16,16	0
55	MG	2A	3659	1/1	0.90	1.06	45,45,45,45	0
55	MG	2a	1689	1/1	0.90	0.25	63,63,63,63	0
55	MG	1A	3257	1/1	0.90	0.77	54,54,54,54	0
55	MG	1B	219	1/1	0.90	0.09	51,51,51,51	0
55	MG	1A	3910	1/1	0.90	0.50	44,44,44,44	0
55	MG	1A	3091	1/1	0.90	0.52	18,18,18,18	0
55	MG	1A	3102	1/1	0.90	0.77	39,39,39,39	0
55	MG	2A	3037	1/1	0.90	0.25	39,39,39,39	0
55	MG	2A	3745	1/1	0.90	0.61	48,48,48,48	0
55	MG	2A	3243	1/1	0.90	0.85	28,28,28,28	0
55	MG	2a	1802	1/1	0.90	0.18	95,95,95,95	0
55	MG	2A	3342	1/1	0.90	0.20	45,45,45,45	0
55	MG	1a	1840	1/1	0.90	0.23	81,81,81,81	0
55	MG	1a	1724	1/1	0.90	0.45	70,70,70,70	0
55	MG	2A	3512	1/1	0.90	0.10	50,50,50,50	0
55	MG	2A	3729	1/1	0.90	0.12	66,66,66,66	0
55	MG	1g	3001	1/1	0.90	0.24	35,35,35,35	0
55	MG	2A	3026	1/1	0.90	0.63	36,36,36,36	0
55	MG	2A	3803	1/1	0.90	0.10	83,83,83,83	0
55	MG	2A	3374	1/1	0.90	0.17	30,30,30,30	0
55	MG	1A	3716	1/1	0.90	0.34	23,23,23,23	0
55	MG	2A	3766	1/1	0.90	0.05	74,74,74,74	0
55	MG	2A	3663	1/1	0.90	0.16	25,25,25,25	0
55	MG	1A	3103	1/1	0.90	0.32	29,29,29,29	0
55	MG	2A	3921	1/1	0.90	0.64	40,40,40,40	0
55	MG	1A	3749	1/1	0.90	0.16	61,61,61,61	0
55	MG	1A	3083	1/1	0.90	1.79	33,33,33,33	0
55	MG	1A	3461	1/1	0.90	0.07	32,32,32,32	0
55	MG	2A	3643	1/1	0.90	1.04	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
55	MG	15	102	1/1	0.90	0.37	33,33,33,33	0
55	MG	2A	3471	1/1	0.90	0.14	61,61,61,61	0
55	MG	2A	3507	1/1	0.90	0.17	38,38,38,38	0
55	MG	2A	3569	1/1	0.90	0.76	46,46,46,46	0
55	MG	2a	1774	1/1	0.90	0.23	81,81,81,81	0
55	MG	2X	102	1/1	0.90	0.20	66,66,66,66	0
55	MG	1A	3840	1/1	0.90	0.28	36,36,36,36	0
55	MG	2a	1795	1/1	0.90	0.34	53,53,53,53	0
55	MG	2A	3749	1/1	0.90	0.38	56,56,56,56	0
55	MG	2A	3572	1/1	0.90	0.09	67,67,67,67	0
55	MG	27	102	1/1	0.90	0.11	48,48,48,48	0
55	MG	2A	3180	1/1	0.90	0.34	51,51,51,51	0
55	MG	1D	304	1/1	0.90	0.52	34,34,34,34	0
55	MG	2A	3651	1/1	0.90	0.21	47,47,47,47	0
55	MG	1A	3561	1/1	0.90	0.58	18,18,18,18	0
55	MG	1a	1743	1/1	0.90	0.31	58,58,58,58	0
55	MG	2A	3774	1/1	0.90	0.12	49,49,49,49	0
55	MG	1A	3680	1/1	0.90	0.21	27,27,27,27	0
55	MG	2A	3298	1/1	0.90	0.11	59,59,59,59	0
55	MG	1a	1730	1/1	0.90	0.35	48,48,48,48	0
55	MG	1B	209	1/1	0.90	0.16	41,41,41,41	0
55	MG	1a	1621	1/1	0.90	0.24	38,38,38,38	0
55	MG	2A	3472	1/1	0.90	0.13	68,68,68,68	0
55	MG	2A	3488	1/1	0.90	0.13	64,64,64,64	0
55	MG	2A	3768	1/1	0.90	0.14	42,42,42,42	0
55	MG	2A	3731	1/1	0.91	0.23	65,65,65,65	0
55	MG	1A	3384	1/1	0.91	0.12	46,46,46,46	0
55	MG	2A	3581	1/1	0.91	0.11	55,55,55,55	0
55	MG	2A	3642	1/1	0.91	0.21	53,53,53,53	0
55	MG	2A	3377	1/1	0.91	0.08	36,36,36,36	0
55	MG	2A	3912	1/1	0.91	0.91	38,38,38,38	0
55	MG	2A	3738	1/1	0.91	0.10	60,60,60,60	0
55	MG	1A	3413	1/1	0.91	0.22	39,39,39,39	0
55	MG	1A	3317	1/1	0.91	0.18	13,13,13,13	0
55	MG	1A	3756	1/1	0.91	0.12	14,14,14,14	0
55	MG	2A	3799	1/1	0.91	0.60	72,72,72,72	0
55	MG	1A	3777	1/1	0.91	0.14	57,57,57,57	0
55	MG	1A	3243	1/1	0.91	0.19	34,34,34,34	0
55	MG	2a	1728	1/1	0.91	0.20	79,79,79,79	0
55	MG	1a	1634	1/1	0.91	0.21	38,38,38,38	0
55	MG	2A	3593	1/1	0.91	0.39	37,37,37,37	0
55	MG	2B	3019	1/1	0.91	0.07	63,63,63,63	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3318	1/1	0.91	0.45	32,32,32,32	0
55	MG	1A	3877	1/1	0.91	0.15	61,61,61,61	0
55	MG	2A	3392	1/1	0.91	0.22	41,41,41,41	0
55	MG	2A	3649	1/1	0.91	0.17	26,26,26,26	0
55	MG	1A	3135	1/1	0.91	0.28	22,22,22,22	0
55	MG	2l	3001	1/1	0.91	0.08	45,45,45,45	0
55	MG	1a	1805	1/1	0.91	0.21	66,66,66,66	0
55	MG	2a	1761	1/1	0.91	0.12	77,77,77,77	0
55	MG	1A	3858	1/1	0.91	0.12	51,51,51,51	0
55	MG	2A	3692	1/1	0.91	0.12	46,46,46,46	0
55	MG	2A	3175	1/1	0.91	0.24	42,42,42,42	0
55	MG	2A	3034	1/1	0.91	0.30	40,40,40,40	0
55	MG	2A	3334	1/1	0.91	0.18	47,47,47,47	0
55	MG	1a	1782	1/1	0.91	0.38	68,68,68,68	0
55	MG	1A	3389	1/1	0.91	0.10	8,8,8,8	0
55	MG	2A	3590	1/1	0.91	0.89	43,43,43,43	0
55	MG	1a	1773	1/1	0.91	0.28	43,43,43,43	0
55	MG	1A	3398	1/1	0.91	0.29	55,55,55,55	0
55	MG	2A	3039	1/1	0.91	0.10	45,45,45,45	0
55	MG	2A	3804	1/1	0.91	0.06	54,54,54,54	0
55	MG	1e	3001	1/1	0.91	0.15	36,36,36,36	0
55	MG	1A	3862	1/1	0.91	0.67	42,42,42,42	0
55	MG	1X	101	1/1	0.91	0.42	32,32,32,32	0
55	MG	1a	1797	1/1	0.91	0.16	72,72,72,72	0
55	MG	1a	1711	1/1	0.91	0.19	72,72,72,72	0
55	MG	1h	8001	1/1	0.91	0.13	64,64,64,64	0
55	MG	1A	3110	1/1	0.91	0.26	40,40,40,40	0
55	MG	2a	1703	1/1	0.91	0.20	60,60,60,60	0
55	MG	2D	313	1/1	0.91	0.43	34,34,34,34	0
55	MG	1A	3249	1/1	0.91	0.22	24,24,24,24	0
55	MG	1A	3037	1/1	0.91	0.60	30,30,30,30	0
55	MG	2A	3900	1/1	0.91	0.23	69,69,69,69	0
55	MG	2U	203	1/1	0.91	0.17	42,42,42,42	0
55	MG	2a	1781	1/1	0.91	0.09	73,73,73,73	0
55	MG	1A	3911	1/1	0.91	0.19	61,61,61,61	0
55	MG	2A	3625	1/1	0.91	0.16	66,66,66,66	0
55	MG	2A	3719	1/1	0.91	0.10	25,25,25,25	0
55	MG	1A	3228	1/1	0.91	0.18	37,37,37,37	0
55	MG	2a	1763	1/1	0.91	0.21	73,73,73,73	0
55	MG	2a	1630	1/1	0.91	0.11	56,56,56,56	0
55	MG	2A	3562	1/1	0.91	0.70	39,39,39,39	0
55	MG	2A	3160	1/1	0.91	0.20	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3552	1/1	0.91	0.21	12,12,12,12	0
55	MG	2a	1835	1/1	0.91	0.45	87,87,87,87	0
55	MG	1A	3902	1/1	0.91	0.24	55,55,55,55	0
55	MG	2A	3498	1/1	0.91	0.16	38,38,38,38	0
55	MG	2A	3493	1/1	0.91	0.11	53,53,53,53	0
55	MG	1A	3072	1/1	0.91	0.34	37,37,37,37	0
55	MG	1A	3719	1/1	0.91	0.31	22,22,22,22	0
55	MG	1A	3321	1/1	0.91	0.14	17,17,17,17	0
55	MG	1A	3706	1/1	0.91	0.19	20,20,20,20	0
55	MG	2A	3272	1/1	0.91	0.47	54,54,54,54	0
55	MG	2a	1700	1/1	0.91	0.31	68,68,68,68	0
55	MG	1A	3728	1/1	0.91	0.37	61,61,61,61	0
55	MG	2A	3571	1/1	0.91	0.17	50,50,50,50	0
55	MG	2A	3295	1/1	0.91	0.38	32,32,32,32	0
55	MG	2A	3831	1/1	0.91	0.20	64,64,64,64	0
55	MG	1a	1720	1/1	0.91	0.24	79,79,79,79	0
55	MG	2a	1739	1/1	0.91	1.65	82,82,82,82	0
55	MG	1A	3392	1/1	0.91	0.15	50,50,50,50	0
55	MG	1a	1717	1/1	0.91	0.19	49,49,49,49	0
55	MG	2A	3325	1/1	0.91	0.20	76,76,76,76	0
55	MG	1A	3477	1/1	0.91	0.18	8,8,8,8	0
55	MG	1A	3793	1/1	0.91	1.02	36,36,36,36	0
55	MG	2a	1771	1/1	0.91	0.07	83,83,83,83	0
55	MG	2A	3020	1/1	0.91	0.51	43,43,43,43	0
55	MG	1a	1820	1/1	0.91	0.24	65,65,65,65	0
55	MG	1A	3444	1/1	0.91	0.59	32,32,32,32	0
55	MG	1W	3002	1/1	0.91	0.24	27,27,27,27	0
55	MG	2A	3509	1/1	0.91	0.13	63,63,63,63	0
55	MG	2B	3024	1/1	0.91	0.23	62,62,62,62	0
55	MG	2A	3959	1/1	0.91	1.02	44,44,44,44	0
55	MG	1A	3292	1/1	0.91	0.15	40,40,40,40	0
55	MG	2A	3964	1/1	0.91	0.29	42,42,42,42	0
55	MG	2a	1623	1/1	0.91	0.61	41,41,41,41	0
55	MG	1D	307	1/1	0.91	0.78	24,24,24,24	0
55	MG	2a	1659	1/1	0.91	0.41	74,74,74,74	0
55	MG	1A	3007	1/1	0.91	0.15	26,26,26,26	0
55	MG	2D	307	1/1	0.91	0.79	41,41,41,41	0
55	MG	1a	1732	1/1	0.91	0.24	75,75,75,75	0
55	MG	1A	3772	1/1	0.91	0.14	41,41,41,41	0
55	MG	2A	3393	1/1	0.91	0.10	74,74,74,74	0
55	MG	2A	3324	1/1	0.91	0.19	28,28,28,28	0
55	MG	1A	3905	1/1	0.91	0.17	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
55	MG	1A	3143	1/1	0.91	0.20	29,29,29,29	0
55	MG	2A	3491	1/1	0.91	0.21	38,38,38,38	0
55	MG	2A	3303	1/1	0.91	0.19	55,55,55,55	0
55	MG	1a	1610	1/1	0.91	0.55	33,33,33,33	0
55	MG	2A	3706	1/1	0.91	0.18	70,70,70,70	0
55	MG	1A	3244	1/1	0.91	0.32	30,30,30,30	0
55	MG	1F	314	1/1	0.91	0.25	47,47,47,47	0
55	MG	2W	3001	1/1	0.91	0.19	27,27,27,27	0
55	MG	2A	3660	1/1	0.91	0.74	59,59,59,59	0
55	MG	2A	3273	1/1	0.91	0.47	50,50,50,50	0
55	MG	2a	1839	1/1	0.91	0.16	62,62,62,62	0
55	MG	1a	1774	1/1	0.91	0.42	66,66,66,66	0
55	MG	2A	3119	1/1	0.91	0.27	35,35,35,35	0
55	MG	2A	3483	1/1	0.91	0.12	36,36,36,36	0
55	MG	2A	3241	1/1	0.91	0.13	72,72,72,72	0
55	MG	1A	3622	1/1	0.91	0.10	57,57,57,57	0
55	MG	1A	3881	1/1	0.91	0.06	57,57,57,57	0
55	MG	2A	3523	1/1	0.91	0.41	38,38,38,38	0
55	MG	2A	3348	1/1	0.91	0.07	56,56,56,56	0
55	MG	2A	3788	1/1	0.91	0.11	94,94,94,94	0
55	MG	1A	3237	1/1	0.91	0.20	23,23,23,23	0
55	MG	2Q	203	1/1	0.91	0.90	51,51,51,51	0
55	MG	2a	1727	1/1	0.91	0.15	62,62,62,62	0
55	MG	2A	3558	1/1	0.91	0.23	15,15,15,15	0
55	MG	2A	3191	1/1	0.91	0.44	45,45,45,45	0
55	MG	1A	3472	1/1	0.91	0.06	28,28,28,28	0
55	MG	2A	3866	1/1	0.91	0.38	49,49,49,49	0
55	MG	2a	1744	1/1	0.91	0.27	72,72,72,72	0
55	MG	2A	3937	1/1	0.91	0.18	40,40,40,40	0
55	MG	1A	3240	1/1	0.91	0.76	17,17,17,17	0
55	MG	1U	202	1/1	0.91	0.50	27,27,27,27	0
55	MG	2A	3908	1/1	0.91	0.16	56,56,56,56	0
55	MG	1A	3543	1/1	0.91	0.13	52,52,52,52	0
55	MG	1A	3760	1/1	0.91	0.19	51,51,51,51	0
55	MG	2A	3549	1/1	0.91	0.20	65,65,65,65	0
55	MG	2a	1618	1/1	0.91	0.35	96,96,96,96	0
55	MG	1F	302	1/1	0.91	0.40	29,29,29,29	0
55	MG	2A	3396	1/1	0.91	0.17	49,49,49,49	0
55	MG	1A	3142	1/1	0.91	0.28	44,44,44,44	0
55	MG	1A	3903	1/1	0.91	0.19	36,36,36,36	0
55	MG	2A	3052	1/1	0.91	0.70	47,47,47,47	0
55	MG	2A	3612	1/1	0.91	0.53	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	1723	1/1	0.91	0.33	55,55,55,55	0
55	MG	2a	1746	1/1	0.92	0.10	87,87,87,87	0
55	MG	2A	3405	1/1	0.92	0.17	51,51,51,51	0
55	MG	2A	3897	1/1	0.92	0.14	52,52,52,52	0
55	MG	2A	3966	1/1	0.92	0.42	46,46,46,46	0
55	MG	2A	3158	1/1	0.92	0.15	37,37,37,37	0
55	MG	2A	3592	1/1	0.92	0.82	43,43,43,43	0
55	MG	1A	3798	1/1	0.92	0.23	60,60,60,60	0
55	MG	2a	1734	1/1	0.92	0.15	79,79,79,79	0
55	MG	2A	3538	1/1	0.92	0.21	52,52,52,52	0
55	MG	1A	3457	1/1	0.92	0.14	41,41,41,41	0
55	MG	1A	3058	1/1	0.92	0.08	49,49,49,49	0
55	MG	1A	3901	1/1	0.92	0.12	29,29,29,29	0
55	MG	1a	1834	1/1	0.92	0.33	60,60,60,60	0
55	MG	2A	3059	1/1	0.92	0.06	67,67,67,67	0
55	MG	10	103	1/1	0.92	0.34	45,45,45,45	0
55	MG	2A	3494	1/1	0.92	0.20	34,34,34,34	0
55	MG	2A	3687	1/1	0.92	0.12	80,80,80,80	0
55	MG	1a	1780	1/1	0.92	0.10	45,45,45,45	0
55	MG	1a	1742	1/1	0.92	0.26	60,60,60,60	0
55	MG	2A	3048	1/1	0.92	0.50	68,68,68,68	0
55	MG	2A	3862	1/1	0.92	0.08	63,63,63,63	0
55	MG	1A	3605	1/1	0.92	0.50	44,44,44,44	0
55	MG	1A	3909	1/1	0.92	0.12	58,58,58,58	0
55	MG	2A	3704	1/1	0.92	0.13	69,69,69,69	0
55	MG	2A	3057	1/1	0.92	0.16	24,24,24,24	0
55	MG	1A	3476	1/1	0.92	0.14	41,41,41,41	0
55	MG	2A	3133	1/1	0.92	0.20	28,28,28,28	0
55	MG	1a	1627	1/1	0.92	0.10	46,46,46,46	0
55	MG	1A	3615	1/1	0.92	0.20	52,52,52,52	0
55	MG	1A	3301	1/1	0.92	0.11	32,32,32,32	0
55	MG	1A	3857	1/1	0.92	0.21	52,52,52,52	0
55	MG	2A	3949	1/1	0.92	1.10	37,37,37,37	0
55	MG	2A	3102	1/1	0.92	0.37	45,45,45,45	0
55	MG	2a	1720	1/1	0.92	0.29	60,60,60,60	0
55	MG	1a	1705	1/1	0.92	0.12	48,48,48,48	0
55	MG	2A	3794	1/1	0.92	0.13	46,46,46,46	0
55	MG	2A	3634	1/1	0.92	0.06	68,68,68,68	0
55	MG	1A	3364	1/1	0.92	0.13	54,54,54,54	0
55	MG	2A	3611	1/1	0.92	0.24	47,47,47,47	0
55	MG	2A	3815	1/1	0.92	0.20	47,47,47,47	0
55	MG	2A	3865	1/1	0.92	0.11	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
55	MG	1A	3341	1/1	0.92	0.11	29,29,29,29	0
55	MG	1A	3270	1/1	0.92	1.52	43,43,43,43	0
55	MG	2A	3956	1/1	0.92	0.62	34,34,34,34	0
55	MG	2A	3526	1/1	0.92	0.22	60,60,60,60	0
55	MG	2A	3889	1/1	0.92	0.14	57,57,57,57	0
55	MG	1a	1736	1/1	0.92	0.16	42,42,42,42	0
55	MG	2A	3942	1/1	0.92	0.20	30,30,30,30	0
55	MG	2A	3613	1/1	0.92	0.12	33,33,33,33	0
55	MG	2A	3858	1/1	0.92	0.50	51,51,51,51	0
55	MG	1A	3405	1/1	0.92	0.13	51,51,51,51	0
55	MG	1a	1790	1/1	0.92	0.10	76,76,76,76	0
55	MG	1A	3053	1/1	0.92	0.81	18,18,18,18	0
55	MG	2a	1614	1/1	0.92	0.15	32,32,32,32	0
55	MG	1a	1636	1/1	0.92	0.31	62,62,62,62	0
55	MG	1A	3640	1/1	0.92	0.55	35,35,35,35	0
55	MG	1A	3512	1/1	0.92	0.34	59,59,59,59	0
55	MG	2A	3205	1/1	0.92	0.67	42,42,42,42	0
55	MG	1A	3159	1/1	0.92	0.60	16,16,16,16	0
55	MG	2A	3661	1/1	0.92	0.75	37,37,37,37	0
55	MG	1A	3607	1/1	0.92	0.14	16,16,16,16	0
55	MG	2a	1789	1/1	0.92	0.65	51,51,51,51	0
55	MG	1A	3951	1/1	0.92	0.37	50,50,50,50	0
55	MG	1A	3078	1/1	0.92	0.88	30,30,30,30	0
55	MG	1A	3872	1/1	0.92	0.45	86,86,86,86	0
55	MG	1a	1688	1/1	0.92	0.12	68,68,68,68	0
55	MG	1A	3612	1/1	0.92	0.10	50,50,50,50	0
55	MG	1a	1768	1/1	0.92	0.19	75,75,75,75	0
55	MG	1D	312	1/1	0.92	0.29	24,24,24,24	0
55	MG	1A	3026	1/1	0.92	0.65	22,22,22,22	0
55	MG	1a	1716	1/1	0.92	0.05	71,71,71,71	0
55	MG	2A	3544	1/1	0.92	0.11	29,29,29,29	0
55	MG	2a	1776	1/1	0.92	0.31	60,60,60,60	0
55	MG	1A	3090	1/1	0.92	0.28	22,22,22,22	0
55	MG	2A	3165	1/1	0.92	0.09	55,55,55,55	0
55	MG	2o	102	1/1	0.92	0.20	38,38,38,38	0
55	MG	1A	3435	1/1	0.92	0.06	47,47,47,47	0
55	MG	2Q	201	1/1	0.92	0.08	79,79,79,79	0
55	MG	1A	3176	1/1	0.92	0.54	20,20,20,20	0
55	MG	1A	3451	1/1	0.92	0.26	48,48,48,48	0
55	MG	1A	3039	1/1	0.92	0.11	35,35,35,35	0
55	MG	1A	3004	1/1	0.92	0.20	29,29,29,29	0
55	MG	1A	3070	1/1	0.92	0.47	24,24,24,24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3023	1/1	0.92	0.62	33,33,33,33	0
55	MG	1Y	502	1/1	0.92	0.14	90,90,90,90	0
55	MG	1A	3498	1/1	0.92	0.30	46,46,46,46	0
55	MG	2a	1701	1/1	0.92	0.27	84,84,84,84	0
55	MG	1A	3505	1/1	0.92	0.26	48,48,48,48	0
55	MG	2A	3497	1/1	0.92	0.30	31,31,31,31	0
55	MG	2A	3565	1/1	0.92	0.61	33,33,33,33	0
55	MG	1A	3490	1/1	0.92	0.23	17,17,17,17	0
55	MG	2A	3740	1/1	0.92	0.26	86,86,86,86	0
55	MG	2A	3458	1/1	0.92	0.10	46,46,46,46	0
55	MG	1A	3519	1/1	0.92	0.32	27,27,27,27	0
55	MG	2A	3474	1/1	0.92	0.07	38,38,38,38	0
55	MG	2A	3415	1/1	0.92	0.32	46,46,46,46	0
55	MG	1A	3443	1/1	0.92	0.07	45,45,45,45	0
55	MG	2A	3639	1/1	0.92	0.27	36,36,36,36	0
55	MG	1A	3262	1/1	0.92	0.34	44,44,44,44	0
55	MG	1G	3003	1/1	0.92	0.08	43,43,43,43	0
55	MG	2E	302	1/1	0.92	0.08	31,31,31,31	0
55	MG	1a	1721	1/1	0.92	0.16	49,49,49,49	0
55	MG	1A	3314	1/1	0.92	0.09	43,43,43,43	0
55	MG	2F	301	1/1	0.92	0.23	47,47,47,47	0
55	MG	1A	3236	1/1	0.92	0.28	22,22,22,22	0
55	MG	2A	3746	1/1	0.92	0.29	63,63,63,63	0
55	MG	2F	305	1/1	0.92	0.36	45,45,45,45	0
55	MG	2A	3077	1/1	0.92	0.29	47,47,47,47	0
55	MG	2A	3333	1/1	0.92	0.13	40,40,40,40	0
55	MG	2A	3223	1/1	0.92	0.33	48,48,48,48	0
55	MG	2A	3141	1/1	0.92	0.23	35,35,35,35	0
55	MG	1a	1655	1/1	0.92	0.16	35,35,35,35	0
55	MG	2a	1756	1/1	0.92	0.12	67,67,67,67	0
55	MG	2a	1699	1/1	0.92	0.12	53,53,53,53	0
55	MG	1A	3568	1/1	0.92	0.08	19,19,19,19	0
55	MG	2A	3769	1/1	0.92	0.08	62,62,62,62	0
55	MG	1A	3876	1/1	0.92	0.13	19,19,19,19	0
55	MG	1o	101	1/1	0.92	0.28	42,42,42,42	0
55	MG	2A	3903	1/1	0.92	0.16	58,58,58,58	0
55	MG	2A	3013	1/1	0.92	0.21	31,31,31,31	0
55	MG	1A	3655	1/1	0.92	0.51	41,41,41,41	0
55	MG	2a	1829	1/1	0.92	0.12	64,64,64,64	0
55	MG	2A	3818	1/1	0.92	0.19	50,50,50,50	0
55	MG	1A	3834	1/1	0.92	0.06	60,60,60,60	0
55	MG	2A	3739	1/1	0.92	0.15	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3153	1/1	0.92	0.12	52,52,52,52	0
55	MG	1A	3268	1/1	0.92	0.13	32,32,32,32	0
55	MG	2A	3406	1/1	0.92	0.19	45,45,45,45	0
55	MG	2A	3150	1/1	0.92	1.25	34,34,34,34	0
55	MG	1A	3817	1/1	0.92	0.51	35,35,35,35	0
55	MG	1B	226	1/1	0.92	0.07	49,49,49,49	0
55	MG	2a	1740	1/1	0.92	0.37	71,71,71,71	0
55	MG	1A	3385	1/1	0.92	0.18	47,47,47,47	0
55	MG	1F	307	1/1	0.92	0.67	25,25,25,25	0
55	MG	2A	3761	1/1	0.92	0.15	58,58,58,58	0
55	MG	2A	3698	1/1	0.92	0.07	44,44,44,44	0
55	MG	2b	3001	1/1	0.92	0.13	68,68,68,68	0
55	MG	2A	3103	1/1	0.92	0.25	40,40,40,40	0
55	MG	1A	3863	1/1	0.92	0.18	66,66,66,66	0
55	MG	2A	3064	1/1	0.92	0.19	36,36,36,36	0
55	MG	1A	3617	1/1	0.92	0.16	54,54,54,54	0
55	MG	2A	3955	1/1	0.92	0.25	46,46,46,46	0
55	MG	2A	3684	1/1	0.92	0.23	61,61,61,61	0
55	MG	2a	1800	1/1	0.92	0.30	68,68,68,68	0
55	MG	2A	3713	1/1	0.92	0.25	34,34,34,34	0
55	MG	1A	3591	1/1	0.93	0.32	60,60,60,60	0
55	MG	1B	224	1/1	0.93	0.14	63,63,63,63	0
55	MG	2U	202	1/1	0.93	0.78	39,39,39,39	0
55	MG	1A	3761	1/1	0.93	0.45	30,30,30,30	0
55	MG	2a	1780	1/1	0.93	0.14	93,93,93,93	0
55	MG	1A	3252	1/1	0.93	2.05	41,41,41,41	0
55	MG	2A	3149	1/1	0.93	1.04	43,43,43,43	0
55	MG	2A	3550	1/1	0.93	0.14	53,53,53,53	0
55	MG	2A	3322	1/1	0.93	0.10	62,62,62,62	0
55	MG	2A	3192	1/1	0.93	0.86	44,44,44,44	0
55	MG	2D	311	1/1	0.93	0.39	24,24,24,24	0
55	MG	2A	3390	1/1	0.93	0.19	41,41,41,41	0
55	MG	1A	3459	1/1	0.93	0.14	8,8,8,8	0
55	MG	2a	1794	1/1	0.93	0.04	92,92,92,92	0
55	MG	1A	3692	1/1	0.93	0.14	29,29,29,29	0
55	MG	1A	3036	1/1	0.93	0.10	56,56,56,56	0
55	MG	2a	1772	1/1	0.93	0.07	57,57,57,57	0
55	MG	1E	302	1/1	0.93	0.63	18,18,18,18	0
55	MG	1a	1836	1/1	0.93	0.13	53,53,53,53	0
55	MG	1a	1612	1/1	0.93	0.20	60,60,60,60	0
55	MG	1A	3106	1/1	0.93	0.28	27,27,27,27	0
55	MG	2a	1706	1/1	0.93	0.11	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2P	201	1/1	0.93	0.62	31,31,31,31	0
55	MG	1A	3920	1/1	0.93	0.75	33,33,33,33	0
55	MG	2A	3388	1/1	0.93	0.21	56,56,56,56	0
55	MG	2a	1775	1/1	0.93	0.07	54,54,54,54	0
55	MG	1E	305	1/1	0.93	0.14	25,25,25,25	0
55	MG	1A	3867	1/1	0.93	0.31	48,48,48,48	0
55	MG	1A	3475	1/1	0.93	0.34	37,37,37,37	0
55	MG	2A	3308	1/1	0.93	0.15	36,36,36,36	0
55	MG	1A	3945	1/1	0.93	0.24	22,22,22,22	0
55	MG	1a	1792	1/1	0.93	0.24	60,60,60,60	0
55	MG	1A	3610	1/1	0.93	0.70	30,30,30,30	0
55	MG	2A	3920	1/1	0.93	0.52	54,54,54,54	0
55	MG	1A	3275	1/1	0.93	0.16	11,11,11,11	0
55	MG	2A	3047	1/1	0.93	0.19	39,39,39,39	0
55	MG	1G	3002	1/1	0.93	0.08	49,49,49,49	0
55	MG	2a	1840	1/1	0.93	0.09	59,59,59,59	0
55	MG	1a	1739	1/1	0.93	0.18	67,67,67,67	0
55	MG	2A	3503	1/1	0.93	0.23	62,62,62,62	0
55	MG	2A	3696	1/1	0.93	0.13	48,48,48,48	0
55	MG	1A	3064	1/1	0.93	0.22	20,20,20,20	0
55	MG	1A	3005	1/1	0.93	0.18	20,20,20,20	0
55	MG	1a	1843	1/1	0.93	0.23	57,57,57,57	0
55	MG	2A	3685	1/1	0.93	0.15	56,56,56,56	0
55	MG	1a	1619	1/1	0.93	0.17	52,52,52,52	0
55	MG	2a	1642	1/1	0.93	0.33	80,80,80,80	0
55	MG	2A	3118	1/1	0.93	0.30	44,44,44,44	0
55	MG	2a	1705	1/1	0.93	0.76	63,63,63,63	0
55	MG	2A	3432	1/1	0.93	0.11	38,38,38,38	0
55	MG	1a	1752	1/1	0.93	0.21	86,86,86,86	0
55	MG	1A	3598	1/1	0.93	0.22	61,61,61,61	0
55	MG	2A	3733	1/1	0.93	0.25	62,62,62,62	0
55	MG	2A	3268	1/1	0.93	0.22	55,55,55,55	0
55	MG	1D	309	1/1	0.93	0.43	27,27,27,27	0
55	MG	15	106	1/1	0.93	0.11	50,50,50,50	0
55	MG	1A	3558	1/1	0.93	0.82	19,19,19,19	0
55	MG	1A	3419	1/1	0.93	0.22	39,39,39,39	0
55	MG	1A	3739	1/1	0.93	0.09	49,49,49,49	0
55	MG	2A	3913	1/1	0.93	0.14	55,55,55,55	0
55	MG	1A	3137	1/1	0.93	0.22	33,33,33,33	0
55	MG	1F	310	1/1	0.93	0.12	18,18,18,18	0
55	MG	2A	3042	1/1	0.93	0.46	29,29,29,29	0
55	MG	1A	3020	1/1	0.93	0.36	22,22,22,22	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3871	1/1	0.93	0.63	39,39,39,39	0
55	MG	1a	1646	1/1	0.93	0.59	47,47,47,47	0
55	MG	18	3302	1/1	0.93	0.77	24,24,24,24	0
55	MG	2A	3449	1/1	0.93	0.10	50,50,50,50	0
55	MG	1A	3751	1/1	0.93	0.51	21,21,21,21	0
55	MG	1a	1749	1/1	0.93	0.22	68,68,68,68	0
55	MG	2A	3091	1/1	0.93	0.79	38,38,38,38	0
55	MG	2A	3114	1/1	0.93	0.16	43,43,43,43	0
55	MG	2a	1685	1/1	0.93	0.09	47,47,47,47	0
55	MG	1A	3815	1/1	0.93	0.06	57,57,57,57	0
55	MG	1a	1613	1/1	0.93	0.15	26,26,26,26	0
55	MG	2A	3484	1/1	0.93	0.12	25,25,25,25	0
55	MG	2A	3087	1/1	0.93	0.46	43,43,43,43	0
55	MG	2A	3062	1/1	0.93	0.34	40,40,40,40	0
55	MG	2A	3247	1/1	0.93	0.53	48,48,48,48	0
55	MG	1A	3956	1/1	0.93	0.54	21,21,21,21	0
55	MG	2A	3587	1/1	0.93	0.19	38,38,38,38	0
55	MG	2A	3880	1/1	0.93	0.10	58,58,58,58	0
55	MG	1A	3713	1/1	0.93	0.20	22,22,22,22	0
55	MG	2A	3280	1/1	0.93	0.10	33,33,33,33	0
55	MG	2A	3525	1/1	0.93	0.35	33,33,33,33	0
55	MG	1a	1697	1/1	0.93	0.12	53,53,53,53	0
55	MG	2A	3173	1/1	0.93	0.12	69,69,69,69	0
55	MG	1A	3434	1/1	0.93	0.13	20,20,20,20	0
55	MG	1a	1603	1/1	0.93	0.23	49,49,49,49	0
55	MG	2A	3823	1/1	0.93	0.06	60,60,60,60	0
55	MG	2A	3221	1/1	0.93	0.33	30,30,30,30	0
55	MG	2N	203	1/1	0.93	0.50	90,90,90,90	0
55	MG	2a	1682	1/1	0.93	0.46	73,73,73,73	0
55	MG	2a	1753	1/1	0.93	0.23	102,102,102,102	0
55	MG	1A	3596	1/1	0.93	0.13	46,46,46,46	0
55	MG	2A	3825	1/1	0.93	0.12	67,67,67,67	0
55	MG	1A	3826	1/1	0.93	0.07	60,60,60,60	0
55	MG	2A	3870	1/1	0.93	0.26	48,48,48,48	0
55	MG	1A	3814	1/1	0.93	0.16	41,41,41,41	0
55	MG	2a	1790	1/1	0.93	0.11	57,57,57,57	0
55	MG	1A	3335	1/1	0.93	0.40	36,36,36,36	0
55	MG	1R	203	1/1	0.93	0.21	31,31,31,31	0
55	MG	2A	3664	1/1	0.93	0.21	51,51,51,51	0
55	MG	2A	3181	1/1	0.93	0.63	36,36,36,36	0
55	MG	2A	3188	1/1	0.93	0.33	39,39,39,39	0
55	MG	2a	1645	1/1	0.93	0.45	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3890	1/1	0.93	0.21	21,21,21,21	0
55	MG	2A	3723	1/1	0.93	0.55	65,65,65,65	0
55	MG	1A	3671	1/1	0.93	0.13	42,42,42,42	0
55	MG	2H	8002	1/1	0.93	1.36	90,90,90,90	0
55	MG	2a	1786	1/1	0.93	0.30	52,52,52,52	0
55	MG	1A	3539	1/1	0.93	0.08	17,17,17,17	0
55	MG	1A	3513	1/1	0.93	0.16	46,46,46,46	0
55	MG	2A	3203	1/1	0.93	0.20	36,36,36,36	0
55	MG	1U	205	1/1	0.93	0.31	22,22,22,22	0
55	MG	1a	1760	1/1	0.93	0.16	76,76,76,76	0
55	MG	2a	1603	1/1	0.93	0.09	93,93,93,93	0
55	MG	2A	3171	1/1	0.93	0.25	40,40,40,40	0
55	MG	1a	1691	1/1	0.93	0.21	59,59,59,59	0
55	MG	2A	3440	1/1	0.93	0.25	27,27,27,27	0
55	MG	1a	1804	1/1	0.93	0.15	52,52,52,52	0
55	MG	2A	3066	1/1	0.93	0.77	46,46,46,46	0
55	MG	1H	202	1/1	0.93	0.14	51,51,51,51	0
55	MG	1A	3380	1/1	0.93	0.10	23,23,23,23	0
55	MG	1A	3766	1/1	0.93	0.17	24,24,24,24	0
55	MG	1a	1660	1/1	0.93	0.31	57,57,57,57	0
55	MG	2A	3376	1/1	0.93	0.12	58,58,58,58	0
55	MG	1A	3164	1/1	0.93	0.30	23,23,23,23	0
55	MG	1a	1776	1/1	0.93	0.07	66,66,66,66	0
55	MG	2A	3384	1/1	0.93	0.17	35,35,35,35	0
55	MG	2A	3629	1/1	0.93	0.29	48,48,48,48	0
55	MG	1A	3947	1/1	0.93	0.55	24,24,24,24	0
55	MG	1A	3658	1/1	0.93	0.08	27,27,27,27	0
55	MG	1a	1652	1/1	0.93	0.40	41,41,41,41	0
55	MG	1a	1702	1/1	0.93	0.08	46,46,46,46	0
55	MG	1A	3445	1/1	0.93	0.24	19,19,19,19	0
55	MG	2A	3882	1/1	0.93	0.72	64,64,64,64	0
55	MG	1A	3129	1/1	0.93	0.20	17,17,17,17	0
55	MG	2A	3893	1/1	0.93	1.02	55,55,55,55	0
55	MG	1D	314	1/1	0.93	0.29	42,42,42,42	0
55	MG	2a	1714	1/1	0.93	0.21	55,55,55,55	0
55	MG	2A	3681	1/1	0.93	0.26	82,82,82,82	0
55	MG	2A	3717	1/1	0.93	0.20	43,43,43,43	0
55	MG	2A	3702	1/1	0.93	0.37	50,50,50,50	0
55	MG	2a	1718	1/1	0.93	0.11	38,38,38,38	0
55	MG	2a	1812	1/1	0.93	0.11	69,69,69,69	0
55	MG	1a	1620	1/1	0.93	0.14	77,77,77,77	0
55	MG	2A	3410	1/1	0.93	0.08	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1F	313	1/1	0.93	0.20	4,4,4,4	0
55	MG	2A	3718	1/1	0.93	0.20	44,44,44,44	0
55	MG	1A	3191	1/1	0.93	0.45	31,31,31,31	0
55	MG	2A	3065	1/1	0.93	0.17	12,12,12,12	0
55	MG	2A	3617	1/1	0.93	0.13	59,59,59,59	0
55	MG	1A	3358	1/1	0.93	0.10	33,33,33,33	0
55	MG	2A	3050	1/1	0.93	0.88	48,48,48,48	0
55	MG	1A	3626	1/1	0.93	0.12	68,68,68,68	0
55	MG	2a	1745	1/1	0.93	0.09	70,70,70,70	0
55	MG	2A	3773	1/1	0.93	0.10	46,46,46,46	0
55	MG	2A	3246	1/1	0.93	0.36	56,56,56,56	0
55	MG	1a	1783	1/1	0.93	0.09	60,60,60,60	0
55	MG	1A	3709	1/1	0.93	0.10	31,31,31,31	0
55	MG	1A	3888	1/1	0.93	0.13	60,60,60,60	0
55	MG	2A	3423	1/1	0.93	0.11	49,49,49,49	0
55	MG	2A	3344	1/1	0.93	0.12	49,49,49,49	0
55	MG	2a	1762	1/1	0.93	0.13	71,71,71,71	0
55	MG	1A	3585	1/1	0.93	0.20	29,29,29,29	0
55	MG	1A	3015	1/1	0.93	0.52	33,33,33,33	0
55	MG	2A	3894	1/1	0.93	0.31	38,38,38,38	0
55	MG	25	102	1/1	0.94	0.25	41,41,41,41	0
55	MG	15	103	1/1	0.94	0.18	19,19,19,19	0
55	MG	1A	3115	1/1	0.94	0.14	23,23,23,23	0
55	MG	1A	3700	1/1	0.94	0.11	48,48,48,48	0
55	MG	1A	3464	1/1	0.94	0.12	38,38,38,38	0
55	MG	2A	3935	1/1	0.94	0.44	49,49,49,49	0
55	MG	15	101	1/1	0.94	0.76	19,19,19,19	0
55	MG	1A	3698	1/1	0.94	0.12	25,25,25,25	0
55	MG	1A	3294	1/1	0.94	0.13	22,22,22,22	0
55	MG	1a	1623	1/1	0.94	0.13	63,63,63,63	0
55	MG	2A	3274	1/1	0.94	1.04	51,51,51,51	0
55	MG	1D	306	1/1	0.94	0.12	17,17,17,17	0
55	MG	2a	1683	1/1	0.94	0.76	48,48,48,48	0
55	MG	2A	3906	1/1	0.94	0.28	79,79,79,79	0
55	MG	2D	309	1/1	0.94	0.70	47,47,47,47	0
55	MG	2A	3820	1/1	0.94	0.10	36,36,36,36	0
55	MG	1A	3397	1/1	0.94	0.19	77,77,77,77	0
55	MG	2A	3873	1/1	0.94	0.16	80,80,80,80	0
55	MG	2A	3691	1/1	0.94	0.10	49,49,49,49	0
55	MG	2A	3277	1/1	0.94	0.46	39,39,39,39	0
55	MG	2A	3113	1/1	0.94	0.17	35,35,35,35	0
55	MG	1A	3695	1/1	0.94	0.13	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
55	MG	10	104	1/1	0.94	0.07	34,34,34,34	0
55	MG	2a	1798	1/1	0.94	0.11	46,46,46,46	0
55	MG	1a	1831	1/1	0.94	0.33	66,66,66,66	0
55	MG	1A	3921	1/1	0.94	0.19	35,35,35,35	0
55	MG	2A	3389	1/1	0.94	0.18	25,25,25,25	0
55	MG	1A	3537	1/1	0.94	0.43	54,54,54,54	0
55	MG	1A	3548	1/1	0.94	0.12	27,27,27,27	0
55	MG	2a	1723	1/1	0.94	0.07	73,73,73,73	0
55	MG	2A	3963	1/1	0.94	0.18	64,64,64,64	0
55	MG	1A	3702	1/1	0.94	0.14	43,43,43,43	0
55	MG	1A	3489	1/1	0.94	0.14	23,23,23,23	0
55	MG	1A	3799	1/1	0.94	0.09	35,35,35,35	0
55	MG	2A	3122	1/1	0.94	0.07	44,44,44,44	0
55	MG	1A	3063	1/1	0.94	0.19	41,41,41,41	0
55	MG	2A	3522	1/1	0.94	0.14	32,32,32,32	0
55	MG	1A	3125	1/1	0.94	0.76	26,26,26,26	0
55	MG	1A	3710	1/1	0.94	0.15	36,36,36,36	0
55	MG	2A	3425	1/1	0.94	0.07	32,32,32,32	0
55	MG	1A	3371	1/1	0.94	0.06	17,17,17,17	0
55	MG	2A	3071	1/1	0.94	0.27	43,43,43,43	0
55	MG	2A	3131	1/1	0.94	0.14	44,44,44,44	0
55	MG	1A	3118	1/1	0.94	0.09	35,35,35,35	0
55	MG	1a	1616	1/1	0.94	0.54	75,75,75,75	0
55	MG	2A	3343	1/1	0.94	0.15	39,39,39,39	0
55	MG	2A	3269	1/1	0.94	0.39	51,51,51,51	0
55	MG	2a	1602	1/1	0.94	0.13	60,60,60,60	0
55	MG	2A	3864	1/1	0.94	0.42	47,47,47,47	0
55	MG	28	102	1/1	0.94	0.08	60,60,60,60	0
55	MG	2A	3017	1/1	0.94	0.66	36,36,36,36	0
55	MG	1a	1713	1/1	0.94	0.15	36,36,36,36	0
55	MG	2a	1805	1/1	0.94	0.30	66,66,66,66	0
55	MG	2E	301	1/1	0.94	0.18	63,63,63,63	0
55	MG	2A	3437	1/1	0.94	0.10	44,44,44,44	0
55	MG	11	104	1/1	0.94	0.18	24,24,24,24	0
55	MG	2A	3403	1/1	0.94	0.11	68,68,68,68	0
55	MG	1A	3734	1/1	0.94	0.07	26,26,26,26	0
55	MG	1W	3003	1/1	0.94	0.33	21,21,21,21	0
55	MG	2a	1773	1/1	0.94	0.18	84,84,84,84	0
55	MG	1W	3001	1/1	0.94	0.20	14,14,14,14	0
55	MG	1A	3065	1/1	0.94	0.35	11,11,11,11	0
55	MG	2A	3589	1/1	0.94	0.47	43,43,43,43	0
55	MG	1B	220	1/1	0.94	0.06	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3929	1/1	0.94	0.18	25,25,25,25	0
55	MG	2a	1647	1/1	0.94	0.27	67,67,67,67	0
55	MG	2A	3965	1/1	0.94	0.51	42,42,42,42	0
55	MG	1A	3560	1/1	0.94	0.21	34,34,34,34	0
55	MG	1a	1745	1/1	0.94	0.28	61,61,61,61	0
55	MG	1A	3030	1/1	0.94	0.26	10,10,10,10	0
55	MG	1A	3664	1/1	0.94	0.21	31,31,31,31	0
55	MG	2A	3197	1/1	0.94	0.17	52,52,52,52	0
55	MG	1A	3368	1/1	0.94	0.13	13,13,13,13	0
55	MG	2A	3901	1/1	0.94	0.35	54,54,54,54	0
55	MG	1A	3092	1/1	0.94	0.21	11,11,11,11	0
55	MG	1a	1706	1/1	0.94	0.20	44,44,44,44	0
55	MG	1A	3843	1/1	0.94	0.91	25,25,25,25	0
55	MG	2a	1770	1/1	0.94	0.13	72,72,72,72	0
55	MG	2A	3213	1/1	0.94	0.54	37,37,37,37	0
56	ZN	2n	101	1/1	0.94	0.07	96,96,96,96	0
55	MG	1A	3891	1/1	0.94	0.21	34,34,34,34	0
55	MG	2A	3674	1/1	0.94	0.24	55,55,55,55	0
55	MG	1A	3280	1/1	0.94	0.14	13,13,13,13	0
55	MG	1A	3221	1/1	0.94	0.40	34,34,34,34	0
55	MG	2A	3186	1/1	0.94	0.84	50,50,50,50	0
55	MG	2A	3812	1/1	0.94	0.06	53,53,53,53	0
55	MG	2A	3606	1/1	0.94	0.71	66,66,66,66	0
55	MG	2A	3925	1/1	0.94	0.50	24,24,24,24	0
55	MG	1F	306	1/1	0.94	0.53	26,26,26,26	0
55	MG	1A	3742	1/1	0.94	0.07	77,77,77,77	0
55	MG	2A	3121	1/1	0.94	0.16	60,60,60,60	0
55	MG	1A	3678	1/1	0.94	0.10	32,32,32,32	0
55	MG	2A	3876	1/1	0.94	0.27	38,38,38,38	0
55	MG	1a	1815	1/1	0.94	0.09	93,93,93,93	0
55	MG	2a	1791	1/1	0.94	0.09	47,47,47,47	0
55	MG	2a	1814	1/1	0.94	0.05	66,66,66,66	0
55	MG	2A	3284	1/1	0.94	0.08	79,79,79,79	0
55	MG	2A	3255	1/1	0.94	0.22	35,35,35,35	0
55	MG	1A	3955	1/1	0.94	0.19	19,19,19,19	0
55	MG	1A	3344	1/1	0.94	0.10	21,21,21,21	0
55	MG	2A	3854	1/1	0.94	0.18	35,35,35,35	0
55	MG	1A	3665	1/1	0.94	0.43	23,23,23,23	0
55	MG	1A	3047	1/1	0.94	0.14	31,31,31,31	0
55	MG	2F	309	1/1	0.94	0.74	42,42,42,42	0
55	MG	1A	3865	1/1	0.94	0.14	48,48,48,48	0
55	MG	1A	3082	1/1	0.94	0.96	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3923	1/1	0.94	0.11	26,26,26,26	0
55	MG	2E	303	1/1	0.94	1.14	37,37,37,37	0
55	MG	2V	203	1/1	0.94	0.52	58,58,58,58	0
55	MG	2a	1657	1/1	0.94	0.67	46,46,46,46	0
55	MG	1A	3551	1/1	0.94	0.21	47,47,47,47	0
55	MG	2A	3145	1/1	0.94	0.12	42,42,42,42	0
55	MG	1A	3188	1/1	0.94	0.24	33,33,33,33	0
55	MG	2a	1726	1/1	0.94	0.51	46,46,46,46	0
55	MG	1A	3128	1/1	0.94	0.20	22,22,22,22	0
55	MG	1A	3520	1/1	0.94	0.15	35,35,35,35	0
55	MG	1A	3720	1/1	0.94	0.14	40,40,40,40	0
55	MG	1A	3426	1/1	0.94	0.10	15,15,15,15	0
55	MG	2a	1730	1/1	0.94	0.16	81,81,81,81	0
55	MG	1A	3075	1/1	0.94	0.57	21,21,21,21	0
55	MG	2a	1680	1/1	0.94	0.13	82,82,82,82	0
55	MG	1a	1808	1/1	0.94	0.18	67,67,67,67	0
55	MG	2A	3576	1/1	0.94	0.22	25,25,25,25	0
55	MG	1A	3557	1/1	0.94	0.95	32,32,32,32	0
55	MG	1a	1624	1/1	0.94	0.44	49,49,49,49	0
55	MG	1A	3156	1/1	0.94	0.21	20,20,20,20	0
55	MG	2a	1632	1/1	0.94	0.08	55,55,55,55	0
55	MG	2A	3847	1/1	0.94	0.12	52,52,52,52	0
55	MG	1A	3285	1/1	0.94	0.20	12,12,12,12	0
55	MG	2A	3832	1/1	0.94	0.98	39,39,39,39	0
55	MG	1A	3367	1/1	0.94	0.11	24,24,24,24	0
55	MG	1a	1667	1/1	0.94	0.41	63,63,63,63	0
55	MG	2A	3074	1/1	0.94	0.44	46,46,46,46	0
55	MG	2A	3506	1/1	0.94	0.13	55,55,55,55	0
55	MG	2A	3356	1/1	0.94	0.14	29,29,29,29	0
55	MG	2A	3957	1/1	0.94	0.11	61,61,61,61	0
55	MG	2A	3448	1/1	0.94	0.09	41,41,41,41	0
55	MG	1A	3436	1/1	0.94	0.15	11,11,11,11	0
55	MG	2d	503	1/1	0.94	0.34	77,77,77,77	0
55	MG	2a	1610	1/1	0.94	0.20	79,79,79,79	0
55	MG	1A	3663	1/1	0.94	0.12	77,77,77,77	0
55	MG	2A	3652	1/1	0.94	0.15	40,40,40,40	0
55	MG	2a	1688	1/1	0.94	0.29	71,71,71,71	0
55	MG	2A	3730	1/1	0.94	0.35	43,43,43,43	0
55	MG	2A	3933	1/1	0.94	0.19	36,36,36,36	0
55	MG	1A	3328	1/1	0.94	0.12	45,45,45,45	0
55	MG	1A	3823	1/1	0.94	0.09	60,60,60,60	0
55	MG	1A	3169	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( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3830	1/1	0.94	0.12	71,71,71,71	0
55	MG	2A	3249	1/1	0.94	0.14	67,67,67,67	0
55	MG	2A	3365	1/1	0.94	0.18	72,72,72,72	0
55	MG	2A	3968	1/1	0.94	1.08	34,34,34,34	0
55	MG	1A	3383	1/1	0.94	0.20	13,13,13,13	0
55	MG	2A	3193	1/1	0.94	0.32	45,45,45,45	0
55	MG	2A	3537	1/1	0.94	0.21	65,65,65,65	0
55	MG	1F	301	1/1	0.94	0.21	17,17,17,17	0
55	MG	1A	3536	1/1	0.94	0.15	40,40,40,40	0
55	MG	2A	3645	1/1	0.94	0.28	33,33,33,33	0
55	MG	2A	3214	1/1	0.94	0.58	32,32,32,32	0
55	MG	1a	1802	1/1	0.94	0.07	67,67,67,67	0
55	MG	2A	3789	1/1	0.94	0.11	41,41,41,41	0
55	MG	1A	3267	1/1	0.94	0.18	20,20,20,20	0
55	MG	2A	3198	1/1	0.94	0.25	49,49,49,49	0
55	MG	2A	3883	1/1	0.94	0.23	71,71,71,71	0
55	MG	1A	3112	1/1	0.94	0.35	46,46,46,46	0
55	MG	2A	3225	1/1	0.94	0.18	30,30,30,30	0
55	MG	1A	3583	1/1	0.94	0.16	21,21,21,21	0
55	MG	1A	3853	1/1	0.94	0.07	47,47,47,47	0
55	MG	2A	3909	1/1	0.94	0.06	58,58,58,58	0
55	MG	1A	3725	1/1	0.94	0.19	29,29,29,29	0
55	MG	1A	3503	1/1	0.94	0.10	60,60,60,60	0
55	MG	1A	3563	1/1	0.94	0.47	28,28,28,28	0
55	MG	2A	3668	1/1	0.94	0.34	44,44,44,44	0
55	MG	2A	3477	1/1	0.94	0.29	32,32,32,32	0
55	MG	1A	3770	1/1	0.94	0.06	45,45,45,45	0
55	MG	1A	3099	1/1	0.94	0.32	29,29,29,29	0
55	MG	2A	3092	1/1	0.94	0.38	47,47,47,47	0
55	MG	2A	3454	1/1	0.94	0.12	38,38,38,38	0
55	MG	1D	301	1/1	0.94	0.18	21,21,21,21	0
55	MG	2A	3254	1/1	0.94	0.49	74,74,74,74	0
55	MG	1A	3162	1/1	0.94	0.15	45,45,45,45	0
55	MG	2A	3869	1/1	0.94	0.09	50,50,50,50	0
55	MG	2A	3570	1/1	0.94	0.51	53,53,53,53	0
55	MG	2A	3381	1/1	0.94	0.34	47,47,47,47	0
55	MG	1a	1796	1/1	0.94	0.17	57,57,57,57	0
55	MG	1B	225	1/1	0.94	0.19	36,36,36,36	0
55	MG	2a	1679	1/1	0.94	0.67	27,27,27,27	0
55	MG	1A	3055	1/1	0.94	0.24	36,36,36,36	0
55	MG	1A	3484	1/1	0.94	0.18	38,38,38,38	0
55	MG	1V	202	1/1	0.94	0.44	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
55	MG	1A	3686	1/1	0.94	0.10	22,22,22,22	0
55	MG	2A	3843	1/1	0.94	0.10	38,38,38,38	0
55	MG	1A	3141	1/1	0.94	0.12	36,36,36,36	0
55	MG	1A	3415	1/1	0.94	0.07	49,49,49,49	0
55	MG	1a	1649	1/1	0.94	0.28	47,47,47,47	0
55	MG	1A	3108	1/1	0.94	0.94	24,24,24,24	0
55	MG	1a	1714	1/1	0.94	0.06	49,49,49,49	0
55	MG	2A	3204	1/1	0.94	0.49	31,31,31,31	0
55	MG	2A	3561	1/1	0.94	0.58	55,55,55,55	0
55	MG	1A	3446	1/1	0.94	0.07	76,76,76,76	0
55	MG	2A	3757	1/1	0.94	0.23	60,60,60,60	0
55	MG	2B	3013	1/1	0.94	0.07	66,66,66,66	0
55	MG	2A	3756	1/1	0.94	0.55	49,49,49,49	0
55	MG	1A	3059	1/1	0.94	0.12	51,51,51,51	0
55	MG	2A	3918	1/1	0.94	0.26	70,70,70,70	0
55	MG	1a	1694	1/1	0.94	0.32	48,48,48,48	0
55	MG	1A	3139	1/1	0.94	0.36	33,33,33,33	0
55	MG	1A	3329	1/1	0.94	0.08	67,67,67,67	0
55	MG	1A	3482	1/1	0.94	0.18	37,37,37,37	0
55	MG	1A	3522	1/1	0.94	0.14	71,71,71,71	0
55	MG	1A	3747	1/1	0.94	0.20	27,27,27,27	0
55	MG	1A	3154	1/1	0.94	0.83	41,41,41,41	0
55	MG	1A	3069	1/1	0.94	0.48	17,17,17,17	0
55	MG	1A	3521	1/1	0.94	0.31	19,19,19,19	0
55	MG	1A	3848	1/1	0.94	0.17	63,63,63,63	0
55	MG	1A	3349	1/1	0.94	0.12	31,31,31,31	0
55	MG	1a	1769	1/1	0.94	0.27	62,62,62,62	0
55	MG	2a	1769	1/1	0.94	0.40	83,83,83,83	0
55	MG	1A	3390	1/1	0.94	0.11	36,36,36,36	0
55	MG	1a	1651	1/1	0.94	0.16	43,43,43,43	0
55	MG	1A	3150	1/1	0.94	0.12	41,41,41,41	0
55	MG	2A	3286	1/1	0.94	0.13	61,61,61,61	0
55	MG	2A	3444	1/1	0.94	0.11	36,36,36,36	0
55	MG	2A	3936	1/1	0.94	0.21	35,35,35,35	0
55	MG	18	3303	1/1	0.94	0.07	56,56,56,56	0
55	MG	1A	3288	1/1	0.94	0.38	7,7,7,7	0
55	MG	1A	3679	1/1	0.94	0.17	36,36,36,36	0
55	MG	2A	3962	1/1	0.94	0.33	32,32,32,32	0
55	MG	1a	1818	1/1	0.94	0.14	72,72,72,72	0
55	MG	2A	3101	1/1	0.94	0.45	36,36,36,36	0
55	MG	2A	3839	1/1	0.94	0.09	28,28,28,28	0
55	MG	2A	3638	1/1	0.94	0.07	51,51,51,51	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3201	1/1	0.94	0.24	29,29,29,29	0
55	MG	1A	3748	1/1	0.94	0.13	49,49,49,49	0
55	MG	1A	3511	1/1	0.94	0.22	46,46,46,46	0
55	MG	2A	3836	1/1	0.94	0.13	79,79,79,79	0
55	MG	2A	3725	1/1	0.95	0.15	40,40,40,40	0
55	MG	2A	3801	1/1	0.95	0.13	57,57,57,57	0
55	MG	2A	3552	1/1	0.95	0.75	40,40,40,40	0
55	MG	1A	3479	1/1	0.95	0.09	39,39,39,39	0
55	MG	1A	3738	1/1	0.95	0.12	19,19,19,19	0
55	MG	1A	3828	1/1	0.95	0.12	52,52,52,52	0
55	MG	1A	3736	1/1	0.95	0.18	33,33,33,33	0
55	MG	1A	3131	1/1	0.95	0.30	19,19,19,19	0
55	MG	1A	3886	1/1	0.95	0.08	38,38,38,38	0
55	MG	1a	1617	1/1	0.95	0.19	93,93,93,93	0
55	MG	2a	1604	1/1	0.95	0.14	81,81,81,81	0
55	MG	1A	3016	1/1	0.95	0.73	15,15,15,15	0
55	MG	2A	3517	1/1	0.95	0.16	48,48,48,48	0
55	MG	1A	3753	1/1	0.95	0.35	49,49,49,49	0
55	MG	2F	303	1/1	0.95	0.88	40,40,40,40	0
55	MG	2A	3728	1/1	0.95	0.12	37,37,37,37	0
55	MG	1A	3439	1/1	0.95	0.05	49,49,49,49	0
55	MG	1A	3943	1/1	0.95	0.93	34,34,34,34	0
55	MG	2A	3339	1/1	0.95	0.09	34,34,34,34	0
55	MG	2A	3848	1/1	0.95	0.16	40,40,40,40	0
55	MG	1a	1781	1/1	0.95	0.21	63,63,63,63	0
55	MG	2a	1792	1/1	0.95	0.14	56,56,56,56	0
55	MG	1A	3954	1/1	0.95	0.33	21,21,21,21	0
55	MG	2a	1797	1/1	0.95	0.10	75,75,75,75	0
55	MG	1a	1678	1/1	0.95	0.05	46,46,46,46	0
55	MG	1a	1654	1/1	0.95	0.39	46,46,46,46	0
55	MG	2A	3707	1/1	0.95	0.11	26,26,26,26	0
55	MG	2a	1698	1/1	0.95	0.06	75,75,75,75	0
55	MG	1a	1762	1/1	0.95	0.13	54,54,54,54	0
55	MG	2A	3516	1/1	0.95	0.05	65,65,65,65	0
55	MG	2a	1826	1/1	0.95	0.25	85,85,85,85	0
55	MG	1a	1683	1/1	0.95	0.22	72,72,72,72	0
55	MG	1A	3422	1/1	0.95	0.15	42,42,42,42	0
55	MG	1A	3608	1/1	0.95	0.06	49,49,49,49	0
55	MG	2A	3361	1/1	0.95	0.10	26,26,26,26	0
55	MG	2A	3886	1/1	0.95	0.17	55,55,55,55	0
55	MG	1A	3627	1/1	0.95	0.11	62,62,62,62	0
55	MG	1A	3915	1/1	0.95	0.19	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3632	1/1	0.95	0.26	16,16,16,16	0
55	MG	2A	3633	1/1	0.95	0.14	17,17,17,17	0
55	MG	2A	3786	1/1	0.95	0.31	50,50,50,50	0
55	MG	2A	3341	1/1	0.95	0.40	32,32,32,32	0
55	MG	1a	1622	1/1	0.95	0.25	59,59,59,59	0
55	MG	2A	3386	1/1	0.95	0.08	44,44,44,44	0
55	MG	2A	3736	1/1	0.95	0.08	52,52,52,52	0
55	MG	25	104	1/1	0.95	0.95	33,33,33,33	0
55	MG	2a	1737	1/1	0.95	0.17	73,73,73,73	0
55	MG	2a	1638	1/1	0.95	0.29	50,50,50,50	0
55	MG	2a	1750	1/1	0.95	0.12	72,72,72,72	0
55	MG	2A	3041	1/1	0.95	0.11	46,46,46,46	0
55	MG	1A	3844	1/1	0.95	0.06	53,53,53,53	0
55	MG	1A	3160	1/1	0.95	0.90	23,23,23,23	0
55	MG	1A	3006	1/1	0.95	0.16	21,21,21,21	0
55	MG	2D	305	1/1	0.95	0.46	33,33,33,33	0
55	MG	2A	3540	1/1	0.95	0.13	49,49,49,49	0
55	MG	1A	3541	1/1	0.95	0.08	41,41,41,41	0
55	MG	1A	3755	1/1	0.95	0.10	58,58,58,58	0
55	MG	1A	3050	1/1	0.95	0.47	29,29,29,29	0
55	MG	2A	3147	1/1	0.95	0.42	38,38,38,38	0
55	MG	1a	1718	1/1	0.95	0.08	48,48,48,48	0
55	MG	1A	3499	1/1	0.95	0.07	33,33,33,33	0
55	MG	2a	1708	1/1	0.95	0.13	76,76,76,76	0
55	MG	2B	3020	1/1	0.95	0.07	58,58,58,58	0
55	MG	1A	3735	1/1	0.95	0.20	63,63,63,63	0
55	MG	1A	3217	1/1	0.95	0.16	62,62,62,62	0
55	MG	1a	1811	1/1	0.95	0.11	61,61,61,61	0
55	MG	1A	3830	1/1	0.95	0.81	21,21,21,21	0
55	MG	2A	3418	1/1	0.95	0.04	60,60,60,60	0
55	MG	2A	3546	1/1	0.95	0.13	52,52,52,52	0
55	MG	2A	3770	1/1	0.95	0.20	47,47,47,47	0
55	MG	29	102	1/1	0.95	1.40	48,48,48,48	0
55	MG	2A	3607	1/1	0.95	0.09	74,74,74,74	0
55	MG	1A	3391	1/1	0.95	0.24	30,30,30,30	0
55	MG	2A	3442	1/1	0.95	0.15	20,20,20,20	0
55	MG	1A	3559	1/1	0.95	0.52	15,15,15,15	0
55	MG	2A	3082	1/1	0.95	0.17	50,50,50,50	0
55	MG	2A	3798	1/1	0.95	0.18	60,60,60,60	0
55	MG	1A	3949	1/1	0.95	0.56	14,14,14,14	0
55	MG	2A	3960	1/1	0.95	0.36	44,44,44,44	0
55	MG	2A	3096	1/1	0.95	0.16	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1B	212	1/1	0.95	0.05	59,59,59,59	0
55	MG	1A	3247	1/1	0.95	0.25	41,41,41,41	0
55	MG	2a	1731	1/1	0.95	0.10	62,62,62,62	0
55	MG	1A	3417	1/1	0.95	0.11	32,32,32,32	0
55	MG	1A	3057	1/1	0.95	0.26	16,16,16,16	0
55	MG	2A	3138	1/1	0.95	0.28	40,40,40,40	0
55	MG	2A	3902	1/1	0.95	0.22	87,87,87,87	0
55	MG	2A	3328	1/1	0.95	0.24	39,39,39,39	0
55	MG	2A	3296	1/1	0.95	0.23	54,54,54,54	0
55	MG	1A	3845	1/1	0.95	0.15	47,47,47,47	0
55	MG	1A	3215	1/1	0.95	0.35	23,23,23,23	0
55	MG	1A	3880	1/1	0.95	0.23	54,54,54,54	0
55	MG	1A	3442	1/1	0.95	0.14	25,25,25,25	0
55	MG	1a	1701	1/1	0.95	0.07	56,56,56,56	0
55	MG	1B	206	1/1	0.95	0.14	50,50,50,50	0
55	MG	2A	3291	1/1	0.95	0.10	29,29,29,29	0
55	MG	1A	3333	1/1	0.95	0.14	28,28,28,28	0
55	MG	1A	3838	1/1	0.95	0.22	39,39,39,39	0
55	MG	1A	3759	1/1	0.95	0.08	28,28,28,28	0
55	MG	1A	3792	1/1	0.95	0.18	25,25,25,25	0
55	MG	2a	1833	1/1	0.95	0.07	71,71,71,71	0
55	MG	1a	1605	1/1	0.95	0.12	60,60,60,60	0
55	MG	2A	3143	1/1	0.95	0.52	42,42,42,42	0
55	MG	1B	207	1/1	0.95	0.39	41,41,41,41	0
55	MG	1a	1814	1/1	0.95	0.10	54,54,54,54	0
55	MG	2A	3878	1/1	0.95	0.51	43,43,43,43	0
55	MG	2f	8001	1/1	0.95	0.12	75,75,75,75	0
55	MG	2a	1648	1/1	0.95	0.23	42,42,42,42	0
55	MG	1A	3124	1/1	0.95	0.44	28,28,28,28	0
55	MG	2A	3604	1/1	0.95	0.15	49,49,49,49	0
55	MG	2a	1716	1/1	0.95	0.08	55,55,55,55	0
55	MG	2A	3470	1/1	0.95	0.14	26,26,26,26	0
55	MG	1A	3165	1/1	0.95	0.69	25,25,25,25	0
55	MG	2a	1815	1/1	0.95	0.09	75,75,75,75	0
55	MG	1A	3643	1/1	0.95	0.21	40,40,40,40	0
55	MG	2A	3952	1/1	0.95	0.13	27,27,27,27	0
55	MG	2a	1622	1/1	0.95	0.27	51,51,51,51	0
55	MG	2A	3877	1/1	0.95	0.10	26,26,26,26	0
55	MG	1a	1825	1/1	0.95	0.13	71,71,71,71	0
55	MG	2A	3293	1/1	0.95	0.23	7,7,7,7	0
55	MG	2A	3609	1/1	0.95	0.20	64,64,64,64	0
55	MG	2A	3080	1/1	0.95	0.23	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1F	305	1/1	0.95	0.67	18,18,18,18	0
55	MG	1A	3013	1/1	0.95	0.17	17,17,17,17	0
55	MG	1A	3620	1/1	0.95	0.12	58,58,58,58	0
55	MG	2A	3368	1/1	0.95	0.24	51,51,51,51	0
55	MG	1A	3287	1/1	0.95	0.07	26,26,26,26	0
55	MG	1A	3347	1/1	0.95	0.18	13,13,13,13	0
55	MG	1a	1722	1/1	0.95	0.08	63,63,63,63	0
55	MG	1A	3927	1/1	0.95	0.14	27,27,27,27	0
55	MG	2A	3412	1/1	0.95	0.37	68,68,68,68	0
55	MG	2A	3005	1/1	0.95	0.24	37,37,37,37	0
55	MG	2A	3450	1/1	0.95	0.56	28,28,28,28	0
55	MG	2T	203	1/1	0.95	0.76	59,59,59,59	0
55	MG	1A	3547	1/1	0.95	0.11	29,29,29,29	0
55	MG	1A	3758	1/1	0.95	0.20	17,17,17,17	0
55	MG	1A	3535	1/1	0.95	0.14	19,19,19,19	0
55	MG	2A	3802	1/1	0.95	0.07	45,45,45,45	0
55	MG	2A	3043	1/1	0.95	0.52	35,35,35,35	0
55	MG	2A	3627	1/1	0.95	0.20	68,68,68,68	0
55	MG	1a	1819	1/1	0.95	0.06	52,52,52,52	0
55	MG	2A	3289	1/1	0.95	0.14	64,64,64,64	0
55	MG	1N	204	1/1	0.95	0.25	73,73,73,73	0
55	MG	2A	3485	1/1	0.95	0.17	60,60,60,60	0
55	MG	1A	3681	1/1	0.95	0.13	38,38,38,38	0
55	MG	2a	1777	1/1	0.95	0.28	55,55,55,55	0
55	MG	2a	1633	1/1	0.95	0.13	47,47,47,47	0
55	MG	1A	3675	1/1	0.95	0.25	44,44,44,44	0
55	MG	1A	3869	1/1	0.95	0.30	38,38,38,38	0
55	MG	1A	3093	1/1	0.95	0.24	27,27,27,27	0
55	MG	1A	3339	1/1	0.95	0.14	13,13,13,13	0
55	MG	1a	1637	1/1	0.95	1.17	57,57,57,57	0
55	MG	1a	1747	1/1	0.95	0.20	36,36,36,36	0
55	MG	1A	3311	1/1	0.95	0.20	11,11,11,11	0
55	MG	1A	3019	1/1	0.95	0.40	15,15,15,15	0
55	MG	2A	3598	1/1	0.95	0.49	34,34,34,34	0
55	MG	2A	3785	1/1	0.95	0.16	71,71,71,71	0
55	MG	1A	3343	1/1	0.95	0.06	12,12,12,12	0
55	MG	2A	3518	1/1	0.95	0.14	58,58,58,58	0
55	MG	1A	3567	1/1	0.95	0.17	12,12,12,12	0
55	MG	2A	3220	1/1	0.95	0.20	58,58,58,58	0
55	MG	2A	3337	1/1	0.95	0.14	22,22,22,22	0
55	MG	2A	3468	1/1	0.95	0.11	36,36,36,36	0
55	MG	2A	3154	1/1	0.95	0.22	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3884	1/1	0.95	0.14	76,76,76,76	0
55	MG	2a	1704	1/1	0.95	0.21	63,63,63,63	0
55	MG	1A	3523	1/1	0.95	0.13	12,12,12,12	0
55	MG	1A	3084	1/1	0.95	0.08	48,48,48,48	0
55	MG	1B	222	1/1	0.95	0.10	35,35,35,35	0
55	MG	1A	3696	1/1	0.95	0.13	50,50,50,50	0
55	MG	2A	3321	1/1	0.95	0.20	30,30,30,30	0
55	MG	2V	205	1/1	0.95	0.13	59,59,59,59	0
55	MG	1A	3218	1/1	0.95	0.24	46,46,46,46	0
55	MG	2a	1696	1/1	0.95	0.10	38,38,38,38	0
55	MG	2A	3940	1/1	0.95	0.10	48,48,48,48	0
55	MG	2T	201	1/1	0.95	0.14	21,21,21,21	0
55	MG	1A	3440	1/1	0.95	0.09	26,26,26,26	0
55	MG	11	103	1/1	0.95	0.14	44,44,44,44	0
55	MG	10	106	1/1	0.95	0.20	39,39,39,39	0
55	MG	1a	1633	1/1	0.95	0.12	34,34,34,34	0
55	MG	2A	3460	1/1	0.95	0.14	25,25,25,25	0
55	MG	2A	3283	1/1	0.95	0.16	61,61,61,61	0
55	MG	2A	3767	1/1	0.95	0.10	52,52,52,52	0
55	MG	1a	1664	1/1	0.95	0.31	67,67,67,67	0
55	MG	1A	3049	1/1	0.95	0.26	22,22,22,22	0
55	MG	1A	3279	1/1	0.95	0.16	70,70,70,70	0
55	MG	1A	3546	1/1	0.95	0.11	48,48,48,48	0
55	MG	1A	3414	1/1	0.95	0.09	29,29,29,29	0
55	MG	2A	3601	1/1	0.95	0.13	34,34,34,34	0
55	MG	1A	3187	1/1	0.95	0.30	28,28,28,28	0
55	MG	1A	3155	1/1	0.95	0.29	16,16,16,16	0
55	MG	1H	201	1/1	0.95	0.20	47,47,47,47	0
55	MG	1A	3801	1/1	0.95	0.07	83,83,83,83	0
55	MG	1A	3619	1/1	0.95	0.17	45,45,45,45	0
55	MG	2A	3678	1/1	0.95	0.23	53,53,53,53	0
55	MG	1A	3396	1/1	0.95	0.23	35,35,35,35	0
55	MG	1A	3192	1/1	0.95	0.52	31,31,31,31	0
55	MG	1A	3776	1/1	0.95	0.08	46,46,46,46	0
55	MG	2A	3263	1/1	0.95	0.12	44,44,44,44	0
55	MG	1A	3185	1/1	0.95	0.37	25,25,25,25	0
55	MG	1a	1631	1/1	0.95	0.08	61,61,61,61	0
55	MG	1A	3939	1/1	0.95	0.21	24,24,24,24	0
55	MG	1A	3259	1/1	0.95	0.14	17,17,17,17	0
55	MG	1A	3052	1/1	0.95	0.61	34,34,34,34	0
55	MG	2A	3056	1/1	0.95	0.09	54,54,54,54	0
55	MG	2A	3622	1/1	0.95	0.15	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
55	MG	1A	3086	1/1	0.95	0.48	38,38,38,38	0
55	MG	1a	1761	1/1	0.95	0.17	72,72,72,72	0
55	MG	1A	3711	1/1	0.95	0.08	21,21,21,21	0
55	MG	1A	3323	1/1	0.95	0.14	24,24,24,24	0
55	MG	1A	3203	1/1	0.95	0.17	34,34,34,34	0
55	MG	1A	3003	1/1	0.95	0.11	21,21,21,21	0
55	MG	2a	1656	1/1	0.95	0.18	76,76,76,76	0
55	MG	1E	304	1/1	0.95	0.13	25,25,25,25	0
55	MG	2A	3438	1/1	0.95	0.16	38,38,38,38	0
55	MG	1a	1733	1/1	0.95	0.35	67,67,67,67	0
55	MG	1A	3089	1/1	0.95	0.54	26,26,26,26	0
55	MG	2A	3778	1/1	0.95	0.07	63,63,63,63	0
55	MG	2A	3597	1/1	0.95	0.16	52,52,52,52	0
55	MG	2A	3148	1/1	0.95	0.48	35,35,35,35	0
55	MG	1A	3832	1/1	0.95	0.22	10,10,10,10	0
55	MG	1A	3625	1/1	0.95	0.11	69,69,69,69	0
55	MG	1A	3527	1/1	0.95	0.16	40,40,40,40	0
55	MG	2A	3520	1/1	0.95	0.13	54,54,54,54	0
55	MG	1A	3825	1/1	0.95	0.05	18,18,18,18	0
55	MG	1A	3549	1/1	0.95	0.19	40,40,40,40	0
55	MG	1A	3001	1/1	0.95	0.11	23,23,23,23	0
55	MG	1a	1606	1/1	0.95	0.15	53,53,53,53	0
55	MG	1a	1738	1/1	0.95	0.21	50,50,50,50	0
55	MG	1A	3470	1/1	0.95	0.17	20,20,20,20	0
55	MG	2A	3451	1/1	0.95	0.17	30,30,30,30	0
55	MG	2A	3895	1/1	0.95	0.17	55,55,55,55	0
55	MG	1a	1829	1/1	0.95	0.07	84,84,84,84	0
55	MG	2A	3809	1/1	0.95	0.08	35,35,35,35	0
55	MG	1A	3211	1/1	0.95	0.47	20,20,20,20	0
55	MG	1A	3697	1/1	0.95	0.32	37,37,37,37	0
55	MG	1A	3590	1/1	0.95	0.10	47,47,47,47	0
55	MG	1A	3624	1/1	0.95	0.20	58,58,58,58	0
55	MG	1N	203	1/1	0.95	0.48	55,55,55,55	0
55	MG	1a	1604	1/1	0.95	0.18	73,73,73,73	0
55	MG	2a	1649	1/1	0.95	0.13	65,65,65,65	0
55	MG	2A	3242	1/1	0.95	0.22	32,32,32,32	0
55	MG	1F	312	1/1	0.95	0.73	22,22,22,22	0
55	MG	2A	3058	1/1	0.95	0.09	59,59,59,59	0
55	MG	1a	1645	1/1	0.95	0.29	64,64,64,64	0
55	MG	1A	3022	1/1	0.95	0.34	42,42,42,42	0
55	MG	1A	3861	1/1	0.95	0.20	63,63,63,63	0
55	MG	1a	1727	1/1	0.95	0.13	77,77,77,77	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1822	1/1	0.95	0.39	51,51,51,51	0
55	MG	2a	1743	1/1	0.95	0.13	75,75,75,75	0
55	MG	2A	3481	1/1	0.95	0.86	40,40,40,40	0
55	MG	2A	3104	1/1	0.95	0.17	57,57,57,57	0
55	MG	2A	3863	1/1	0.95	0.12	61,61,61,61	0
55	MG	2A	3879	1/1	0.95	0.11	38,38,38,38	0
55	MG	1A	3953	1/1	0.95	0.63	22,22,22,22	0
55	MG	1A	3189	1/1	0.95	0.94	30,30,30,30	0
55	MG	2A	3373	1/1	0.95	0.10	27,27,27,27	0
55	MG	2F	302	1/1	0.96	0.38	35,35,35,35	0
55	MG	2A	3054	1/1	0.96	0.17	31,31,31,31	0
55	MG	1A	3897	1/1	0.96	0.12	45,45,45,45	0
55	MG	1A	3931	1/1	0.96	0.10	32,32,32,32	0
55	MG	1A	3324	1/1	0.96	0.06	52,52,52,52	0
55	MG	2A	3662	1/1	0.96	0.18	46,46,46,46	0
55	MG	2A	3411	1/1	0.96	0.20	49,49,49,49	0
55	MG	2A	3183	1/1	0.96	0.16	43,43,43,43	0
55	MG	2a	1819	1/1	0.96	0.14	61,61,61,61	0
55	MG	1A	3708	1/1	0.96	0.05	32,32,32,32	0
55	MG	1A	3248	1/1	0.96	0.33	39,39,39,39	0
55	MG	1a	1729	1/1	0.96	0.47	43,43,43,43	0
55	MG	2a	1601	1/1	0.96	0.10	66,66,66,66	0
55	MG	2A	3363	1/1	0.96	0.22	50,50,50,50	0
55	MG	2A	3688	1/1	0.96	0.18	51,51,51,51	0
55	MG	2A	3647	1/1	0.96	0.87	37,37,37,37	0
55	MG	2A	3514	1/1	0.96	0.16	59,59,59,59	0
55	MG	2A	3346	1/1	0.96	0.09	35,35,35,35	0
55	MG	2A	3632	1/1	0.96	0.07	74,74,74,74	0
55	MG	2A	3796	1/1	0.96	0.19	79,79,79,79	0
55	MG	2A	3577	1/1	0.96	0.06	69,69,69,69	0
55	MG	2A	3545	1/1	0.96	0.19	39,39,39,39	0
55	MG	2T	202	1/1	0.96	0.07	56,56,56,56	0
55	MG	2A	3094	1/1	0.96	0.94	42,42,42,42	0
55	MG	2A	3505	1/1	0.96	0.16	47,47,47,47	0
55	MG	2A	3217	1/1	0.96	0.48	32,32,32,32	0
55	MG	1B	221	1/1	0.96	0.07	33,33,33,33	0
55	MG	2A	3185	1/1	0.96	0.47	51,51,51,51	0
55	MG	2A	3023	1/1	0.96	0.69	44,44,44,44	0
55	MG	2A	3838	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3332	1/1	0.96	0.16	53,53,53,53	0
55	MG	1A	3937	1/1	0.96	0.41	19,19,19,19	0
55	MG	1A	3690	1/1	0.96	0.54	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3724	1/1	0.96	0.05	63,63,63,63	0
56	ZN	1n	501	1/1	0.96	0.12	75,75,75,75	0
55	MG	17	102	1/1	0.96	0.16	28,28,28,28	0
55	MG	1A	3014	1/1	0.96	0.18	28,28,28,28	0
55	MG	2A	3695	1/1	0.96	0.21	39,39,39,39	0
55	MG	2a	1807	1/1	0.96	0.08	55,55,55,55	0
55	MG	1a	1638	1/1	0.96	0.20	30,30,30,30	0
55	MG	1A	3787	1/1	0.96	0.10	23,23,23,23	0
55	MG	2A	3115	1/1	0.96	0.30	31,31,31,31	0
55	MG	2A	3928	1/1	0.96	0.10	35,35,35,35	0
55	MG	1A	3944	1/1	0.96	0.75	28,28,28,28	0
56	ZN	2Y	202	1/1	0.96	0.05	80,80,80,80	0
55	MG	1a	1665	1/1	0.96	0.49	75,75,75,75	0
55	MG	2A	3166	1/1	0.96	0.40	36,36,36,36	0
55	MG	1A	3308	1/1	0.96	0.13	17,17,17,17	0
55	MG	1A	3510	1/1	0.96	0.04	57,57,57,57	0
55	MG	1A	3701	1/1	0.96	0.07	33,33,33,33	0
55	MG	1A	3272	1/1	0.96	0.77	22,22,22,22	0
55	MG	2a	1768	1/1	0.96	0.22	59,59,59,59	0
55	MG	2A	3288	1/1	0.96	0.12	24,24,24,24	0
55	MG	2A	3366	1/1	0.96	0.12	25,25,25,25	0
55	MG	13	101	1/1	0.96	0.19	30,30,30,30	0
55	MG	2A	3111	1/1	0.96	0.50	44,44,44,44	0
55	MG	1A	3403	1/1	0.96	0.09	40,40,40,40	0
55	MG	2a	1758	1/1	0.96	0.12	75,75,75,75	0
55	MG	1A	3029	1/1	0.96	0.10	21,21,21,21	0
55	MG	2A	3855	1/1	0.96	0.04	64,64,64,64	0
55	MG	1A	3485	1/1	0.96	0.72	30,30,30,30	0
55	MG	1A	3117	1/1	0.96	0.04	72,72,72,72	0
55	MG	1A	3438	1/1	0.96	0.06	33,33,33,33	0
55	MG	1a	1728	1/1	0.96	0.08	69,69,69,69	0
55	MG	1T	202	1/1	0.96	0.50	60,60,60,60	0
55	MG	1A	3420	1/1	0.96	0.09	48,48,48,48	0
55	MG	1A	3922	1/1	0.96	0.12	31,31,31,31	0
55	MG	1a	1830	1/1	0.96	0.20	56,56,56,56	0
55	MG	1A	3813	1/1	0.96	0.15	26,26,26,26	0
55	MG	1a	1719	1/1	0.96	0.05	44,44,44,44	0
55	MG	1A	3276	1/1	0.96	0.10	35,35,35,35	0
55	MG	2A	3584	1/1	0.96	0.88	33,33,33,33	0
55	MG	1A	3226	1/1	0.96	0.23	27,27,27,27	0
55	MG	2A	3420	1/1	0.96	0.09	50,50,50,50	0
55	MG	1A	3067	1/1	0.96	0.27	27,27,27,27	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3406	1/1	0.96	0.09	38,38,38,38	0
55	MG	1A	3816	1/1	0.96	0.22	43,43,43,43	0
55	MG	1a	1793	1/1	0.96	0.16	77,77,77,77	0
55	MG	1A	3025	1/1	0.96	1.08	22,22,22,22	0
55	MG	1A	3714	1/1	0.96	0.15	26,26,26,26	0
55	MG	1A	3703	1/1	0.96	0.08	17,17,17,17	0
55	MG	1A	3101	1/1	0.96	0.40	24,24,24,24	0
55	MG	1A	3246	1/1	0.96	0.32	32,32,32,32	0
55	MG	2A	3306	1/1	0.96	0.14	46,46,46,46	0
55	MG	1A	3241	1/1	0.96	0.82	21,21,21,21	0
55	MG	2F	306	1/1	0.96	0.48	34,34,34,34	0
55	MG	1D	310	1/1	0.96	0.28	10,10,10,10	0
55	MG	1A	3291	1/1	0.96	0.19	45,45,45,45	0
55	MG	1a	1817	1/1	0.96	0.11	65,65,65,65	0
55	MG	2A	3846	1/1	0.96	0.09	56,56,56,56	0
55	MG	1A	3044	1/1	0.96	0.16	21,21,21,21	0
55	MG	1A	3361	1/1	0.96	0.12	35,35,35,35	0
55	MG	1a	1696	1/1	0.96	0.29	63,63,63,63	0
55	MG	2A	3722	1/1	0.96	0.18	63,63,63,63	0
55	MG	2A	3762	1/1	0.96	0.15	69,69,69,69	0
55	MG	2D	306	1/1	0.96	0.44	33,33,33,33	0
55	MG	10	101	1/1	0.96	0.13	36,36,36,36	0
55	MG	1A	3764	1/1	0.96	0.05	45,45,45,45	0
55	MG	1A	3811	1/1	0.96	0.07	13,13,13,13	0
55	MG	1A	3428	1/1	0.96	0.10	12,12,12,12	0
55	MG	2a	1674	1/1	0.96	0.22	31,31,31,31	0
55	MG	1A	3571	1/1	0.96	0.09	55,55,55,55	0
55	MG	1A	3887	1/1	0.96	0.25	71,71,71,71	0
55	MG	2A	3852	1/1	0.96	0.28	50,50,50,50	0
55	MG	2a	1707	1/1	0.96	0.07	51,51,51,51	0
55	MG	2a	1817	1/1	0.96	0.21	68,68,68,68	0
55	MG	1A	3507	1/1	0.96	0.18	47,47,47,47	0
55	MG	1N	202	1/1	0.96	0.51	32,32,32,32	0
55	MG	1a	1839	1/1	0.96	0.13	56,56,56,56	0
55	MG	15	105	1/1	0.96	0.56	36,36,36,36	0
55	MG	2A	3362	1/1	0.96	0.11	32,32,32,32	0
55	MG	1A	3418	1/1	0.96	0.09	53,53,53,53	0
55	MG	1A	3478	1/1	0.96	0.11	36,36,36,36	0
55	MG	1A	3757	1/1	0.96	0.16	9,9,9,9	0
55	MG	11	101	1/1	0.96	0.14	26,26,26,26	0
55	MG	2a	1687	1/1	0.96	0.18	67,67,67,67	0
55	MG	1A	3849	1/1	0.96	0.08	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3357	1/1	0.96	0.31	40,40,40,40	0
55	MG	1A	3737	1/1	0.96	0.07	53,53,53,53	0
55	MG	1A	3359	1/1	0.96	0.12	46,46,46,46	0
55	MG	1A	3555	1/1	0.96	0.14	27,27,27,27	0
55	MG	19	102	1/1	0.96	0.24	50,50,50,50	0
55	MG	1A	3183	1/1	0.96	0.51	39,39,39,39	0
55	MG	1A	3011	1/1	0.96	0.13	27,27,27,27	0
55	MG	1A	3454	1/1	0.96	0.14	9,9,9,9	0
55	MG	1A	3653	1/1	0.96	0.64	21,21,21,21	0
55	MG	1A	3802	1/1	0.96	0.12	26,26,26,26	0
55	MG	1A	3056	1/1	0.96	0.13	50,50,50,50	0
55	MG	1A	3327	1/1	0.96	0.14	23,23,23,23	0
55	MG	1A	3216	1/1	0.96	0.34	21,21,21,21	0
55	MG	1A	3925	1/1	0.96	0.35	26,26,26,26	0
55	MG	2A	3654	1/1	0.96	0.28	37,37,37,37	0
55	MG	1A	3431	1/1	0.96	0.10	14,14,14,14	0
55	MG	1A	3935	1/1	0.96	0.72	20,20,20,20	0
55	MG	1A	3604	1/1	0.96	0.09	25,25,25,25	0
55	MG	2A	3398	1/1	0.96	0.18	47,47,47,47	0
55	MG	2a	1609	1/1	0.96	0.21	78,78,78,78	0
55	MG	1A	3448	1/1	0.96	0.17	41,41,41,41	0
55	MG	2A	3574	1/1	0.96	0.07	47,47,47,47	0
55	MG	1A	3245	1/1	0.96	0.09	65,65,65,65	0
55	MG	1A	3178	1/1	0.96	0.12	34,34,34,34	0
55	MG	1A	3704	1/1	0.96	0.07	57,57,57,57	0
55	MG	1a	1824	1/1	0.96	0.13	42,42,42,42	0
55	MG	1A	3667	1/1	0.96	0.09	41,41,41,41	0
55	MG	2A	3573	1/1	0.96	0.21	27,27,27,27	0
55	MG	1A	3502	1/1	0.96	0.30	36,36,36,36	0
55	MG	2A	3583	1/1	0.96	0.07	50,50,50,50	0
55	MG	2A	3385	1/1	0.96	0.12	40,40,40,40	0
55	MG	2a	1691	1/1	0.96	0.30	59,59,59,59	0
55	MG	1a	1725	1/1	0.96	0.23	47,47,47,47	0
55	MG	1A	3251	1/1	0.96	0.69	16,16,16,16	0
55	MG	1A	3360	1/1	0.96	0.12	16,16,16,16	0
55	MG	2A	3353	1/1	0.96	0.14	24,24,24,24	0
55	MG	1A	3395	1/1	0.96	0.38	34,34,34,34	0
55	MG	1A	3098	1/1	0.96	0.50	34,34,34,34	0
55	MG	1A	3948	1/1	0.96	0.56	24,24,24,24	0
55	MG	1A	3854	1/1	0.96	0.25	38,38,38,38	0
55	MG	1a	1737	1/1	0.96	0.10	67,67,67,67	0
55	MG	2A	3790	1/1	0.96	0.09	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3409	1/1	0.96	0.17	46,46,46,46	0
55	MG	2a	1695	1/1	0.96	0.06	48,48,48,48	0
55	MG	1A	3683	1/1	0.96	0.06	73,73,73,73	0
55	MG	2A	3896	1/1	0.96	0.29	45,45,45,45	0
55	MG	1A	3875	1/1	0.96	0.44	26,26,26,26	0
55	MG	1a	1842	1/1	0.96	0.11	56,56,56,56	0
55	MG	2A	3383	1/1	0.96	0.07	46,46,46,46	0
55	MG	2A	3805	1/1	0.96	0.09	73,73,73,73	0
55	MG	2a	1692	1/1	0.96	0.14	61,61,61,61	0
55	MG	1A	3008	1/1	0.96	0.15	32,32,32,32	0
55	MG	1A	3204	1/1	0.96	0.18	31,31,31,31	0
55	MG	1A	3565	1/1	0.96	0.14	42,42,42,42	0
55	MG	1A	3336	1/1	0.96	0.12	37,37,37,37	0
55	MG	2A	3428	1/1	0.96	0.35	62,62,62,62	0
55	MG	2A	3211	1/1	0.96	0.42	40,40,40,40	0
55	MG	1A	3284	1/1	0.96	0.32	34,34,34,34	0
55	MG	1A	3186	1/1	0.96	0.65	24,24,24,24	0
55	MG	1A	3408	1/1	0.96	0.08	54,54,54,54	0
55	MG	1A	3462	1/1	0.96	0.25	50,50,50,50	0
55	MG	1A	3202	1/1	0.96	0.63	29,29,29,29	0
55	MG	1B	210	1/1	0.96	0.51	52,52,52,52	0
55	MG	2a	1693	1/1	0.96	0.29	67,67,67,67	0
55	MG	2A	3276	1/1	0.96	0.47	41,41,41,41	0
55	MG	2D	310	1/1	0.96	0.27	40,40,40,40	0
55	MG	2A	3095	1/1	0.96	0.18	17,17,17,17	0
55	MG	1A	3606	1/1	0.96	0.10	23,23,23,23	0
55	MG	2A	3443	1/1	0.96	0.07	25,25,25,25	0
55	MG	2N	201	1/1	0.96	0.20	72,72,72,72	0
55	MG	1A	3885	1/1	0.96	0.10	47,47,47,47	0
55	MG	1A	3637	1/1	0.96	0.12	36,36,36,36	0
55	MG	2a	1667	1/1	0.96	0.39	52,52,52,52	0
55	MG	1A	3171	1/1	0.96	0.29	24,24,24,24	0
55	MG	2A	3236	1/1	0.96	0.07	91,91,91,91	0
55	MG	1A	3932	1/1	0.96	0.64	24,24,24,24	0
55	MG	2A	3089	1/1	0.96	0.39	49,49,49,49	0
55	MG	1A	3907	1/1	0.96	0.80	20,20,20,20	0
55	MG	2A	3358	1/1	0.96	0.10	23,23,23,23	0
55	MG	1A	3577	1/1	0.96	0.16	20,20,20,20	0
55	MG	1A	3768	1/1	0.96	0.12	25,25,25,25	0
55	MG	2a	1733	1/1	0.96	0.42	47,47,47,47	0
55	MG	2A	3579	1/1	0.96	0.13	37,37,37,37	0
55	MG	2A	3285	1/1	0.96	0.10	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3129	1/1	0.96	0.99	33,33,33,33	0
55	MG	1A	3833	1/1	0.96	0.15	17,17,17,17	0
55	MG	1a	1693	1/1	0.96	0.24	44,44,44,44	0
55	MG	1A	3908	1/1	0.96	0.34	14,14,14,14	0
55	MG	1A	3238	1/1	0.96	0.24	20,20,20,20	0
55	MG	2A	3653	1/1	0.96	0.37	76,76,76,76	0
55	MG	2A	3340	1/1	0.96	0.12	39,39,39,39	0
55	MG	1A	3767	1/1	0.96	0.06	42,42,42,42	0
55	MG	1A	3670	1/1	0.96	0.45	36,36,36,36	0
55	MG	1A	3179	1/1	0.96	0.15	51,51,51,51	0
55	MG	1R	204	1/1	0.96	0.21	19,19,19,19	0
55	MG	2A	3697	1/1	0.96	0.28	33,33,33,33	0
55	MG	2a	1742	1/1	0.96	0.17	51,51,51,51	0
55	MG	1a	1822	1/1	0.96	0.40	74,74,74,74	0
55	MG	1A	3618	1/1	0.96	0.50	24,24,24,24	0
55	MG	2A	3476	1/1	0.96	0.14	56,56,56,56	0
55	MG	1A	3775	1/1	0.96	0.14	52,52,52,52	0
55	MG	2A	3436	1/1	0.96	0.07	47,47,47,47	0
55	MG	2A	3737	1/1	0.96	0.08	43,43,43,43	0
55	MG	1A	3779	1/1	0.96	0.15	17,17,17,17	0
55	MG	2A	3139	1/1	0.96	0.32	38,38,38,38	0
55	MG	2a	1811	1/1	0.96	0.06	60,60,60,60	0
55	MG	1a	1695	1/1	0.96	0.14	53,53,53,53	0
55	MG	1F	303	1/1	0.96	0.45	56,56,56,56	0
55	MG	2A	3536	1/1	0.96	0.30	58,58,58,58	0
55	MG	2A	3816	1/1	0.96	0.10	42,42,42,42	0
55	MG	1A	3114	1/1	0.97	0.36	18,18,18,18	0
55	MG	1a	1798	1/1	0.97	0.10	48,48,48,48	0
55	MG	2A	3486	1/1	0.97	0.33	59,59,59,59	0
55	MG	2A	3309	1/1	0.97	0.10	41,41,41,41	0
55	MG	2A	3445	1/1	0.97	0.12	55,55,55,55	0
55	MG	1A	3153	1/1	0.97	0.82	26,26,26,26	0
55	MG	1A	3712	1/1	0.97	0.12	11,11,11,11	0
55	MG	2A	3292	1/1	0.97	0.07	38,38,38,38	0
55	MG	2A	3582	1/1	0.97	0.12	29,29,29,29	0
55	MG	1A	3376	1/1	0.97	0.13	26,26,26,26	0
55	MG	1A	3304	1/1	0.97	0.10	34,34,34,34	0
55	MG	1A	3666	1/1	0.97	0.10	42,42,42,42	0
55	MG	1A	3740	1/1	0.97	0.12	46,46,46,46	0
55	MG	1A	3167	1/1	0.97	0.54	33,33,33,33	0
55	MG	2A	3446	1/1	0.97	0.16	22,22,22,22	0
55	MG	2A	3323	1/1	0.97	0.19	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3928	1/1	0.97	0.64	33,33,33,33	0
55	MG	2A	3313	1/1	0.97	0.10	36,36,36,36	0
55	MG	1a	1657	1/1	0.97	0.10	67,67,67,67	0
55	MG	1A	3471	1/1	0.97	0.09	46,46,46,46	0
55	MG	27	101	1/1	0.97	0.68	38,38,38,38	0
55	MG	2A	3208	1/1	0.97	0.11	38,38,38,38	0
55	MG	1Q	202	1/1	0.97	0.11	19,19,19,19	0
55	MG	1A	3837	1/1	0.97	0.12	9,9,9,9	0
55	MG	2A	3780	1/1	0.97	0.13	29,29,29,29	0
55	MG	2A	3841	1/1	0.97	0.09	25,25,25,25	0
55	MG	2A	3172	1/1	0.97	0.20	54,54,54,54	0
55	MG	2a	1760	1/1	0.97	0.10	52,52,52,52	0
55	MG	2A	3700	1/1	0.97	0.14	58,58,58,58	0
55	MG	1A	3250	1/1	0.97	0.12	44,44,44,44	0
55	MG	25	101	1/1	0.97	0.11	48,48,48,48	0
55	MG	1a	1707	1/1	0.97	0.17	54,54,54,54	0
55	MG	1A	3726	1/1	0.97	0.12	44,44,44,44	0
55	MG	1A	3554	1/1	0.97	0.15	56,56,56,56	0
55	MG	1A	3741	1/1	0.97	0.73	29,29,29,29	0
55	MG	2a	1652	1/1	0.97	0.20	43,43,43,43	0
55	MG	2A	3455	1/1	0.97	0.32	62,62,62,62	0
55	MG	1U	203	1/1	0.97	0.14	32,32,32,32	0
55	MG	1A	3796	1/1	0.97	0.13	33,33,33,33	0
55	MG	1A	3531	1/1	0.97	0.08	42,42,42,42	0
55	MG	2A	3375	1/1	0.97	0.10	21,21,21,21	0
55	MG	1A	3441	1/1	0.97	0.16	16,16,16,16	0
55	MG	2A	3813	1/1	0.97	0.11	21,21,21,21	0
55	MG	2A	3496	1/1	0.97	0.10	43,43,43,43	0
55	MG	1a	1787	1/1	0.97	0.06	60,60,60,60	0
55	MG	1A	3508	1/1	0.97	0.07	46,46,46,46	0
55	MG	2A	3002	1/1	0.97	0.13	38,38,38,38	0
55	MG	1A	3370	1/1	0.97	0.06	45,45,45,45	0
55	MG	1A	3207	1/1	0.97	0.60	27,27,27,27	0
55	MG	1A	3277	1/1	0.97	0.16	37,37,37,37	0
55	MG	1A	3095	1/1	0.97	0.28	21,21,21,21	0
55	MG	2A	3430	1/1	0.97	0.07	71,71,71,71	0
55	MG	1P	203	1/1	0.97	0.68	9,9,9,9	0
55	MG	2A	3489	1/1	0.97	0.34	38,38,38,38	0
55	MG	1A	3449	1/1	0.97	0.11	45,45,45,45	0
55	MG	1A	3644	1/1	0.97	0.09	30,30,30,30	0
55	MG	2A	3551	1/1	0.97	0.09	60,60,60,60	0
55	MG	2A	3275	1/1	0.97	0.23	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
55	MG	2A	3822	1/1	0.97	0.06	53,53,53,53	0
55	MG	1A	3302	1/1	0.97	0.19	43,43,43,43	0
55	MG	1A	3818	1/1	0.97	0.15	40,40,40,40	0
55	MG	1a	1827	1/1	0.97	0.08	49,49,49,49	0
55	MG	2A	3407	1/1	0.97	0.12	32,32,32,32	0
55	MG	1A	3705	1/1	0.97	0.13	58,58,58,58	0
55	MG	2A	3256	1/1	0.97	0.52	45,45,45,45	0
55	MG	1A	3318	1/1	0.97	0.09	9,9,9,9	0
55	MG	2A	3282	1/1	0.97	0.16	41,41,41,41	0
55	MG	2A	3240	1/1	0.97	0.41	37,37,37,37	0
55	MG	1A	3312	1/1	0.97	0.10	36,36,36,36	0
55	MG	2A	3755	1/1	0.97	0.27	35,35,35,35	0
55	MG	2A	3478	1/1	0.97	0.13	58,58,58,58	0
55	MG	2A	3953	1/1	0.97	0.38	48,48,48,48	0
55	MG	1A	3281	1/1	0.97	0.09	58,58,58,58	0
55	MG	1A	3582	1/1	0.97	0.34	14,14,14,14	0
55	MG	2A	3859	1/1	0.97	0.30	62,62,62,62	0
55	MG	1A	3298	1/1	0.97	0.08	34,34,34,34	0
55	MG	1A	3028	1/1	0.97	0.39	19,19,19,19	0
55	MG	1A	3346	1/1	0.97	0.14	12,12,12,12	0
55	MG	1A	3487	1/1	0.97	0.16	21,21,21,21	0
55	MG	1a	1607	1/1	0.97	0.06	74,74,74,74	0
55	MG	2A	3400	1/1	0.97	0.08	29,29,29,29	0
55	MG	2F	304	1/1	0.97	0.60	45,45,45,45	0
55	MG	2A	3382	1/1	0.97	0.11	37,37,37,37	0
55	MG	2A	3464	1/1	0.97	0.14	37,37,37,37	0
55	MG	1A	3220	1/1	0.97	0.81	27,27,27,27	0
55	MG	1A	3797	1/1	0.97	0.45	37,37,37,37	0
55	MG	2a	1608	1/1	0.97	0.20	88,88,88,88	0
55	MG	2A	3530	1/1	0.97	0.29	37,37,37,37	0
55	MG	2U	204	1/1	0.97	0.50	44,44,44,44	0
55	MG	1A	3181	1/1	0.97	0.48	34,34,34,34	0
55	MG	2A	3453	1/1	0.97	0.11	36,36,36,36	0
55	MG	2A	3851	1/1	0.97	0.17	66,66,66,66	0
55	MG	2B	3022	1/1	0.97	0.33	68,68,68,68	0
55	MG	1A	3060	1/1	0.97	0.16	22,22,22,22	0
55	MG	2A	3435	1/1	0.97	0.13	42,42,42,42	0
55	MG	2A	3401	1/1	0.97	0.14	36,36,36,36	0
55	MG	1a	1709	1/1	0.97	0.09	37,37,37,37	0
55	MG	2Q	204	1/1	0.97	0.17	32,32,32,32	0
55	MG	2A	3140	1/1	0.97	0.23	51,51,51,51	0
55	MG	2A	3808	1/1	0.97	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
55	MG	1A	3305	1/1	0.97	0.11	47,47,47,47	0
55	MG	2A	3947	1/1	0.97	0.17	33,33,33,33	0
55	MG	1A	3282	1/1	0.97	0.09	18,18,18,18	0
55	MG	1A	3210	1/1	0.97	0.38	28,28,28,28	0
55	MG	2A	3824	1/1	0.97	0.18	47,47,47,47	0
55	MG	2A	3479	1/1	0.97	0.09	53,53,53,53	0
55	MG	2A	3910	1/1	0.97	0.19	37,37,37,37	0
55	MG	1A	3745	1/1	0.97	0.14	28,28,28,28	0
55	MG	1A	3100	1/1	0.97	0.16	43,43,43,43	0
55	MG	1F	311	1/1	0.97	0.37	11,11,11,11	0
55	MG	1A	3526	1/1	0.97	0.06	28,28,28,28	0
55	MG	1A	3533	1/1	0.97	0.09	25,25,25,25	0
55	MG	2A	3135	1/1	0.97	0.17	30,30,30,30	0
55	MG	1A	3659	1/1	0.97	0.12	6,6,6,6	0
55	MG	1A	3483	1/1	0.97	0.10	62,62,62,62	0
55	MG	2A	3840	1/1	0.97	0.14	39,39,39,39	0
55	MG	2A	3352	1/1	0.97	0.09	48,48,48,48	0
55	MG	2A	3349	1/1	0.97	0.11	42,42,42,42	0
55	MG	2A	3163	1/1	0.97	0.54	38,38,38,38	0
55	MG	1A	3407	1/1	0.97	0.38	34,34,34,34	0
55	MG	2A	3327	1/1	0.97	0.13	34,34,34,34	0
55	MG	1A	3913	1/1	0.97	0.21	27,27,27,27	0
55	MG	1A	3254	1/1	0.97	0.42	41,41,41,41	0
55	MG	2A	3209	1/1	0.97	0.58	36,36,36,36	0
55	MG	1A	3206	1/1	0.97	0.34	18,18,18,18	0
55	MG	1A	3465	1/1	0.97	0.05	48,48,48,48	0
55	MG	2A	3063	1/1	0.97	0.14	32,32,32,32	0
55	MG	2a	1653	1/1	0.97	0.26	70,70,70,70	0
55	MG	2A	3310	1/1	0.97	0.05	69,69,69,69	0
55	MG	1A	3379	1/1	0.97	0.14	13,13,13,13	0
55	MG	1A	3642	1/1	0.97	0.51	29,29,29,29	0
55	MG	2A	3887	1/1	0.97	0.08	76,76,76,76	0
55	MG	2A	3076	1/1	0.97	0.39	36,36,36,36	0
55	MG	2A	3266	1/1	0.97	0.53	41,41,41,41	0
55	MG	2Q	202	1/1	0.97	0.17	34,34,34,34	0
55	MG	1A	3338	1/1	0.97	0.10	17,17,17,17	0
55	MG	2A	3167	1/1	0.97	0.20	35,35,35,35	0
55	MG	1A	3773	1/1	0.97	0.10	20,20,20,20	0
55	MG	2A	3290	1/1	0.97	0.14	29,29,29,29	0
55	MG	2A	3253	1/1	0.97	0.21	56,56,56,56	0
55	MG	1A	3540	1/1	0.97	0.22	32,32,32,32	0
55	MG	1a	1703	1/1	0.97	0.16	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
55	MG	1A	3941	1/1	0.97	0.11	48,48,48,48	0
55	MG	2a	1729	1/1	0.97	0.33	65,65,65,65	0
55	MG	1N	201	1/1	0.97	0.17	39,39,39,39	0
55	MG	2A	3826	1/1	0.97	0.05	43,43,43,43	0
55	MG	2A	3338	1/1	0.97	0.17	51,51,51,51	0
55	MG	2A	3371	1/1	0.97	0.08	45,45,45,45	0
55	MG	2A	3602	1/1	0.97	0.16	53,53,53,53	0
55	MG	1A	3545	1/1	0.97	0.11	40,40,40,40	0
55	MG	2A	3364	1/1	0.97	0.13	37,37,37,37	0
55	MG	1a	1821	1/1	0.97	0.05	70,70,70,70	0
55	MG	1A	3365	1/1	0.97	0.07	33,33,33,33	0
55	MG	2A	3665	1/1	0.97	0.13	38,38,38,38	0
55	MG	1A	3134	1/1	0.97	0.17	24,24,24,24	0
55	MG	2A	3162	1/1	0.97	0.20	33,33,33,33	0
55	MG	1A	3366	1/1	0.97	0.08	27,27,27,27	0
55	MG	1A	3147	1/1	0.97	0.71	30,30,30,30	0
55	MG	2a	1824	1/1	0.97	0.59	65,65,65,65	0
55	MG	1B	202	1/1	0.97	0.24	52,52,52,52	0
55	MG	1A	3409	1/1	0.97	0.33	21,21,21,21	0
55	MG	2B	3004	1/1	0.97	0.20	67,67,67,67	0
55	MG	2A	3500	1/1	0.97	0.12	45,45,45,45	0
55	MG	1A	3491	1/1	0.97	0.10	21,21,21,21	0
55	MG	1A	3193	1/1	0.97	0.44	20,20,20,20	0
55	MG	1A	3588	1/1	0.97	0.79	31,31,31,31	0
55	MG	1A	3936	1/1	0.97	0.12	41,41,41,41	0
55	MG	2A	3189	1/1	0.97	0.48	43,43,43,43	0
55	MG	2A	3088	1/1	0.97	0.66	44,44,44,44	0
55	MG	2A	3355	1/1	0.97	0.05	54,54,54,54	0
55	MG	1A	3628	1/1	0.97	0.14	10,10,10,10	0
55	MG	1a	1698	1/1	0.97	0.07	37,37,37,37	0
55	MG	2A	3686	1/1	0.97	0.15	39,39,39,39	0
55	MG	1A	3820	1/1	0.97	0.06	53,53,53,53	0
55	MG	2a	1837	1/1	0.97	0.17	51,51,51,51	0
55	MG	2A	3144	1/1	0.97	0.62	33,33,33,33	0
55	MG	1A	3595	1/1	0.97	0.12	27,27,27,27	0
55	MG	1A	3730	1/1	0.97	0.14	61,61,61,61	0
55	MG	2A	3427	1/1	0.97	0.20	44,44,44,44	0
55	MG	1A	3839	1/1	0.97	0.09	11,11,11,11	0
55	MG	1A	3410	1/1	0.97	0.15	8,8,8,8	0
55	MG	2A	3914	1/1	0.97	0.22	57,57,57,57	0
55	MG	2A	3759	1/1	0.97	0.15	28,28,28,28	0
55	MG	1A	3468	1/1	0.97	0.17	24,24,24,24	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3930	1/1	0.97	0.54	36,36,36,36	0
55	MG	1A	3194	1/1	0.97	0.17	39,39,39,39	0
55	MG	1B	223	1/1	0.97	0.23	61,61,61,61	0
55	MG	1A	3694	1/1	0.97	0.14	31,31,31,31	0
55	MG	1A	3906	1/1	0.97	0.08	14,14,14,14	0
55	MG	1A	3088	1/1	0.97	0.68	24,24,24,24	0
55	MG	1A	3432	1/1	0.97	0.20	8,8,8,8	0
55	MG	1t	3001	1/1	0.97	0.28	69,69,69,69	0
55	MG	2A	3614	1/1	0.97	0.04	62,62,62,62	0
55	MG	1A	3684	1/1	0.97	0.24	41,41,41,41	0
55	MG	1A	3769	1/1	0.97	0.04	30,30,30,30	0
55	MG	2A	3715	1/1	0.97	0.06	37,37,37,37	0
55	MG	2A	3018	1/1	0.97	0.28	41,41,41,41	0
55	MG	2A	3787	1/1	0.97	0.13	20,20,20,20	0
55	MG	1A	3437	1/1	0.97	0.07	9,9,9,9	0
55	MG	1a	1823	1/1	0.97	0.24	51,51,51,51	0
55	MG	1A	3293	1/1	0.97	0.09	45,45,45,45	0
55	MG	1A	3326	1/1	0.97	0.07	32,32,32,32	0
55	MG	2A	3835	1/1	0.97	0.10	41,41,41,41	0
55	MG	1a	1784	1/1	0.97	0.21	74,74,74,74	0
55	MG	2B	3021	1/1	0.97	0.09	45,45,45,45	0
55	MG	1D	313	1/1	0.97	0.43	24,24,24,24	0
55	MG	1B	216	1/1	0.97	0.09	29,29,29,29	0
55	MG	1a	1816	1/1	0.97	0.10	51,51,51,51	0
55	MG	2A	3287	1/1	0.97	0.12	24,24,24,24	0
55	MG	2A	3588	1/1	0.97	0.18	24,24,24,24	0
55	MG	1a	1803	1/1	0.97	0.13	40,40,40,40	0
55	MG	1A	3035	1/1	0.97	0.11	16,16,16,16	0
55	MG	1A	3212	1/1	0.97	0.32	21,21,21,21	0
55	MG	2A	3314	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3474	1/1	0.97	0.97	18,18,18,18	0
55	MG	1A	3113	1/1	0.97	0.14	21,21,21,21	0
55	MG	1F	309	1/1	0.97	0.57	21,21,21,21	0
55	MG	2A	3265	1/1	0.97	0.26	50,50,50,50	0
55	MG	1T	201	1/1	0.97	0.10	30,30,30,30	0
55	MG	1A	3952	1/1	0.97	0.43	23,23,23,23	0
55	MG	2A	3771	1/1	0.97	0.15	46,46,46,46	0
55	MG	2A	3237	1/1	0.97	0.17	41,41,41,41	0
55	MG	1A	3043	1/1	0.97	0.41	10,10,10,10	0
55	MG	2A	3297	1/1	0.97	0.12	40,40,40,40	0
55	MG	1A	3295	1/1	0.97	0.08	18,18,18,18	0
55	MG	1A	3286	1/1	0.97	0.20	17,17,17,17	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3356	1/1	0.97	0.15	20,20,20,20	0
55	MG	2A	3301	1/1	0.97	0.11	52,52,52,52	0
55	MG	1A	3874	1/1	0.97	0.07	27,27,27,27	0
55	MG	1A	3373	1/1	0.97	0.11	7,7,7,7	0
55	MG	2A	3547	1/1	0.97	0.05	50,50,50,50	0
55	MG	1A	3819	1/1	0.97	0.05	23,23,23,23	0
55	MG	1A	3647	1/1	0.97	0.13	28,28,28,28	0
55	MG	28	101	1/1	0.97	0.82	36,36,36,36	0
55	MG	1A	3611	1/1	0.97	0.14	60,60,60,60	0
55	MG	2A	3072	1/1	0.97	0.30	39,39,39,39	0
55	MG	1a	1735	1/1	0.97	0.08	41,41,41,41	0
55	MG	1b	3001	1/1	0.97	0.06	79,79,79,79	0
55	MG	2V	201	1/1	0.97	0.25	40,40,40,40	0
55	MG	2A	3157	1/1	0.97	0.15	51,51,51,51	0
55	MG	2A	3329	1/1	0.97	0.10	43,43,43,43	0
55	MG	2A	3387	1/1	0.97	0.13	35,35,35,35	0
55	MG	2F	307	1/1	0.97	0.09	30,30,30,30	0
55	MG	2A	3244	1/1	0.97	0.52	29,29,29,29	0
55	MG	2A	3752	1/1	0.97	0.07	31,31,31,31	0
55	MG	1A	3310	1/1	0.97	0.16	17,17,17,17	0
55	MG	2A	3475	1/1	0.97	0.24	39,39,39,39	0
55	MG	2A	3657	1/1	0.97	0.16	45,45,45,45	0
55	MG	1a	1764	1/1	0.97	0.11	75,75,75,75	0
55	MG	2A	3367	1/1	0.97	0.11	36,36,36,36	0
55	MG	2A	3125	1/1	0.97	0.18	44,44,44,44	0
55	MG	1a	1687	1/1	0.97	0.12	31,31,31,31	0
55	MG	1A	3227	1/1	0.97	0.59	28,28,28,28	0
55	MG	2A	3067	1/1	0.97	0.25	41,41,41,41	0
55	MG	1A	3425	1/1	0.97	0.16	10,10,10,10	0
55	MG	1A	3340	1/1	0.97	0.10	20,20,20,20	0
55	MG	2A	3610	1/1	0.97	0.13	35,35,35,35	0
55	MG	1A	3852	1/1	0.97	0.20	29,29,29,29	0
55	MG	2A	3216	1/1	0.97	0.29	37,37,37,37	0
55	MG	2A	3467	1/1	0.97	0.17	30,30,30,30	0
55	MG	1A	3808	1/1	0.97	0.12	14,14,14,14	0
55	MG	1A	3136	1/1	0.97	0.24	31,31,31,31	0
55	MG	2A	3465	1/1	0.97	0.08	32,32,32,32	0
55	MG	1A	3597	1/1	0.97	0.30	67,67,67,67	0
55	MG	1a	1800	1/1	0.97	0.24	45,45,45,45	0
55	MG	1A	3785	1/1	0.97	0.14	8,8,8,8	0
55	MG	1A	3896	1/1	0.97	0.12	35,35,35,35	0
55	MG	1A	3387	1/1	0.97	0.04	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
55	MG	1A	3423	1/1	0.97	0.14	9,9,9,9	0
55	MG	2A	3758	1/1	0.97	0.11	32,32,32,32	0
55	MG	2A	3904	1/1	0.97	0.14	35,35,35,35	0
55	MG	2A	3416	1/1	0.97	0.12	21,21,21,21	0
55	MG	2A	3369	1/1	0.97	0.13	28,28,28,28	0
55	MG	1B	218	1/1	0.97	0.15	51,51,51,51	0
55	MG	1A	3116	1/1	0.97	0.09	35,35,35,35	0
55	MG	1A	3412	1/1	0.97	0.04	50,50,50,50	0
55	MG	1A	3354	1/1	0.98	0.09	12,12,12,12	0
55	MG	1A	3337	1/1	0.98	0.18	25,25,25,25	0
55	MG	1A	3042	1/1	0.98	0.54	1,1,1,1	0
55	MG	2A	3307	1/1	0.98	0.09	57,57,57,57	0
55	MG	2D	301	1/1	0.98	0.30	46,46,46,46	0
55	MG	2A	3422	1/1	0.98	0.07	60,60,60,60	0
55	MG	1A	3795	1/1	0.98	0.19	27,27,27,27	0
55	MG	1a	1786	1/1	0.98	0.04	69,69,69,69	0
55	MG	1A	3517	1/1	0.98	0.13	21,21,21,21	0
55	MG	2a	1644	1/1	0.98	0.27	46,46,46,46	0
55	MG	1a	1699	1/1	0.98	0.09	33,33,33,33	0
55	MG	2A	3075	1/1	0.98	0.33	50,50,50,50	0
55	MG	2A	3085	1/1	0.98	0.28	52,52,52,52	0
55	MG	2A	3499	1/1	0.98	0.29	28,28,28,28	0
55	MG	2A	3898	1/1	0.98	0.09	24,24,24,24	0
55	MG	1a	1639	1/1	0.98	0.13	63,63,63,63	0
55	MG	2A	3646	1/1	0.98	0.21	40,40,40,40	0
55	MG	1a	1767	1/1	0.98	0.05	78,78,78,78	0
55	MG	1D	302	1/1	0.98	0.21	22,22,22,22	0
55	MG	1A	3842	1/1	0.98	0.16	39,39,39,39	0
55	MG	1A	3831	1/1	0.98	0.11	13,13,13,13	0
55	MG	2F	308	1/1	0.98	0.68	34,34,34,34	0
55	MG	2A	3408	1/1	0.98	0.12	29,29,29,29	0
55	MG	1A	3107	1/1	0.98	0.42	20,20,20,20	0
55	MG	2A	3853	1/1	0.98	0.09	53,53,53,53	0
55	MG	2A	3045	1/1	0.98	0.12	28,28,28,28	0
55	MG	1A	3157	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3693	1/1	0.98	0.07	37,37,37,37	0
55	MG	2A	3391	1/1	0.98	0.35	63,63,63,63	0
55	MG	2A	3345	1/1	0.98	0.13	21,21,21,21	0
55	MG	20	103	1/1	0.98	0.11	64,64,64,64	0
55	MG	1A	3123	1/1	0.98	0.37	24,24,24,24	0
55	MG	2A	3264	1/1	0.98	0.23	16,16,16,16	0
55	MG	2A	3060	1/1	0.98	0.33	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3575	1/1	0.98	0.07	29,29,29,29	0
55	MG	2A	3480	1/1	0.98	0.06	39,39,39,39	0
55	MG	1A	3803	1/1	0.98	0.06	46,46,46,46	0
55	MG	1A	3581	1/1	0.98	0.25	24,24,24,24	0
55	MG	1A	3542	1/1	0.98	0.14	49,49,49,49	0
55	MG	2A	3712	1/1	0.98	0.06	44,44,44,44	0
55	MG	2a	1710	1/1	0.98	0.20	49,49,49,49	0
55	MG	1A	3529	1/1	0.98	0.13	34,34,34,34	0
55	MG	1A	3835	1/1	0.98	0.10	14,14,14,14	0
55	MG	1A	3433	1/1	0.98	0.08	22,22,22,22	0
55	MG	2a	1725	1/1	0.98	0.19	58,58,58,58	0
55	MG	2A	3127	1/1	0.98	0.32	29,29,29,29	0
55	MG	2A	3219	1/1	0.98	0.20	68,68,68,68	0
55	MG	2A	3035	1/1	0.98	0.10	41,41,41,41	0
55	MG	2A	3772	1/1	0.98	0.08	50,50,50,50	0
55	MG	1A	3225	1/1	0.98	0.10	25,25,25,25	0
55	MG	1A	3045	1/1	0.98	0.12	13,13,13,13	0
55	MG	1A	3530	1/1	0.98	0.11	53,53,53,53	0
55	MG	1A	3168	1/1	0.98	0.12	31,31,31,31	0
55	MG	1R	201	1/1	0.98	0.17	20,20,20,20	0
55	MG	1A	3424	1/1	0.98	0.09	45,45,45,45	0
55	MG	1A	3394	1/1	0.98	0.10	18,18,18,18	0
55	MG	1A	3919	1/1	0.98	0.14	9,9,9,9	0
55	MG	1A	3097	1/1	0.98	0.44	23,23,23,23	0
55	MG	2A	3748	1/1	0.98	0.05	50,50,50,50	0
55	MG	1A	3894	1/1	0.98	0.06	13,13,13,13	0
55	MG	1A	3452	1/1	0.98	0.18	40,40,40,40	0
55	MG	1A	3806	1/1	0.98	0.09	37,37,37,37	0
55	MG	1A	3629	1/1	0.98	0.09	55,55,55,55	0
55	MG	1A	3633	1/1	0.98	0.07	40,40,40,40	0
55	MG	2A	3107	1/1	0.98	0.43	40,40,40,40	0
55	MG	1A	3378	1/1	0.98	0.17	17,17,17,17	0
55	MG	1A	3158	1/1	0.98	0.13	28,28,28,28	0
55	MG	1A	3524	1/1	0.98	0.26	24,24,24,24	0
55	MG	1A	3111	1/1	0.98	0.15	29,29,29,29	0
55	MG	2A	3600	1/1	0.98	0.21	29,29,29,29	0
55	MG	1A	3351	1/1	0.98	0.14	11,11,11,11	0
55	MG	2A	3210	1/1	0.98	0.41	37,37,37,37	0
55	MG	1A	3676	1/1	0.98	0.05	25,25,25,25	0
55	MG	1E	301	1/1	0.98	0.13	9,9,9,9	0
55	MG	1A	3404	1/1	0.98	0.06	38,38,38,38	0
55	MG	2V	202	1/1	0.98	0.40	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3450	1/1	0.98	0.09	63,63,63,63	0
55	MG	2A	3028	1/1	0.98	0.59	38,38,38,38	0
55	MG	2A	3357	1/1	0.98	0.10	23,23,23,23	0
55	MG	1A	3296	1/1	0.98	0.11	36,36,36,36	0
55	MG	1A	3421	1/1	0.98	0.21	29,29,29,29	0
55	MG	2A	3079	1/1	0.98	0.35	41,41,41,41	0
55	MG	2A	3239	1/1	0.98	0.18	29,29,29,29	0
55	MG	2A	3360	1/1	0.98	0.12	26,26,26,26	0
55	MG	1A	3355	1/1	0.98	0.04	10,10,10,10	0
55	MG	2A	3810	1/1	0.98	0.10	27,27,27,27	0
55	MG	1A	3369	1/1	0.98	0.11	12,12,12,12	0
55	MG	2A	3905	1/1	0.98	0.09	51,51,51,51	0
55	MG	2A	3136	1/1	0.98	0.13	34,34,34,34	0
55	MG	1A	3024	1/1	0.98	0.12	19,19,19,19	0
55	MG	2a	1715	1/1	0.98	0.07	44,44,44,44	0
55	MG	1A	3674	1/1	0.98	0.06	27,27,27,27	0
55	MG	1A	3587	1/1	0.98	0.29	29,29,29,29	0
55	MG	1a	1625	1/1	0.98	0.25	54,54,54,54	0
55	MG	1A	3688	1/1	0.98	0.13	23,23,23,23	0
55	MG	1A	3375	1/1	0.98	0.16	24,24,24,24	0
55	MG	2A	3161	1/1	0.98	0.22	31,31,31,31	0
55	MG	1A	3299	1/1	0.98	0.10	28,28,28,28	0
55	MG	1A	3388	1/1	0.98	0.04	45,45,45,45	0
55	MG	1a	1812	1/1	0.98	0.07	50,50,50,50	0
55	MG	1A	3895	1/1	0.98	0.06	21,21,21,21	0
55	MG	1A	3334	1/1	0.98	0.19	29,29,29,29	0
55	MG	1A	3306	1/1	0.98	0.04	31,31,31,31	0
55	MG	2a	1841	1/1	0.98	0.07	87,87,87,87	0
55	MG	2a	1821	1/1	0.98	0.06	46,46,46,46	0
55	MG	2A	3431	1/1	0.98	0.20	20,20,20,20	0
55	MG	2A	3616	1/1	0.98	0.55	35,35,35,35	0
55	MG	2A	3792	1/1	0.98	0.12	51,51,51,51	0
55	MG	1A	3235	1/1	0.98	0.10	27,27,27,27	0
55	MG	1A	3630	1/1	0.98	0.09	46,46,46,46	0
55	MG	1A	3283	1/1	0.98	0.13	9,9,9,9	0
55	MG	1A	3924	1/1	0.98	0.21	16,16,16,16	0
55	MG	1A	3851	1/1	0.98	0.14	43,43,43,43	0
55	MG	1A	3693	1/1	0.98	0.10	20,20,20,20	0
55	MG	2A	3227	1/1	0.98	0.41	49,49,49,49	0
55	MG	1A	3430	1/1	0.98	0.14	29,29,29,29	0
56	ZN	29	103	1/1	0.98	0.10	66,66,66,66	0
55	MG	2A	3943	1/1	0.98	0.19	38,38,38,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	ZN	1Y	501	1/1	0.98	0.10	43,43,43,43	0
55	MG	2A	3426	1/1	0.98	0.07	66,66,66,66	0
55	MG	1A	3525	1/1	0.98	0.14	33,33,33,33	0
55	MG	1A	3399	1/1	0.98	0.06	30,30,30,30	0
55	MG	2A	3414	1/1	0.98	0.10	70,70,70,70	0
55	MG	1A	3342	1/1	0.98	0.08	30,30,30,30	0
55	MG	1A	3393	1/1	0.98	0.09	34,34,34,34	0
55	MG	2A	3222	1/1	0.98	0.38	42,42,42,42	0
55	MG	2A	3117	1/1	0.98	0.27	36,36,36,36	0
55	MG	2A	3424	1/1	0.98	0.12	72,72,72,72	0
55	MG	2A	3267	1/1	0.98	0.49	44,44,44,44	0
55	MG	1A	3495	1/1	0.98	0.24	33,33,33,33	0
55	MG	2A	3926	1/1	0.98	0.11	50,50,50,50	0
55	MG	1A	3416	1/1	0.98	0.07	38,38,38,38	0
55	MG	1A	3829	1/1	0.98	0.15	50,50,50,50	0
55	MG	2A	3229	1/1	0.98	0.10	29,29,29,29	0
55	MG	2a	1816	1/1	0.98	0.41	66,66,66,66	0
55	MG	1A	3926	1/1	0.98	0.04	52,52,52,52	0
55	MG	2A	3671	1/1	0.98	0.05	52,52,52,52	0
55	MG	1A	3827	1/1	0.98	0.12	57,57,57,57	0
55	MG	2A	3429	1/1	0.98	0.14	23,23,23,23	0
55	MG	1A	3569	1/1	0.98	0.09	17,17,17,17	0
55	MG	2A	3224	1/1	0.98	0.51	31,31,31,31	0
55	MG	1A	3682	1/1	0.98	0.18	39,39,39,39	0
55	MG	1A	3889	1/1	0.98	0.35	34,34,34,34	0
55	MG	2A	3793	1/1	0.98	0.04	52,52,52,52	0
55	MG	1A	3315	1/1	0.98	0.13	10,10,10,10	0
55	MG	2A	3927	1/1	0.98	0.22	28,28,28,28	0
55	MG	2A	3797	1/1	0.98	0.12	36,36,36,36	0
55	MG	2A	3844	1/1	0.98	0.20	65,65,65,65	0
55	MG	1A	3363	1/1	0.98	0.06	19,19,19,19	0
55	MG	1A	3319	1/1	0.98	0.06	52,52,52,52	0
55	MG	1A	3868	1/1	0.98	0.12	29,29,29,29	0
55	MG	1A	3641	1/1	0.98	0.30	36,36,36,36	0
55	MG	2A	3014	1/1	0.98	0.15	23,23,23,23	0
55	MG	2A	3463	1/1	0.98	0.16	36,36,36,36	0
55	MG	1A	3836	1/1	0.98	0.09	27,27,27,27	0
55	MG	2A	3807	1/1	0.98	0.11	55,55,55,55	0
55	MG	2A	3934	1/1	0.98	0.10	45,45,45,45	0
55	MG	2A	3016	1/1	0.98	0.50	38,38,38,38	0
55	MG	1V	203	1/1	0.98	0.17	29,29,29,29	0
55	MG	1a	1692	1/1	0.98	0.21	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3303	1/1	0.98	0.15	27,27,27,27	0
55	MG	2A	3578	1/1	0.98	0.29	43,43,43,43	0
55	MG	2B	3001	1/1	0.98	0.26	51,51,51,51	0
55	MG	1A	3492	1/1	0.98	0.19	28,28,28,28	0
55	MG	2A	3003	1/1	0.98	0.20	34,34,34,34	0
55	MG	1A	3353	1/1	0.98	0.10	13,13,13,13	0
55	MG	1A	3576	1/1	0.98	0.12	13,13,13,13	0
55	MG	1A	3790	1/1	0.98	0.06	36,36,36,36	0
56	ZN	15	104	1/1	0.98	0.08	37,37,37,37	0
55	MG	1a	1726	1/1	0.98	0.04	68,68,68,68	0
55	MG	1A	3898	1/1	0.98	0.08	58,58,58,58	0
55	MG	1A	3362	1/1	0.98	0.29	38,38,38,38	0
55	MG	2A	3021	1/1	0.98	0.68	44,44,44,44	0
55	MG	1D	305	1/1	0.98	0.13	42,42,42,42	0
55	MG	2A	3890	1/1	0.98	0.23	43,43,43,43	0
55	MG	1A	3594	1/1	0.98	0.25	16,16,16,16	0
55	MG	1A	3377	1/1	0.98	0.14	16,16,16,16	0
55	MG	2I	8001	1/1	0.98	0.07	51,51,51,51	0
55	MG	2A	3015	1/1	0.98	0.50	44,44,44,44	0
55	MG	1A	3076	1/1	0.98	0.26	17,17,17,17	0
55	MG	2A	3084	1/1	0.98	0.53	38,38,38,38	0
55	MG	1A	3652	1/1	0.98	0.13	31,31,31,31	0
55	MG	1A	3807	1/1	0.98	0.08	20,20,20,20	0
55	MG	2A	3228	1/1	0.98	0.14	43,43,43,43	0
55	MG	2A	3090	1/1	0.98	0.07	46,46,46,46	0
55	MG	1A	3289	1/1	0.98	0.12	24,24,24,24	0
55	MG	1A	3746	1/1	0.98	0.10	48,48,48,48	0
55	MG	1a	1712	1/1	0.98	0.19	83,83,83,83	0
55	MG	1B	201	1/1	0.98	0.45	27,27,27,27	0
55	MG	2a	1818	1/1	0.98	0.16	45,45,45,45	0
55	MG	1A	3382	1/1	0.98	0.12	35,35,35,35	0
55	MG	1A	3261	1/1	0.98	0.16	20,20,20,20	0
55	MG	2a	1823	1/1	0.98	0.05	94,94,94,94	0
55	MG	1A	3309	1/1	0.98	0.14	7,7,7,7	0
55	MG	2A	3281	1/1	0.98	0.08	56,56,56,56	0
55	MG	2A	3399	1/1	0.98	0.07	38,38,38,38	0
55	MG	1A	3794	1/1	0.98	0.07	50,50,50,50	0
55	MG	2B	3012	1/1	0.98	0.07	56,56,56,56	0
55	MG	2A	3716	1/1	0.98	0.11	27,27,27,27	0
55	MG	2B	3002	1/1	0.98	0.05	69,69,69,69	0
55	MG	2A	3821	1/1	0.98	0.05	46,46,46,46	0
55	MG	1A	3707	1/1	0.98	0.08	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3666	1/1	0.98	0.14	51,51,51,51	0
55	MG	1A	3859	1/1	0.98	0.06	35,35,35,35	0
55	MG	2A	3099	1/1	0.98	0.22	43,43,43,43	0
55	MG	1A	3469	1/1	0.98	0.19	41,41,41,41	0
55	MG	2A	3711	1/1	0.98	0.07	51,51,51,51	0
55	MG	1A	3062	1/1	0.98	0.38	17,17,17,17	0
55	MG	1B	214	1/1	0.98	0.06	31,31,31,31	0
55	MG	2a	1712	1/1	0.98	0.18	59,59,59,59	0
55	MG	1A	3300	1/1	0.98	0.09	21,21,21,21	0
55	MG	1A	3600	1/1	0.98	0.35	41,41,41,41	0
55	MG	1A	3068	1/1	0.98	0.50	33,33,33,33	0
55	MG	2R	203	1/1	0.98	0.12	16,16,16,16	0
55	MG	1A	3352	1/1	0.98	0.12	11,11,11,11	0
55	MG	2A	3637	1/1	0.98	0.23	39,39,39,39	0
55	MG	1R	202	1/1	0.98	0.11	26,26,26,26	0
55	MG	1A	3933	1/1	0.99	0.12	17,17,17,17	0
55	MG	2A	3300	1/1	0.99	0.06	31,31,31,31	0
55	MG	1A	3348	1/1	0.99	0.15	11,11,11,11	0
55	MG	1A	3917	1/1	0.99	0.18	23,23,23,23	0
57	SF4	2d	501	8/8	0.99	0.14	54,68,91,93	0
55	MG	1A	3345	1/1	0.99	0.14	4,4,4,4	0
55	MG	1A	3810	1/1	0.99	0.03	35,35,35,35	0
55	MG	1A	3200	1/1	0.99	0.37	23,23,23,23	0
55	MG	1A	3429	1/1	0.99	0.18	18,18,18,18	0
55	MG	1A	3331	1/1	0.99	0.20	10,10,10,10	0
56	ZN	19	103	1/1	0.99	0.11	40,40,40,40	0
55	MG	1A	3788	1/1	0.99	0.08	25,25,25,25	0
55	MG	10	105	1/1	0.99	0.06	49,49,49,49	0
55	MG	1A	3463	1/1	0.99	0.09	13,13,13,13	0
55	MG	2A	3078	1/1	0.99	0.14	44,44,44,44	0
55	MG	1A	3427	1/1	0.99	0.08	16,16,16,16	0
55	MG	2A	3775	1/1	0.99	0.09	35,35,35,35	0
55	MG	2E	304	1/1	0.99	0.09	16,16,16,16	0
55	MG	1A	3750	1/1	0.99	0.10	14,14,14,14	0
55	MG	1A	3661	1/1	0.99	0.10	27,27,27,27	0
55	MG	1A	3516	1/1	0.99	0.15	19,19,19,19	0
55	MG	1A	3721	1/1	0.99	0.07	18,18,18,18	0
55	MG	1A	3222	1/1	0.99	0.25	30,30,30,30	0
55	MG	1A	3205	1/1	0.99	0.10	14,14,14,14	0
55	MG	23	101	1/1	0.99	0.25	56,56,56,56	0
55	MG	1A	3791	1/1	0.99	0.11	38,38,38,38	0
55	MG	1A	3573	1/1	0.99	0.22	10,10,10,10	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	ZN	25	105	1/1	0.99	0.06	51,51,51,51	0
55	MG	2A	3354	1/1	0.99	0.09	39,39,39,39	0
55	MG	1A	3223	1/1	0.99	0.09	31,31,31,31	0
55	MG	2a	1711	1/1	0.99	0.03	62,62,62,62	0
55	MG	1A	3578	1/1	0.99	0.25	26,26,26,26	0
55	MG	1A	3824	1/1	0.99	0.04	23,23,23,23	0
55	MG	1A	3460	1/1	0.99	0.15	16,16,16,16	0
55	MG	1A	3689	1/1	0.99	0.11	20,20,20,20	0
55	MG	2A	3024	1/1	0.99	0.09	31,31,31,31	0
55	MG	2A	3312	1/1	0.99	0.10	23,23,23,23	0
55	MG	1a	1710	1/1	0.99	0.06	38,38,38,38	0
55	MG	1P	202	1/1	0.99	0.22	17,17,17,17	0
55	MG	1A	3087	1/1	0.99	0.08	30,30,30,30	0
55	MG	1A	3208	1/1	0.99	0.34	16,16,16,16	0
56	ZN	16	101	1/1	0.99	0.11	34,34,34,34	0
55	MG	1A	3771	1/1	0.99	0.16	20,20,20,20	0
55	MG	1Q	201	1/1	0.99	0.05	27,27,27,27	0
55	MG	1A	3821	1/1	0.99	0.12	33,33,33,33	0
55	MG	1A	3260	1/1	0.99	0.13	10,10,10,10	0
55	MG	2A	3170	1/1	0.99	0.36	48,48,48,48	0
55	MG	2A	3433	1/1	0.99	0.20	33,33,33,33	0
55	MG	1A	3892	1/1	0.99	0.16	27,27,27,27	0
55	MG	1Q	204	1/1	0.99	0.15	28,28,28,28	0
55	MG	1A	3614	1/1	0.99	0.42	32,32,32,32	0
55	MG	1A	3601	1/1	0.99	0.24	57,57,57,57	0
55	MG	1B	213	1/1	0.99	0.15	21,21,21,21	0
55	MG	1a	1700	1/1	0.99	0.04	75,75,75,75	0
55	MG	2A	3196	1/1	0.99	0.17	29,29,29,29	0
55	MG	2A	3946	1/1	0.99	0.08	24,24,24,24	0
55	MG	1A	3273	1/1	0.99	0.14	21,21,21,21	0
55	MG	1A	3473	1/1	0.99	0.04	20,20,20,20	0
55	MG	1A	3316	1/1	0.99	0.02	36,36,36,36	0
55	MG	1A	3079	1/1	0.99	0.21	36,36,36,36	0
55	MG	1A	3386	1/1	0.99	0.12	18,18,18,18	0
55	MG	2A	3278	1/1	0.99	0.29	38,38,38,38	0
55	MG	1D	308	1/1	0.99	0.46	27,27,27,27	0
55	MG	2A	3044	1/1	0.99	0.21	26,26,26,26	0
55	MG	1A	3805	1/1	0.99	0.04	34,34,34,34	0
55	MG	1A	3307	1/1	0.99	0.12	12,12,12,12	0
55	MG	1A	3572	1/1	0.99	0.19	34,34,34,34	0
55	MG	2A	3760	1/1	0.99	0.16	31,31,31,31	0
55	MG	2A	3379	1/1	0.99	0.14	15,15,15,15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3822	1/1	0.99	0.09	50,50,50,50	0
55	MG	1A	3381	1/1	0.99	0.13	19,19,19,19	0
55	MG	1P	201	1/1	0.99	0.08	23,23,23,23	0
56	ZN	26	101	1/1	0.99	0.08	57,57,57,57	0
55	MG	1A	3765	1/1	0.99	0.05	38,38,38,38	0
55	MG	1A	3105	1/1	0.99	0.35	33,33,33,33	0
55	MG	2A	3190	1/1	0.99	0.19	35,35,35,35	0
55	MG	2A	3234	1/1	0.99	0.11	29,29,29,29	0
55	MG	2a	1831	1/1	0.99	0.22	67,67,67,67	0
55	MG	2A	3238	1/1	0.99	0.37	30,30,30,30	0
55	MG	2A	3053	1/1	0.99	0.23	37,37,37,37	0
55	MG	2A	3899	1/1	0.99	0.05	29,29,29,29	0
55	MG	1A	3066	1/1	0.99	0.40	23,23,23,23	0
55	MG	1A	3870	1/1	0.99	0.09	47,47,47,47	0
55	MG	2A	3529	1/1	0.99	0.18	21,21,21,21	0
55	MG	1A	3942	1/1	0.99	0.20	10,10,10,10	0
55	MG	1A	3021	1/1	0.99	0.21	26,26,26,26	0
55	MG	1A	3278	1/1	0.99	0.10	42,42,42,42	0
55	MG	1A	3458	1/1	0.99	0.12	14,14,14,14	0
55	MG	1A	3400	1/1	0.99	0.06	35,35,35,35	0
55	MG	1A	3500	1/1	0.99	0.09	44,44,44,44	0
55	MG	2A	3128	1/1	0.99	0.14	39,39,39,39	0
55	MG	1A	3017	1/1	0.99	0.32	9,9,9,9	0
57	SF4	1d	302	8/8	0.99	0.13	46,61,71,75	0
55	MG	1A	3496	1/1	0.99	0.08	40,40,40,40	0
55	MG	2A	3305	1/1	0.99	0.10	31,31,31,31	0
55	MG	1A	3841	1/1	0.99	0.06	20,20,20,20	0
55	MG	1A	3447	1/1	0.99	0.08	29,29,29,29	0
55	MG	2A	3105	1/1	0.99	0.47	39,39,39,39	0
55	MG	1A	3234	1/1	0.99	0.05	66,66,66,66	0
55	MG	2A	3315	1/1	0.99	0.18	25,25,25,25	0
55	MG	1A	3350	1/1	0.99	0.16	14,14,14,14	0
55	MG	1A	3232	1/1	0.99	0.16	16,16,16,16	0
55	MG	2A	3351	1/1	0.99	0.22	22,22,22,22	0
55	MG	1E	303	1/1	0.99	0.15	11,11,11,11	0
55	MG	1A	3856	1/1	0.99	0.12	34,34,34,34	0
55	MG	2D	302	1/1	0.99	0.37	28,28,28,28	0
55	MG	2A	3215	1/1	0.99	0.34	38,38,38,38	0
55	MG	2A	3134	1/1	0.99	0.10	40,40,40,40	0
55	MG	1A	3662	1/1	0.99	0.06	36,36,36,36	0
55	MG	1A	3401	1/1	0.99	0.11	21,21,21,21	0
55	MG	1A	3263	1/1	1.00	0.09	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3402	1/1	1.00	0.09	12,12,12,12	0
55	MG	1A	3130	1/1	1.00	0.08	14,14,14,14	0
55	MG	1A	3850	1/1	1.00	0.24	43,43,43,43	0
55	MG	1A	3180	1/1	1.00	0.20	24,24,24,24	0
55	MG	1A	3121	1/1	1.00	0.11	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.