



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 11:16 pm BST

PDB ID : 4Z8C  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome bound to translation inhibitor oncocin  
Authors : Roy, R.N.; Lomakin, I.B.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : 2015-04-08  
Resolution : 2.90 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

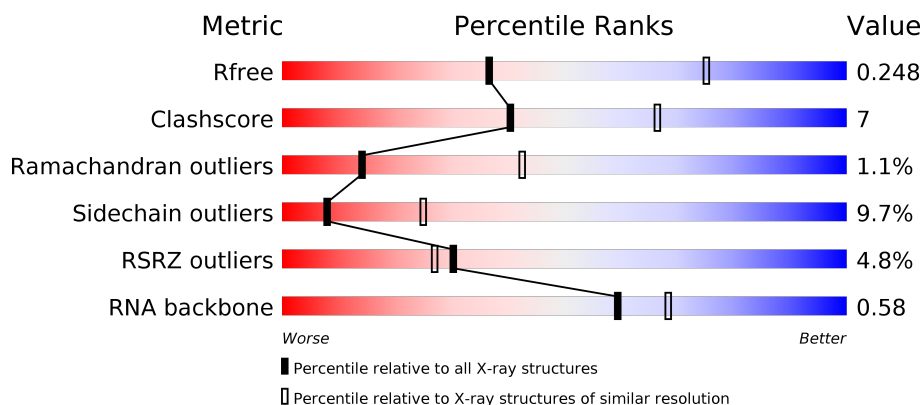
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	 67% 23% 6%
1	2A	2915	 62% 29% 5%
2	1B	121	 72% 25%
2	2B	121	 55% 38% 6%

*Continued on next page...*

Continued from previous page...

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




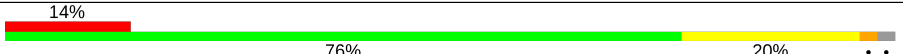
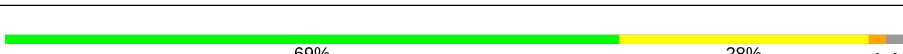
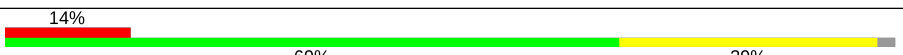
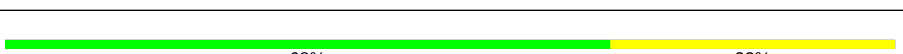
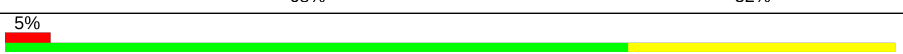

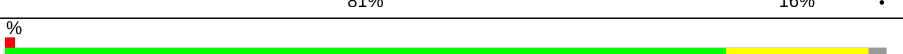

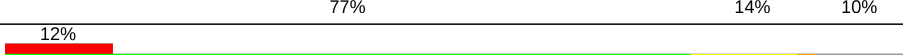
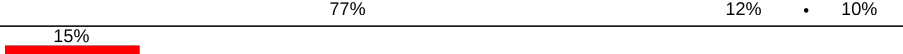
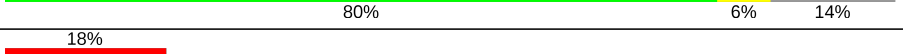





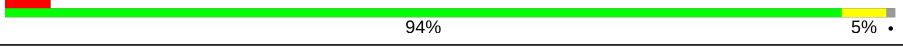
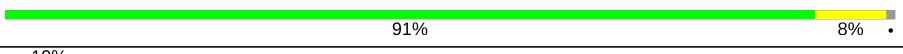

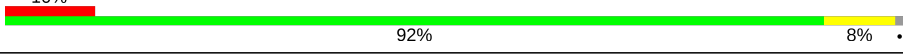
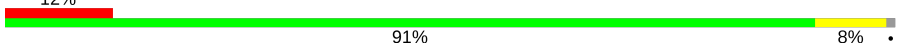

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	% 68% 18% 10% .
16	1U	118	79% 18% . .
16	2U	118	81% 16% . .
17	1V	101	80% 16% . .
17	2V	101	3% 68% 27% . .
18	1W	113	2% 83% 15% . .
18	2W	113	2% 83% 14% . .
19	1X	96	% 80% 19% .
19	2X	96	3% 76% 21% . .
20	1Y	110	% 71% 25% . .
20	2Y	110	5% 74% 21% . .
21	1Z	206	71% 17% . 10%
21	2Z	206	3% 60% 25% 5% 10%
22	10	85	69% 16% . 12%
22	20	85	13% 72% 15% . 12%
23	11	98	2% 73% 23% . .
23	21	98	6% 73% 21% . .
24	12	72	4% 76% 17% . .
24	22	72	% 82% 14% . .
25	13	60	78% 18% . .
25	23	60	88% 8% . .
26	14	71	10% 55% 28% 13% . .
26	24	71	14% 55% 31% 10% . .
27	15	60	2% 90% 7% . .
27	25	60	82% 12% 5% .

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	19	
55	2z	19	

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
56	MG	15	101	-	-	-	X
56	MG	1A	3028	-	-	-	X
56	MG	1A	3035	-	-	-	X
56	MG	1A	3044	-	-	-	X
56	MG	1A	3057	-	-	-	X
56	MG	1A	3132	-	-	-	X
56	MG	1A	3392	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3417	-	-	-	X
56	MG	1A	3464	-	-	-	X
56	MG	1A	3508	-	-	-	X
56	MG	1A	3977	-	-	-	X
56	MG	1D	304	-	-	-	X
56	MG	1F	308	-	-	-	X
56	MG	1H	8002	-	-	-	X
56	MG	1N	3002	-	-	-	X
56	MG	1Q	3003	-	-	-	X
56	MG	1a	1765	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3554	-	-	-	X
56	MG	2A	3562	-	-	-	X
56	MG	2a	3173	-	-	-	X
56	MG	2a	3241	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288378 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	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

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

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

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- 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
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	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
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	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
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	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
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- 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
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	3			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	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
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	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
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	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
			715	447	140	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
			671	424	133	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			811	519	148	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	84	Total	C	N	O	S	0	0	0
			642	409	119	112	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	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
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called Initiator Methionine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
54	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 55 is a protein called Oncocin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	13	Total	C	N	O	0	0	0
			108	72	20	16			
55	2z	13	Total	C	N	O	0	0	0
			108	72	20	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	4	Total	Mg	0	0
			4	4		
56	17	1	Total	Mg	0	0
			1	1		
56	1z	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	5	Total	Mg	0	0
			5	5		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	1	Total	Mg	0	0
			1	1		
56	18	3	Total	Mg	0	0
			3	3		
56	1o	2	Total	Mg	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	2h	1	Total 1	Mg 1	0	0
56	1P	6	Total 6	Mg 6	0	0
56	2B	11	Total 11	Mg 11	0	0
56	1q	4	Total 4	Mg 4	0	0
56	2a	263	Total 263	Mg 263	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1E	5	Total 5	Mg 5	0	0
56	2z	1	Total 1	Mg 1	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	6	Total 6	Mg 6	0	0
56	16	2	Total 2	Mg 2	0	0
56	28	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1021	Total 1021	Mg 1021	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	2	Total 2	Mg 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	12	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	1D	14	Total 14	Mg 14	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	1	Total 1	Mg 1	0	0
56	1a	276	Total 276	Mg 276	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	4	Total 4	Mg 4	0	0
56	1x	8	Total 8	Mg 8	0	0
56	1R	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	2U	1	Total 1	Mg 1	0	0
56	1G	3	Total 3	Mg 3	0	0
56	2O	3	Total 3	Mg 3	0	0
56	11	1	Total 1	Mg 1	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1H	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2x	4	Total 4	Mg 4	0	0
56	1Z	2	Total 2	Mg 2	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1O	2	Total 2	Mg 2	0	0
56	1r	2	Total 2	Mg 2	0	0
56	19	3	Total 3	Mg 3	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1F	8	Total 8	Mg 8	0	0
56	10	7	Total 7	Mg 7	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	2A	566	Total 566	Mg 566	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	24	Total 24	Mg 24	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

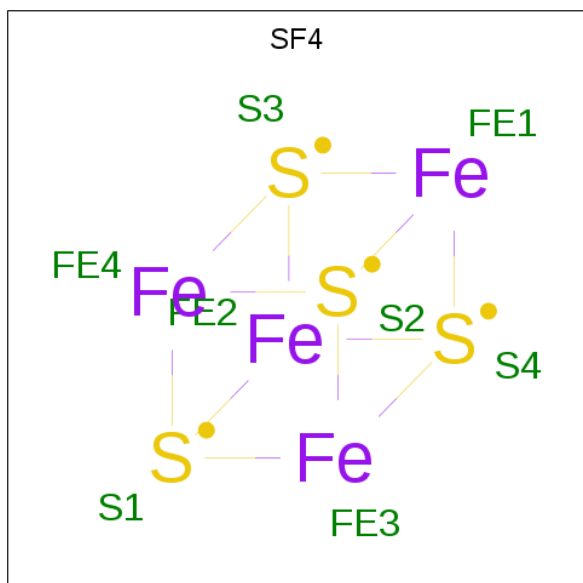
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2088	Total	O	0	0
			2088	2088		
59	1B	38	Total	O	0	0
			38	38		
59	1D	22	Total	O	0	0
			22	22		
59	1E	25	Total	O	0	0
			25	25		
59	1F	16	Total	O	0	0
			16	16		
59	1G	6	Total	O	0	0
			6	6		
59	1H	5	Total	O	0	0
			5	5		
59	1I	1	Total	O	0	0
			1	1		
59	1N	5	Total	O	0	0
			5	5		
59	1O	4	Total	O	0	0
			4	4		
59	1P	21	Total	O	0	0
			21	21		
59	1Q	9	Total	O	0	0
			9	9		
59	1R	9	Total	O	0	0
			9	9		
59	1S	1	Total	O	0	0
			1	1		
59	1T	11	Total	O	0	0
			11	11		
59	1U	13	Total	O	0	0
			13	13		
59	1V	2	Total	O	0	0
			2	2		
59	1W	9	Total	O	0	0
			9	9		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	5	Total 5	O 5	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	3	Total 3	O 3	0	0
59	10	10	Total 10	O 10	0	0
59	11	4	Total 4	O 4	0	0
59	12	1	Total 1	O 1	0	0
59	13	4	Total 4	O 4	0	0
59	15	5	Total 5	O 5	0	0
59	16	8	Total 8	O 8	0	0
59	17	8	Total 8	O 8	0	0
59	18	13	Total 13	O 13	0	0
59	19	2	Total 2	O 2	0	0
59	1a	319	Total 319	O 319	0	0
59	1b	2	Total 2	O 2	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	4	Total 4	O 4	0	0
59	1e	2	Total 2	O 2	0	0
59	1f	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1m	1	Total 1	O 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1o	3	Total 3	O 3	0	0
59	1p	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	1	Total 1	O 1	0	0
59	1x	7	Total 7	O 7	0	0
59	1z	2	Total 2	O 2	0	0
59	2A	801	Total 801	O 801	0	0
59	2B	13	Total 13	O 13	0	0
59	2D	20	Total 20	O 20	0	0
59	2E	10	Total 10	O 10	0	0
59	2F	7	Total 7	O 7	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	4	Total 4	O 4	0	0
59	2P	4	Total 4	O 4	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
59	2T	3	Total 3	O 3	0	0
59	2U	2	Total 2	O 2	0	0
59	2V	2	Total 2	O 2	0	0
59	2W	2	Total 2	O 2	0	0
59	2X	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

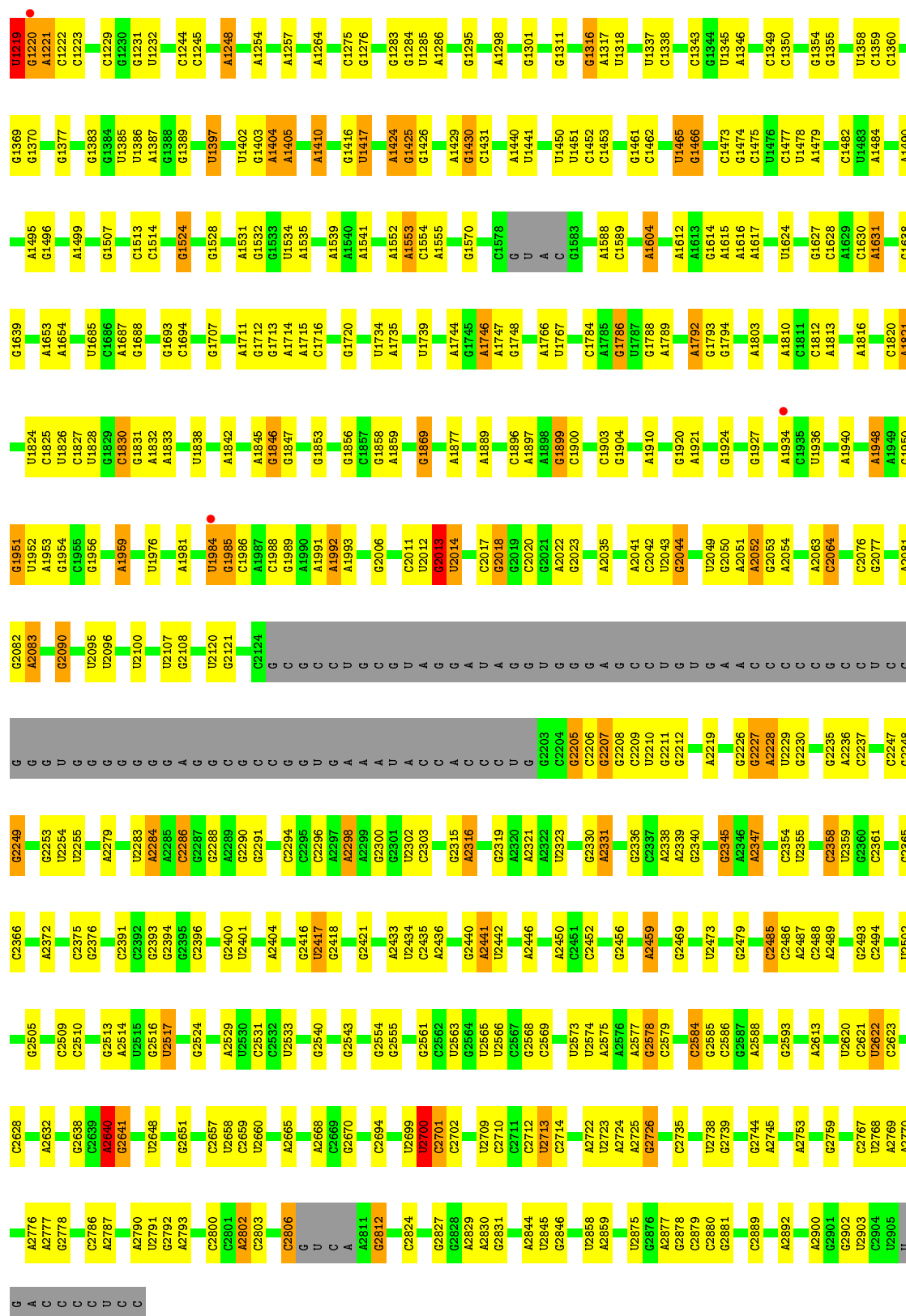
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2Y	1	Total 1	O 1	0	0
59	2Z	2	Total 2	O 2	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	27	2	Total 2	O 2	0	0
59	28	4	Total 4	O 4	0	0
59	2a	371	Total 371	O 371	0	0
59	2c	2	Total 2	O 2	0	0
59	2e	3	Total 3	O 3	0	0
59	2h	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2j	1	Total 1	O 1	0	0
59	2k	3	Total 3	O 3	0	0
59	2l	3	Total 3	O 3	0	0
59	2m	1	Total 1	O 1	0	0
59	2n	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	2	Total 2	O 2	0	0
59	2q	2	Total 2	O 2	0	0

*Continued on next page...*

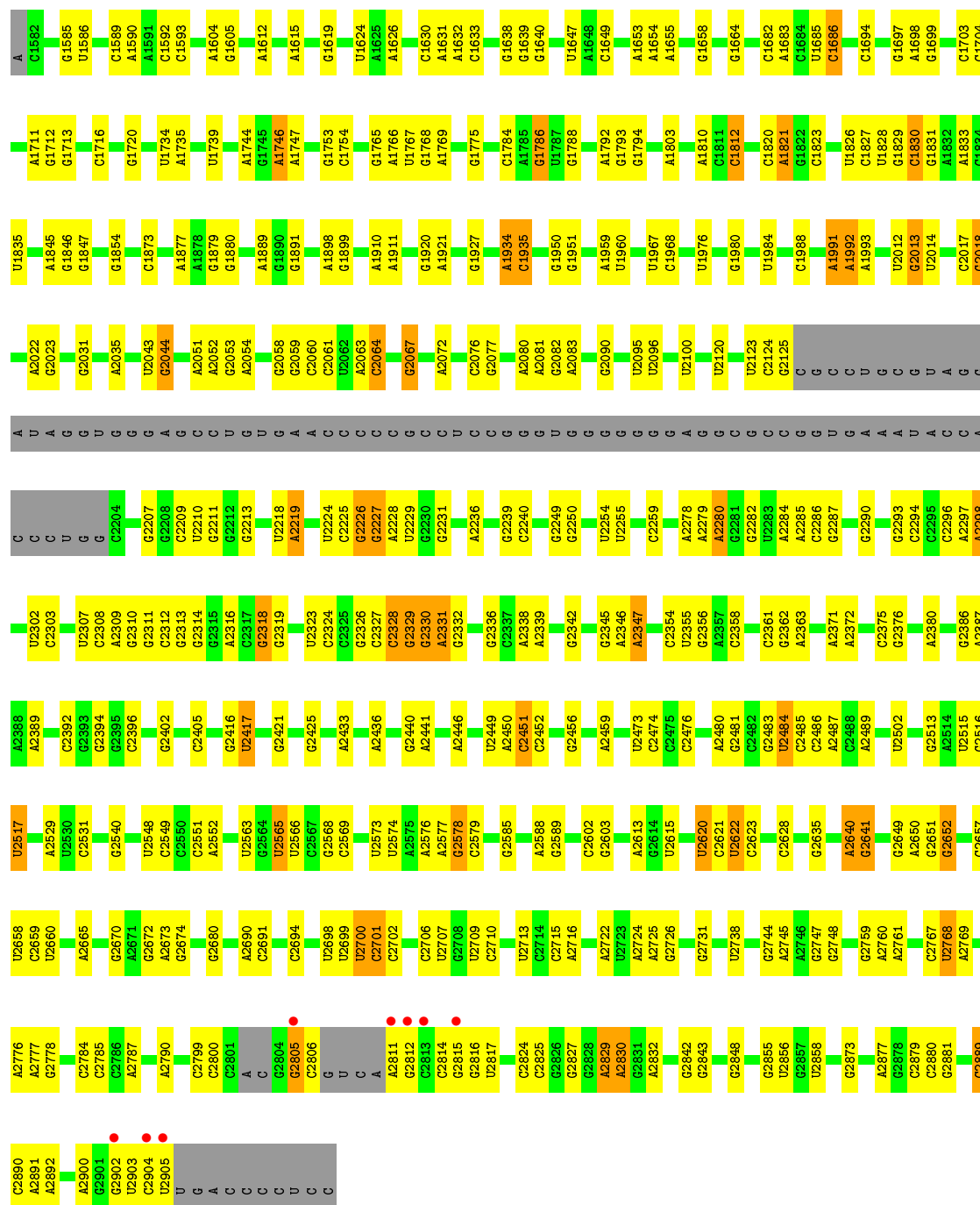
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2r	1	Total	O	0	0
			1	1		
59	2t	3	Total	O	0	0
			3	3		
59	2x	3	Total	O	0	0
			3	3		
59	2z	1	Total	O	0	0
			1	1		





U1451	A1346	U	U1128	A1066	C960	A865	G756	A655	C555	G436	G298	A187	U88	G
C1452	G1354	G	A1129	G1067	G961	U872	G763	A658	A556	G437	A299	A193	G93	U
G1461	G1355	A	A1130	U1068	A962	U873	G763	C658	G557	A438	A300	G193	G94	C
C1462	G1356	C1222	A1131	G1069	A963	U874	C767	C659	U558	A448	A301	G200	G95	A
U1465	U1357	G1231	A1132	U1071	G964	U879	C768	A661	C559	A454	C309	A201	G96	G6
G1466	U1358	U1232	G1134	A1072	U967	U885	C769	G662	C560	A468	C310	G202	U97	A7
U1470	C1359	U1135	U1135	A1073	C968	C886	U770	C664	C561	C469	C311	A204	G98	U8
G1473	U1361	G1234	A1141	G1075	G972	G894	C776	C668	A568	C470	C320	A206	G99	G9
C1475	U1142	G1076	U1142	C777	G973	A895	C778	C669	A	G471	C321	A209	U11	U11
U1477	U1143	U1078	U1143	G779	G976	U895	C779	A670	G572	C478	A322	A210	A12	A12
A1490	U1150	U1080	U1150	U786	G984	G898	U786	G675	G573	C479	A323	A217	G103	A13
G1494	G1151	G1081	G1151	G806	A985	G899	G806	A678	G585	C480	A324	G228	C104	G14
A1495	U1152	G1082	U1152	A807	G988	G900	A807	C587	C587	C481	G330	A221	U105	G15
G1496	U1153	U1083	U1153	U808	A989	G901	U808	U588	U588	A482	G331	G222	G113	G22
G1501	C1154	G1084	C1154	G809	G990	C902	G809	A679	A589	G493	G332	U223	G114	G23
A1506	G1155	U1085	G1155	G811	G991	C903	G811	G681	U590	G494	A333	U224	A115	U24
C1510	A1156	G1086	A1156	G816	G992	G905	G816	G	A593	A495	A334	C225	A116	G25
G1512	U1157	G1087	U1157	G820	G993	G908	G820	C	A594	A496	A343	G228	U27	A27
C1513	U1158	G1088	U1158	A820	G1000	G909	A820	C	A595	A497	A344	A232	G128	U28
A1517	C1161	A1090	C1161	A821	A1001	A909	A821	C	A596	G501	A345	G131	G29	G29
G1528	G1162	A1091	G1162	G822	U1002	G910	G822	C	C596	A504	A346	A232	C33	C30
U1534	C1163	C1005	C1163	G823	C1005	G920	G823	C	A597	A505	A347	G135	G136	C33
A1535	U1167	G1018	U1167	U825	G1018	G921	U825	A	U598	G506	A350	G235	G137	G34
C1538	G1170	C1019	G1170	A828	C1019	A924	A828	C	A600	A507	A351	G237	A138	C44
U1542	U1171	C1097	U1171	A829	G1097	G925	A829	C	A608	A508	A352	C241	G141	C45
A1553	C1179	A1102	C1179	A834	A1025	G926	A834	C	C609	A516	A353	G242	G151	G49
C1554	G1180	G1103	G1180	A835	A1026	G927	A835	C	U610	G517	A354	A253	C152	A50
A1555	U1181	G1104	U1181	C836	C1037	G928	C836	C	C611	G518	G360	G253	G153	G53
G1557	G1182	U1105	G1182	C837	G1038	G929	C837	C	A609	G524	G361	A258	C154	A54
U1561	U1183	C1039	U1183	G838	C1039	G930	G838	C	U628	A527	G364	G259	U155	C55
G1562	U1184	G1107	U1184	C841	C1040	C935	C841	C	A625	U528	G365	A260	U	G56
C1573	U1185	C1109	U1185	C842	A1041	A936	C842	C	U630	A529	G375	U264	U	U57
A1574	U1186	U1110	U1186	C843	G1042	G937	C843	C	A631	G530	G385	U265	G159	G59
G1575	A1187	U1111	A1187	C846	G1047	C938	C846	C	C627	A531	G386	C285	G166	A62
U1579	U1194	G1112	U1194	A846	C1049	C939	A846	C	U628	A532	G387	G286	G170	G66
U	C1195	A1113	C1195	A851	C1050	A941	A851	C	A630	A533	G398	G287	C171	C67
	U1195	A1114	U1195	C852	G1056	A945	C852	C	A631	G536	G408	U271	U173	G68
	C1198	G1116	C1198	U853	U1057	A946	U853	C	C634	A540	U409	G272	G177	U70
	U1199	G1117	U1199	G855	U1057	C947	G855	C	C635	C541	U410	G273	A178	A71
	A1200	U1118	A1200	G855	C1058	C948	G855	C	U543	C411	G412	G274	A179	A72
	U1211	G1119	U1211	C858	U1059	U948	C858	C	C544	G417	G417	G282	C180	G73
	U1212	C1120	U1212	C859	G1060	A954	C859	C	A550	G424	G424	G283	U181	G78
	G1216	G1121	G1216	A855	G1062	A955	A855	C	A551	G428	G428	G287	G182	G79
	A	A1122	A	A956	C1063	A956	A956	C	A552	U431	U431	G288	A183	G80
	U1126	U1126	U1126	C963	U1064	C963	C963	C	G554				A184	G81
	U1127	U1127	U1127	G864	A1065		G864	C	A651					A82



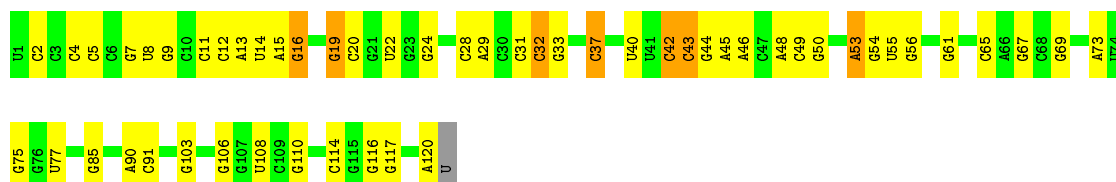
- Molecule 2: 5S ribosomal RNA

Chain 1B: 72% 25% ..

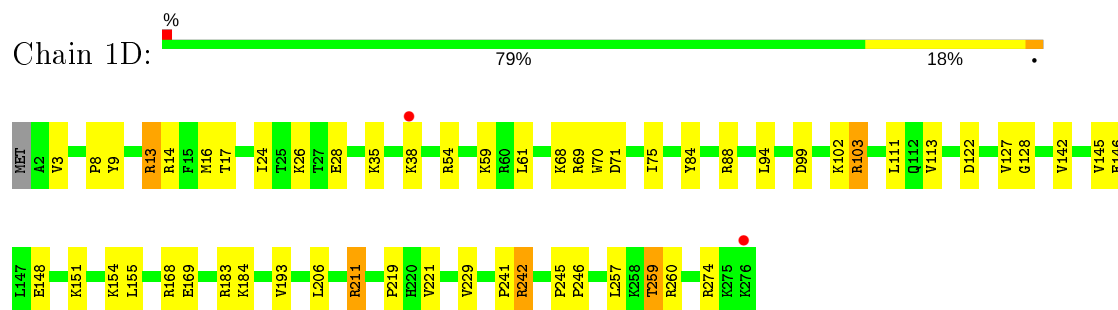


- Molecule 2: 5S ribosomal RNA

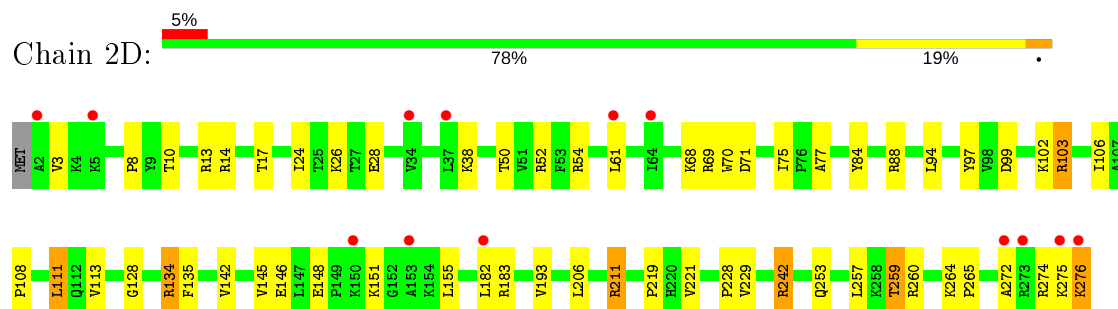
Chain 2B: 55% 38% 6% .



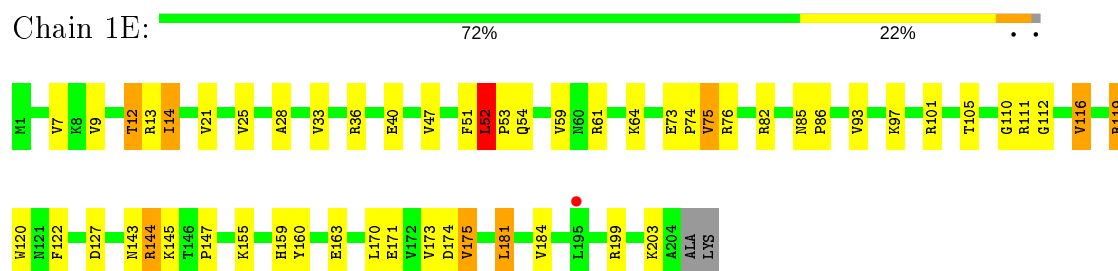
- Molecule 3: 50S ribosomal protein L2



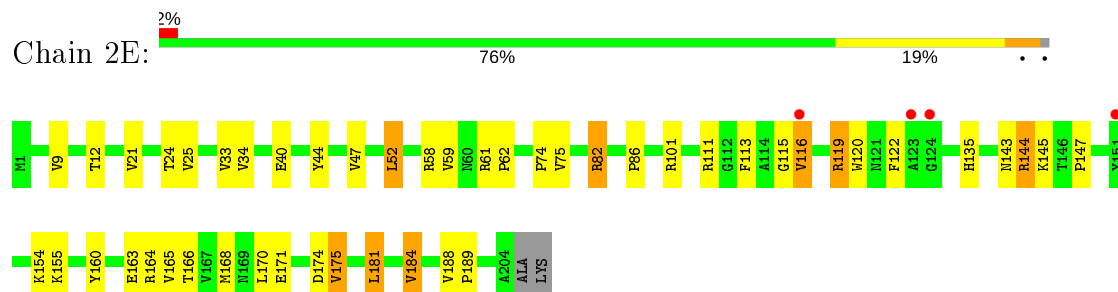
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

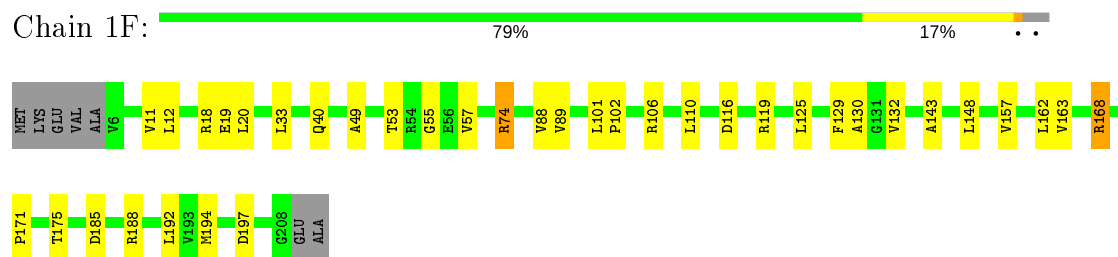


- Molecule 4: 50S ribosomal protein L3

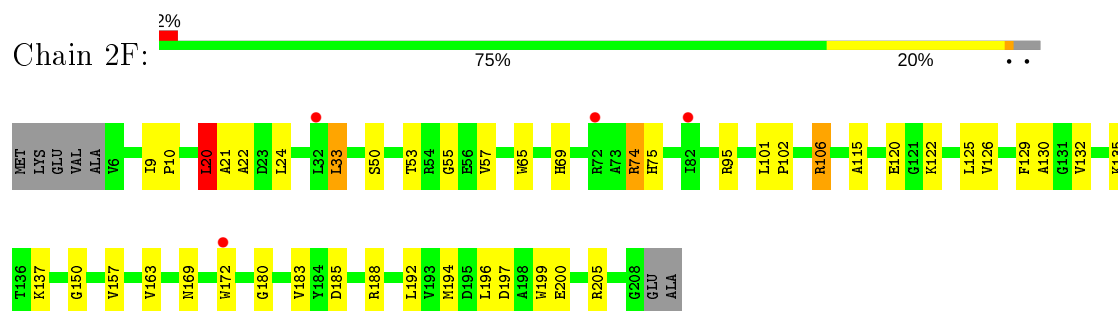


- Molecule 5: 50S ribosomal protein L4

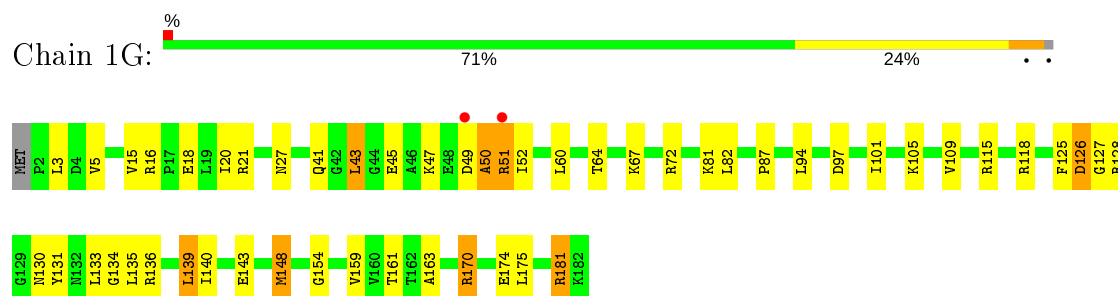




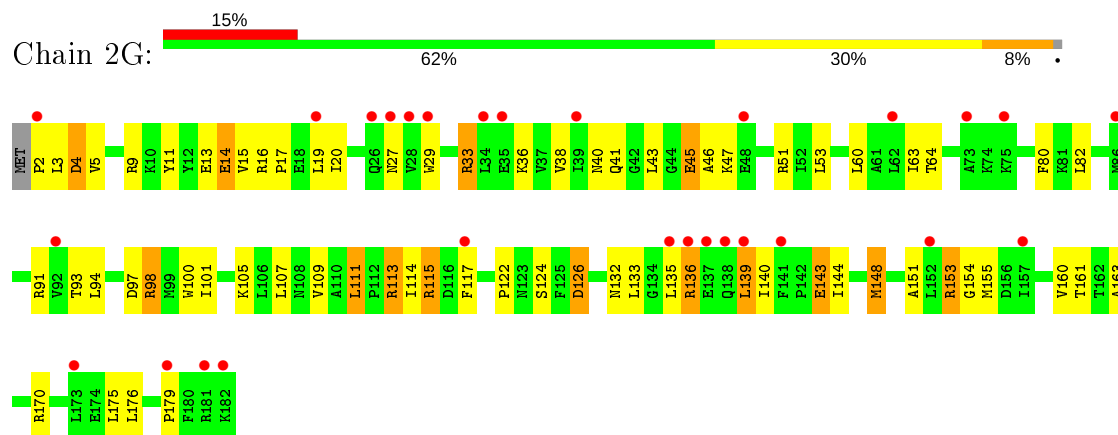
- Molecule 5: 50S ribosomal protein L4



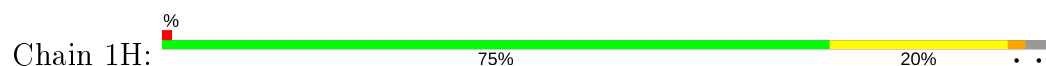
- Molecule 6: 50S ribosomal protein L5

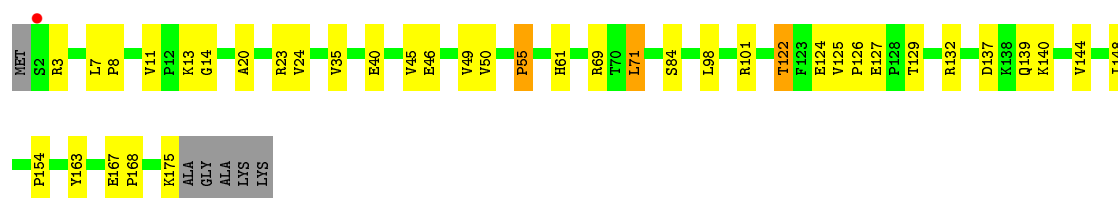


- Molecule 6: 50S ribosomal protein L5

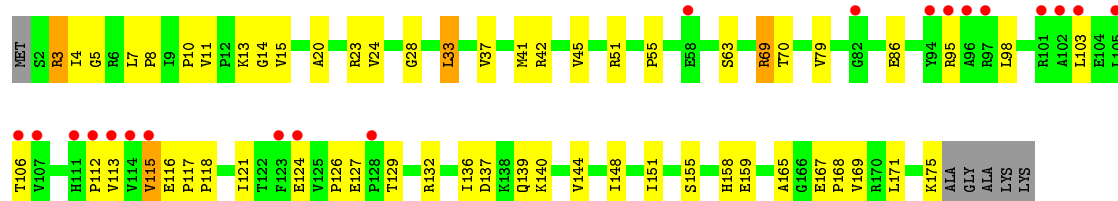


- Molecule 7: 50S ribosomal protein L6

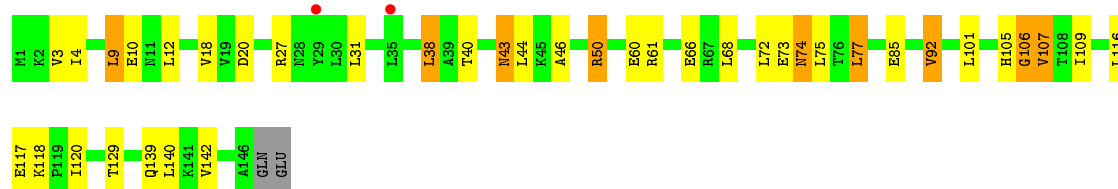
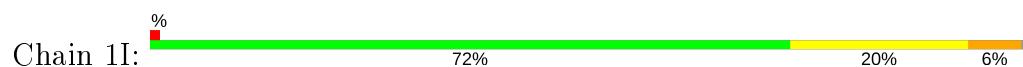




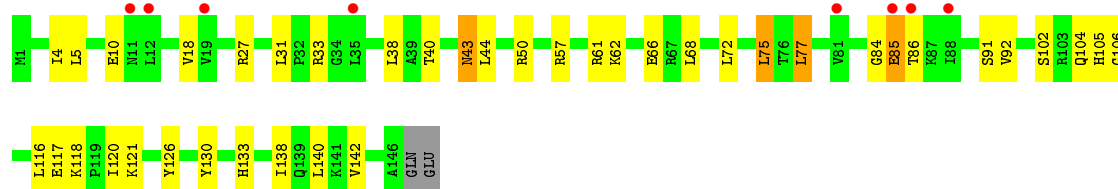
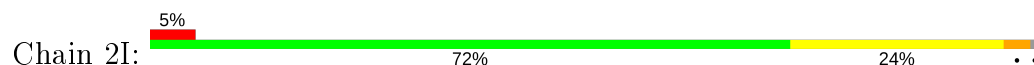
• Molecule 7: 50S ribosomal protein L6



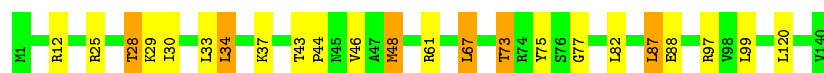
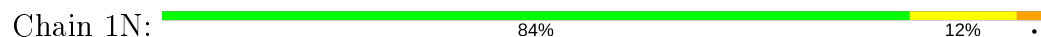
• Molecule 8: 50S ribosomal protein L9



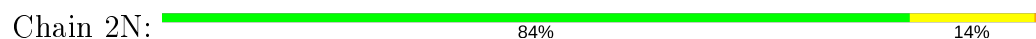
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13

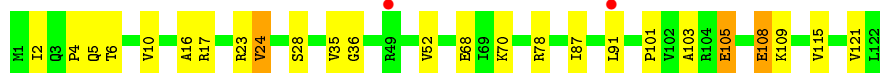
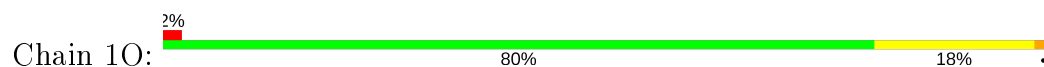


• Molecule 9: 50S ribosomal protein L13

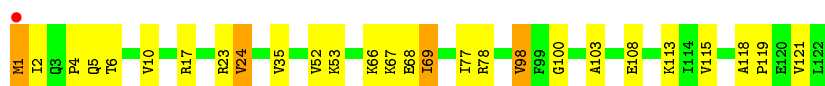
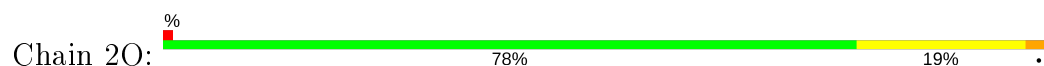




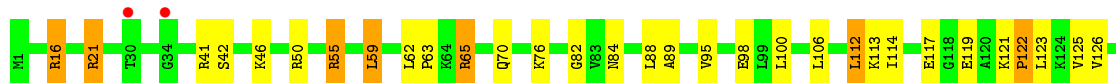
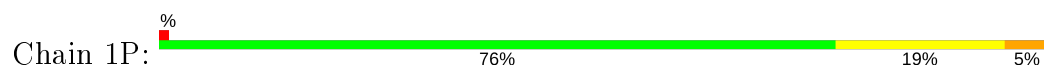
- Molecule 10: 50S ribosomal protein L14



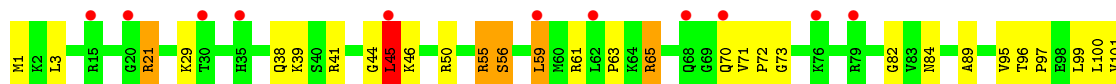
- Molecule 10: 50S ribosomal protein L14



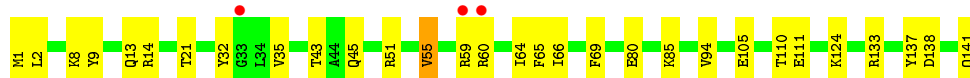
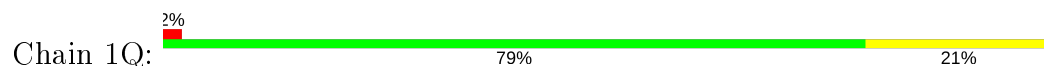
- Molecule 11: 50S ribosomal protein L15



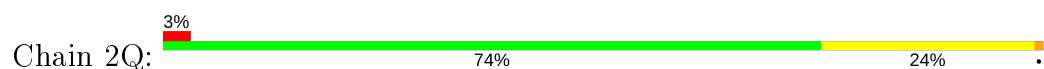
- Molecule 11: 50S ribosomal protein L15

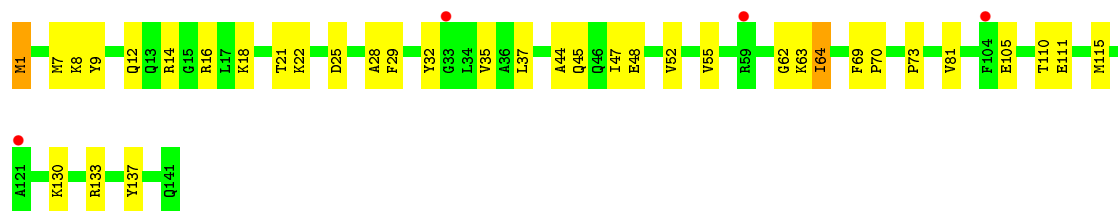


- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16





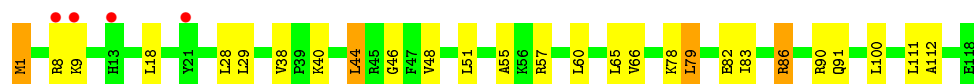
- Molecule 13: 50S ribosomal protein L17

Chain 1R: 80% 18% •



- Molecule 13: 50S ribosomal protein L17

Chain 2R: 3% 77% 19% •



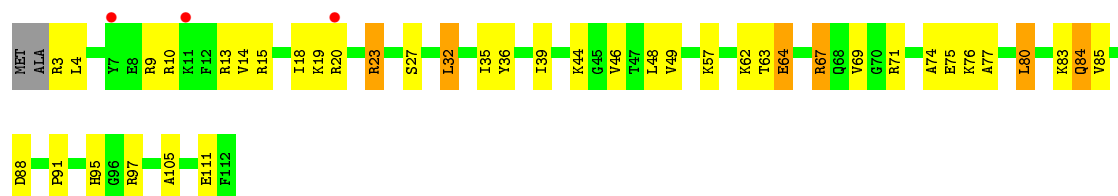
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 75% 21% • •



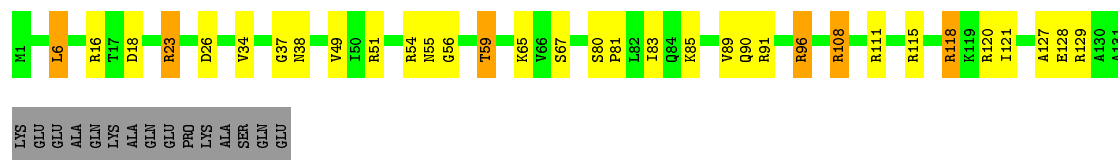
- Molecule 14: 50S ribosomal protein L18

Chain 2S: 3% 62% 31% 5% •

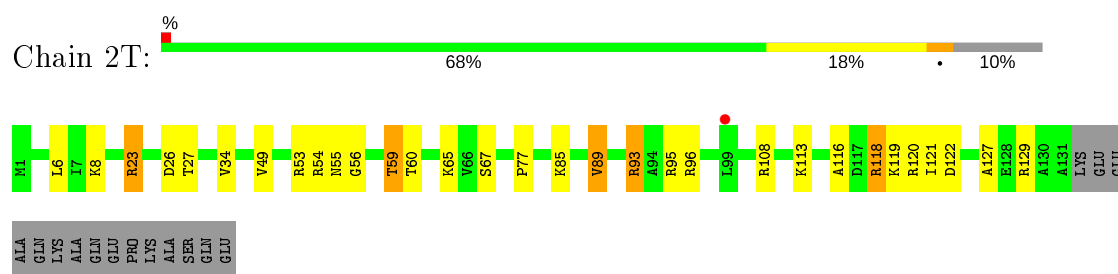


- Molecule 15: 50S ribosomal protein L19

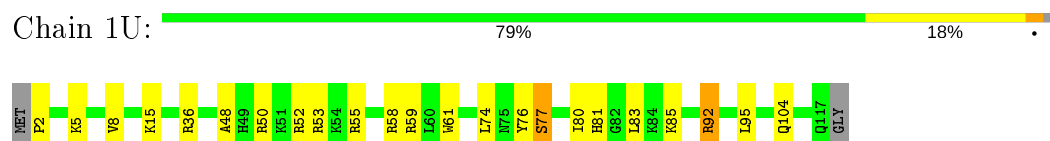
Chain 1T: 67% 18% 10% •



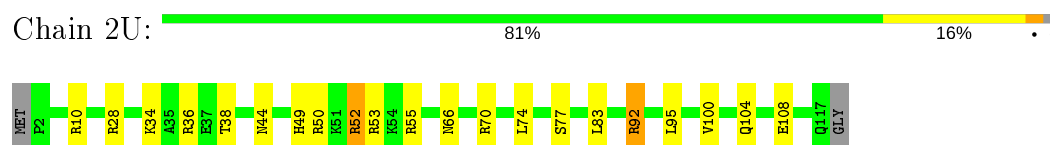
- Molecule 15: 50S ribosomal protein L19



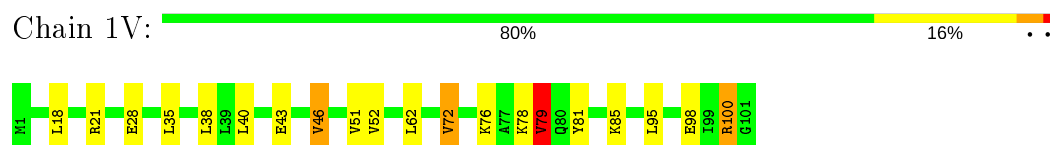
- Molecule 16: 50S ribosomal protein L20



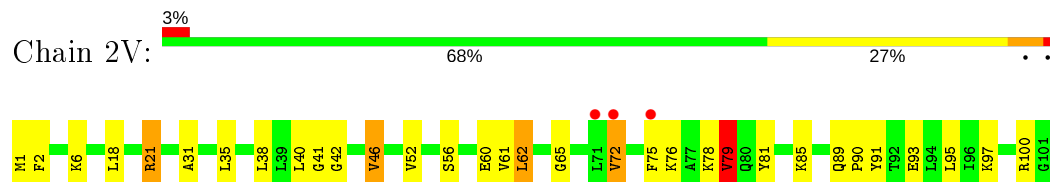
- Molecule 16: 50S ribosomal protein L20



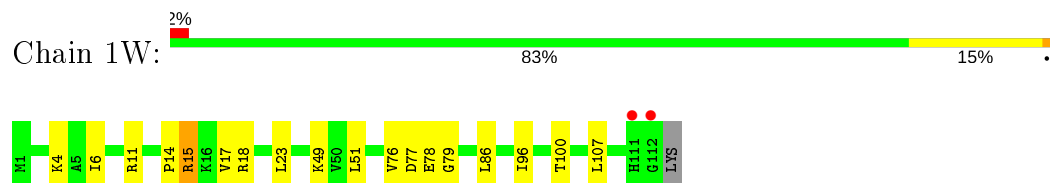
- Molecule 17: 50S ribosomal protein L21



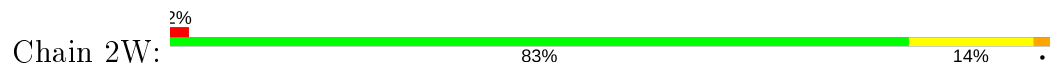
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22

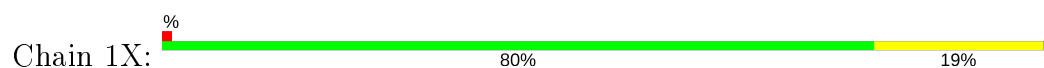


- Molecule 18: 50S ribosomal protein L22

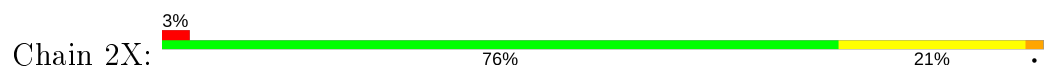




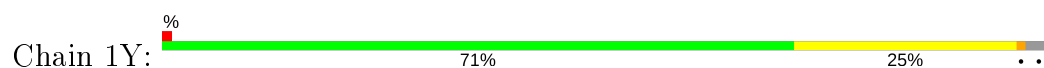
- Molecule 19: 50S ribosomal protein L23



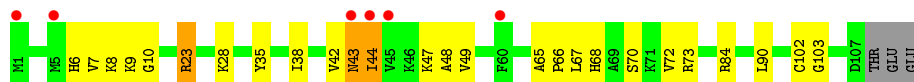
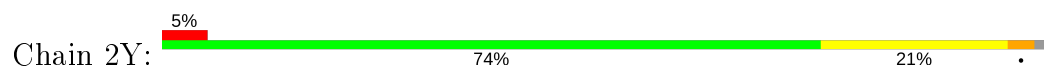
- Molecule 19: 50S ribosomal protein L23



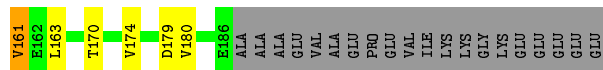
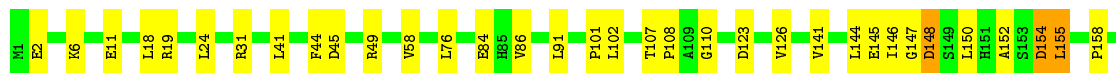
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

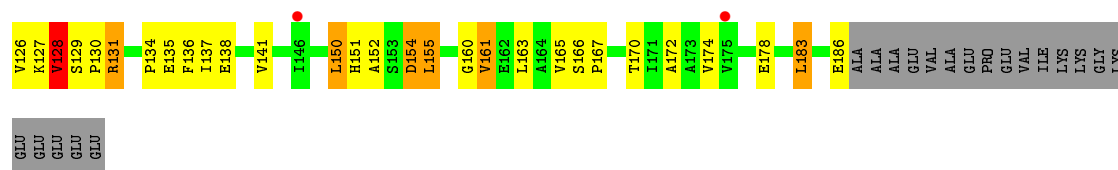


- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25





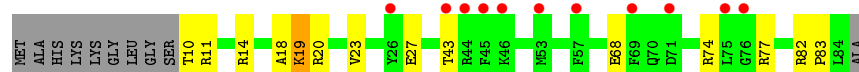
- Molecule 22: 50S ribosomal protein L27

Chain 10: 69% 16% 12%



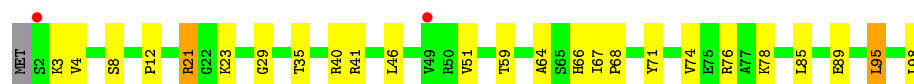
- Molecule 22: 50S ribosomal protein L27

Chain 20: 13% 72% 15% 12%



- Molecule 23: 50S ribosomal protein L28

Chain 11: 2% 73% 23%



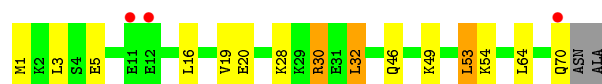
- Molecule 23: 50S ribosomal protein L28

Chain 21: 6% 73% 21%



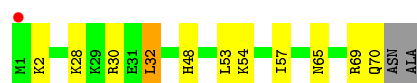
- Molecule 24: 50S ribosomal protein L29

Chain 12: 4% 76% 17%




- Molecule 24: 50S ribosomal protein L29

Chain 22: 82% 14%



- Molecule 25: 50S ribosomal protein L30

Chain 13:  78% 18% ..



- Molecule 25: 50S ribosomal protein L30

Chain 23:  88% 8% ..



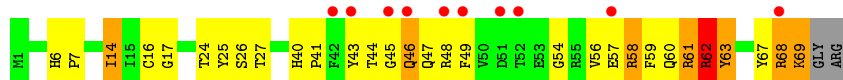
- Molecule 26: 50S ribosomal protein L31

Chain 14:  10% 55% 28% 13% ..




- Molecule 26: 50S ribosomal protein L31

Chain 24:  14% 55% 31% 10% ..




- Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 90% 7% ..




- Molecule 27: 50S ribosomal protein L32

Chain 25:  82% 12% 5% .



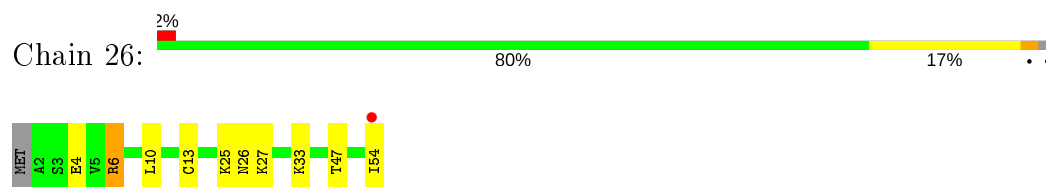
- Molecule 28: 50S ribosomal protein L33

Chain 16:  85% 9% ..

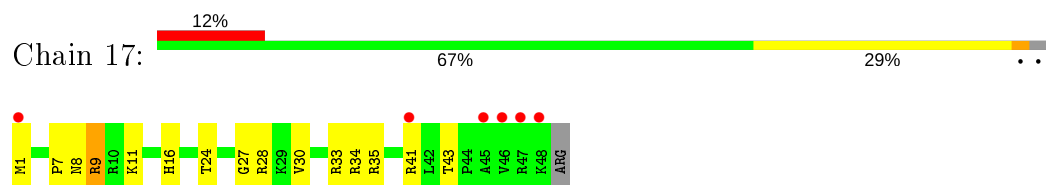




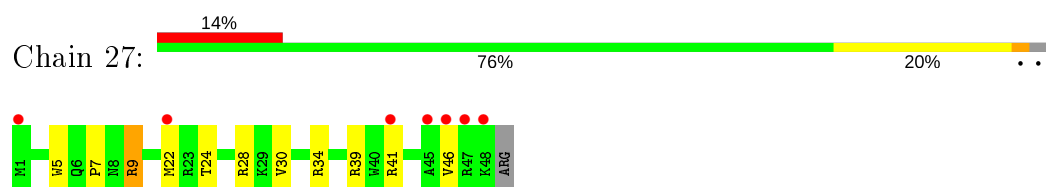
## • Molecule 28: 50S ribosomal protein L33



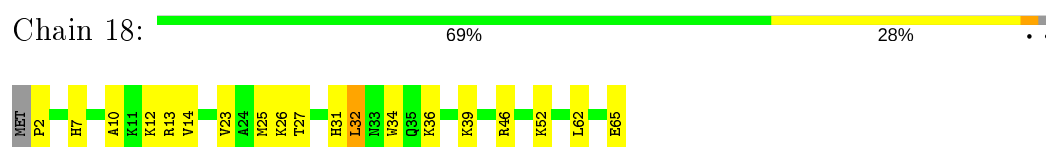
## • Molecule 29: 50S ribosomal protein L34



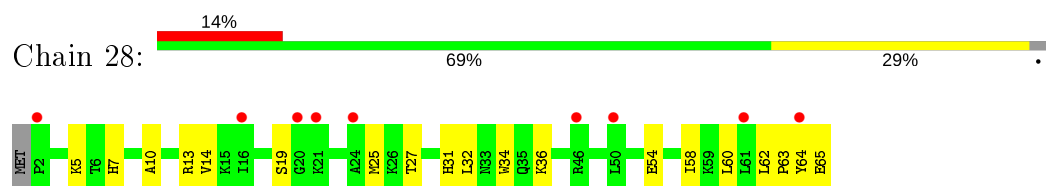
## • Molecule 29: 50S ribosomal protein L34



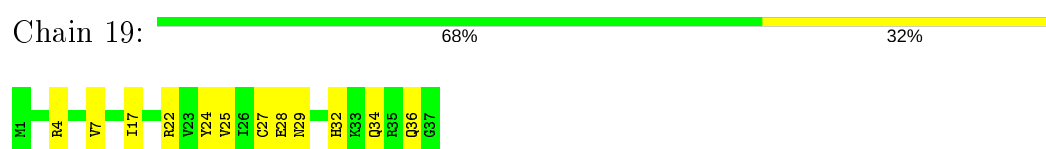
## • Molecule 30: 50S ribosomal protein L35



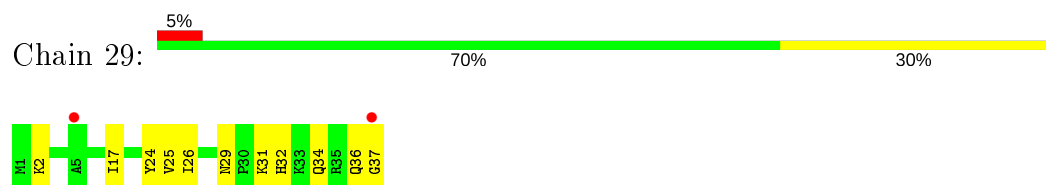
## • Molecule 30: 50S ribosomal protein L35



## • Molecule 31: 50S ribosomal protein L36



## • Molecule 31: 50S ribosomal protein L36



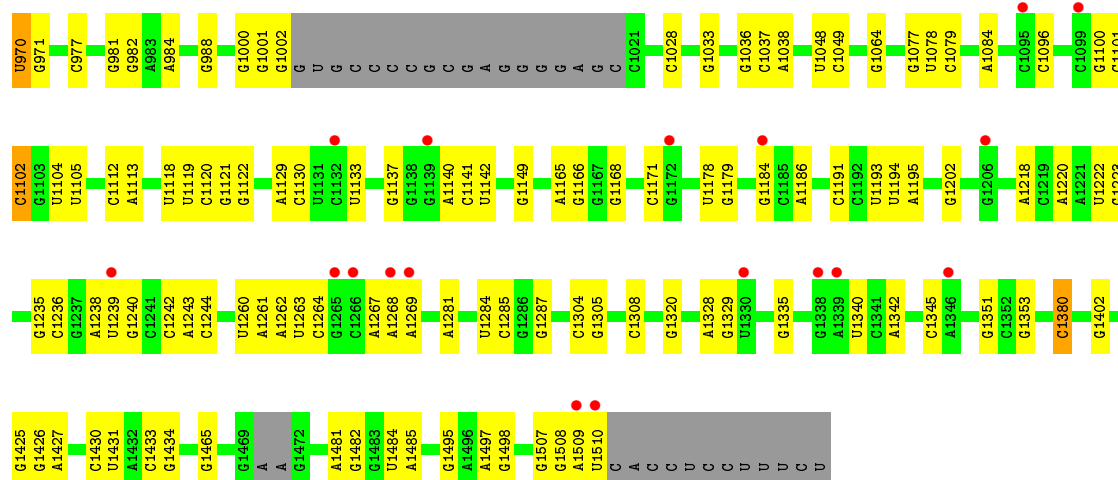
Chain 1a:

81% 16%

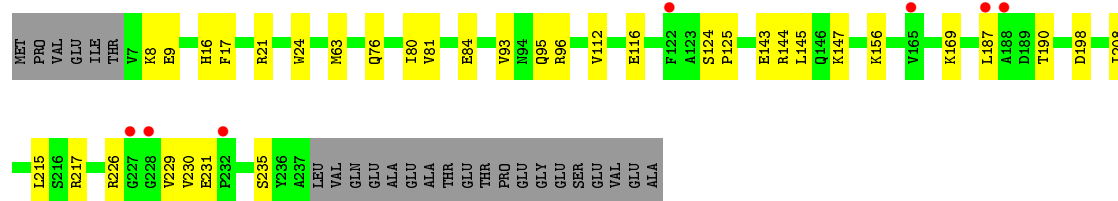
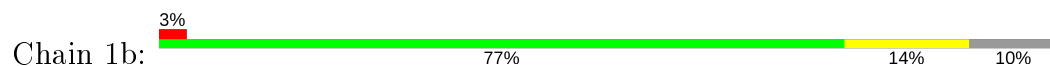
Category	Percentage
1352	0%
1353	0%
1383	0%
1402	0%
1425	0%
1426	0%
1433	0%
1465	0%
1469	0%
1472	0%
1475	0%
1481	0%
1482	0%
1483	0%
1484	0%
1495	0%
1507	0%
1508	0%
1509	0%
1517	0%
1518	0%
1519	0%
1520	0%
1521	0%
1522	0%
1523	0%
1524	0%
1525	0%
1526	0%
1527	0%
1528	0%
1529	0%
1530	0%
1531	0%
1532	0%
1533	0%
1534	0%
1535	0%
1536	0%
1537	0%
1538	0%
1539	0%
1540	0%
1541	0%
1542	0%
1543	0%
1544	0%
1545	0%
1546	0%
1547	0%
1548	0%
1549	0%
1550	0%
1551	0%
1552	0%
1553	0%
1554	0%
1555	0%
1556	0%
1557	0%
1558	0%
1559	0%
1560	0%
1561	0%
1562	0%
1563	0%
1564	0%
1565	0%
1566	0%
1567	0%
1568	0%
1569	0%
1570	0%
1571	0%
1572	0%
1573	0%
1574	0%
1575	0%
1576	0%
1577	0%
1578	0%
1579	0%
1580	0%
1581	0%
1582	0%
1583	0%
1584	0%
1585	0%
1586	0%
1587	0%
1588	0%
1589	0%
1590	0%
1591	0%
1592	0%
1593	0%
1594	0%
1595	0%
1596	0%
1597	0%
1598	0%
1599	0%
1600	0%
1601	0%
1602	0%
1603	0%
1604	0%
1605	0%
1606	0%
1607	0%
1608	0%
1609	0%
1610	0%
1611	0%
1612	0%
1613	0%
1614	0%
1615	0%
1616	0%
1617	0%
1618	0%
1619	0%
1620	0%
1621	0%
1622	0%
1623	0%
1624	0%
1625	0%
1626	0%
1627	0%
1628	0%
1629	0%
1630	0%
1631	0%
1632	0%
1633	0%
1634	0%
1635	0%
1636	0%
1637	0%
1638	0%
1639	0%
1640	0%
1641	0%
1642	0%
1643	0%
1644	0%
1645	0%
1646	0%
1647	0%
1648	0%
1649	0%
1650	0%
1651	0%
1652	0%
1653	0%
1654	0%
1655	0%
1656	0%
1657	0%
1658	0%
1659	0%
1660	0%
1661	0%
1662	0%
1663	0%
1664	0%
1665	0%
1666	0%
1667	0%
1668	0%
1669	0%
1670	0%
1671	0%
1672	0%
1673	0%
1674	0%
1675	0%
1676	0%
1677	0%
1678	0%
1679	0%
1680	0%
1681	0%
1682	0%
1683	0%
1684	0%
1685	0%
1686	0%
1687	0%
1688	0%
1689	0%
1690</	

Chain 2a:

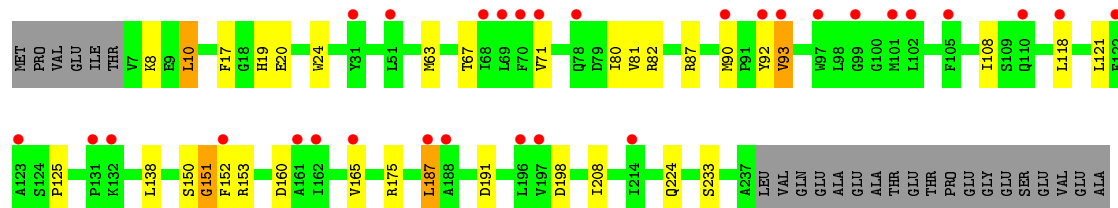
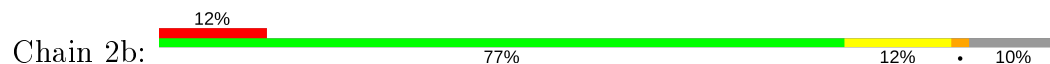
81% 16%



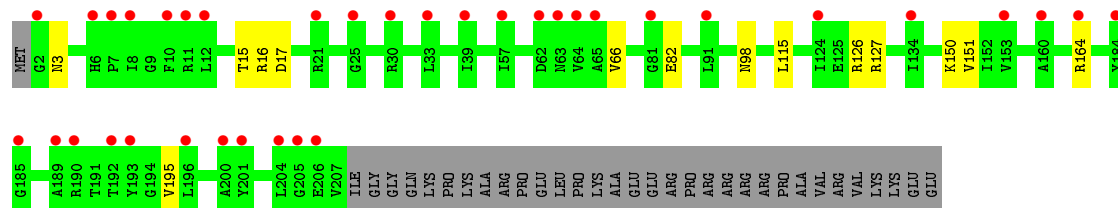
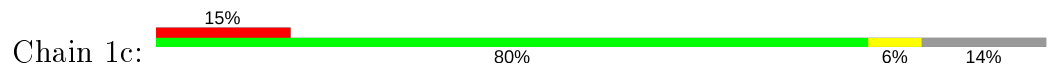
• Molecule 33: 30S ribosomal protein S2



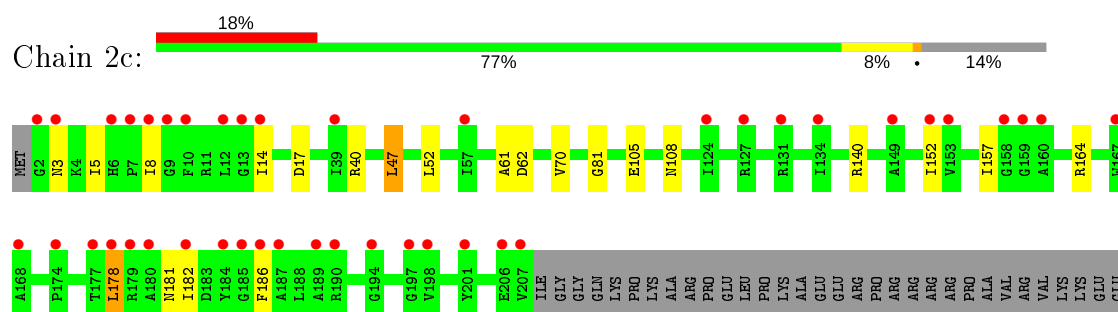
• Molecule 33: 30S ribosomal protein S2



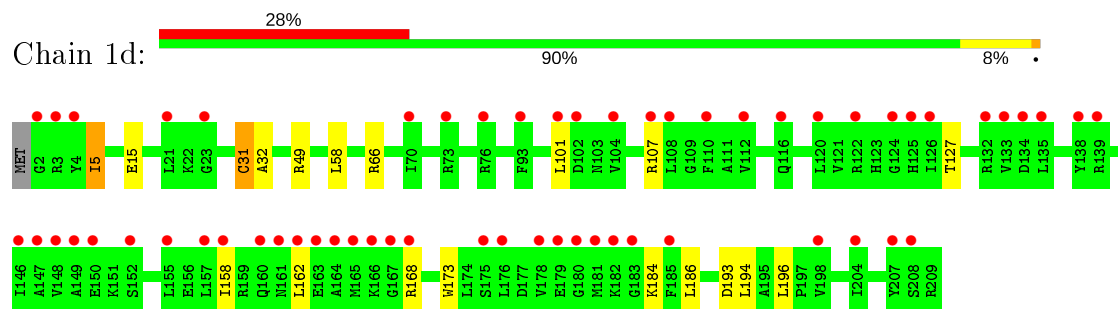
• Molecule 34: 30S ribosomal protein S3



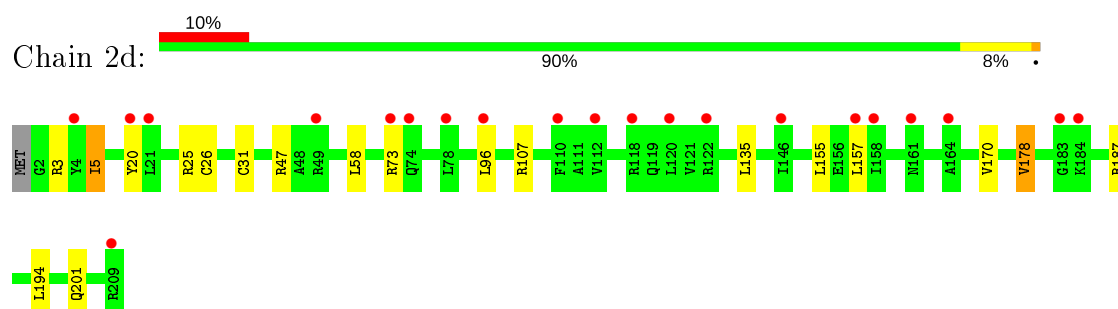
• Molecule 34: 30S ribosomal protein S3



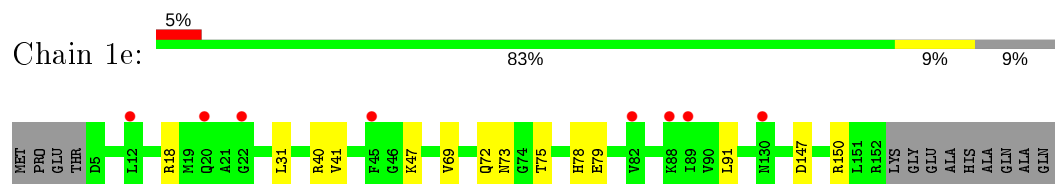
- Molecule 35: 30S ribosomal protein S4



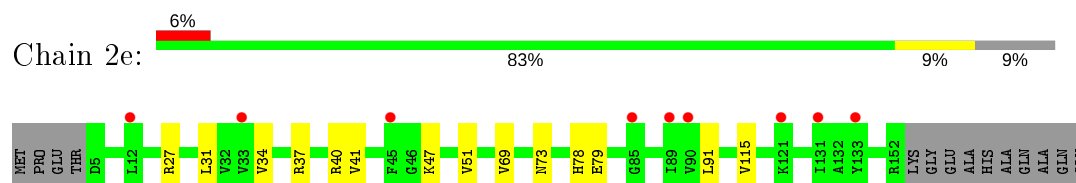
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6





- Molecule 37: 30S ribosomal protein S6

Chain 2f: 91% 8%



- Molecule 38: 30S ribosomal protein S7

Chain 1g: 10% 87% 12%



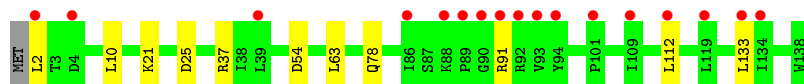
- Molecule 38: 30S ribosomal protein S7

Chain 2g: 10% 92% 8%



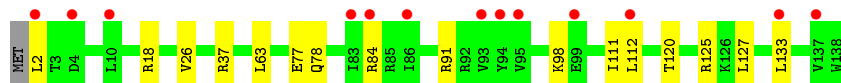
- Molecule 39: 30S ribosomal protein S8

Chain 1h: 12% 91% 8%



- Molecule 39: 30S ribosomal protein S8

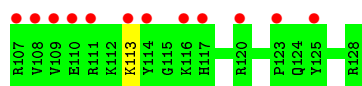
Chain 2h: 9% 88% 12%



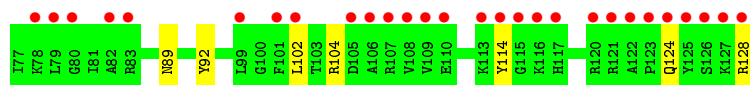
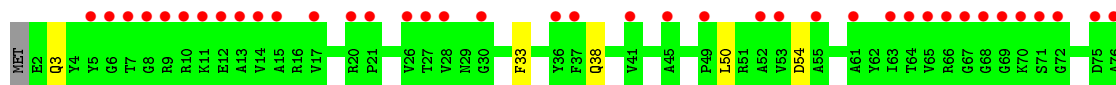
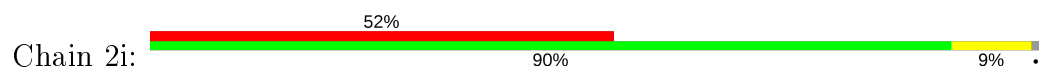
- Molecule 40: 30S ribosomal protein S9

Chain 1i: 31% 89% 10%

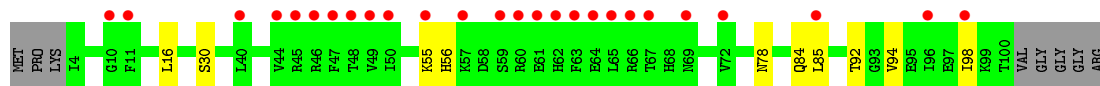
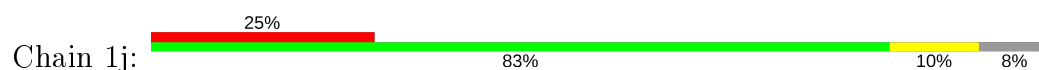




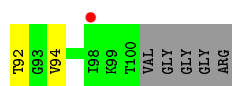
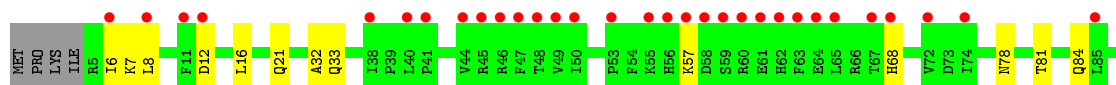
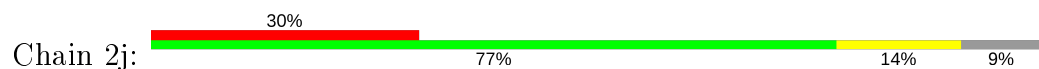
- Molecule 40: 30S ribosomal protein S9



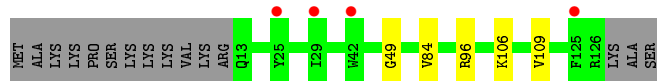
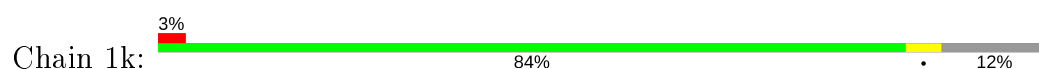
- Molecule 41: 30S ribosomal protein S10



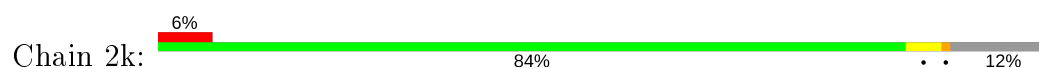
- Molecule 41: 30S ribosomal protein S10



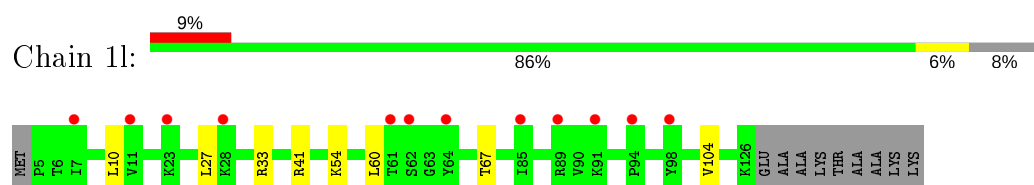
- Molecule 42: 30S ribosomal protein S11



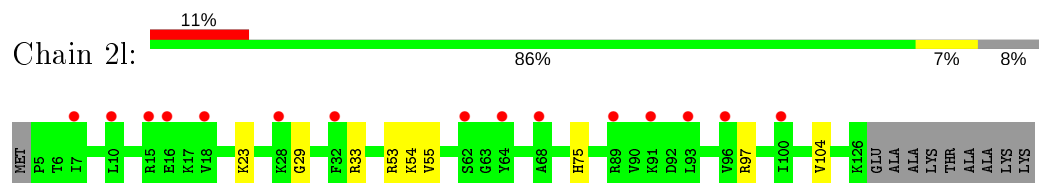
- Molecule 42: 30S ribosomal protein S11



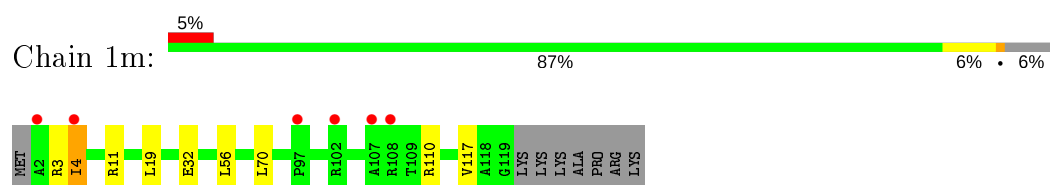
- Molecule 43: 30S ribosomal protein S12



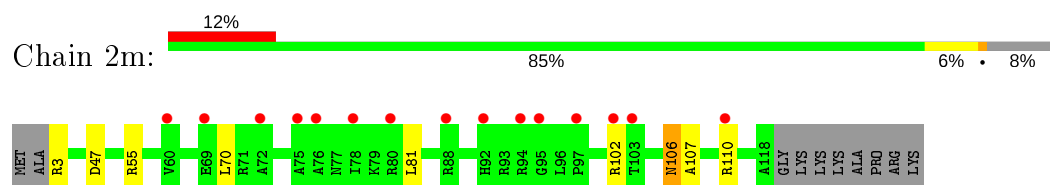
- Molecule 43: 30S ribosomal protein S12



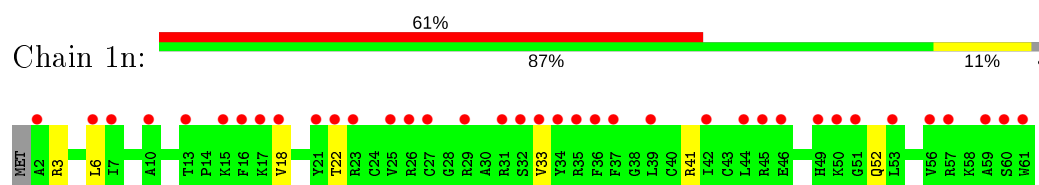
- Molecule 44: 30S ribosomal protein S13



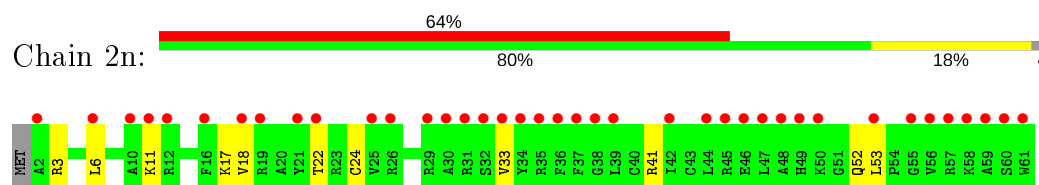
- Molecule 44: 30S ribosomal protein S13



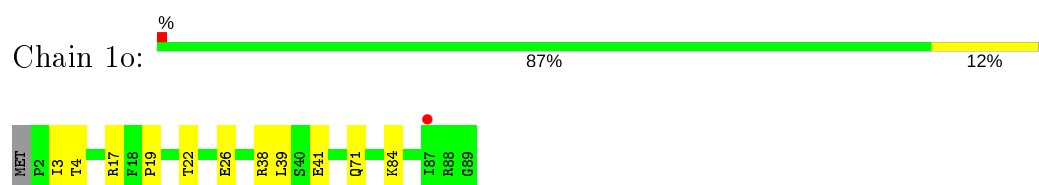
- Molecule 45: 30S ribosomal protein S14 type Z



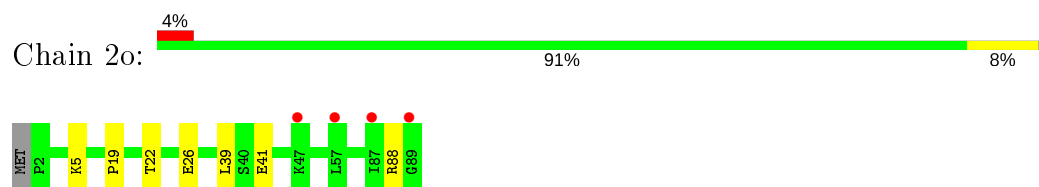
- Molecule 45: 30S ribosomal protein S14 type Z



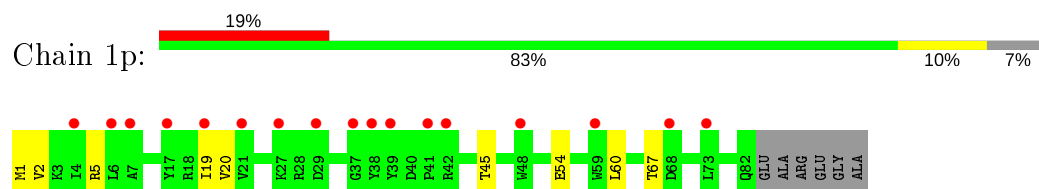
- Molecule 46: 30S ribosomal protein S15



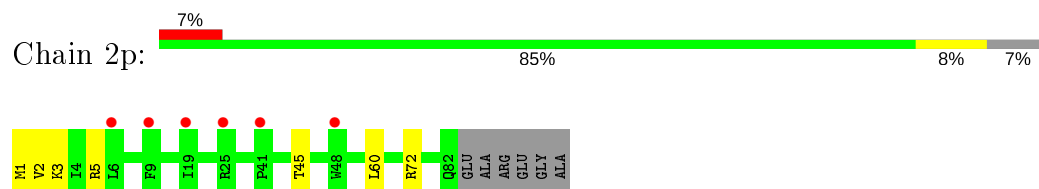
## • Molecule 46: 30S ribosomal protein S15



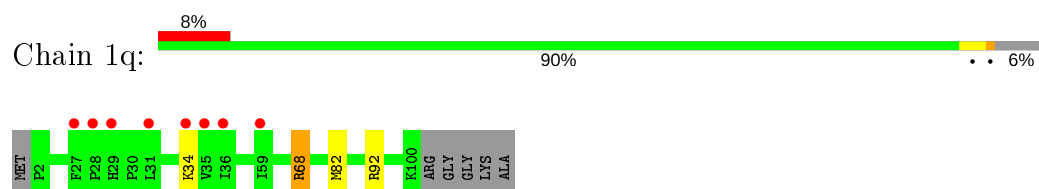
## • Molecule 47: 30S ribosomal protein S16



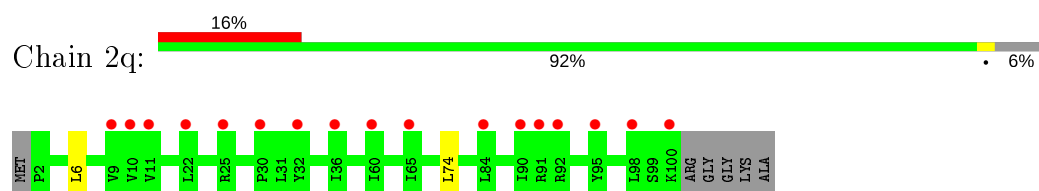
## • Molecule 47: 30S ribosomal protein S16



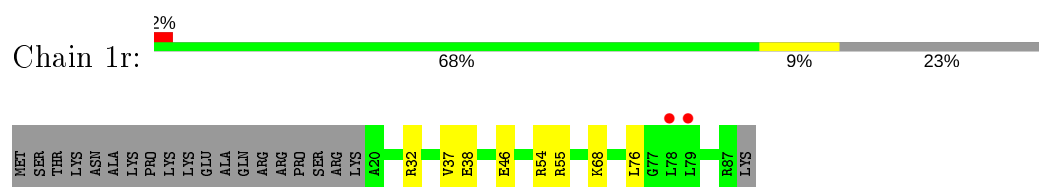
## • Molecule 48: 30S ribosomal protein S17



## • Molecule 48: 30S ribosomal protein S17



## • Molecule 49: 30S ribosomal protein S18

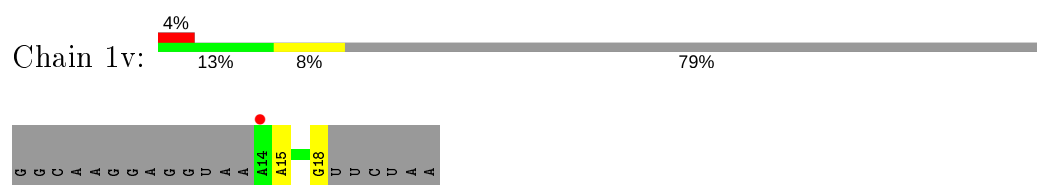


## • Molecule 49: 30S ribosomal protein S18





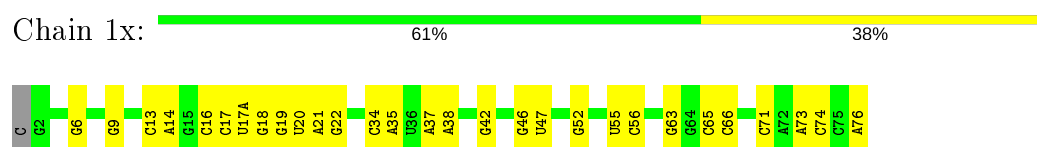




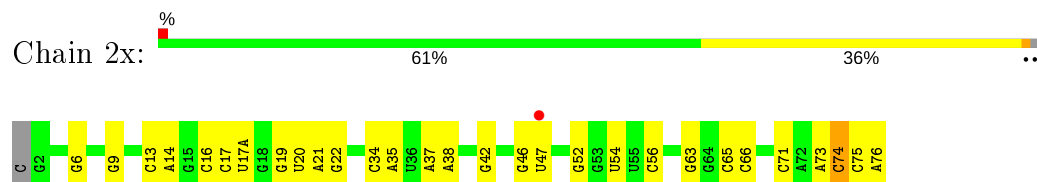
- Molecule 53: mRNA



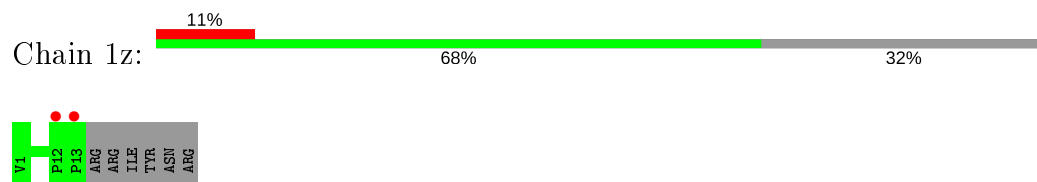
- Molecule 54: Initiator Methionine tRNA



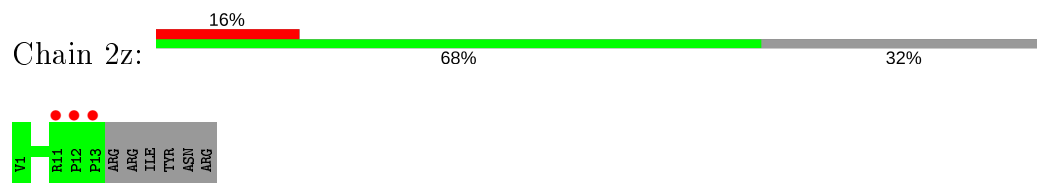
- Molecule 54: Initiator Methionine tRNA



- Molecule 55: Oncocin



- Molecule 55: Oncocin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.14Å 450.73Å 623.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.98 – 2.90 311.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (59.98-2.90) 98.0 (311.74-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.203 , 0.248 0.204 , 0.248	Depositor DCC
$R_{free}$ test set	70488 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	288378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, SF4, MG, 5MC, 4SU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1A	0.34	0/66249	0.77	19/103407 (0.0%)
1	2A	0.28	0/67298	0.76	12/105044 (0.0%)
2	1B	0.28	0/2877	0.79	0/4488
2	2B	0.30	0/2878	0.79	0/4490
3	1D	0.29	0/2186	0.49	0/2944
3	2D	0.28	0/2192	0.49	0/2951
4	1E	0.36	0/1592	0.51	1/2149 (0.0%)
4	2E	0.26	0/1592	0.49	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.25	0/1615	0.48	0/2188
6	1G	0.23	0/1450	0.46	0/1959
6	2G	0.26	0/1449	0.49	0/1958
7	1H	0.25	0/1356	0.46	0/1834
7	2H	0.24	0/1356	0.45	0/1834
8	1I	0.24	0/1100	0.49	0/1501
8	2I	0.23	0/1076	0.49	0/1471
9	1N	0.27	0/1144	0.46	0/1543
9	2N	0.25	0/1144	0.46	0/1543
10	1O	0.28	0/943	0.48	0/1269
10	2O	0.27	0/943	0.49	0/1269
11	1P	0.27	0/1156	0.50	0/1537
11	2P	0.27	0/1152	0.49	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.27	0/1143	0.47	0/1527
13	1R	0.26	0/982	0.50	0/1312
13	2R	0.25	0/982	0.47	0/1312
14	1S	0.25	0/887	0.48	0/1180
14	2S	0.27	0/880	0.52	0/1172
15	1T	0.27	0/1105	0.45	0/1477
15	2T	0.26	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.45	0/1301
16	2U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.28	0/782	0.46	0/1049
17	2V	0.25	0/782	0.44	0/1049
18	1W	0.28	0/897	0.44	0/1205
18	2W	0.26	0/897	0.44	0/1205
19	1X	0.28	0/764	0.46	0/1025
19	2X	0.26	0/764	0.48	1/1025 (0.1%)
20	1Y	0.28	0/819	0.51	0/1095
20	2Y	0.25	0/819	0.47	0/1095
21	1Z	0.25	0/1502	0.45	0/2041
21	2Z	0.24	0/1486	0.44	0/2022
22	10	0.28	0/606	0.50	0/808
22	20	0.26	0/606	0.47	0/808
23	11	0.26	0/762	0.45	0/1014
23	21	0.25	0/762	0.43	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.25	0/590	0.40	0/781
25	13	0.26	0/474	0.43	0/635
25	23	0.24	0/469	0.44	0/630
26	14	0.29	0/571	0.59	0/768
26	24	0.29	0/545	0.58	0/737
27	15	0.29	0/469	0.51	0/635
27	25	0.25	0/469	0.48	0/635
28	16	0.29	0/460	0.43	0/613
28	26	0.26	0/456	0.45	0/608
29	17	0.28	0/426	0.43	0/561
29	27	0.27	0/426	0.44	0/561
30	18	0.29	0/525	0.47	0/691
30	28	0.26	0/525	0.43	0/691
31	19	0.29	0/310	0.44	0/407
31	29	0.25	0/310	0.43	0/407
32	1a	0.25	0/35537	0.77	7/55456 (0.0%)
32	2a	0.25	2/35680 (0.0%)	0.78	33/55681 (0.1%)
33	1b	0.25	0/1820	0.51	0/2468
33	2b	2.71	8/1728 (0.5%)	0.68	3/2352 (0.1%)
34	1c	0.23	0/1504	0.44	0/2047
34	2c	0.25	0/1435	0.51	2/1960 (0.1%)
35	1d	0.24	0/1648	0.48	0/2222
35	2d	0.25	0/1659	0.45	0/2230
36	1e	0.25	0/1145	0.49	0/1543
36	2e	0.26	0/1111	0.50	0/1504
37	1f	0.24	0/819	0.45	0/1111
37	2f	0.24	0/830	0.44	0/1125
38	1g	0.23	0/1198	0.42	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.24	0/1185	0.42	0/1602
39	1h	0.23	0/1108	0.45	0/1494
39	2h	0.23	0/1094	0.47	0/1478
40	1i	0.25	0/995	0.49	0/1339
40	2i	0.26	0/949	0.50	0/1284
41	1j	0.24	0/695	0.55	0/950
41	2j	0.25	0/690	0.50	0/943
42	1k	0.24	0/840	0.45	0/1138
42	2k	0.25	0/844	0.51	1/1145 (0.1%)
43	1l	0.24	0/936	0.46	0/1263
43	2l	0.25	0/934	0.51	1/1262 (0.1%)
44	1m	0.23	0/933	0.49	0/1254
44	2m	0.27	0/913	0.47	0/1230
45	1n	0.29	0/491	0.50	0/653
45	2n	0.27	0/467	0.41	0/624
46	1o	0.24	0/726	0.47	0/970
46	2o	0.23	0/739	0.44	0/985
47	1p	0.22	0/686	0.46	0/926
47	2p	0.23	0/693	0.47	0/935
48	1q	0.25	0/824	0.46	0/1105
48	2q	0.24	0/836	0.44	0/1117
49	1r	0.25	0/560	0.48	0/746
49	2r	0.23	0/560	0.44	0/746
50	1s	0.24	0/657	0.52	0/890
50	2s	0.26	0/661	0.53	0/893
51	1t	0.22	0/714	0.52	0/948
51	2t	0.23	0/733	0.44	0/969
52	1u	0.21	0/191	0.45	0/252
52	2u	0.24	0/203	0.42	0/266
53	1v	0.39	0/122	1.03	0/188
53	2v	0.41	0/122	1.09	0/188
54	1x	0.41	0/1725	1.03	10/2689 (0.4%)
54	2x	0.41	0/1725	1.04	11/2689 (0.4%)
55	1z	0.29	0/114	0.54	0/158
55	2z	0.24	0/114	0.48	0/158
All	All	0.35	10/306296 (0.0%)	0.71	101/458216 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
41	2j	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	58.43	2.27	1.39
33	2b	92	TYR	CD2-CE2	54.24	2.20	1.39
33	2b	92	TYR	CE2-CZ	42.19	1.93	1.38
33	2b	92	TYR	CE1-CZ	41.20	1.92	1.38
33	2b	92	TYR	CG-CD1	33.29	1.82	1.39

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.60	157.16	122.30
32	2a	1102	C	N1-C2-O2	14.44	127.57	118.90
32	2a	1137	G	N3-C2-N2	13.03	129.02	119.90
32	2a	1137	G	N1-C2-N2	-12.03	105.38	116.20
32	2a	1137	G	C4-N9-C1'	11.15	141.00	126.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	Peptide
41	2j	32	ALA	Peptide

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

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	59154	0	29830	434	0
1	2A	60091	0	30300	592	0
2	1B	2572	0	1306	18	0
2	2B	2573	0	1306	34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	38	0
3	2D	2142	0	2229	39	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	27	0
5	1F	1584	0	1625	21	0
5	2F	1580	0	1619	25	0
6	1G	1425	0	1443	28	0
6	2G	1424	0	1434	48	0
7	1H	1330	0	1407	19	0
7	2H	1330	0	1407	31	0
8	1I	1085	0	1114	17	0
8	2I	1061	0	1080	24	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	11	0
10	1O	933	0	996	16	0
10	2O	933	0	996	17	0
11	1P	1139	0	1223	27	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1178	19	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	8	0
13	2R	968	0	1033	12	0
14	1S	877	0	938	18	0
14	2S	870	0	923	23	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	10	0
16	2U	959	0	1019	15	0
17	1V	771	0	830	9	0
17	2V	771	0	830	18	0
18	1W	886	0	940	10	0
18	2W	886	0	940	8	0
19	1X	750	0	814	13	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	18	0
21	1Z	1470	0	1478	20	0
21	2Z	1454	0	1452	41	0
22	10	598	0	614	11	0
22	20	598	0	614	11	0
23	11	755	0	826	16	0
23	21	755	0	826	15	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	6	0
24	22	588	0	643	4	0
25	13	469	0	518	8	0
25	23	464	0	514	2	0
26	14	558	0	544	20	0
26	24	532	0	503	23	0
27	15	455	0	465	7	0
27	25	455	0	465	9	0
28	16	453	0	473	5	0
28	26	449	0	469	6	0
29	17	418	0	467	10	0
29	27	418	0	467	8	0
30	18	517	0	582	16	0
30	28	517	0	582	14	0
31	19	307	0	335	8	0
31	29	307	0	335	8	0
32	1a	31750	0	16028	0	0
32	2a	31877	0	16086	0	0
33	1b	1786	0	1744	0	0
33	2b	1697	0	1574	0	0
34	1c	1480	0	1400	0	0
34	2c	1412	0	1246	0	0
35	1d	1618	0	1579	0	0
35	2d	1630	0	1633	0	0
36	1e	1129	0	1184	0	0
36	2e	1095	0	1124	0	0
37	1f	806	0	793	0	0
37	2f	817	0	808	0	0
38	1g	1183	0	1165	0	0
38	2g	1167	0	1119	0	0
39	1h	1088	0	1126	0	0
39	2h	1074	0	1100	0	0
40	1i	976	0	973	0	0
40	2i	932	0	891	0	0
41	1j	682	0	598	0	0
41	2j	678	0	612	0	0
42	1k	826	0	829	0	0
42	2k	829	0	825	0	0
43	1l	920	0	958	0	0
43	2l	918	0	947	0	0
44	1m	923	0	962	0	0
44	2m	903	0	923	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	482	0	507	0	0
45	2n	459	0	467	0	0
46	1o	715	0	729	0	0
46	2o	728	0	760	0	0
47	1p	671	0	679	0	0
47	2p	677	0	686	0	0
48	1q	811	0	858	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	642	0	629	0	0
50	2s	646	0	644	0	0
51	1t	712	0	759	0	0
51	2t	731	0	807	0	0
52	1u	187	0	186	0	0
52	2u	199	0	208	0	0
53	1v	109	0	55	0	0
53	2v	109	0	55	0	0
54	1x	1625	0	829	0	0
54	2x	1625	0	829	0	0
55	1z	108	0	116	0	0
55	2z	108	0	116	0	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	1	0	0	0	0
56	18	3	0	0	0	0
56	19	3	0	0	0	0
56	1A	1021	0	0	0	0
56	1B	24	0	0	0	0
56	1D	14	0	0	0	0
56	1E	5	0	0	0	0
56	1F	8	0	0	0	0
56	1G	3	0	0	0	0
56	1H	2	0	0	0	0
56	1N	6	0	0	0	0
56	1O	2	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	4	0	0	0	0
56	1T	5	0	0	0	0
56	1U	5	0	0	0	0
56	1V	1	0	0	0	0
56	1W	5	0	0	0	0
56	1X	2	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	276	0	0	0	0
56	1b	2	0	0	0	0
56	1d	2	0	0	0	0
56	1e	3	0	0	0	0
56	1f	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	2	0	0	0	0
56	1q	4	0	0	0	0
56	1r	2	0	0	0	0
56	1t	1	0	0	0	0
56	1x	8	0	0	0	0
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	566	0	0	0	0
56	2B	11	0	0	0	0
56	2D	6	0	0	0	0
56	2E	4	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2U	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	263	0	0	0	0
56	2d	1	0	0	0	0
56	2f	1	0	0	0	0
56	2h	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2q	2	0	0	0	0
56	2t	1	0	0	0	0
56	2x	4	0	0	0	0
56	2z	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	10	0	0	1	0
59	11	4	0	0	0	0
59	12	1	0	0	0	0
59	13	4	0	0	1	0
59	15	5	0	0	0	0
59	16	8	0	0	1	0
59	17	8	0	0	2	0
59	18	13	0	0	0	0
59	19	2	0	0	0	0
59	1A	2088	0	0	61	0
59	1B	38	0	0	4	0
59	1D	22	0	0	0	0
59	1E	25	0	0	4	0
59	1F	16	0	0	0	0
59	1G	6	0	0	0	0
59	1H	5	0	0	1	0
59	1I	1	0	0	0	0
59	1N	5	0	0	0	0
59	1O	4	0	0	0	0
59	1P	21	0	0	1	0
59	1Q	9	0	0	0	0
59	1R	9	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1S	1	0	0	0	0
59	1T	11	0	0	2	0
59	1U	13	0	0	0	0
59	1V	2	0	0	0	0
59	1W	9	0	0	0	0
59	1X	5	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	3	0	0	0	0
59	1a	319	0	0	0	0
59	1b	2	0	0	0	0
59	1c	1	0	0	0	0
59	1d	4	0	0	0	0
59	1e	2	0	0	0	0
59	1f	1	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1m	1	0	0	0	0
59	1o	3	0	0	0	0
59	1p	1	0	0	0	0
59	1s	1	0	0	0	0
59	1v	1	0	0	0	0
59	1x	7	0	0	0	0
59	1z	2	0	0	0	0
59	20	3	0	0	0	0
59	21	1	0	0	0	0
59	23	2	0	0	0	0
59	25	1	0	0	0	0
59	27	2	0	0	0	0
59	28	4	0	0	0	0
59	2A	801	0	0	45	0
59	2B	13	0	0	0	0
59	2D	20	0	0	1	0
59	2E	10	0	0	1	0
59	2F	7	0	0	0	0
59	2N	1	0	0	0	0
59	2O	4	0	0	0	0
59	2P	4	0	0	0	0
59	2Q	2	0	0	0	0
59	2R	3	0	0	0	0
59	2T	3	0	0	0	0
59	2U	2	0	0	1	0
59	2V	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2W	2	0	0	0	0
59	2X	3	0	0	0	0
59	2Y	1	0	0	0	0
59	2Z	2	0	0	0	0
59	2a	371	0	0	0	0
59	2c	2	0	0	0	0
59	2e	3	0	0	0	0
59	2h	1	0	0	0	0
59	2i	2	0	0	0	0
59	2j	1	0	0	0	0
59	2k	3	0	0	0	0
59	2l	3	0	0	0	0
59	2m	1	0	0	0	0
59	2n	1	0	0	0	0
59	2o	1	0	0	0	0
59	2p	2	0	0	0	0
59	2q	2	0	0	0	0
59	2r	1	0	0	0	0
59	2t	3	0	0	0	0
59	2x	3	0	0	0	0
59	2z	1	0	0	0	0
All	All	288378	0	189976	1793	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1793 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)
1:2A:1098:C:N3	1:2A:1099:A:C8	2.28	1.01
1:2A:1096:G:C5	1:2A:1097:C:C5	2.56	0.94
1:2A:1151:G:C2	1:2A:1152:G:N7	2.38	0.92
1:2A:1096:G:C4	1:2A:1097:C:C5	2.61	0.88
1:2A:1151:G:H2'	1:2A:1152:G:H5'	1.55	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	34	66
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61
4	2E	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	29	61
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	61
5	2F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	61
6	1G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	6	24
6	2G	179/182 (98%)	159 (89%)	16 (9%)	4 (2%)	6	24
7	1H	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	13	40
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	13	40
8	1I	144/148 (97%)	124 (86%)	15 (10%)	5 (4%)	3	14
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	36
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	22	54
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	54
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	22	54
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	22	54
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	48
14	2S	108/112 (96%)	97 (90%)	6 (6%)	5 (5%)	2	9
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	45
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	45
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	14	42
19	2X	93/96 (97%)	91 (98%)	0	2 (2%)	6	24
20	1Y	105/110 (96%)	98 (93%)	5 (5%)	2 (2%)	8	28
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	184/206 (89%)	172 (94%)	12 (6%)	0	100	100
21	2Z	184/206 (89%)	172 (94%)	11 (6%)	1 (0%)	29	61
22	10	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	11	36
22	20	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	42
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	51 (76%)	8 (12%)	8 (12%)	0	1
26	24	67/71 (94%)	53 (79%)	7 (10%)	7 (10%)	0	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	24
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	195 (85%)	28 (12%)	6 (3%)	5	20
33	2b	229/256 (90%)	190 (83%)	33 (14%)	6 (3%)	5	20
34	1c	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	10	34
34	2c	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	4	18
35	1d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	10	34
35	2d	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	10	34
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	11	36
36	2e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	7	26
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	12	37
38	2g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	12	37
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	9	32
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	19	51
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	4	16
41	2j	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	14	42
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	48
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	48
43	1l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	17	48
44	2m	114/126 (90%)	100 (88%)	12 (10%)	2 (2%)	8	29
45	1n	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	3	15
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	31
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	13	40
46	2o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	6	23
47	1p	80/88 (91%)	66 (82%)	14 (18%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	45
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
51	1t	94/106 (89%)	84 (89%)	7 (7%)	3 (3%)	4	16
51	2t	94/106 (89%)	83 (88%)	7 (7%)	4 (4%)	2	10
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
55	1z	11/19 (58%)	11 (100%)	0	0	100	100
55	2z	11/19 (58%)	11 (100%)	0	0	100	100
All	All	11432/12166 (94%)	10579 (92%)	731 (6%)	122 (1%)	14	42

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	126	ASP
7	1H	126	PRO
14	1S	60	GLY
22	10	13	GLY
26	14	45	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	197 (92%)	18 (8%)	11	31
3	2D	216/218 (99%)	198 (92%)	18 (8%)	11	32
4	1E	164/166 (99%)	147 (90%)	17 (10%)	7	21

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	146 (89%)	18 (11%)	6	19
5	1F	160/166 (96%)	148 (92%)	12 (8%)	13	37
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11	32
6	1G	143/156 (92%)	129 (90%)	14 (10%)	8	24
6	2G	142/156 (91%)	126 (89%)	16 (11%)	6	18
7	1H	144/148 (97%)	135 (94%)	9 (6%)	18	46
7	2H	144/148 (97%)	135 (94%)	9 (6%)	18	46
8	1I	110/124 (89%)	92 (84%)	18 (16%)	2	7
8	2I	104/124 (84%)	97 (93%)	7 (7%)	16	43
9	1N	118/119 (99%)	107 (91%)	11 (9%)	9	27
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10	31
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	57
10	2O	100/100 (100%)	92 (92%)	8 (8%)	12	33
11	1P	116/116 (100%)	103 (89%)	13 (11%)	6	18
11	2P	115/116 (99%)	100 (87%)	15 (13%)	4	12
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	39
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4	13
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	10
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	33
14	2S	85/88 (97%)	73 (86%)	12 (14%)	3	10
15	1T	115/127 (91%)	104 (90%)	11 (10%)	8	25
15	2T	113/127 (89%)	103 (91%)	10 (9%)	10	30
16	1U	93/94 (99%)	82 (88%)	11 (12%)	5	16
16	2U	93/94 (99%)	86 (92%)	7 (8%)	13	37
17	1V	80/82 (98%)	66 (82%)	14 (18%)	2	6
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	10
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	43
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	34
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	77
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	66

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	26	59
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14	40
21	1Z	159/179 (89%)	144 (91%)	15 (9%)	8	26
21	2Z	156/179 (87%)	138 (88%)	18 (12%)	5	17
22	10	60/67 (90%)	55 (92%)	5 (8%)	11	32
22	20	60/67 (90%)	58 (97%)	2 (3%)	38	72
23	11	80/83 (96%)	75 (94%)	5 (6%)	18	46
23	21	80/83 (96%)	74 (92%)	6 (8%)	13	37
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	14
24	22	65/67 (97%)	60 (92%)	5 (8%)	13	35
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	34
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	49
26	14	60/63 (95%)	50 (83%)	10 (17%)	2	6
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	9
27	15	50/52 (96%)	48 (96%)	2 (4%)	31	65
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	49
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	66
28	26	50/52 (96%)	48 (96%)	2 (4%)	31	65
29	17	41/42 (98%)	38 (93%)	3 (7%)	14	38
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	79
30	18	54/55 (98%)	48 (89%)	6 (11%)	6	19
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	52
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	177/220 (80%)	148 (84%)	29 (16%)	2	7
33	2b	158/220 (72%)	130 (82%)	28 (18%)	2	5
34	1c	127/188 (68%)	116 (91%)	11 (9%)	10	30
34	2c	108/188 (57%)	92 (85%)	16 (15%)	3	9
35	1d	161/181 (89%)	143 (89%)	18 (11%)	6	18
35	2d	164/181 (91%)	146 (89%)	18 (11%)	6	19
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	106/123 (86%)	95 (90%)	11 (10%)	7	21
37	1f	83/90 (92%)	78 (94%)	5 (6%)	19	49
37	2f	86/90 (96%)	78 (91%)	8 (9%)	9	27
38	1g	111/127 (87%)	94 (85%)	17 (15%)	2	8
38	2g	107/127 (84%)	97 (91%)	10 (9%)	9	27
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	25
39	2h	111/119 (93%)	95 (86%)	16 (14%)	3	9
40	1i	89/99 (90%)	78 (88%)	11 (12%)	4	14
40	2i	80/99 (81%)	69 (86%)	11 (14%)	3	10
41	1j	60/92 (65%)	53 (88%)	7 (12%)	5	16
41	2j	62/92 (67%)	49 (79%)	13 (21%)	1	3
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	57
42	2k	82/99 (83%)	77 (94%)	5 (6%)	18	48
43	1l	95/109 (87%)	87 (92%)	8 (8%)	11	31
43	2l	94/109 (86%)	86 (92%)	8 (8%)	10	31
44	1m	90/101 (89%)	81 (90%)	9 (10%)	7	23
44	2m	87/101 (86%)	79 (91%)	8 (9%)	9	27
45	1n	47/50 (94%)	42 (89%)	5 (11%)	6	20
45	2n	43/50 (86%)	33 (77%)	10 (23%)	1	2
46	1o	75/80 (94%)	65 (87%)	10 (13%)	4	11
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17	45
47	1p	67/74 (90%)	58 (87%)	9 (13%)	4	11
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	22
48	1q	91/97 (94%)	87 (96%)	4 (4%)	28	61
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	81
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	11
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	15
50	1s	65/80 (81%)	55 (85%)	10 (15%)	2	8
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	29
51	1t	66/82 (80%)	59 (89%)	7 (11%)	6	20
51	2t	71/82 (87%)	68 (96%)	3 (4%)	30	63

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
55	1z	13/19 (68%)	13 (100%)	0	100	100
55	2z	13/19 (68%)	13 (100%)	0	100	100
All	All	9161/10104 (91%)	8276 (90%)	885 (10%)	8	25

5 of 885 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	1o	3	ILE
5	2F	197	ASP
41	2j	33	GLN
47	1p	5	ARG
3	2D	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
3	2D	253	GLN
15	2T	58	ASN
44	2m	77	ASN
5	2F	69	HIS
8	2I	43	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	357 (13%)	17 (0%)
1	2A	2781/2915 (95%)	405 (14%)	26 (0%)
2	1B	119/121 (98%)	13 (10%)	2 (1%)
2	2B	119/121 (98%)	23 (19%)	2 (1%)
32	1a	1472/1521 (96%)	238 (16%)	0
32	2a	1479/1521 (97%)	240 (16%)	0
53	1v	4/24 (16%)	2 (50%)	0
53	2v	4/24 (16%)	2 (50%)	0
54	1x	75/77 (97%)	26 (34%)	0
54	2x	75/77 (97%)	26 (34%)	0
All	All	8865/9316 (95%)	1332 (15%)	47 (0%)

5 of 1332 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	12	A
1	1A	14	G
1	1A	33	C
1	1A	44	C

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	424	G
1	2A	1047	G
1	2A	2700	U
1	2A	669	C
1	2A	1087	G

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

8 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$
54	PSU	2x	55	54	17,21,22	1.53	3 (17%)	20,30,33	3.16	5 (25%)
54	5MU	2x	54	54	15,22,23	1.09	1 (6%)	16,32,35	1.71	2 (12%)
54	5MC	2x	32	54	15,22,23	1.27	1 (6%)	19,32,35	1.34	2 (10%)
54	4SU	1x	8	54	14,21,22	1.42	2 (14%)	15,30,33	2.44	2 (13%)
54	4SU	2x	8	54	14,21,22	1.29	2 (14%)	15,30,33	2.36	2 (13%)
54	5MC	1x	32	54	15,22,23	1.33	1 (6%)	19,32,35	1.39	3 (15%)
54	5MU	1x	54	54	15,22,23	1.08	2 (13%)	16,32,35	2.02	2 (12%)
54	PSU	1x	55	54	17,21,22	1.58	3 (17%)	20,30,33	3.22	6 (30%)

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
54	PSU	2x	55	54	-	3/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/5/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/5/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/5/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/5/25/26	0/2/2/2
54	PSU	1x	55	54	-	3/7/25/26	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	32	5MC	C5-C4	4.78	1.48	1.41
54	2x	32	5MC	C5-C4	4.54	1.48	1.41
54	1x	55	PSU	C5-C1'	-4.23	1.48	1.52
54	1x	8	4SU	C4-S4	-3.82	1.60	1.67
54	2x	8	4SU	C4-S4	-3.74	1.60	1.67

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	55	PSU	N1-C2-N3	-8.94	121.32	128.43
54	2x	55	PSU	N1-C2-N3	-8.85	121.40	128.43
54	1x	8	4SU	C2-N3-C4	8.18	127.00	115.15
54	2x	8	4SU	C2-N3-C4	7.76	126.41	115.15
54	1x	54	5MU	C4-N3-C2	7.51	121.49	115.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	1x	55	PSU	C3'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	1x	55	PSU	O4'-C4'-C5'-O5'
54	1x	55	PSU	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2352 ligands modelled in this entry, 2350 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	$\# Z  > 2$
58	SF4	1d	501	35	0,12,12	0.00	-	-		
58	SF4	2d	501	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
58	SF4	1d	501	35	-	-	0/6/5/5
58	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2746/2915 (94%)	0.69	10 (0%) 92 93	24, 41, 87, 115	0
1	2A	2790/2915 (95%)	0.25	16 (0%) 89 89	26, 45, 94, 113	0
2	1B	120/121 (99%)	0.49	0 100 100	40, 66, 79, 96	0
2	2B	120/121 (99%)	-0.13	0 100 100	45, 72, 82, 98	0
3	1D	275/276 (99%)	0.56	2 (0%) 87 87	21, 40, 58, 81	0
3	2D	275/276 (99%)	0.54	13 (4%) 31 28	21, 42, 60, 81	0
4	1E	204/206 (99%)	0.37	1 (0%) 91 91	17, 37, 64, 79	0
4	2E	204/206 (99%)	0.40	4 (1%) 65 63	26, 52, 72, 83	0
5	1F	203/210 (96%)	0.39	0 100 100	22, 50, 77, 92	0
5	2F	203/210 (96%)	0.13	4 (1%) 65 63	25, 54, 78, 92	0
6	1G	181/182 (99%)	0.20	2 (1%) 80 80	54, 71, 84, 98	0
6	2G	181/182 (99%)	0.83	28 (15%) 2 1	59, 76, 88, 99	0
7	1H	174/180 (96%)	0.37	1 (0%) 89 89	49, 64, 79, 86	0
7	2H	174/180 (96%)	0.51	20 (11%) 4 3	52, 70, 82, 88	0
8	1I	146/148 (98%)	0.12	2 (1%) 75 75	47, 75, 87, 93	0
8	2I	146/148 (98%)	0.30	8 (5%) 25 21	48, 77, 87, 93	0
9	1N	140/140 (100%)	0.60	0 100 100	30, 46, 70, 78	0
9	2N	140/140 (100%)	0.27	0 100 100	33, 50, 72, 80	0
10	1O	122/122 (100%)	0.54	2 (1%) 72 71	31, 42, 64, 70	0
10	2O	122/122 (100%)	0.24	1 (0%) 86 86	34, 45, 64, 71	0
11	1P	149/150 (99%)	0.52	2 (1%) 77 77	25, 53, 75, 85	0
11	2P	149/150 (99%)	0.72	12 (8%) 12 9	29, 57, 77, 87	0
12	1Q	141/141 (100%)	0.57	3 (2%) 63 61	32, 50, 65, 84	0
12	2Q	141/141 (100%)	0.31	4 (2%) 53 49	36, 53, 68, 84	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%)	0.52	0 100 100	27, 40, 56, 67	0
13	2R	118/118 (100%)	0.47	4 (3%) 45 40	29, 43, 57, 69	0
14	1S	110/112 (98%)	0.29	0 100 100	49, 63, 74, 82	0
14	2S	110/112 (98%)	0.08	3 (2%) 54 50	54, 67, 78, 84	0
15	1T	131/146 (89%)	0.38	0 100 100	35, 48, 80, 88	0
15	2T	131/146 (89%)	0.23	1 (0%) 86 86	37, 50, 78, 87	0
16	1U	116/118 (98%)	0.61	0 100 100	29, 39, 57, 78	0
16	2U	116/118 (98%)	0.23	0 100 100	31, 44, 61, 78	0
17	1V	101/101 (100%)	0.44	0 100 100	30, 51, 69, 78	0
17	2V	101/101 (100%)	-0.08	3 (2%) 50 45	33, 57, 72, 79	0
18	1W	112/113 (99%)	0.54	2 (1%) 68 67	28, 37, 59, 90	0
18	2W	112/113 (99%)	0.24	2 (1%) 68 67	30, 40, 60, 90	0
19	1X	95/96 (98%)	0.55	1 (1%) 80 80	31, 47, 68, 80	0
19	2X	95/96 (98%)	0.22	3 (3%) 47 43	35, 50, 71, 81	0
20	1Y	107/110 (97%)	0.18	1 (0%) 84 84	31, 49, 74, 84	0
20	2Y	107/110 (97%)	0.72	6 (5%) 24 20	55, 72, 84, 96	0
21	1Z	186/206 (90%)	-0.06	0 100 100	40, 62, 79, 96	0
21	2Z	186/206 (90%)	0.26	6 (3%) 47 43	67, 81, 94, 101	0
22	10	75/85 (88%)	0.34	0 100 100	23, 38, 53, 67	0
22	20	75/85 (88%)	1.17	11 (14%) 2 1	43, 63, 73, 78	0
23	11	97/98 (98%)	0.59	2 (2%) 63 61	21, 42, 71, 80	0
23	21	97/98 (98%)	0.52	6 (6%) 20 16	33, 54, 77, 86	0
24	12	70/72 (97%)	0.53	3 (4%) 35 31	42, 59, 74, 89	0
24	22	70/72 (97%)	-0.03	1 (1%) 75 75	46, 63, 75, 87	0
25	13	59/60 (98%)	0.45	0 100 100	32, 46, 67, 80	0
25	23	59/60 (98%)	0.39	0 100 100	36, 49, 72, 82	0
26	14	69/71 (97%)	0.31	7 (10%) 7 5	68, 84, 100, 103	0
26	24	69/71 (97%)	0.77	10 (14%) 2 1	73, 86, 100, 104	0
27	15	59/60 (98%)	0.54	1 (1%) 70 69	21, 40, 60, 78	0
27	25	59/60 (98%)	0.19	0 100 100	24, 43, 62, 79	0
28	16	53/54 (98%)	0.23	0 100 100	36, 48, 63, 68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.05	1 (1%) 66 65	39, 51, 65, 70	0
29	17	48/49 (97%)	1.23	6 (12%) 3 3	26, 31, 67, 76	0
29	27	48/49 (97%)	1.11	7 (14%) 2 1	28, 33, 67, 78	0
30	18	64/65 (98%)	0.72	0 100 100	32, 40, 51, 64	0
30	28	64/65 (98%)	1.16	9 (14%) 2 2	34, 43, 54, 67	0
31	19	37/37 (100%)	0.64	0 100 100	40, 49, 66, 69	0
31	29	37/37 (100%)	0.77	2 (5%) 25 22	44, 53, 67, 71	0
32	1a	1477/1521 (97%)	0.32	17 (1%) 79 79	33, 72, 99, 116	0
32	2a	1483/1521 (97%)	0.35	20 (1%) 77 77	43, 78, 102, 119	0
33	1b	231/256 (90%)	0.12	7 (3%) 50 45	60, 83, 95, 105	0
33	2b	231/256 (90%)	0.78	30 (12%) 3 2	71, 88, 97, 101	0
34	1c	206/239 (86%)	0.84	36 (17%) 1 1	70, 84, 91, 99	0
34	2c	206/239 (86%)	0.82	42 (20%) 1 0	72, 86, 93, 100	0
35	1d	208/209 (99%)	1.28	59 (28%) 0 0	55, 78, 91, 101	0
35	2d	208/209 (99%)	0.66	21 (10%) 7 5	58, 75, 87, 90	0
36	1e	148/162 (91%)	0.61	8 (5%) 25 22	47, 65, 77, 94	0
36	2e	148/162 (91%)	0.59	9 (6%) 21 17	56, 74, 86, 91	0
37	1f	100/101 (99%)	0.36	5 (5%) 28 25	57, 75, 85, 89	0
37	2f	100/101 (99%)	-0.20	0 100 100	60, 76, 86, 90	0
38	1g	155/156 (99%)	0.55	15 (9%) 7 6	66, 80, 93, 101	0
38	2g	155/156 (99%)	0.42	15 (9%) 7 6	69, 81, 94, 99	0
39	1h	137/138 (99%)	0.72	17 (12%) 4 3	56, 68, 80, 85	0
39	2h	137/138 (99%)	0.61	13 (9%) 8 6	58, 75, 83, 89	0
40	1i	127/128 (99%)	1.44	40 (31%) 0 0	66, 87, 94, 99	0
40	2i	127/128 (99%)	2.37	67 (52%) 0 0	65, 88, 96, 100	0
41	1j	97/105 (92%)	1.16	26 (26%) 0 0	65, 86, 96, 104	0
41	2j	96/105 (91%)	1.53	32 (33%) 0 0	75, 92, 99, 103	0
42	1k	114/129 (88%)	0.42	4 (3%) 44 38	45, 69, 82, 94	0
42	2k	114/129 (88%)	0.37	8 (7%) 16 12	52, 76, 88, 91	0
43	1l	122/132 (92%)	0.53	12 (9%) 7 5	47, 65, 76, 88	0
43	2l	122/132 (92%)	0.88	15 (12%) 4 3	52, 67, 77, 85	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	118/126 (93%)	0.44	6 (5%) 28 24	64, 82, 89, 95	0
44	2m	116/126 (92%)	0.52	15 (12%) 3 2	66, 84, 91, 94	0
45	1n	60/61 (98%)	2.36	37 (61%) 0 0	69, 81, 88, 93	0
45	2n	60/61 (98%)	2.74	39 (65%) 0 0	71, 83, 89, 95	0
46	1o	88/89 (98%)	0.27	1 (1%) 80 80	49, 68, 84, 91	0
46	2o	88/89 (98%)	0.28	4 (4%) 33 29	56, 73, 85, 94	0
47	1p	82/88 (93%)	1.17	17 (20%) 1 0	66, 79, 92, 96	0
47	2p	82/88 (93%)	0.75	6 (7%) 15 11	59, 71, 83, 96	0
48	1q	99/105 (94%)	0.59	8 (8%) 12 9	51, 68, 81, 84	0
48	2q	99/105 (94%)	1.09	17 (17%) 1 1	57, 72, 83, 86	0
49	1r	68/88 (77%)	0.39	2 (2%) 51 47	56, 71, 84, 91	0
49	2r	68/88 (77%)	0.69	5 (7%) 14 11	65, 75, 89, 94	0
50	1s	84/93 (90%)	0.00	0 100 100	71, 83, 92, 98	0
50	2s	83/93 (89%)	1.37	22 (26%) 0 0	80, 92, 101, 108	0
51	1t	96/106 (90%)	0.92	20 (20%) 1 0	61, 74, 88, 90	0
51	2t	96/106 (90%)	0.40	3 (3%) 49 44	54, 73, 85, 90	0
52	1u	23/27 (85%)	1.13	5 (21%) 0 0	71, 80, 85, 87	0
52	2u	23/27 (85%)	2.46	12 (52%) 0 0	72, 82, 87, 89	0
53	1v	5/24 (20%)	1.22	1 (20%) 1 0	57, 67, 94, 101	0
53	2v	5/24 (20%)	2.34	3 (60%) 0 0	61, 70, 95, 102	0
54	1x	72/77 (93%)	0.26	0 100 100	35, 68, 87, 102	0
54	2x	72/77 (93%)	0.23	1 (1%) 75 75	38, 72, 89, 103	0
55	1z	13/19 (68%)	0.95	2 (15%) 2 1	26, 37, 63, 72	0
55	2z	13/19 (68%)	1.75	3 (23%) 0 0	28, 39, 65, 74	0
All	All	20522/21482 (95%)	0.50	980 (4%) 30 27	17, 62, 93, 119	0

The worst 5 of 980 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	9.6
40	2i	7	THR	7.9
38	1g	79	ARG	7.8
52	2u	14	TRP	7.7
26	24	49	PHE	7.6

## 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
54	PSU	2x	55	20/21	0.86	0.13	69,77,85,97	0
54	4SU	2x	8	20/21	0.92	0.15	70,77,94,99	0
54	PSU	1x	55	20/21	0.92	0.18	62,73,83,85	0
54	5MU	1x	54	21/22	0.94	0.17	57,66,80,87	0
54	5MU	2x	54	21/22	0.94	0.17	75,81,92,101	0
54	4SU	1x	8	20/21	0.95	0.20	51,69,76,81	0
54	5MC	2x	32	21/22	0.96	0.22	61,77,79,91	0
54	5MC	1x	32	21/22	0.97	0.20	48,59,69,81	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
56	MG	2A	3455	1/1	0.31	0.26	69,69,69,69	0
56	MG	2A	3210	1/1	0.31	0.17	63,63,63,63	0
56	MG	2a	3030	1/1	0.42	0.26	73,73,73,73	0
56	MG	2A	3061	1/1	0.43	0.28	68,68,68,68	0
56	MG	1A	3429	1/1	0.47	0.32	70,70,70,70	0
56	MG	1A	3145	1/1	0.48	0.19	77,77,77,77	0
56	MG	2A	3443	1/1	0.48	0.23	56,56,56,56	0
56	MG	2a	3014	1/1	0.52	0.12	65,65,65,65	0
56	MG	2a	3031	1/1	0.52	0.17	65,65,65,65	0
56	MG	1A	3521	1/1	0.53	0.33	75,75,75,75	0
56	MG	2a	3185	1/1	0.56	0.16	67,67,67,67	0
56	MG	2a	3254	1/1	0.56	0.23	71,71,71,71	0
56	MG	2G	3001	1/1	0.57	0.18	58,58,58,58	0
56	MG	1A	3023	1/1	0.58	0.20	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3034	1/1	0.59	0.24	73,73,73,73	0
56	MG	1A	3164	1/1	0.59	0.15	64,64,64,64	0
56	MG	1A	3032	1/1	0.60	0.16	63,63,63,63	0
56	MG	2B	3001	1/1	0.60	0.20	65,65,65,65	0
56	MG	1A	3417	1/1	0.62	0.47	58,58,58,58	0
56	MG	2A	3365	1/1	0.62	0.13	63,63,63,63	0
56	MG	2a	3235	1/1	0.62	0.14	68,68,68,68	0
56	MG	1A	3392	1/1	0.63	0.76	52,52,52,52	0
56	MG	2A	3381	1/1	0.63	0.20	64,64,64,64	0
56	MG	1A	3520	1/1	0.63	0.14	75,75,75,75	0
56	MG	2A	3445	1/1	0.63	0.16	71,71,71,71	0
56	MG	2a	3073	1/1	0.64	0.14	61,61,61,61	0
56	MG	2A	3145	1/1	0.64	0.22	77,77,77,77	0
56	MG	2a	3043	1/1	0.64	0.20	65,65,65,65	0
56	MG	1A	3780	1/1	0.64	0.14	43,43,43,43	0
56	MG	1A	3527	1/1	0.64	0.19	41,41,41,41	0
56	MG	1k	3001	1/1	0.64	0.17	70,70,70,70	0
56	MG	1f	3001	1/1	0.65	0.13	68,68,68,68	0
56	MG	1A	3126	1/1	0.65	0.17	53,53,53,53	0
56	MG	1a	1676	1/1	0.65	0.11	74,74,74,74	0
56	MG	1A	3070	1/1	0.65	0.17	72,72,72,72	0
56	MG	2a	3075	1/1	0.65	0.16	72,72,72,72	0
56	MG	1A	3035	1/1	0.66	0.66	53,53,53,53	0
56	MG	1A	3057	1/1	0.66	0.70	50,50,50,50	0
56	MG	2A	3113	1/1	0.66	0.18	64,64,64,64	0
56	MG	1A	3394	1/1	0.66	0.46	56,56,56,56	0
56	MG	15	101	1/1	0.66	0.48	58,58,58,58	0
56	MG	1A	3082	1/1	0.67	0.17	56,56,56,56	0
56	MG	1a	1732	1/1	0.67	0.24	74,74,74,74	0
56	MG	1F	307	1/1	0.68	0.26	59,59,59,59	0
56	MG	2a	3214	1/1	0.68	0.20	97,97,97,97	0
56	MG	1A	3132	1/1	0.68	0.73	51,51,51,51	0
56	MG	2A	3213	1/1	0.68	0.15	59,59,59,59	0
56	MG	2a	3161	1/1	0.68	0.12	102,102,102,102	0
56	MG	2a	3096	1/1	0.68	0.22	80,80,80,80	0
56	MG	2A	3501	1/1	0.68	0.15	85,85,85,85	0
56	MG	1A	3445	1/1	0.69	0.29	63,63,63,63	0
56	MG	1P	201	1/1	0.69	0.40	47,47,47,47	0
56	MG	2A	3076	1/1	0.69	0.20	60,60,60,60	0
56	MG	1A	3552	1/1	0.69	0.22	50,50,50,50	0
56	MG	2A	3401	1/1	0.69	0.14	48,48,48,48	0
56	MG	2a	3072	1/1	0.69	0.12	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
56	MG	1A	3166	1/1	0.69	0.15	55,55,55,55	0
56	MG	2A	3036	1/1	0.69	0.10	74,74,74,74	0
56	MG	1A	3349	1/1	0.70	0.17	73,73,73,73	0
56	MG	1T	203	1/1	0.70	0.18	61,61,61,61	0
56	MG	2A	3460	1/1	0.70	0.10	54,54,54,54	0
56	MG	2A	3352	1/1	0.70	0.16	68,68,68,68	0
56	MG	1A	3296	1/1	0.70	0.18	55,55,55,55	0
56	MG	2A	3353	1/1	0.70	0.14	61,61,61,61	0
56	MG	12	3001	1/1	0.70	0.39	61,61,61,61	0
56	MG	2A	3515	1/1	0.70	0.09	63,63,63,63	0
56	MG	1A	3338	1/1	0.70	0.34	54,54,54,54	0
56	MG	1A	3815	1/1	0.70	0.13	67,67,67,67	0
56	MG	1A	3399	1/1	0.70	0.30	58,58,58,58	0
56	MG	1A	3498	1/1	0.71	0.37	67,67,67,67	0
56	MG	1D	304	1/1	0.71	0.53	58,58,58,58	0
56	MG	1A	3357	1/1	0.71	0.21	68,68,68,68	0
56	MG	1A	3961	1/1	0.71	0.22	60,60,60,60	0
56	MG	1A	3508	1/1	0.71	0.43	57,57,57,57	0
56	MG	2A	3195	1/1	0.71	0.16	48,48,48,48	0
56	MG	1A	3560	1/1	0.71	0.13	45,45,45,45	0
56	MG	2A	3122	1/1	0.71	0.18	66,66,66,66	0
56	MG	2a	3159	1/1	0.71	0.20	85,85,85,85	0
56	MG	1N	3002	1/1	0.71	0.51	48,48,48,48	0
56	MG	2a	3092	1/1	0.71	0.19	87,87,87,87	0
56	MG	2a	3070	1/1	0.71	0.14	69,69,69,69	0
56	MG	2a	3255	1/1	0.72	0.18	70,70,70,70	0
56	MG	1a	1873	1/1	0.72	0.09	52,52,52,52	0
56	MG	1A	3923	1/1	0.72	0.24	53,53,53,53	0
56	MG	2a	3259	1/1	0.72	0.23	56,56,56,56	0
56	MG	2A	3551	1/1	0.72	0.23	57,57,57,57	0
56	MG	1a	1627	1/1	0.72	0.14	67,67,67,67	0
56	MG	1A	3977	1/1	0.72	0.56	53,53,53,53	0
56	MG	1A	3165	1/1	0.73	0.26	53,53,53,53	0
56	MG	2A	3008	1/1	0.73	0.12	64,64,64,64	0
56	MG	1A	3439	1/1	0.73	0.12	51,51,51,51	0
56	MG	1A	3433	1/1	0.73	0.15	71,71,71,71	0
56	MG	1a	1705	1/1	0.73	0.09	73,73,73,73	0
56	MG	2a	3008	1/1	0.73	0.19	67,67,67,67	0
56	MG	2F	304	1/1	0.73	0.24	53,53,53,53	0
56	MG	1A	3924	1/1	0.73	0.14	66,66,66,66	0
56	MG	2A	3106	1/1	0.73	0.14	59,59,59,59	0
56	MG	1A	3442	1/1	0.73	0.38	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3326	1/1	0.73	0.21	42,42,42,42	0
56	MG	1A	3043	1/1	0.74	0.37	52,52,52,52	0
56	MG	2A	3194	1/1	0.74	0.14	44,44,44,44	0
56	MG	1a	1623	1/1	0.74	0.19	72,72,72,72	0
56	MG	1A	3111	1/1	0.74	0.22	68,68,68,68	0
56	MG	1a	1751	1/1	0.74	0.18	61,61,61,61	0
56	MG	1a	1677	1/1	0.74	0.11	66,66,66,66	0
56	MG	2A	3117	1/1	0.74	0.14	53,53,53,53	0
56	MG	2A	3011	1/1	0.74	0.35	61,61,61,61	0
56	MG	2A	3287	1/1	0.74	0.14	56,56,56,56	0
56	MG	2a	3116	1/1	0.74	0.12	62,62,62,62	0
56	MG	2A	3027	1/1	0.74	0.90	51,51,51,51	0
56	MG	2A	3258	1/1	0.74	0.13	30,30,30,30	0
56	MG	2A	3250	1/1	0.75	0.17	64,64,64,64	0
56	MG	2A	3257	1/1	0.75	0.20	62,62,62,62	0
56	MG	2a	3056	1/1	0.75	0.12	85,85,85,85	0
56	MG	10	105	1/1	0.75	0.17	53,53,53,53	0
56	MG	2A	3001	1/1	0.75	0.21	45,45,45,45	0
56	MG	1A	3464	1/1	0.75	1.11	76,76,76,76	0
56	MG	1o	3001	1/1	0.75	0.16	74,74,74,74	0
56	MG	1a	1626	1/1	0.75	0.12	80,80,80,80	0
56	MG	1A	3884	1/1	0.75	0.14	53,53,53,53	0
56	MG	2A	3334	1/1	0.75	0.18	58,58,58,58	0
56	MG	2l	201	1/1	0.75	0.10	63,63,63,63	0
56	MG	2a	3256	1/1	0.76	0.13	94,94,94,94	0
56	MG	1A	3838	1/1	0.76	0.22	66,66,66,66	0
56	MG	2A	3229	1/1	0.76	0.22	55,55,55,55	0
56	MG	1A	3513	1/1	0.76	0.34	57,57,57,57	0
56	MG	2A	3091	1/1	0.76	0.23	49,49,49,49	0
56	MG	1A	3833	1/1	0.76	0.15	78,78,78,78	0
56	MG	2A	3483	1/1	0.76	0.18	54,54,54,54	0
56	MG	2a	3261	1/1	0.76	0.24	74,74,74,74	0
56	MG	1A	3385	1/1	0.76	0.19	59,59,59,59	0
56	MG	2a	3156	1/1	0.76	0.10	72,72,72,72	0
56	MG	1a	1614	1/1	0.77	0.34	68,68,68,68	0
56	MG	1A	3377	1/1	0.77	0.24	61,61,61,61	0
56	MG	1a	1757	1/1	0.77	0.14	63,63,63,63	0
56	MG	2a	3241	1/1	0.77	0.41	95,95,95,95	0
56	MG	1z	101	1/1	0.77	0.40	76,76,76,76	0
56	MG	1A	3363	1/1	0.77	0.19	68,68,68,68	0
56	MG	1a	1723	1/1	0.77	0.16	85,85,85,85	0
56	MG	2A	3554	1/1	0.77	2.24	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3562	1/1	0.77	0.64	49,49,49,49	0
56	MG	1A	3959	1/1	0.77	0.08	79,79,79,79	0
56	MG	1A	3018	1/1	0.77	0.12	59,59,59,59	0
57	ZN	24	501	1/1	0.77	0.10	125,125,125,125	0
56	MG	2a	3100	1/1	0.77	0.15	66,66,66,66	0
56	MG	1a	1776	1/1	0.77	0.18	69,69,69,69	0
56	MG	1Q	3003	1/1	0.77	0.75	51,51,51,51	0
56	MG	2A	3235	1/1	0.78	0.17	52,52,52,52	0
56	MG	1A	3261	1/1	0.78	0.35	62,62,62,62	0
56	MG	2a	3173	1/1	0.78	0.55	74,74,74,74	0
56	MG	2A	3332	1/1	0.78	0.13	38,38,38,38	0
56	MG	2A	3103	1/1	0.78	0.36	53,53,53,53	0
56	MG	1A	3050	1/1	0.78	0.27	48,48,48,48	0
56	MG	2A	3540	1/1	0.78	0.34	58,58,58,58	0
56	MG	2A	3209	1/1	0.78	0.19	45,45,45,45	0
56	MG	1A	3936	1/1	0.78	0.20	64,64,64,64	0
56	MG	1A	3002	1/1	0.78	0.24	53,53,53,53	0
56	MG	1a	1702	1/1	0.78	0.34	82,82,82,82	0
56	MG	2a	3077	1/1	0.78	0.12	59,59,59,59	0
56	MG	2A	3141	1/1	0.78	0.15	74,74,74,74	0
56	MG	1A	3822	1/1	0.78	0.15	46,46,46,46	0
56	MG	1A	3044	1/1	0.78	1.11	45,45,45,45	0
56	MG	1A	3028	1/1	0.78	0.43	46,46,46,46	0
56	MG	2A	3047	1/1	0.78	0.21	65,65,65,65	0
56	MG	2A	3509	1/1	0.78	0.18	62,62,62,62	0
56	MG	2A	3342	1/1	0.78	0.25	63,63,63,63	0
56	MG	2A	3126	1/1	0.79	0.11	50,50,50,50	0
56	MG	1A	3079	1/1	0.79	0.15	58,58,58,58	0
56	MG	2a	3138	1/1	0.79	0.13	81,81,81,81	0
56	MG	1B	221	1/1	0.79	0.17	68,68,68,68	0
56	MG	1B	204	1/1	0.79	0.28	54,54,54,54	0
56	MG	2A	3074	1/1	0.79	0.27	57,57,57,57	0
56	MG	1r	3001	1/1	0.79	0.15	69,69,69,69	0
56	MG	2a	3123	1/1	0.79	0.15	81,81,81,81	0
56	MG	1A	3027	1/1	0.79	0.34	54,54,54,54	0
56	MG	1A	3709	1/1	0.79	0.20	45,45,45,45	0
56	MG	2A	3511	1/1	0.79	0.14	52,52,52,52	0
56	MG	2a	3108	1/1	0.79	0.09	62,62,62,62	0
56	MG	1A	3570	1/1	0.79	0.18	66,66,66,66	0
56	MG	2A	3096	1/1	0.79	0.17	40,40,40,40	0
56	MG	1A	3106	1/1	0.79	0.15	64,64,64,64	0
56	MG	1A	3619	1/1	0.79	0.14	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2B	3003	1/1	0.79	0.21	73,73,73,73	0
56	MG	2q	202	1/1	0.79	0.25	69,69,69,69	0
56	MG	1A	3704	1/1	0.79	0.18	18,18,18,18	0
56	MG	1A	3013	1/1	0.79	0.26	70,70,70,70	0
56	MG	1A	3606	1/1	0.79	0.19	32,32,32,32	0
56	MG	1a	1628	1/1	0.79	0.15	61,61,61,61	0
56	MG	1a	1765	1/1	0.79	0.51	57,57,57,57	0
56	MG	1a	1694	1/1	0.79	0.17	78,78,78,78	0
56	MG	2A	3465	1/1	0.79	0.17	31,31,31,31	0
56	MG	1F	308	1/1	0.80	0.62	55,55,55,55	0
56	MG	2A	3254	1/1	0.80	0.28	40,40,40,40	0
56	MG	2A	3388	1/1	0.80	0.21	45,45,45,45	0
56	MG	1A	3857	1/1	0.80	0.21	32,32,32,32	0
56	MG	1A	3575	1/1	0.80	0.21	41,41,41,41	0
56	MG	1A	3610	1/1	0.80	0.10	37,37,37,37	0
56	MG	1A	3778	1/1	0.80	0.20	23,23,23,23	0
56	MG	1A	3119	1/1	0.80	0.35	65,65,65,65	0
56	MG	2A	3092	1/1	0.80	0.12	54,54,54,54	0
56	MG	1A	3440	1/1	0.80	0.10	66,66,66,66	0
56	MG	1A	3451	1/1	0.80	0.88	66,66,66,66	0
56	MG	1H	8002	1/1	0.80	0.43	79,79,79,79	0
56	MG	10	101	1/1	0.80	0.14	61,61,61,61	0
56	MG	1W	3002	1/1	0.80	0.21	55,55,55,55	0
56	MG	2a	3001	1/1	0.80	0.19	60,60,60,60	0
56	MG	2a	3170	1/1	0.80	0.14	77,77,77,77	0
56	MG	2a	3058	1/1	0.80	0.18	87,87,87,87	0
56	MG	2A	3364	1/1	0.80	0.15	60,60,60,60	0
56	MG	2A	3110	1/1	0.80	0.17	45,45,45,45	0
56	MG	1a	1609	1/1	0.80	0.20	63,63,63,63	0
56	MG	1a	1703	1/1	0.80	0.14	62,62,62,62	0
56	MG	1A	3031	1/1	0.80	0.35	61,61,61,61	0
56	MG	2A	3131	1/1	0.80	0.17	52,52,52,52	0
56	MG	1A	3327	1/1	0.80	0.13	73,73,73,73	0
56	MG	1A	4017	1/1	0.80	0.93	60,60,60,60	0
56	MG	2a	3162	1/1	0.80	0.20	75,75,75,75	0
56	MG	2a	3011	1/1	0.80	0.23	67,67,67,67	0
56	MG	1a	1822	1/1	0.80	0.15	52,52,52,52	0
56	MG	1A	3083	1/1	0.80	0.32	56,56,56,56	0
56	MG	2A	3071	1/1	0.80	0.18	68,68,68,68	0
56	MG	1A	3396	1/1	0.80	0.24	67,67,67,67	0
56	MG	1A	3005	1/1	0.80	0.23	58,58,58,58	0
56	MG	2a	3023	1/1	0.81	0.17	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1783	1/1	0.81	0.16	57,57,57,57	0
56	MG	2a	3210	1/1	0.81	0.11	62,62,62,62	0
56	MG	1A	3511	1/1	0.81	0.13	76,76,76,76	0
56	MG	1a	1745	1/1	0.81	0.18	79,79,79,79	0
56	MG	2a	3091	1/1	0.81	0.24	61,61,61,61	0
56	MG	1A	3421	1/1	0.81	0.14	47,47,47,47	0
56	MG	2a	3015	1/1	0.81	0.14	67,67,67,67	0
56	MG	2A	3087	1/1	0.81	0.21	59,59,59,59	0
56	MG	1b	3002	1/1	0.81	0.12	76,76,76,76	0
56	MG	2a	3157	1/1	0.81	0.14	74,74,74,74	0
56	MG	15	105	1/1	0.81	0.10	49,49,49,49	0
56	MG	2a	3180	1/1	0.81	0.18	61,61,61,61	0
56	MG	1A	3665	1/1	0.81	0.20	22,22,22,22	0
56	MG	2a	3125	1/1	0.81	0.10	60,60,60,60	0
56	MG	2a	3038	1/1	0.81	0.17	57,57,57,57	0
56	MG	1A	3322	1/1	0.81	0.64	50,50,50,50	0
56	MG	1N	3006	1/1	0.81	0.64	71,71,71,71	0
56	MG	1A	3499	1/1	0.81	0.16	62,62,62,62	0
56	MG	1a	1775	1/1	0.81	0.34	80,80,80,80	0
56	MG	2a	3152	1/1	0.81	0.15	84,84,84,84	0
56	MG	1A	3409	1/1	0.81	0.12	51,51,51,51	0
56	MG	1t	3001	1/1	0.81	0.14	54,54,54,54	0
56	MG	1A	3290	1/1	0.81	0.49	37,37,37,37	0
56	MG	2a	3018	1/1	0.81	0.20	49,49,49,49	0
56	MG	2A	3228	1/1	0.81	0.19	57,57,57,57	0
56	MG	2A	3473	1/1	0.81	0.14	64,64,64,64	0
56	MG	1a	1773	1/1	0.81	0.22	77,77,77,77	0
56	MG	1A	3095	1/1	0.81	0.29	50,50,50,50	0
56	MG	1A	3372	1/1	0.81	0.53	57,57,57,57	0
56	MG	2a	3153	1/1	0.81	0.11	67,67,67,67	0
56	MG	1a	1717	1/1	0.81	0.10	63,63,63,63	0
56	MG	2A	3039	1/1	0.81	0.20	49,49,49,49	0
56	MG	2A	3564	1/1	0.81	0.19	59,59,59,59	0
56	MG	2A	3240	1/1	0.81	0.15	63,63,63,63	0
56	MG	1A	3408	1/1	0.81	0.25	42,42,42,42	0
56	MG	1B	213	1/1	0.81	0.18	110,110,110,110	0
56	MG	2A	3389	1/1	0.81	0.24	77,77,77,77	0
56	MG	1A	3450	1/1	0.81	0.19	45,45,45,45	0
56	MG	1A	3953	1/1	0.81	0.30	71,71,71,71	0
56	MG	2A	3187	1/1	0.81	1.31	49,49,49,49	0
56	MG	1A	3467	1/1	0.81	0.22	71,71,71,71	0
56	MG	2a	3052	1/1	0.81	0.08	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
56	MG	1A	3197	1/1	0.81	0.13	50,50,50,50	0
56	MG	1A	3120	1/1	0.81	0.49	41,41,41,41	0
56	MG	1a	1706	1/1	0.82	0.22	64,64,64,64	0
56	MG	2B	3004	1/1	0.82	0.14	75,75,75,75	0
56	MG	2A	3006	1/1	0.82	0.10	64,64,64,64	0
56	MG	1A	3457	1/1	0.82	0.15	72,72,72,72	0
56	MG	2A	3031	1/1	0.82	0.15	51,51,51,51	0
56	MG	2A	3398	1/1	0.82	0.17	50,50,50,50	0
56	MG	1a	1771	1/1	0.82	0.15	63,63,63,63	0
56	MG	1A	3328	1/1	0.82	0.11	65,65,65,65	0
56	MG	1A	3939	1/1	0.82	0.39	69,69,69,69	0
56	MG	2A	3049	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3266	1/1	0.82	0.13	71,71,71,71	0
56	MG	1A	3479	1/1	0.82	0.41	38,38,38,38	0
56	MG	1a	1704	1/1	0.82	0.18	54,54,54,54	0
56	MG	1A	3632	1/1	0.82	0.21	25,25,25,25	0
56	MG	2A	3555	1/1	0.82	0.51	36,36,36,36	0
56	MG	2A	3513	1/1	0.82	0.14	61,61,61,61	0
56	MG	1A	3278	1/1	0.82	0.13	56,56,56,56	0
56	MG	1A	3523	1/1	0.82	0.17	59,59,59,59	0
56	MG	1A	3482	1/1	0.82	0.17	48,48,48,48	0
56	MG	1a	1800	1/1	0.82	0.17	57,57,57,57	0
56	MG	2a	3036	1/1	0.82	0.26	72,72,72,72	0
56	MG	1A	3675	1/1	0.82	0.11	79,79,79,79	0
56	MG	2A	3218	1/1	0.82	0.56	62,62,62,62	0
56	MG	1r	3002	1/1	0.82	0.22	55,55,55,55	0
56	MG	1a	1689	1/1	0.82	0.11	65,65,65,65	0
56	MG	2a	3026	1/1	0.82	0.25	64,64,64,64	0
56	MG	1a	1617	1/1	0.82	0.29	78,78,78,78	0
56	MG	2a	3086	1/1	0.82	0.22	64,64,64,64	0
56	MG	1A	3486	1/1	0.82	0.14	67,67,67,67	0
56	MG	1A	3966	1/1	0.82	0.99	47,47,47,47	0
56	MG	1a	1802	1/1	0.82	0.14	76,76,76,76	0
56	MG	2A	3493	1/1	0.82	0.22	58,58,58,58	0
56	MG	1A	3446	1/1	0.82	0.31	62,62,62,62	0
56	MG	1A	3270	1/1	0.82	0.18	34,34,34,34	0
56	MG	1A	3033	1/1	0.82	0.13	57,57,57,57	0
56	MG	1A	3167	1/1	0.82	0.26	35,35,35,35	0
56	MG	1A	3434	1/1	0.82	0.20	70,70,70,70	0
56	MG	2A	3510	1/1	0.82	0.15	34,34,34,34	0
56	MG	2A	3486	1/1	0.82	0.18	57,57,57,57	0
56	MG	1A	3066	1/1	0.82	0.61	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1672	1/1	0.82	0.15	58,58,58,58	0
56	MG	1A	3645	1/1	0.82	0.21	23,23,23,23	0
56	MG	2A	3034	1/1	0.82	0.26	54,54,54,54	0
56	MG	1A	3995	1/1	0.82	0.88	42,42,42,42	0
56	MG	2A	3358	1/1	0.82	0.27	59,59,59,59	0
56	MG	1A	3564	1/1	0.82	0.19	35,35,35,35	0
56	MG	1A	3060	1/1	0.82	0.54	67,67,67,67	0
56	MG	2A	3104	1/1	0.82	0.54	54,54,54,54	0
56	MG	1a	1690	1/1	0.82	0.16	63,63,63,63	0
56	MG	1A	3755	1/1	0.82	0.11	66,66,66,66	0
56	MG	1A	3769	1/1	0.82	0.20	90,90,90,90	0
56	MG	1A	3647	1/1	0.83	0.22	74,74,74,74	0
56	MG	1A	3855	1/1	0.83	0.20	84,84,84,84	0
56	MG	2a	3221	1/1	0.83	0.12	66,66,66,66	0
56	MG	2A	3301	1/1	0.83	0.15	38,38,38,38	0
56	MG	1A	3516	1/1	0.83	0.26	53,53,53,53	0
56	MG	1A	3170	1/1	0.83	0.23	44,44,44,44	0
56	MG	2F	305	1/1	0.83	0.11	41,41,41,41	0
56	MG	2A	3315	1/1	0.83	0.22	55,55,55,55	0
56	MG	1A	3105	1/1	0.83	0.22	61,61,61,61	0
56	MG	2a	3201	1/1	0.83	0.37	88,88,88,88	0
56	MG	2B	3007	1/1	0.83	0.25	56,56,56,56	0
56	MG	2A	3369	1/1	0.83	0.15	31,31,31,31	0
56	MG	1A	3163	1/1	0.83	0.14	32,32,32,32	0
56	MG	1a	1876	1/1	0.83	0.12	80,80,80,80	0
56	MG	2x	3002	1/1	0.83	0.14	65,65,65,65	0
56	MG	2A	3086	1/1	0.83	0.30	49,49,49,49	0
56	MG	1A	3583	1/1	0.83	0.10	55,55,55,55	0
56	MG	1A	3547	1/1	0.83	0.17	54,54,54,54	0
56	MG	1A	3124	1/1	0.83	0.58	56,56,56,56	0
56	MG	1A	3226	1/1	0.83	0.10	41,41,41,41	0
56	MG	1A	3648	1/1	0.83	0.13	20,20,20,20	0
56	MG	1a	1807	1/1	0.83	0.17	60,60,60,60	0
56	MG	2a	3047	1/1	0.83	0.22	63,63,63,63	0
56	MG	1A	3420	1/1	0.83	0.11	56,56,56,56	0
56	MG	1n	502	1/1	0.83	0.23	67,67,67,67	0
56	MG	1a	1649	1/1	0.83	0.37	63,63,63,63	0
56	MG	1B	223	1/1	0.83	0.13	59,59,59,59	0
56	MG	2A	3239	1/1	0.83	0.11	60,60,60,60	0
56	MG	1A	3427	1/1	0.83	0.15	53,53,53,53	0
56	MG	1a	1828	1/1	0.83	0.11	61,61,61,61	0
56	MG	1A	3352	1/1	0.83	0.12	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3368	1/1	0.83	0.21	29,29,29,29	0
56	MG	2a	3146	1/1	0.83	0.15	57,57,57,57	0
56	MG	2A	3038	1/1	0.83	0.11	58,58,58,58	0
56	MG	1A	3470	1/1	0.83	0.13	52,52,52,52	0
56	MG	2A	3295	1/1	0.83	0.14	48,48,48,48	0
56	MG	1A	3405	1/1	0.83	0.14	54,54,54,54	0
56	MG	2A	3232	1/1	0.83	0.23	54,54,54,54	0
56	MG	1A	3230	1/1	0.83	0.55	46,46,46,46	0
56	MG	1a	1651	1/1	0.83	0.26	54,54,54,54	0
56	MG	1a	1862	1/1	0.83	0.13	65,65,65,65	0
56	MG	1A	3361	1/1	0.83	0.19	66,66,66,66	0
56	MG	1A	3459	1/1	0.83	0.41	46,46,46,46	0
56	MG	2A	3309	1/1	0.83	0.18	31,31,31,31	0
56	MG	2A	3271	1/1	0.83	0.15	27,27,27,27	0
56	MG	1A	3895	1/1	0.83	0.22	24,24,24,24	0
56	MG	1a	1643	1/1	0.83	0.14	76,76,76,76	0
56	MG	1a	1792	1/1	0.83	0.10	54,54,54,54	0
56	MG	2A	3530	1/1	0.83	0.12	46,46,46,46	0
56	MG	2x	3003	1/1	0.83	0.12	73,73,73,73	0
56	MG	2l	203	1/1	0.83	0.23	60,60,60,60	0
56	MG	1a	1854	1/1	0.83	0.10	82,82,82,82	0
56	MG	1a	1741	1/1	0.84	0.15	63,63,63,63	0
56	MG	1a	1724	1/1	0.84	0.09	76,76,76,76	0
56	MG	2A	3112	1/1	0.84	0.13	39,39,39,39	0
56	MG	2a	3044	1/1	0.84	0.21	71,71,71,71	0
56	MG	1A	3379	1/1	0.84	0.28	61,61,61,61	0
56	MG	1a	1721	1/1	0.84	0.14	59,59,59,59	0
56	MG	1A	3172	1/1	0.84	0.61	44,44,44,44	0
56	MG	1d	502	1/1	0.84	0.13	76,76,76,76	0
56	MG	1A	3751	1/1	0.84	0.13	39,39,39,39	0
56	MG	1A	3883	1/1	0.84	0.59	58,58,58,58	0
56	MG	1A	3489	1/1	0.84	0.11	51,51,51,51	0
56	MG	2A	3371	1/1	0.84	0.13	56,56,56,56	0
56	MG	18	102	1/1	0.84	0.29	57,57,57,57	0
56	MG	1A	3067	1/1	0.84	0.18	46,46,46,46	0
56	MG	2a	3046	1/1	0.84	0.09	65,65,65,65	0
56	MG	1A	3705	1/1	0.84	0.39	34,34,34,34	0
56	MG	2A	3238	1/1	0.84	0.14	60,60,60,60	0
56	MG	10	104	1/1	0.84	0.22	43,43,43,43	0
56	MG	1a	1760	1/1	0.84	0.13	85,85,85,85	0
56	MG	2a	3082	1/1	0.84	0.13	61,61,61,61	0
56	MG	2A	3328	1/1	0.84	0.19	57,57,57,57	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3471	1/1	0.84	0.09	74,74,74,74	0
56	MG	1A	3039	1/1	0.84	0.30	49,49,49,49	0
56	MG	2A	3013	1/1	0.84	0.18	68,68,68,68	0
56	MG	2A	3380	1/1	0.84	0.27	74,74,74,74	0
56	MG	1A	3785	1/1	0.84	0.13	72,72,72,72	0
56	MG	2A	3169	1/1	0.84	0.25	33,33,33,33	0
56	MG	1A	3221	1/1	0.84	0.15	37,37,37,37	0
56	MG	1A	3281	1/1	0.84	0.42	53,53,53,53	0
56	MG	2a	3079	1/1	0.84	0.06	69,69,69,69	0
56	MG	1a	1750	1/1	0.84	0.37	64,64,64,64	0
56	MG	1A	3509	1/1	0.84	0.23	71,71,71,71	0
56	MG	2A	3148	1/1	0.84	0.26	63,63,63,63	0
56	MG	2a	3158	1/1	0.84	0.10	74,74,74,74	0
56	MG	2A	3156	1/1	0.84	0.17	49,49,49,49	0
56	MG	2A	3236	1/1	0.84	0.06	91,91,91,91	0
56	MG	2A	3041	1/1	0.84	0.41	53,53,53,53	0
56	MG	2A	3114	1/1	0.84	0.14	57,57,57,57	0
56	MG	2A	3142	1/1	0.84	0.20	50,50,50,50	0
56	MG	1A	3118	1/1	0.84	0.16	68,68,68,68	0
56	MG	1G	3002	1/1	0.84	0.16	61,61,61,61	0
56	MG	1T	202	1/1	0.84	0.13	55,55,55,55	0
56	MG	1a	1642	1/1	0.84	0.12	69,69,69,69	0
56	MG	1a	1608	1/1	0.84	0.28	59,59,59,59	0
56	MG	1A	3330	1/1	0.84	0.13	41,41,41,41	0
56	MG	2a	3006	1/1	0.84	0.10	62,62,62,62	0
56	MG	2A	3405	1/1	0.84	0.18	63,63,63,63	0
56	MG	1A	3262	1/1	0.84	0.06	66,66,66,66	0
56	MG	1A	3242	1/1	0.84	0.12	33,33,33,33	0
56	MG	1B	209	1/1	0.84	0.33	62,62,62,62	0
56	MG	2a	3020	1/1	0.84	0.17	49,49,49,49	0
56	MG	2A	3556	1/1	0.84	0.19	62,62,62,62	0
56	MG	1A	3462	1/1	0.84	0.08	57,57,57,57	0
56	MG	2A	3083	1/1	0.84	0.14	49,49,49,49	0
56	MG	2a	3228	1/1	0.84	0.39	69,69,69,69	0
56	MG	2A	3241	1/1	0.84	0.17	65,65,65,65	0
56	MG	1A	3024	1/1	0.84	0.20	63,63,63,63	0
56	MG	2a	3027	1/1	0.84	0.28	70,70,70,70	0
56	MG	1A	3918	1/1	0.85	0.39	71,71,71,71	0
56	MG	2A	3508	1/1	0.85	0.21	56,56,56,56	0
56	MG	2A	3217	1/1	0.85	0.11	56,56,56,56	0
56	MG	1A	3522	1/1	0.85	0.13	69,69,69,69	0
56	MG	1A	3613	1/1	0.85	0.19	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3403	1/1	0.85	0.08	59,59,59,59	0
56	MG	1A	3472	1/1	0.85	0.68	83,83,83,83	0
56	MG	1A	3526	1/1	0.85	0.21	32,32,32,32	0
56	MG	2A	3452	1/1	0.85	0.16	69,69,69,69	0
56	MG	2A	3174	1/1	0.85	0.13	45,45,45,45	0
56	MG	1H	8001	1/1	0.85	0.09	58,58,58,58	0
56	MG	1A	3881	1/1	0.85	0.11	55,55,55,55	0
56	MG	1A	3875	1/1	0.85	0.29	83,83,83,83	0
56	MG	1A	3130	1/1	0.85	0.36	58,58,58,58	0
56	MG	1A	3054	1/1	0.85	0.18	47,47,47,47	0
56	MG	1A	3862	1/1	0.85	0.21	62,62,62,62	0
56	MG	1A	4018	1/1	0.85	0.94	50,50,50,50	0
56	MG	1A	3865	1/1	0.85	0.25	68,68,68,68	0
56	MG	1a	1607	1/1	0.85	0.10	78,78,78,78	0
56	MG	1A	3846	1/1	0.85	0.08	78,78,78,78	0
56	MG	1D	310	1/1	0.85	0.23	57,57,57,57	0
56	MG	2a	3104	1/1	0.85	0.15	62,62,62,62	0
56	MG	1A	3668	1/1	0.85	0.12	60,60,60,60	0
56	MG	2A	3102	1/1	0.85	0.14	52,52,52,52	0
56	MG	1a	1621	1/1	0.85	0.24	68,68,68,68	0
56	MG	2a	3206	1/1	0.85	0.09	63,63,63,63	0
56	MG	1A	3380	1/1	0.85	0.39	63,63,63,63	0
56	MG	1A	3779	1/1	0.85	0.27	54,54,54,54	0
56	MG	2A	3162	1/1	0.85	0.26	50,50,50,50	0
56	MG	2a	3022	1/1	0.85	0.71	73,73,73,73	0
56	MG	1b	3001	1/1	0.85	0.11	83,83,83,83	0
56	MG	2a	3207	1/1	0.85	0.16	73,73,73,73	0
56	MG	1A	3549	1/1	0.85	0.19	48,48,48,48	0
56	MG	2a	3035	1/1	0.85	0.10	69,69,69,69	0
56	MG	1A	3274	1/1	0.85	0.21	41,41,41,41	0
56	MG	1A	3367	1/1	0.85	0.11	66,66,66,66	0
56	MG	1A	3026	1/1	0.85	0.14	53,53,53,53	0
56	MG	1A	3243	1/1	0.85	0.84	46,46,46,46	0
56	MG	2A	3118	1/1	0.85	0.22	75,75,75,75	0
56	MG	1a	1707	1/1	0.85	0.11	67,67,67,67	0
56	MG	1A	3757	1/1	0.85	0.11	39,39,39,39	0
56	MG	1A	3128	1/1	0.85	0.14	56,56,56,56	0
56	MG	2A	3211	1/1	0.85	0.29	63,63,63,63	0
56	MG	1a	1821	1/1	0.85	0.07	49,49,49,49	0
56	MG	1A	3100	1/1	0.85	0.12	48,48,48,48	0
56	MG	1A	3955	1/1	0.85	0.15	63,63,63,63	0
56	MG	1A	3149	1/1	0.85	0.17	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3300	1/1	0.85	0.18	32,32,32,32	0
56	MG	1B	205	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3997	1/1	0.85	0.22	50,50,50,50	0
56	MG	2A	3333	1/1	0.85	0.16	51,51,51,51	0
56	MG	1A	3183	1/1	0.85	0.73	44,44,44,44	0
56	MG	2A	3523	1/1	0.86	0.39	56,56,56,56	0
56	MG	1a	1875	1/1	0.86	0.25	82,82,82,82	0
56	MG	1A	3297	1/1	0.86	0.30	70,70,70,70	0
56	MG	2A	3321	1/1	0.86	0.15	35,35,35,35	0
56	MG	1B	201	1/1	0.86	0.10	50,50,50,50	0
56	MG	1A	3131	1/1	0.86	0.56	42,42,42,42	0
56	MG	2A	3256	1/1	0.86	0.15	34,34,34,34	0
56	MG	2A	3225	1/1	0.86	0.13	63,63,63,63	0
56	MG	1A	3360	1/1	0.86	0.22	47,47,47,47	0
56	MG	1a	1618	1/1	0.86	0.13	64,64,64,64	0
56	MG	1A	3077	1/1	0.86	0.23	69,69,69,69	0
56	MG	1A	3185	1/1	0.86	0.10	41,41,41,41	0
56	MG	1A	3146	1/1	0.86	0.18	65,65,65,65	0
56	MG	1a	1849	1/1	0.86	0.10	53,53,53,53	0
56	MG	1A	3654	1/1	0.86	0.18	67,67,67,67	0
56	MG	1G	3001	1/1	0.86	0.17	48,48,48,48	0
56	MG	2A	3216	1/1	0.86	0.43	45,45,45,45	0
56	MG	1x	107	1/1	0.86	0.39	61,61,61,61	0
56	MG	1A	3519	1/1	0.86	0.31	62,62,62,62	0
56	MG	1A	3219	1/1	0.86	0.26	59,59,59,59	0
56	MG	1A	3101	1/1	0.86	0.29	55,55,55,55	0
56	MG	1A	3390	1/1	0.86	0.73	40,40,40,40	0
56	MG	1A	3052	1/1	0.86	0.13	59,59,59,59	0
56	MG	2A	3449	1/1	0.86	0.12	60,60,60,60	0
56	MG	1a	1602	1/1	0.86	0.35	64,64,64,64	0
56	MG	2a	3205	1/1	0.86	0.22	74,74,74,74	0
56	MG	2A	3269	1/1	0.86	0.15	41,41,41,41	0
56	MG	1A	3913	1/1	0.86	0.16	64,64,64,64	0
56	MG	1A	3306	1/1	0.86	0.26	41,41,41,41	0
56	MG	2A	3246	1/1	0.86	0.17	36,36,36,36	0
56	MG	2a	3216	1/1	0.86	0.26	56,56,56,56	0
56	MG	2A	3559	1/1	0.86	0.32	54,54,54,54	0
56	MG	1A	3468	1/1	0.86	0.24	57,57,57,57	0
56	MG	1A	3703	1/1	0.86	0.15	49,49,49,49	0
56	MG	1A	3332	1/1	0.86	0.12	55,55,55,55	0
56	MG	1A	3889	1/1	0.86	0.36	60,60,60,60	0
56	MG	1A	3268	1/1	0.86	0.14	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3150	1/1	0.86	0.15	34,34,34,34	0
56	MG	1A	3605	1/1	0.86	0.20	33,33,33,33	0
56	MG	2A	3341	1/1	0.86	0.17	52,52,52,52	0
56	MG	2a	3191	1/1	0.86	0.12	54,54,54,54	0
56	MG	2B	3002	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3009	1/1	0.86	0.42	60,60,60,60	0
56	MG	1A	3640	1/1	0.86	0.20	24,24,24,24	0
56	MG	2A	3005	1/1	0.86	0.13	54,54,54,54	0
56	MG	1A	3607	1/1	0.86	0.20	40,40,40,40	0
56	MG	2A	3097	1/1	0.86	0.14	51,51,51,51	0
56	MG	2A	3497	1/1	0.86	0.18	54,54,54,54	0
56	MG	1A	3600	1/1	0.86	0.20	54,54,54,54	0
56	MG	2a	3134	1/1	0.86	0.12	59,59,59,59	0
56	MG	1A	3301	1/1	0.86	0.17	53,53,53,53	0
56	MG	1A	3378	1/1	0.86	0.48	69,69,69,69	0
56	MG	1a	1640	1/1	0.86	0.20	51,51,51,51	0
56	MG	1A	3888	1/1	0.86	0.48	42,42,42,42	0
56	MG	1A	3614	1/1	0.86	0.23	37,37,37,37	0
56	MG	1A	3238	1/1	0.86	0.99	45,45,45,45	0
56	MG	1x	106	1/1	0.86	0.21	63,63,63,63	0
56	MG	1A	3359	1/1	0.86	0.31	53,53,53,53	0
56	MG	1A	3534	1/1	0.86	0.23	35,35,35,35	0
56	MG	13	102	1/1	0.86	0.14	56,56,56,56	0
56	MG	1A	3745	1/1	0.86	0.68	71,71,71,71	0
56	MG	1A	3980	1/1	0.86	0.43	50,50,50,50	0
56	MG	2a	3065	1/1	0.86	0.32	80,80,80,80	0
56	MG	1A	3725	1/1	0.87	0.19	42,42,42,42	0
56	MG	1A	3448	1/1	0.87	0.17	49,49,49,49	0
56	MG	1A	3007	1/1	0.87	0.28	56,56,56,56	0
56	MG	2a	3024	1/1	0.87	0.18	76,76,76,76	0
56	MG	1A	3246	1/1	0.87	0.20	58,58,58,58	0
56	MG	1A	3388	1/1	0.87	0.10	53,53,53,53	0
56	MG	2A	3018	1/1	0.87	0.18	50,50,50,50	0
56	MG	2a	3240	1/1	0.87	0.23	81,81,81,81	0
56	MG	1A	3685	1/1	0.87	0.26	73,73,73,73	0
56	MG	2A	3484	1/1	0.87	0.13	82,82,82,82	0
56	MG	2A	3306	1/1	0.87	0.19	48,48,48,48	0
56	MG	17	101	1/1	0.87	0.28	57,57,57,57	0
56	MG	1A	3320	1/1	0.87	0.06	93,93,93,93	0
56	MG	1A	3404	1/1	0.87	0.34	48,48,48,48	0
56	MG	1A	4010	1/1	0.87	0.57	41,41,41,41	0
56	MG	2A	3522	1/1	0.87	0.11	70,70,70,70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	219	1/1	0.87	0.08	60,60,60,60	0
56	MG	1A	3142	1/1	0.87	0.58	57,57,57,57	0
56	MG	2D	302	1/1	0.87	0.19	54,54,54,54	0
56	MG	1x	108	1/1	0.87	0.15	70,70,70,70	0
56	MG	1A	3992	1/1	0.87	0.16	55,55,55,55	0
56	MG	1A	3428	1/1	0.87	0.11	65,65,65,65	0
56	MG	1A	3734	1/1	0.87	0.21	38,38,38,38	0
56	MG	1A	3235	1/1	0.87	0.17	46,46,46,46	0
56	MG	15	104	1/1	0.87	0.27	62,62,62,62	0
56	MG	1B	208	1/1	0.87	0.26	56,56,56,56	0
56	MG	2A	3198	1/1	0.87	0.18	41,41,41,41	0
56	MG	1a	1725	1/1	0.87	0.18	59,59,59,59	0
56	MG	1A	3840	1/1	0.87	0.17	63,63,63,63	0
56	MG	1A	3402	1/1	0.87	0.15	58,58,58,58	0
56	MG	2a	3238	1/1	0.87	0.15	55,55,55,55	0
56	MG	1a	1748	1/1	0.87	0.21	52,52,52,52	0
56	MG	1A	3965	1/1	0.87	0.44	53,53,53,53	0
56	MG	1A	3400	1/1	0.87	0.15	45,45,45,45	0
56	MG	1A	3542	1/1	0.87	0.15	26,26,26,26	0
56	MG	1A	3135	1/1	0.87	0.33	64,64,64,64	0
56	MG	1A	3890	1/1	0.87	0.21	37,37,37,37	0
56	MG	1a	1630	1/1	0.87	0.28	56,56,56,56	0
56	MG	1A	3958	1/1	0.87	0.17	64,64,64,64	0
56	MG	1A	3539	1/1	0.87	0.22	44,44,44,44	0
56	MG	2A	3407	1/1	0.87	0.19	40,40,40,40	0
56	MG	1A	3729	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3298	1/1	0.87	0.13	49,49,49,49	0
56	MG	2a	3217	1/1	0.87	0.12	83,83,83,83	0
56	MG	1A	3818	1/1	0.87	0.16	61,61,61,61	0
56	MG	18	101	1/1	0.87	0.11	63,63,63,63	0
56	MG	2a	3139	1/1	0.87	0.12	70,70,70,70	0
56	MG	1a	1662	1/1	0.87	0.15	61,61,61,61	0
56	MG	1A	3715	1/1	0.87	0.15	63,63,63,63	0
56	MG	2a	3029	1/1	0.87	0.27	69,69,69,69	0
56	MG	1A	3878	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3233	1/1	0.87	0.19	34,34,34,34	0
56	MG	1A	3365	1/1	0.87	0.24	46,46,46,46	0
56	MG	1A	3121	1/1	0.87	0.85	38,38,38,38	0
56	MG	2a	3013	1/1	0.87	0.15	72,72,72,72	0
56	MG	1D	311	1/1	0.87	0.47	55,55,55,55	0
56	MG	1A	3503	1/1	0.87	0.12	62,62,62,62	0
56	MG	2A	3264	1/1	0.87	0.10	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3234	1/1	0.87	0.40	48,48,48,48	0
56	MG	1A	3098	1/1	0.87	0.18	52,52,52,52	0
56	MG	2a	3016	1/1	0.87	0.17	65,65,65,65	0
56	MG	2a	3231	1/1	0.87	0.17	75,75,75,75	0
56	MG	1A	3682	1/1	0.87	0.14	51,51,51,51	0
56	MG	1A	3984	1/1	0.87	0.12	47,47,47,47	0
56	MG	2a	3037	1/1	0.87	0.15	53,53,53,53	0
56	MG	1A	3010	1/1	0.88	0.22	42,42,42,42	0
56	MG	2A	3179	1/1	0.88	0.13	46,46,46,46	0
56	MG	2a	3187	1/1	0.88	0.24	59,59,59,59	0
56	MG	1A	3014	1/1	0.88	0.34	53,53,53,53	0
56	MG	2a	3087	1/1	0.88	0.13	55,55,55,55	0
56	MG	2D	304	1/1	0.88	0.29	42,42,42,42	0
56	MG	1a	1722	1/1	0.88	0.21	54,54,54,54	0
56	MG	1F	304	1/1	0.88	0.54	43,43,43,43	0
56	MG	2A	3268	1/1	0.88	0.17	55,55,55,55	0
56	MG	2A	3158	1/1	0.88	0.18	47,47,47,47	0
56	MG	1A	3133	1/1	0.88	0.33	59,59,59,59	0
56	MG	2A	3035	1/1	0.88	0.12	58,58,58,58	0
56	MG	1A	3699	1/1	0.88	0.12	47,47,47,47	0
56	MG	2A	3030	1/1	0.88	0.09	50,50,50,50	0
56	MG	2a	3098	1/1	0.88	0.30	50,50,50,50	0
56	MG	1A	3615	1/1	0.88	0.18	39,39,39,39	0
56	MG	2a	3093	1/1	0.88	0.10	50,50,50,50	0
56	MG	1A	3985	1/1	0.88	0.17	66,66,66,66	0
56	MG	1a	1726	1/1	0.88	0.20	54,54,54,54	0
56	MG	1A	3331	1/1	0.88	0.21	57,57,57,57	0
56	MG	1A	3494	1/1	0.88	0.34	51,51,51,51	0
56	MG	2B	3011	1/1	0.88	0.18	83,83,83,83	0
56	MG	2a	3176	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	3698	1/1	0.88	0.07	48,48,48,48	0
56	MG	1A	3658	1/1	0.88	0.19	18,18,18,18	0
56	MG	1A	3200	1/1	0.88	0.12	46,46,46,46	0
56	MG	1A	3461	1/1	0.88	0.25	71,71,71,71	0
56	MG	1a	1754	1/1	0.88	0.10	81,81,81,81	0
56	MG	1A	3874	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3088	1/1	0.88	0.17	51,51,51,51	0
56	MG	1A	3263	1/1	0.88	0.14	37,37,37,37	0
56	MG	2A	3021	1/1	0.88	0.27	58,58,58,58	0
56	MG	2A	3542	1/1	0.88	0.15	42,42,42,42	0
56	MG	2A	3227	1/1	0.88	0.17	47,47,47,47	0
56	MG	2A	3119	1/1	0.88	0.14	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3657	1/1	0.88	0.17	49,49,49,49	0
56	MG	2A	3056	1/1	0.88	0.13	38,38,38,38	0
56	MG	2A	3273	1/1	0.88	0.06	41,41,41,41	0
56	MG	1A	3563	1/1	0.88	0.14	46,46,46,46	0
56	MG	1A	3102	1/1	0.88	0.13	60,60,60,60	0
56	MG	2A	3395	1/1	0.88	0.18	33,33,33,33	0
56	MG	1a	1667	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3514	1/1	0.88	0.13	60,60,60,60	0
56	MG	1A	3758	1/1	0.88	0.12	65,65,65,65	0
56	MG	1A	3845	1/1	0.88	0.12	42,42,42,42	0
56	MG	2A	3448	1/1	0.88	0.14	56,56,56,56	0
56	MG	2A	3173	1/1	0.88	0.12	52,52,52,52	0
56	MG	2A	3082	1/1	0.88	0.19	41,41,41,41	0
56	MG	2A	3147	1/1	0.88	0.17	42,42,42,42	0
56	MG	2A	3557	1/1	0.88	0.09	64,64,64,64	0
56	MG	1A	3726	1/1	0.88	0.25	64,64,64,64	0
56	MG	2A	3361	1/1	0.88	0.20	54,54,54,54	0
56	MG	1A	3697	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3299	1/1	0.88	0.18	46,46,46,46	0
56	MG	2A	3495	1/1	0.88	0.12	71,71,71,71	0
56	MG	1A	3020	1/1	0.88	0.12	54,54,54,54	0
56	MG	2A	3255	1/1	0.88	0.15	52,52,52,52	0
56	MG	1A	3355	1/1	0.88	0.14	53,53,53,53	0
56	MG	1N	3003	1/1	0.88	0.20	42,42,42,42	0
56	MG	1A	3284	1/1	0.88	0.10	41,41,41,41	0
56	MG	2O	201	1/1	0.88	0.10	48,48,48,48	0
56	MG	2A	3499	1/1	0.88	0.14	47,47,47,47	0
56	MG	1A	3406	1/1	0.88	0.10	50,50,50,50	0
56	MG	1a	1701	1/1	0.88	0.17	54,54,54,54	0
56	MG	1A	3507	1/1	0.88	0.88	64,64,64,64	0
56	MG	2A	3127	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3310	1/1	0.88	0.14	31,31,31,31	0
56	MG	1A	3683	1/1	0.88	0.22	58,58,58,58	0
56	MG	2A	3003	1/1	0.88	0.11	53,53,53,53	0
56	MG	1a	1611	1/1	0.88	0.10	78,78,78,78	0
56	MG	1A	3867	1/1	0.88	0.21	30,30,30,30	0
56	MG	1A	3415	1/1	0.88	0.12	50,50,50,50	0
56	MG	1a	1727	1/1	0.88	0.13	54,54,54,54	0
56	MG	1U	201	1/1	0.88	0.20	51,51,51,51	0
56	MG	1a	1691	1/1	0.88	0.12	27,27,27,27	0
56	MG	1A	3381	1/1	0.88	0.17	47,47,47,47	0
56	MG	1a	1710	1/1	0.88	0.18	71,71,71,71	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1O	3001	1/1	0.88	0.26	45,45,45,45	0
56	MG	1A	3387	1/1	0.88	1.26	56,56,56,56	0
56	MG	1A	4001	1/1	0.88	0.81	43,43,43,43	0
56	MG	1A	3123	1/1	0.88	0.18	44,44,44,44	0
56	MG	1A	3676	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3143	1/1	0.88	0.11	48,48,48,48	0
56	MG	1a	1610	1/1	0.88	0.13	53,53,53,53	0
56	MG	1F	301	1/1	0.88	0.12	52,52,52,52	0
56	MG	2a	3141	1/1	0.88	0.18	73,73,73,73	0
56	MG	2x	3001	1/1	0.88	0.14	66,66,66,66	0
56	MG	1A	3129	1/1	0.88	0.67	40,40,40,40	0
56	MG	1a	1769	1/1	0.89	0.09	87,87,87,87	0
56	MG	1A	4013	1/1	0.89	0.22	49,49,49,49	0
56	MG	1A	3103	1/1	0.89	0.22	50,50,50,50	0
56	MG	1A	3847	1/1	0.89	0.17	46,46,46,46	0
56	MG	1D	308	1/1	0.89	0.21	35,35,35,35	0
56	MG	1A	3633	1/1	0.89	0.22	71,71,71,71	0
56	MG	2a	3063	1/1	0.89	0.11	77,77,77,77	0
56	MG	1T	204	1/1	0.89	0.20	67,67,67,67	0
56	MG	1A	3092	1/1	0.89	0.60	49,49,49,49	0
56	MG	1A	3598	1/1	0.89	0.17	51,51,51,51	0
56	MG	1A	3410	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3067	1/1	0.89	0.18	52,52,52,52	0
56	MG	1a	1744	1/1	0.89	0.18	61,61,61,61	0
56	MG	2A	3323	1/1	0.89	0.10	48,48,48,48	0
56	MG	1A	3065	1/1	0.89	0.33	49,49,49,49	0
56	MG	1A	3567	1/1	0.89	0.20	39,39,39,39	0
56	MG	2a	3229	1/1	0.89	0.18	51,51,51,51	0
56	MG	1a	1794	1/1	0.89	0.16	67,67,67,67	0
56	MG	1A	4008	1/1	0.89	1.42	48,48,48,48	0
56	MG	1A	3876	1/1	0.89	0.23	79,79,79,79	0
56	MG	2A	3028	1/1	0.89	0.14	52,52,52,52	0
56	MG	2A	3040	1/1	0.89	0.15	53,53,53,53	0
56	MG	1A	3144	1/1	0.89	0.37	54,54,54,54	0
56	MG	1a	1679	1/1	0.89	0.20	57,57,57,57	0
56	MG	2A	3402	1/1	0.89	0.39	62,62,62,62	0
56	MG	1A	3099	1/1	0.89	0.12	39,39,39,39	0
56	MG	1A	3302	1/1	0.89	0.48	41,41,41,41	0
56	MG	1A	3941	1/1	0.89	0.12	65,65,65,65	0
56	MG	1B	211	1/1	0.89	0.24	51,51,51,51	0
56	MG	2a	3121	1/1	0.89	0.19	63,63,63,63	0
56	MG	1A	3374	1/1	0.89	0.78	64,64,64,64	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1869	1/1	0.89	0.16	64,64,64,64	0
56	MG	10	106	1/1	0.89	0.37	61,61,61,61	0
56	MG	1A	3483	1/1	0.89	0.48	54,54,54,54	0
56	MG	1V	201	1/1	0.89	0.31	45,45,45,45	0
56	MG	2A	3252	1/1	0.89	0.17	60,60,60,60	0
56	MG	2A	3502	1/1	0.89	0.13	35,35,35,35	0
56	MG	2A	3184	1/1	0.89	0.20	39,39,39,39	0
56	MG	2A	3533	1/1	0.89	0.22	35,35,35,35	0
56	MG	1A	3998	1/1	0.89	0.27	75,75,75,75	0
56	MG	2A	3294	1/1	0.89	0.17	37,37,37,37	0
56	MG	1a	1606	1/1	0.89	0.13	76,76,76,76	0
56	MG	1a	1657	1/1	0.89	0.10	71,71,71,71	0
56	MG	1A	3350	1/1	0.89	0.14	54,54,54,54	0
56	MG	2A	3055	1/1	0.89	0.30	40,40,40,40	0
56	MG	2F	303	1/1	0.89	0.60	50,50,50,50	0
56	MG	1A	3125	1/1	0.89	0.16	60,60,60,60	0
56	MG	2a	3258	1/1	0.89	0.21	69,69,69,69	0
56	MG	2A	3356	1/1	0.89	0.13	60,60,60,60	0
56	MG	2A	3547	1/1	0.89	0.15	22,22,22,22	0
56	MG	1A	3303	1/1	0.89	0.31	63,63,63,63	0
56	MG	2A	3017	1/1	0.89	0.36	47,47,47,47	0
56	MG	2A	3319	1/1	0.89	0.17	58,58,58,58	0
56	MG	1U	204	1/1	0.89	1.11	42,42,42,42	0
56	MG	2A	3505	1/1	0.89	0.15	57,57,57,57	0
56	MG	1A	3213	1/1	0.89	0.13	33,33,33,33	0
56	MG	1A	3236	1/1	0.89	0.44	46,46,46,46	0
56	MG	1A	3241	1/1	0.89	0.38	42,42,42,42	0
56	MG	1A	3942	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3314	1/1	0.89	0.29	55,55,55,55	0
56	MG	1a	1864	1/1	0.89	0.16	73,73,73,73	0
56	MG	1A	3515	1/1	0.89	0.37	48,48,48,48	0
56	MG	1A	3460	1/1	0.89	0.15	36,36,36,36	0
56	MG	1A	3076	1/1	0.89	0.46	58,58,58,58	0
56	MG	2A	3203	1/1	0.89	0.09	43,43,43,43	0
56	MG	1A	3929	1/1	0.89	0.20	58,58,58,58	0
56	MG	1A	3854	1/1	0.89	0.26	53,53,53,53	0
56	MG	1A	3555	1/1	0.89	0.13	46,46,46,46	0
56	MG	1A	3228	1/1	0.89	0.15	59,59,59,59	0
56	MG	1A	3999	1/1	0.89	0.14	21,21,21,21	0
56	MG	2A	3224	1/1	0.89	0.13	42,42,42,42	0
56	MG	1T	205	1/1	0.89	0.27	65,65,65,65	0
56	MG	2A	3429	1/1	0.89	0.12	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3178	1/1	0.89	0.09	34,34,34,34	0
56	MG	1a	1654	1/1	0.89	0.13	78,78,78,78	0
56	MG	2a	3069	1/1	0.89	0.34	95,95,95,95	0
56	MG	1A	3311	1/1	0.89	0.17	65,65,65,65	0
56	MG	2l	204	1/1	0.89	0.12	64,64,64,64	0
56	MG	1B	203	1/1	0.89	0.22	61,61,61,61	0
56	MG	1A	3323	1/1	0.89	0.35	58,58,58,58	0
56	MG	1A	3544	1/1	0.89	0.13	36,36,36,36	0
56	MG	2A	3010	1/1	0.89	0.10	56,56,56,56	0
56	MG	2A	3023	1/1	0.89	0.18	61,61,61,61	0
56	MG	2A	3288	1/1	0.89	0.15	57,57,57,57	0
56	MG	2A	3410	1/1	0.89	0.22	56,56,56,56	0
56	MG	2a	3051	1/1	0.89	0.11	76,76,76,76	0
56	MG	1A	3458	1/1	0.89	0.23	46,46,46,46	0
56	MG	1U	205	1/1	0.89	1.04	52,52,52,52	0
56	MG	1A	3488	1/1	0.89	0.13	65,65,65,65	0
56	MG	2A	3336	1/1	0.89	0.12	36,36,36,36	0
56	MG	2A	3346	1/1	0.89	0.18	62,62,62,62	0
56	MG	1A	3097	1/1	0.89	0.29	55,55,55,55	0
56	MG	1A	3490	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3431	1/1	0.89	0.28	64,64,64,64	0
56	MG	1A	3722	1/1	0.89	0.19	22,22,22,22	0
56	MG	1A	3220	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3094	1/1	0.89	0.25	46,46,46,46	0
56	MG	2a	3167	1/1	0.89	0.57	80,80,80,80	0
56	MG	2A	3022	1/1	0.89	0.16	51,51,51,51	0
56	MG	2A	3066	1/1	0.89	0.17	55,55,55,55	0
56	MG	1A	3842	1/1	0.89	0.21	56,56,56,56	0
56	MG	1D	301	1/1	0.89	0.18	56,56,56,56	0
56	MG	1D	303	1/1	0.89	0.42	47,47,47,47	0
56	MG	1A	3037	1/1	0.89	0.13	58,58,58,58	0
56	MG	1a	1660	1/1	0.89	0.15	50,50,50,50	0
56	MG	1A	3763	1/1	0.89	0.09	43,43,43,43	0
56	MG	1a	1668	1/1	0.89	0.31	59,59,59,59	0
56	MG	1a	1624	1/1	0.89	0.61	62,62,62,62	0
56	MG	2a	3135	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3344	1/1	0.89	0.10	72,72,72,72	0
56	MG	2A	3474	1/1	0.90	0.22	41,41,41,41	0
56	MG	1A	3621	1/1	0.90	0.14	18,18,18,18	0
56	MG	1a	1687	1/1	0.90	0.16	46,46,46,46	0
56	MG	2A	3080	1/1	0.90	0.16	48,48,48,48	0
56	MG	1a	1644	1/1	0.90	0.14	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3138	1/1	0.90	0.14	54,54,54,54	0
56	MG	2A	3272	1/1	0.90	0.24	46,46,46,46	0
56	MG	2A	3144	1/1	0.90	0.32	51,51,51,51	0
56	MG	1q	201	1/1	0.90	0.18	51,51,51,51	0
56	MG	2E	301	1/1	0.90	0.18	44,44,44,44	0
56	MG	1A	3059	1/1	0.90	0.14	46,46,46,46	0
56	MG	2A	3201	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3368	1/1	0.90	0.25	25,25,25,25	0
56	MG	2A	3400	1/1	0.90	0.49	48,48,48,48	0
56	MG	2a	3163	1/1	0.90	0.13	70,70,70,70	0
56	MG	2A	3487	1/1	0.90	0.08	32,32,32,32	0
56	MG	2a	3155	1/1	0.90	0.10	79,79,79,79	0
56	MG	1A	3273	1/1	0.90	0.18	36,36,36,36	0
56	MG	2A	3418	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3425	1/1	0.90	0.14	63,63,63,63	0
56	MG	2A	3214	1/1	0.90	0.77	43,43,43,43	0
56	MG	1a	1686	1/1	0.90	0.18	49,49,49,49	0
56	MG	1A	4000	1/1	0.90	0.15	61,61,61,61	0
56	MG	2A	3157	1/1	0.90	0.18	43,43,43,43	0
56	MG	1A	3339	1/1	0.90	0.18	56,56,56,56	0
56	MG	1A	3741	1/1	0.90	0.20	19,19,19,19	0
56	MG	2A	3433	1/1	0.90	0.14	65,65,65,65	0
56	MG	1X	102	1/1	0.90	0.46	53,53,53,53	0
56	MG	1A	3783	1/1	0.90	0.18	37,37,37,37	0
56	MG	1a	1638	1/1	0.90	0.11	63,63,63,63	0
56	MG	1A	3721	1/1	0.90	0.19	55,55,55,55	0
56	MG	1A	3514	1/1	0.90	0.19	53,53,53,53	0
56	MG	1A	3280	1/1	0.90	0.14	34,34,34,34	0
56	MG	1A	3455	1/1	0.90	0.17	63,63,63,63	0
56	MG	1a	1827	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3357	1/1	0.90	0.20	65,65,65,65	0
56	MG	1a	1742	1/1	0.90	0.19	51,51,51,51	0
56	MG	2A	3164	1/1	0.90	0.15	64,64,64,64	0
56	MG	2A	3073	1/1	0.90	0.18	55,55,55,55	0
56	MG	2A	3489	1/1	0.90	0.07	63,63,63,63	0
56	MG	2a	3192	1/1	0.90	0.10	60,60,60,60	0
56	MG	1A	3117	1/1	0.90	0.18	48,48,48,48	0
56	MG	2a	3251	1/1	0.90	0.08	57,57,57,57	0
56	MG	1A	3810	1/1	0.90	0.06	48,48,48,48	0
56	MG	2a	3189	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3178	1/1	0.90	0.71	41,41,41,41	0
56	MG	2A	3560	1/1	0.90	0.17	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3358	1/1	0.90	0.69	44,44,44,44	0
56	MG	2a	3066	1/1	0.90	0.10	84,84,84,84	0
56	MG	1A	3045	1/1	0.90	0.10	70,70,70,70	0
56	MG	2A	3093	1/1	0.90	0.10	55,55,55,55	0
56	MG	1Q	3001	1/1	0.90	0.30	38,38,38,38	0
56	MG	2a	3117	1/1	0.90	0.10	58,58,58,58	0
56	MG	2a	3050	1/1	0.90	0.41	93,93,93,93	0
56	MG	1A	3915	1/1	0.90	0.23	58,58,58,58	0
56	MG	1A	4007	1/1	0.90	0.90	36,36,36,36	0
56	MG	1A	3603	1/1	0.90	0.10	60,60,60,60	0
56	MG	1a	1791	1/1	0.90	0.07	99,99,99,99	0
56	MG	2A	3416	1/1	0.90	0.20	48,48,48,48	0
56	MG	1A	3430	1/1	0.90	0.12	62,62,62,62	0
56	MG	1a	1633	1/1	0.90	0.14	38,38,38,38	0
56	MG	1A	3251	1/1	0.90	0.20	30,30,30,30	0
56	MG	1A	3283	1/1	0.90	0.13	44,44,44,44	0
56	MG	1A	3423	1/1	0.90	0.23	57,57,57,57	0
56	MG	2A	3548	1/1	0.90	0.12	40,40,40,40	0
56	MG	2A	3191	1/1	0.90	0.29	40,40,40,40	0
56	MG	1A	3996	1/1	0.90	0.09	40,40,40,40	0
56	MG	2a	3032	1/1	0.90	0.21	50,50,50,50	0
56	MG	2A	3485	1/1	0.90	0.13	38,38,38,38	0
56	MG	1a	1796	1/1	0.90	0.38	86,86,86,86	0
56	MG	1A	3545	1/1	0.90	0.17	17,17,17,17	0
56	MG	1A	3612	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	3820	1/1	0.90	0.11	57,57,57,57	0
56	MG	1A	3249	1/1	0.90	0.25	42,42,42,42	0
56	MG	1Z	8001	1/1	0.90	0.23	69,69,69,69	0
56	MG	1A	3362	1/1	0.90	0.18	56,56,56,56	0
56	MG	2A	3185	1/1	0.90	0.18	52,52,52,52	0
56	MG	1a	1843	1/1	0.90	0.09	74,74,74,74	0
56	MG	2q	201	1/1	0.90	0.16	58,58,58,58	0
56	MG	1A	3305	1/1	0.90	0.20	43,43,43,43	0
56	MG	1A	3518	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3894	1/1	0.90	0.10	41,41,41,41	0
56	MG	2A	3339	1/1	0.90	0.22	31,31,31,31	0
56	MG	1A	3792	1/1	0.90	0.16	79,79,79,79	0
56	MG	1A	3318	1/1	0.90	0.29	52,52,52,52	0
56	MG	2a	3181	1/1	0.90	0.18	47,47,47,47	0
56	MG	1D	313	1/1	0.90	0.57	56,56,56,56	0
56	MG	1W	3005	1/1	0.90	0.53	49,49,49,49	0
56	MG	2A	3490	1/1	0.90	0.29	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3130	1/1	0.90	0.12	39,39,39,39	0
56	MG	1a	1758	1/1	0.90	0.07	82,82,82,82	0
56	MG	1q	203	1/1	0.90	0.25	51,51,51,51	0
56	MG	2a	3198	1/1	0.90	0.06	63,63,63,63	0
56	MG	1A	3371	1/1	0.90	0.15	56,56,56,56	0
56	MG	1A	3525	1/1	0.90	0.16	60,60,60,60	0
56	MG	2a	3025	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3219	1/1	0.90	0.30	44,44,44,44	0
56	MG	2a	3166	1/1	0.90	0.14	66,66,66,66	0
56	MG	2a	3049	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3128	1/1	0.90	0.18	60,60,60,60	0
56	MG	1B	222	1/1	0.90	0.09	70,70,70,70	0
56	MG	1A	3465	1/1	0.90	0.19	44,44,44,44	0
56	MG	1A	3324	1/1	0.90	0.23	57,57,57,57	0
56	MG	2a	3250	1/1	0.90	0.15	61,61,61,61	0
56	MG	2A	3024	1/1	0.90	0.26	43,43,43,43	0
56	MG	1A	3141	1/1	0.90	0.19	66,66,66,66	0
56	MG	1A	3036	1/1	0.90	0.40	55,55,55,55	0
56	MG	1A	3991	1/1	0.90	0.15	52,52,52,52	0
56	MG	1A	3927	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3177	1/1	0.90	0.23	48,48,48,48	0
56	MG	26	101	1/1	0.90	0.11	57,57,57,57	0
56	MG	2A	3249	1/1	0.90	0.14	59,59,59,59	0
56	MG	2a	3055	1/1	0.90	0.05	98,98,98,98	0
56	MG	1A	3207	1/1	0.90	0.10	30,30,30,30	0
56	MG	2a	3248	1/1	0.90	0.15	65,65,65,65	0
56	MG	1x	102	1/1	0.90	0.30	67,67,67,67	0
56	MG	1a	1756	1/1	0.90	0.11	75,75,75,75	0
56	MG	2A	3098	1/1	0.90	0.12	51,51,51,51	0
56	MG	1A	3104	1/1	0.90	0.10	55,55,55,55	0
56	MG	1a	1653	1/1	0.90	0.13	60,60,60,60	0
56	MG	1a	1646	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3973	1/1	0.90	0.44	51,51,51,51	0
56	MG	1F	305	1/1	0.90	0.16	44,44,44,44	0
56	MG	2A	3302	1/1	0.90	0.16	41,41,41,41	0
56	MG	1l	201	1/1	0.90	0.15	58,58,58,58	0
56	MG	1a	1673	1/1	0.90	0.16	71,71,71,71	0
56	MG	1A	4015	1/1	0.90	0.20	15,15,15,15	0
56	MG	2h	3001	1/1	0.90	0.15	62,62,62,62	0
56	MG	1a	1615	1/1	0.90	0.18	55,55,55,55	0
56	MG	1a	1666	1/1	0.90	0.11	71,71,71,71	0
56	MG	2A	3270	1/1	0.90	0.11	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3006	1/1	0.90	0.24	57,57,57,57	0
56	MG	1a	1658	1/1	0.90	0.35	67,67,67,67	0
56	MG	2A	3015	1/1	0.90	0.23	52,52,52,52	0
56	MG	1A	3384	1/1	0.90	0.14	69,69,69,69	0
56	MG	1A	3944	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3863	1/1	0.90	0.20	78,78,78,78	0
56	MG	1a	1820	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3022	1/1	0.90	0.23	59,59,59,59	0
56	MG	1A	3315	1/1	0.90	0.46	49,49,49,49	0
56	MG	2a	3010	1/1	0.90	0.12	74,74,74,74	0
56	MG	1A	3255	1/1	0.90	0.12	58,58,58,58	0
56	MG	1U	202	1/1	0.90	0.84	50,50,50,50	0
56	MG	2a	3118	1/1	0.90	0.17	38,38,38,38	0
56	MG	2a	3097	1/1	0.90	0.21	71,71,71,71	0
56	MG	2A	3025	1/1	0.91	0.45	67,67,67,67	0
56	MG	2A	3292	1/1	0.91	0.19	42,42,42,42	0
56	MG	2a	3184	1/1	0.91	0.14	80,80,80,80	0
56	MG	2A	3527	1/1	0.91	0.26	51,51,51,51	0
56	MG	1A	3398	1/1	0.91	0.55	43,43,43,43	0
56	MG	1D	302	1/1	0.91	0.70	65,65,65,65	0
56	MG	1A	3738	1/1	0.91	0.17	37,37,37,37	0
56	MG	2a	3045	1/1	0.91	0.22	74,74,74,74	0
56	MG	2A	3072	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3981	1/1	0.91	0.24	50,50,50,50	0
56	MG	1A	3096	1/1	0.91	0.36	50,50,50,50	0
56	MG	1A	3375	1/1	0.91	0.61	51,51,51,51	0
56	MG	2A	3282	1/1	0.91	0.11	48,48,48,48	0
56	MG	2A	3176	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	3766	1/1	0.91	0.19	49,49,49,49	0
56	MG	1G	3003	1/1	0.91	0.17	45,45,45,45	0
56	MG	1A	3611	1/1	0.91	0.11	58,58,58,58	0
56	MG	1E	304	1/1	0.91	0.17	57,57,57,57	0
56	MG	1A	3291	1/1	0.91	0.52	48,48,48,48	0
56	MG	2a	3164	1/1	0.91	0.10	82,82,82,82	0
56	MG	1A	3983	1/1	0.91	0.18	55,55,55,55	0
56	MG	2A	3450	1/1	0.91	0.08	62,62,62,62	0
56	MG	1A	3062	1/1	0.91	0.14	48,48,48,48	0
56	MG	1A	3325	1/1	0.91	0.11	74,74,74,74	0
56	MG	1A	3765	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3901	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3247	1/1	0.91	0.53	59,59,59,59	0
56	MG	2a	3145	1/1	0.91	0.10	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3496	1/1	0.91	0.08	42,42,42,42	0
56	MG	1A	3300	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3591	1/1	0.91	0.12	77,77,77,77	0
56	MG	1a	1872	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3221	1/1	0.91	0.09	47,47,47,47	0
56	MG	1a	1708	1/1	0.91	0.12	61,61,61,61	0
56	MG	1l	4000	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3397	1/1	0.91	0.17	66,66,66,66	0
56	MG	1A	3718	1/1	0.91	0.13	41,41,41,41	0
56	MG	1A	3617	1/1	0.91	0.23	27,27,27,27	0
56	MG	1A	3333	1/1	0.91	0.26	70,70,70,70	0
56	MG	2a	3012	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3239	1/1	0.91	0.56	36,36,36,36	0
56	MG	2a	3113	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3182	1/1	0.91	0.27	52,52,52,52	0
56	MG	1Z	8002	1/1	0.91	0.11	67,67,67,67	0
56	MG	1A	3806	1/1	0.91	0.27	61,61,61,61	0
56	MG	1A	3772	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3289	1/1	0.91	0.20	58,58,58,58	0
56	MG	1q	202	1/1	0.91	0.25	62,62,62,62	0
56	MG	1a	1766	1/1	0.91	0.27	60,60,60,60	0
56	MG	1a	1764	1/1	0.91	0.45	68,68,68,68	0
56	MG	1A	3798	1/1	0.91	0.07	61,61,61,61	0
56	MG	1a	1629	1/1	0.91	0.13	49,49,49,49	0
56	MG	2A	3553	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3524	1/1	0.91	0.11	41,41,41,41	0
56	MG	1A	3478	1/1	0.91	0.39	65,65,65,65	0
56	MG	1A	3040	1/1	0.91	0.38	45,45,45,45	0
56	MG	2A	3065	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3207	1/1	0.91	0.11	44,44,44,44	0
56	MG	1a	1781	1/1	0.91	0.28	46,46,46,46	0
56	MG	1A	3807	1/1	0.91	0.13	57,57,57,57	0
56	MG	2a	3067	1/1	0.91	0.10	88,88,88,88	0
56	MG	2a	3257	1/1	0.91	0.16	90,90,90,90	0
56	MG	1A	3003	1/1	0.91	0.19	46,46,46,46	0
56	MG	1A	3089	1/1	0.91	0.44	55,55,55,55	0
56	MG	2A	3477	1/1	0.91	0.20	57,57,57,57	0
56	MG	2a	3168	1/1	0.91	0.08	71,71,71,71	0
56	MG	1a	1865	1/1	0.91	0.18	69,69,69,69	0
56	MG	2A	3053	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3747	1/1	0.91	0.17	29,29,29,29	0
56	MG	2A	3468	1/1	0.91	0.20	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3931	1/1	0.91	0.45	33,33,33,33	0
56	MG	2a	3186	1/1	0.91	0.14	48,48,48,48	0
56	MG	1a	1637	1/1	0.91	0.31	53,53,53,53	0
56	MG	2a	3234	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3932	1/1	0.91	0.34	20,20,20,20	0
56	MG	1A	3541	1/1	0.91	0.07	48,48,48,48	0
56	MG	1A	3988	1/1	0.91	0.74	45,45,45,45	0
56	MG	1a	1867	1/1	0.91	0.12	80,80,80,80	0
56	MG	2A	3516	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3730	1/1	0.91	0.15	30,30,30,30	0
56	MG	1a	1858	1/1	0.91	0.26	52,52,52,52	0
56	MG	1A	3137	1/1	0.91	0.33	51,51,51,51	0
56	MG	2A	3284	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3444	1/1	0.91	0.59	36,36,36,36	0
56	MG	1A	3162	1/1	0.91	0.41	38,38,38,38	0
56	MG	1F	306	1/1	0.91	0.76	33,33,33,33	0
56	MG	1A	3416	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	3115	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3971	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3618	1/1	0.91	0.19	18,18,18,18	0
56	MG	2A	3233	1/1	0.91	0.53	48,48,48,48	0
56	MG	2A	3461	1/1	0.91	0.13	47,47,47,47	0
56	MG	2a	3094	1/1	0.91	0.18	49,49,49,49	0
56	MG	1P	202	1/1	0.91	0.20	55,55,55,55	0
56	MG	1A	3474	1/1	0.91	0.35	39,39,39,39	0
56	MG	1a	1759	1/1	0.91	0.18	70,70,70,70	0
56	MG	1a	1841	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3928	1/1	0.91	0.09	62,62,62,62	0
56	MG	1A	3937	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3655	1/1	0.91	0.30	48,48,48,48	0
56	MG	1A	3505	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3436	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3160	1/1	0.91	0.23	52,52,52,52	0
56	MG	1N	3001	1/1	0.91	0.27	42,42,42,42	0
56	MG	2A	3135	1/1	0.91	0.13	61,61,61,61	0
56	MG	2a	3034	1/1	0.91	0.16	59,59,59,59	0
56	MG	2A	3305	1/1	0.91	0.12	42,42,42,42	0
56	MG	1R	203	1/1	0.91	0.63	43,43,43,43	0
56	MG	1a	1777	1/1	0.91	0.24	28,28,28,28	0
56	MG	2A	3525	1/1	0.91	0.14	63,63,63,63	0
56	MG	1A	3512	1/1	0.91	0.28	60,60,60,60	0
56	MG	1a	1871	1/1	0.91	0.11	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
56	MG	2A	3290	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3276	1/1	0.91	0.28	38,38,38,38	0
56	MG	1A	3974	1/1	0.91	0.13	30,30,30,30	0
56	MG	20	8001	1/1	0.91	0.08	65,65,65,65	0
56	MG	2A	3453	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3968	1/1	0.91	0.61	50,50,50,50	0
56	MG	1A	3777	1/1	0.91	0.13	49,49,49,49	0
56	MG	1a	1868	1/1	0.91	0.12	66,66,66,66	0
56	MG	1a	1675	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3068	1/1	0.91	0.69	44,44,44,44	0
56	MG	1A	3154	1/1	0.91	0.14	28,28,28,28	0
56	MG	1A	3750	1/1	0.91	0.15	21,21,21,21	0
56	MG	1a	1788	1/1	0.91	0.65	76,76,76,76	0
56	MG	1A	3921	1/1	0.91	0.26	55,55,55,55	0
56	MG	1A	3187	1/1	0.91	0.64	46,46,46,46	0
56	MG	2A	3447	1/1	0.91	0.12	62,62,62,62	0
56	MG	2a	3175	1/1	0.91	0.09	62,62,62,62	0
56	MG	1A	3299	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3896	1/1	0.91	0.18	19,19,19,19	0
56	MG	2A	3059	1/1	0.91	0.18	48,48,48,48	0
56	MG	1a	1846	1/1	0.91	0.19	52,52,52,52	0
56	MG	1a	1620	1/1	0.91	0.09	58,58,58,58	0
56	MG	1a	1634	1/1	0.91	0.10	52,52,52,52	0
56	MG	1A	3871	1/1	0.91	0.27	60,60,60,60	0
56	MG	1A	3397	1/1	0.91	0.72	49,49,49,49	0
56	MG	1A	3337	1/1	0.91	0.32	57,57,57,57	0
56	MG	1a	1671	1/1	0.91	0.18	38,38,38,38	0
56	MG	2A	3293	1/1	0.92	0.16	62,62,62,62	0
56	MG	1A	3087	1/1	0.92	0.57	57,57,57,57	0
56	MG	1a	1688	1/1	0.92	0.11	56,56,56,56	0
56	MG	1a	1733	1/1	0.92	0.12	65,65,65,65	0
56	MG	2B	3005	1/1	0.92	0.17	53,53,53,53	0
56	MG	1a	1786	1/1	0.92	0.52	92,92,92,92	0
56	MG	1A	3771	1/1	0.92	0.48	71,71,71,71	0
56	MG	1A	3642	1/1	0.92	0.19	58,58,58,58	0
56	MG	1B	214	1/1	0.92	0.08	68,68,68,68	0
56	MG	1A	3257	1/1	0.92	0.18	44,44,44,44	0
56	MG	2a	3215	1/1	0.92	0.25	56,56,56,56	0
56	MG	1a	1659	1/1	0.92	0.45	63,63,63,63	0
56	MG	1A	3524	1/1	0.92	0.16	54,54,54,54	0
56	MG	1A	3075	1/1	0.92	0.19	71,71,71,71	0
56	MG	1A	3609	1/1	0.92	0.17	22,22,22,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3351	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3832	1/1	0.92	0.12	57,57,57,57	0
56	MG	2a	3204	1/1	0.92	0.14	64,64,64,64	0
56	MG	1A	3821	1/1	0.92	0.28	23,23,23,23	0
56	MG	2A	3190	1/1	0.92	0.21	54,54,54,54	0
56	MG	2A	3347	1/1	0.92	0.10	60,60,60,60	0
56	MG	1a	1801	1/1	0.92	0.20	59,59,59,59	0
56	MG	2A	3029	1/1	0.92	0.24	48,48,48,48	0
56	MG	2a	3196	1/1	0.92	0.17	90,90,90,90	0
56	MG	2A	3033	1/1	0.92	0.33	61,61,61,61	0
56	MG	2a	3230	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3068	1/1	0.92	0.12	39,39,39,39	0
56	MG	1A	3744	1/1	0.92	0.11	53,53,53,53	0
56	MG	2A	3197	1/1	0.92	0.23	57,57,57,57	0
56	MG	1A	3786	1/1	0.92	0.15	57,57,57,57	0
57	ZN	1n	501	1/1	0.92	0.11	84,84,84,84	0
56	MG	2A	3396	1/1	0.92	0.23	40,40,40,40	0
56	MG	1A	3346	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3004	1/1	0.92	0.16	40,40,40,40	0
56	MG	1A	3452	1/1	0.92	0.14	56,56,56,56	0
56	MG	2A	3026	1/1	0.92	0.16	51,51,51,51	0
56	MG	2A	3360	1/1	0.92	0.14	58,58,58,58	0
56	MG	1E	301	1/1	0.92	0.14	15,15,15,15	0
56	MG	2A	3546	1/1	0.92	0.17	44,44,44,44	0
56	MG	2A	3183	1/1	0.92	0.13	56,56,56,56	0
56	MG	2A	3186	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3391	1/1	0.92	0.17	35,35,35,35	0
56	MG	1B	207	1/1	0.92	0.20	33,33,33,33	0
56	MG	1A	3136	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	3962	1/1	0.92	0.99	52,52,52,52	0
56	MG	2A	3322	1/1	0.92	0.14	67,67,67,67	0
56	MG	1e	3001	1/1	0.92	0.13	69,69,69,69	0
56	MG	1A	3982	1/1	0.92	0.31	49,49,49,49	0
56	MG	2A	3550	1/1	0.92	0.50	42,42,42,42	0
56	MG	1a	1682	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3334	1/1	0.92	0.17	72,72,72,72	0
56	MG	2A	3437	1/1	0.92	0.12	57,57,57,57	0
56	MG	1a	1612	1/1	0.92	0.09	65,65,65,65	0
56	MG	1A	3047	1/1	0.92	0.16	67,67,67,67	0
56	MG	2A	3456	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3500	1/1	0.92	0.23	55,55,55,55	0
56	MG	1a	1669	1/1	0.92	0.12	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
56	MG	1N	3004	1/1	0.92	0.23	36,36,36,36	0
56	MG	2a	3060	1/1	0.92	0.20	86,86,86,86	0
56	MG	2A	3084	1/1	0.92	0.21	54,54,54,54	0
56	MG	1A	3189	1/1	0.92	0.20	39,39,39,39	0
56	MG	2a	3137	1/1	0.92	0.10	67,67,67,67	0
56	MG	1a	1709	1/1	0.92	0.16	43,43,43,43	0
56	MG	1a	1678	1/1	0.92	0.07	43,43,43,43	0
56	MG	1A	3749	1/1	0.92	0.12	27,27,27,27	0
56	MG	1A	3466	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3625	1/1	0.92	0.15	22,22,22,22	0
56	MG	2A	3085	1/1	0.92	0.28	53,53,53,53	0
56	MG	10	103	1/1	0.92	0.10	75,75,75,75	0
56	MG	1A	3041	1/1	0.92	0.20	55,55,55,55	0
56	MG	1A	3872	1/1	0.92	0.12	28,28,28,28	0
56	MG	2A	3373	1/1	0.92	0.17	47,47,47,47	0
56	MG	1A	3649	1/1	0.92	0.13	71,71,71,71	0
56	MG	2D	303	1/1	0.92	0.30	49,49,49,49	0
56	MG	2A	3274	1/1	0.92	0.12	64,64,64,64	0
56	MG	1A	3432	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3887	1/1	0.92	0.34	31,31,31,31	0
56	MG	1a	1784	1/1	0.92	0.14	56,56,56,56	0
56	MG	1D	305	1/1	0.92	0.28	39,39,39,39	0
56	MG	1A	3485	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3295	1/1	0.92	0.18	50,50,50,50	0
56	MG	2A	3411	1/1	0.92	0.14	64,64,64,64	0
56	MG	2a	3083	1/1	0.92	0.27	51,51,51,51	0
56	MG	2A	3311	1/1	0.92	0.21	42,42,42,42	0
56	MG	2a	3110	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	3533	1/1	0.92	0.21	51,51,51,51	0
56	MG	1A	3737	1/1	0.92	0.19	24,24,24,24	0
56	MG	2a	3004	1/1	0.92	0.16	46,46,46,46	0
56	MG	1B	220	1/1	0.92	0.15	70,70,70,70	0
56	MG	2A	3442	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3168	1/1	0.92	0.25	42,42,42,42	0
56	MG	1A	3343	1/1	0.92	0.18	77,77,77,77	0
56	MG	1a	1852	1/1	0.92	0.14	70,70,70,70	0
56	MG	2A	3297	1/1	0.92	0.11	58,58,58,58	0
56	MG	2A	3180	1/1	0.92	0.10	37,37,37,37	0
57	ZN	2Y	501	1/1	0.92	0.19	85,85,85,85	0
56	MG	2A	3045	1/1	0.92	0.45	48,48,48,48	0
56	MG	2a	3247	1/1	0.92	0.11	71,71,71,71	0
56	MG	2a	3202	1/1	0.92	0.18	72,72,72,72	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1838	1/1	0.92	0.33	66,66,66,66	0
56	MG	1e	3003	1/1	0.92	0.20	68,68,68,68	0
56	MG	2a	3054	1/1	0.92	0.07	89,89,89,89	0
56	MG	1A	3345	1/1	0.92	0.09	60,60,60,60	0
56	MG	2A	3101	1/1	0.92	0.23	57,57,57,57	0
56	MG	1A	3140	1/1	0.92	0.41	62,62,62,62	0
56	MG	2a	3099	1/1	0.92	0.16	35,35,35,35	0
56	MG	2a	3160	1/1	0.92	0.26	74,74,74,74	0
56	MG	1a	1737	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3053	1/1	0.92	0.23	53,53,53,53	0
56	MG	2A	3354	1/1	0.92	0.12	63,63,63,63	0
56	MG	1A	3046	1/1	0.92	0.32	65,65,65,65	0
56	MG	1A	3113	1/1	0.92	0.14	63,63,63,63	0
56	MG	1A	3536	1/1	0.92	0.21	68,68,68,68	0
56	MG	1A	3437	1/1	0.92	0.25	62,62,62,62	0
56	MG	2B	3009	1/1	0.92	0.24	63,63,63,63	0
56	MG	1A	3009	1/1	0.92	0.28	56,56,56,56	0
56	MG	1A	3008	1/1	0.92	0.47	58,58,58,58	0
56	MG	2A	3329	1/1	0.92	0.15	37,37,37,37	0
56	MG	1a	1793	1/1	0.92	0.10	77,77,77,77	0
56	MG	1a	1698	1/1	0.92	0.14	55,55,55,55	0
56	MG	2A	3317	1/1	0.92	0.15	34,34,34,34	0
56	MG	2A	3308	1/1	0.92	0.16	40,40,40,40	0
56	MG	1a	1763	1/1	0.92	0.36	69,69,69,69	0
56	MG	2A	3048	1/1	0.92	0.18	56,56,56,56	0
56	MG	2A	3503	1/1	0.92	0.09	59,59,59,59	0
57	ZN	2n	501	1/1	0.92	0.12	98,98,98,98	0
56	MG	2A	3430	1/1	0.92	0.29	45,45,45,45	0
56	MG	1A	3759	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3472	1/1	0.92	0.09	39,39,39,39	0
56	MG	2A	3107	1/1	0.92	0.75	45,45,45,45	0
56	MG	2A	3386	1/1	0.92	0.16	30,30,30,30	0
56	MG	1a	1836	1/1	0.92	0.16	41,41,41,41	0
56	MG	1A	3869	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3849	1/1	0.92	0.16	73,73,73,73	0
56	MG	1a	1755	1/1	0.92	0.09	79,79,79,79	0
56	MG	2A	3427	1/1	0.92	0.23	56,56,56,56	0
56	MG	1A	3234	1/1	0.92	0.10	43,43,43,43	0
56	MG	1a	1857	1/1	0.92	0.26	73,73,73,73	0
56	MG	1A	3653	1/1	0.92	0.15	25,25,25,25	0
56	MG	2a	3115	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3492	1/1	0.92	0.09	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3556	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3188	1/1	0.92	0.20	43,43,43,43	0
56	MG	1A	3147	1/1	0.92	0.23	54,54,54,54	0
56	MG	1A	3723	1/1	0.92	0.19	8,8,8,8	0
56	MG	1A	3294	1/1	0.92	0.11	23,23,23,23	0
56	MG	2A	3408	1/1	0.92	0.17	62,62,62,62	0
56	MG	1a	1761	1/1	0.92	0.20	86,86,86,86	0
56	MG	2A	3124	1/1	0.92	0.25	54,54,54,54	0
56	MG	1A	3441	1/1	0.92	0.24	72,72,72,72	0
56	MG	1a	1695	1/1	0.92	0.24	50,50,50,50	0
56	MG	2A	3132	1/1	0.92	0.26	53,53,53,53	0
56	MG	1A	3940	1/1	0.92	0.17	63,63,63,63	0
56	MG	2a	3041	1/1	0.92	0.26	73,73,73,73	0
56	MG	1A	3254	1/1	0.92	0.33	34,34,34,34	0
56	MG	2A	3504	1/1	0.93	0.09	56,56,56,56	0
56	MG	2B	3006	1/1	0.93	0.09	58,58,58,58	0
56	MG	1a	1601	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3140	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3684	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3441	1/1	0.93	0.08	58,58,58,58	0
56	MG	1a	1813	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3278	1/1	0.93	0.12	31,31,31,31	0
56	MG	1A	3767	1/1	0.93	0.20	40,40,40,40	0
56	MG	2A	3032	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3212	1/1	0.93	0.15	23,23,23,23	0
56	MG	2A	3204	1/1	0.93	0.12	44,44,44,44	0
56	MG	2Q	3001	1/1	0.93	0.33	48,48,48,48	0
56	MG	2A	3325	1/1	0.93	0.18	52,52,52,52	0
56	MG	2A	3403	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3211	1/1	0.93	0.13	58,58,58,58	0
56	MG	2a	3174	1/1	0.93	0.19	69,69,69,69	0
56	MG	2A	3279	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3165	1/1	0.93	0.23	49,49,49,49	0
56	MG	2A	3419	1/1	0.93	0.07	56,56,56,56	0
56	MG	1A	3951	1/1	0.93	0.32	70,70,70,70	0
56	MG	1A	3414	1/1	0.93	0.11	65,65,65,65	0
56	MG	2A	3383	1/1	0.93	0.22	66,66,66,66	0
56	MG	1A	3081	1/1	0.93	0.31	58,58,58,58	0
56	MG	2a	3242	1/1	0.93	0.12	61,61,61,61	0
56	MG	1E	302	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3189	1/1	0.93	0.14	34,34,34,34	0
56	MG	1A	3407	1/1	0.93	0.10	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3900	1/1	0.93	0.11	66,66,66,66	0
56	MG	1a	1762	1/1	0.93	0.08	89,89,89,89	0
56	MG	2a	3089	1/1	0.93	0.09	66,66,66,66	0
56	MG	2A	3069	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3287	1/1	0.93	0.35	27,27,27,27	0
56	MG	1A	3107	1/1	0.93	0.26	58,58,58,58	0
56	MG	1A	3568	1/1	0.93	0.22	42,42,42,42	0
56	MG	2A	3415	1/1	0.93	0.16	60,60,60,60	0
56	MG	1A	3502	1/1	0.93	0.34	63,63,63,63	0
56	MG	1A	3731	1/1	0.93	0.22	23,23,23,23	0
56	MG	2a	3151	1/1	0.93	0.15	92,92,92,92	0
56	MG	1A	3064	1/1	0.93	0.41	40,40,40,40	0
56	MG	2E	302	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3017	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3477	1/1	0.93	0.29	66,66,66,66	0
56	MG	2A	3267	1/1	0.93	0.15	39,39,39,39	0
56	MG	2A	3314	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	3976	1/1	0.93	0.28	69,69,69,69	0
56	MG	1A	3449	1/1	0.93	0.31	66,66,66,66	0
56	MG	1A	3531	1/1	0.93	0.22	33,33,33,33	0
56	MG	1A	3826	1/1	0.93	0.16	37,37,37,37	0
56	MG	2F	302	1/1	0.93	0.20	47,47,47,47	0
56	MG	1A	3597	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3544	1/1	0.93	0.18	45,45,45,45	0
56	MG	1a	1855	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3075	1/1	0.93	0.14	59,59,59,59	0
56	MG	2A	3115	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3562	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3557	1/1	0.93	0.19	31,31,31,31	0
56	MG	2A	3159	1/1	0.93	0.19	37,37,37,37	0
56	MG	1A	3279	1/1	0.93	0.20	28,28,28,28	0
56	MG	2A	3134	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3426	1/1	0.93	0.27	46,46,46,46	0
56	MG	1A	4005	1/1	0.93	0.13	58,58,58,58	0
56	MG	1U	203	1/1	0.93	0.50	47,47,47,47	0
56	MG	2a	3219	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	3419	1/1	0.93	0.20	56,56,56,56	0
56	MG	2A	3206	1/1	0.93	0.11	41,41,41,41	0
56	MG	1a	1861	1/1	0.93	0.17	58,58,58,58	0
56	MG	1a	1684	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3338	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3784	1/1	0.93	0.22	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3495	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3443	1/1	0.93	0.48	48,48,48,48	0
56	MG	1A	3139	1/1	0.93	0.41	41,41,41,41	0
56	MG	1A	3447	1/1	0.93	0.15	63,63,63,63	0
56	MG	1A	3700	1/1	0.93	0.06	63,63,63,63	0
56	MG	1A	3877	1/1	0.93	0.13	42,42,42,42	0
56	MG	2A	3320	1/1	0.93	0.15	33,33,33,33	0
56	MG	1A	3114	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	3627	1/1	0.93	0.14	20,20,20,20	0
56	MG	1A	3811	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3318	1/1	0.93	0.23	47,47,47,47	0
56	MG	2a	3165	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3177	1/1	0.93	0.62	39,39,39,39	0
57	ZN	29	501	1/1	0.93	0.16	62,62,62,62	0
56	MG	2a	3090	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3836	1/1	0.93	0.19	35,35,35,35	0
56	MG	1A	3412	1/1	0.93	0.55	45,45,45,45	0
56	MG	1A	3733	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3277	1/1	0.93	0.87	48,48,48,48	0
56	MG	1A	3336	1/1	0.93	0.14	49,49,49,49	0
56	MG	2A	3016	1/1	0.93	0.27	57,57,57,57	0
56	MG	1A	3956	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3906	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3116	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3661	1/1	0.93	0.20	36,36,36,36	0
56	MG	1a	1874	1/1	0.93	0.07	61,61,61,61	0
56	MG	2A	3265	1/1	0.93	0.19	37,37,37,37	0
56	MG	2A	3536	1/1	0.93	0.12	38,38,38,38	0
56	MG	1A	3049	1/1	0.93	0.26	48,48,48,48	0
56	MG	1A	3830	1/1	0.93	0.26	63,63,63,63	0
56	MG	2A	3230	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	3209	1/1	0.93	0.60	40,40,40,40	0
56	MG	2a	3071	1/1	0.93	0.29	59,59,59,59	0
56	MG	2a	3149	1/1	0.93	0.13	65,65,65,65	0
56	MG	2a	3220	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	3127	1/1	0.93	0.50	53,53,53,53	0
56	MG	1A	3266	1/1	0.93	0.10	44,44,44,44	0
56	MG	2a	3005	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3569	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3337	1/1	0.93	0.18	46,46,46,46	0
56	MG	2A	3175	1/1	0.93	0.25	52,52,52,52	0
56	MG	1A	3543	1/1	0.93	0.18	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3044	1/1	0.93	0.75	48,48,48,48	0
56	MG	1x	105	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3641	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3735	1/1	0.93	0.16	36,36,36,36	0
56	MG	2F	301	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3094	1/1	0.93	0.32	51,51,51,51	0
56	MG	1A	4016	1/1	0.93	0.46	37,37,37,37	0
56	MG	2A	3376	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3793	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3497	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3152	1/1	0.93	0.14	50,50,50,50	0
56	MG	2a	3003	1/1	0.93	0.19	57,57,57,57	0
56	MG	2A	3231	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3454	1/1	0.93	0.46	66,66,66,66	0
56	MG	1a	1799	1/1	0.93	0.18	61,61,61,61	0
56	MG	2a	3260	1/1	0.93	0.08	72,72,72,72	0
56	MG	2A	3014	1/1	0.93	0.06	66,66,66,66	0
56	MG	2A	3105	1/1	0.93	0.27	54,54,54,54	0
56	MG	1A	3264	1/1	0.93	0.38	38,38,38,38	0
56	MG	1A	3819	1/1	0.93	0.10	82,82,82,82	0
56	MG	1A	3837	1/1	0.93	0.09	62,62,62,62	0
56	MG	1a	1604	1/1	0.93	0.12	69,69,69,69	0
56	MG	2A	3469	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3038	1/1	0.93	0.10	52,52,52,52	0
56	MG	2a	3102	1/1	0.93	0.24	47,47,47,47	0
56	MG	1A	3732	1/1	0.93	0.22	45,45,45,45	0
56	MG	1A	3042	1/1	0.93	0.83	44,44,44,44	0
56	MG	2A	3367	1/1	0.93	0.17	50,50,50,50	0
56	MG	2A	3565	1/1	0.93	0.15	52,52,52,52	0
56	MG	2a	3114	1/1	0.93	0.23	53,53,53,53	0
56	MG	2A	3446	1/1	0.93	0.10	42,42,42,42	0
56	MG	1a	1665	1/1	0.93	0.14	61,61,61,61	0
56	MG	2a	3128	1/1	0.93	0.11	38,38,38,38	0
56	MG	1A	3122	1/1	0.93	0.23	58,58,58,58	0
56	MG	1A	3056	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3375	1/1	0.93	0.17	48,48,48,48	0
56	MG	2B	3010	1/1	0.93	0.32	50,50,50,50	0
56	MG	1A	3248	1/1	0.93	0.12	26,26,26,26	0
56	MG	2A	3428	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3134	1/1	0.93	0.51	45,45,45,45	0
56	MG	2A	3390	1/1	0.93	0.19	56,56,56,56	0
56	MG	1a	1782	1/1	0.93	0.18	43,43,43,43	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3498	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3353	1/1	0.93	0.23	58,58,58,58	0
56	MG	1A	3761	1/1	0.93	0.10	66,66,66,66	0
56	MG	1A	3639	1/1	0.93	0.12	25,25,25,25	0
56	MG	1A	3493	1/1	0.93	0.15	65,65,65,65	0
56	MG	2a	3019	1/1	0.93	0.12	73,73,73,73	0
56	MG	2a	3236	1/1	0.93	0.15	62,62,62,62	0
56	MG	1A	3341	1/1	0.93	0.10	64,64,64,64	0
56	MG	1A	3110	1/1	0.93	0.71	55,55,55,55	0
56	MG	1A	3804	1/1	0.93	0.12	31,31,31,31	0
56	MG	2A	3512	1/1	0.93	0.10	44,44,44,44	0
56	MG	18	103	1/1	0.93	0.31	52,52,52,52	0
56	MG	1A	3933	1/1	0.93	0.13	42,42,42,42	0
56	MG	1a	1798	1/1	0.93	0.10	71,71,71,71	0
56	MG	1A	3868	1/1	0.93	0.18	44,44,44,44	0
56	MG	1a	1778	1/1	0.93	0.27	57,57,57,57	0
56	MG	2a	3103	1/1	0.93	0.12	69,69,69,69	0
56	MG	1A	3886	1/1	0.93	0.34	33,33,33,33	0
56	MG	1A	3224	1/1	0.93	0.18	35,35,35,35	0
56	MG	1A	3481	1/1	0.93	0.91	40,40,40,40	0
56	MG	1A	3160	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3021	1/1	0.93	1.04	48,48,48,48	0
56	MG	2D	301	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3579	1/1	0.93	0.15	45,45,45,45	0
56	MG	1A	3354	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3616	1/1	0.93	0.15	22,22,22,22	0
56	MG	1B	202	1/1	0.93	0.19	52,52,52,52	0
56	MG	2A	3064	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3602	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3414	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3170	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3530	1/1	0.94	0.26	51,51,51,51	0
56	MG	2O	203	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3917	1/1	0.94	0.15	31,31,31,31	0
56	MG	1a	1720	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3002	1/1	0.94	0.16	47,47,47,47	0
56	MG	1a	1616	1/1	0.94	0.27	74,74,74,74	0
56	MG	1A	3231	1/1	0.94	1.03	49,49,49,49	0
56	MG	2a	3262	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3171	1/1	0.94	0.16	41,41,41,41	0
56	MG	2a	3188	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3084	1/1	0.94	0.12	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3193	1/1	0.94	0.16	23,23,23,23	0
56	MG	2A	3012	1/1	0.94	0.24	53,53,53,53	0
56	MG	2a	3021	1/1	0.94	0.49	60,60,60,60	0
56	MG	1A	3712	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3283	1/1	0.94	0.11	48,48,48,48	0
56	MG	2a	3120	1/1	0.94	0.13	63,63,63,63	0
56	MG	2Y	502	1/1	0.94	0.22	52,52,52,52	0
56	MG	1A	3910	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3078	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3475	1/1	0.94	0.56	53,53,53,53	0
56	MG	2A	3244	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3891	1/1	0.94	0.08	62,62,62,62	0
56	MG	2A	3226	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3473	1/1	0.94	0.85	50,50,50,50	0
56	MG	1A	3029	1/1	0.94	0.14	54,54,54,54	0
56	MG	19	102	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3180	1/1	0.94	0.47	33,33,33,33	0
56	MG	1A	3205	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3313	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3903	1/1	0.94	0.17	19,19,19,19	0
56	MG	1A	3491	1/1	0.94	0.40	61,61,61,61	0
56	MG	1A	3664	1/1	0.94	0.14	15,15,15,15	0
56	MG	1A	3282	1/1	0.94	0.18	52,52,52,52	0
56	MG	2A	3153	1/1	0.94	0.18	33,33,33,33	0
56	MG	1a	1811	1/1	0.94	0.14	55,55,55,55	0
56	MG	1a	1670	1/1	0.94	0.17	43,43,43,43	0
56	MG	2A	3404	1/1	0.94	0.11	43,43,43,43	0
56	MG	2a	3190	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3740	1/1	0.94	0.26	36,36,36,36	0
56	MG	1a	1860	1/1	0.94	0.21	55,55,55,55	0
56	MG	1A	3979	1/1	0.94	0.19	49,49,49,49	0
56	MG	2a	3105	1/1	0.94	0.32	55,55,55,55	0
56	MG	1A	3393	1/1	0.94	0.50	52,52,52,52	0
56	MG	2a	3225	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3143	1/1	0.94	0.26	52,52,52,52	0
56	MG	1a	1823	1/1	0.94	0.18	69,69,69,69	0
56	MG	10	102	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3905	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3628	1/1	0.94	0.19	28,28,28,28	0
56	MG	1A	3151	1/1	0.94	0.08	47,47,47,47	0
56	MG	1a	1736	1/1	0.94	0.22	41,41,41,41	0
56	MG	1a	1715	1/1	0.94	0.07	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3631	1/1	0.94	0.12	19,19,19,19	0
56	MG	1A	3634	1/1	0.94	0.18	56,56,56,56	0
56	MG	2a	3203	1/1	0.94	0.15	69,69,69,69	0
56	MG	10	107	1/1	0.94	0.16	55,55,55,55	0
56	MG	2A	3058	1/1	0.94	0.17	37,37,37,37	0
56	MG	2A	3479	1/1	0.94	0.37	50,50,50,50	0
56	MG	1A	3109	1/1	0.94	0.31	55,55,55,55	0
56	MG	2A	3051	1/1	0.94	0.10	40,40,40,40	0
56	MG	2a	3068	1/1	0.94	0.33	67,67,67,67	0
56	MG	1A	3186	1/1	0.94	0.43	32,32,32,32	0
56	MG	2A	3488	1/1	0.94	0.20	63,63,63,63	0
56	MG	2a	3039	1/1	0.94	0.17	57,57,57,57	0
56	MG	1a	1774	1/1	0.94	0.08	76,76,76,76	0
56	MG	1A	3670	1/1	0.94	0.13	55,55,55,55	0
56	MG	2a	3002	1/1	0.94	0.24	65,65,65,65	0
56	MG	2a	3224	1/1	0.94	0.17	54,54,54,54	0
56	MG	2A	3220	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3624	1/1	0.94	0.18	18,18,18,18	0
56	MG	1A	3943	1/1	0.94	0.17	68,68,68,68	0
56	MG	2a	3246	1/1	0.94	0.07	62,62,62,62	0
56	MG	1A	3061	1/1	0.94	0.18	44,44,44,44	0
56	MG	13	101	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3280	1/1	0.94	0.12	63,63,63,63	0
56	MG	1A	3599	1/1	0.94	0.23	37,37,37,37	0
56	MG	1a	1635	1/1	0.94	0.17	50,50,50,50	0
56	MG	2A	3111	1/1	0.94	0.28	68,68,68,68	0
56	MG	2a	3124	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3475	1/1	0.94	0.18	35,35,35,35	0
56	MG	1a	1787	1/1	0.94	0.16	58,58,58,58	0
56	MG	1E	303	1/1	0.94	1.00	58,58,58,58	0
56	MG	2a	3040	1/1	0.94	0.16	39,39,39,39	0
56	MG	2a	3064	1/1	0.94	0.08	77,77,77,77	0
56	MG	1A	3952	1/1	0.94	0.14	51,51,51,51	0
56	MG	1a	1805	1/1	0.94	0.20	67,67,67,67	0
56	MG	2A	3037	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	3245	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3277	1/1	0.94	0.25	41,41,41,41	0
56	MG	2A	3070	1/1	0.94	0.17	32,32,32,32	0
56	MG	2A	3139	1/1	0.94	0.31	45,45,45,45	0
56	MG	1A	3827	1/1	0.94	0.13	31,31,31,31	0
56	MG	1A	3957	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3986	1/1	0.94	0.84	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3711	1/1	0.94	0.35	48,48,48,48	0
56	MG	1A	3902	1/1	0.94	0.10	45,45,45,45	0
56	MG	15	102	1/1	0.94	0.66	40,40,40,40	0
56	MG	2t	3001	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3724	1/1	0.94	0.20	58,58,58,58	0
56	MG	2a	3171	1/1	0.94	0.11	68,68,68,68	0
56	MG	1R	201	1/1	0.94	0.27	63,63,63,63	0
56	MG	1A	3689	1/1	0.94	0.12	55,55,55,55	0
56	MG	1A	3148	1/1	0.94	0.15	62,62,62,62	0
56	MG	2a	3081	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3019	1/1	0.94	0.13	49,49,49,49	0
56	MG	1a	1812	1/1	0.94	0.23	49,49,49,49	0
56	MG	1a	1848	1/1	0.94	0.21	57,57,57,57	0
56	MG	2A	3307	1/1	0.94	0.20	35,35,35,35	0
56	MG	1A	3692	1/1	0.94	0.14	33,33,33,33	0
56	MG	2A	3435	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3436	1/1	0.94	0.17	61,61,61,61	0
56	MG	1a	1842	1/1	0.94	0.20	73,73,73,73	0
56	MG	1A	3198	1/1	0.94	0.22	28,28,28,28	0
56	MG	2a	3140	1/1	0.94	0.08	63,63,63,63	0
56	MG	1a	1809	1/1	0.94	0.18	62,62,62,62	0
56	MG	2A	3539	1/1	0.94	0.22	35,35,35,35	0
56	MG	2a	3127	1/1	0.94	0.19	61,61,61,61	0
56	MG	2a	3053	1/1	0.94	0.14	85,85,85,85	0
56	MG	2A	3046	1/1	0.94	0.26	64,64,64,64	0
56	MG	1A	3637	1/1	0.94	0.17	47,47,47,47	0
56	MG	2D	306	1/1	0.94	0.08	68,68,68,68	0
56	MG	2a	3048	1/1	0.94	0.17	80,80,80,80	0
56	MG	2A	3078	1/1	0.94	0.20	60,60,60,60	0
56	MG	1a	1797	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3960	1/1	0.94	0.66	53,53,53,53	0
56	MG	1A	3418	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	3788	1/1	0.94	0.16	23,23,23,23	0
56	MG	2A	3193	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3912	1/1	0.94	0.32	40,40,40,40	0
56	MG	2A	3089	1/1	0.94	0.18	40,40,40,40	0
56	MG	1a	1770	1/1	0.94	0.07	67,67,67,67	0
56	MG	2a	3244	1/1	0.94	0.18	67,67,67,67	0
56	MG	1a	1699	1/1	0.94	0.07	71,71,71,71	0
56	MG	1a	1734	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	4002	1/1	0.94	0.90	34,34,34,34	0
56	MG	1a	1700	1/1	0.94	0.10	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3909	1/1	0.94	0.12	62,62,62,62	0
56	MG	2A	3260	1/1	0.94	0.14	72,72,72,72	0
56	MG	1A	4019	1/1	0.94	0.78	47,47,47,47	0
56	MG	1a	1681	1/1	0.94	0.06	55,55,55,55	0
56	MG	1a	1753	1/1	0.94	0.08	70,70,70,70	0
56	MG	1A	3852	1/1	0.94	0.18	16,16,16,16	0
56	MG	1A	3823	1/1	0.94	0.28	43,43,43,43	0
56	MG	1A	3217	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3359	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3138	1/1	0.94	0.58	55,55,55,55	0
56	MG	2A	3393	1/1	0.94	0.13	63,63,63,63	0
56	MG	2A	3243	1/1	0.94	0.17	63,63,63,63	0
56	MG	1A	3671	1/1	0.94	0.32	56,56,56,56	0
56	MG	2A	3355	1/1	0.94	0.20	73,73,73,73	0
56	MG	2A	3440	1/1	0.94	0.29	60,60,60,60	0
56	MG	1A	3275	1/1	0.94	0.09	25,25,25,25	0
56	MG	1A	3920	1/1	0.94	0.15	64,64,64,64	0
56	MG	2A	3563	1/1	0.94	0.70	47,47,47,47	0
56	MG	2E	304	1/1	0.94	0.19	67,67,67,67	0
56	MG	2A	3543	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3776	1/1	0.94	0.14	20,20,20,20	0
56	MG	1A	3364	1/1	0.94	0.16	44,44,44,44	0
56	MG	2A	3261	1/1	0.94	0.18	42,42,42,42	0
56	MG	1a	1685	1/1	0.94	0.16	53,53,53,53	0
56	MG	1A	3252	1/1	0.94	0.15	28,28,28,28	0
56	MG	2A	3077	1/1	0.94	0.20	64,64,64,64	0
56	MG	2A	3506	1/1	0.94	0.32	56,56,56,56	0
56	MG	1A	3794	1/1	0.94	0.14	68,68,68,68	0
56	MG	2A	3521	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3308	1/1	0.94	0.34	50,50,50,50	0
56	MG	1a	1785	1/1	0.94	0.25	63,63,63,63	0
56	MG	1A	3573	1/1	0.94	0.25	47,47,47,47	0
56	MG	1A	3813	1/1	0.94	0.21	56,56,56,56	0
56	MG	2A	3412	1/1	0.94	0.15	63,63,63,63	0
56	MG	1a	1790	1/1	0.94	0.16	71,71,71,71	0
56	MG	1a	1674	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3386	1/1	0.94	0.27	63,63,63,63	0
56	MG	1a	1639	1/1	0.94	0.15	62,62,62,62	0
56	MG	1a	1739	1/1	0.94	0.29	46,46,46,46	0
56	MG	1A	3240	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	3340	1/1	0.94	0.24	47,47,47,47	0
56	MG	1A	3227	1/1	0.94	0.16	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3528	1/1	0.94	0.26	49,49,49,49	0
56	MG	1E	305	1/1	0.94	0.14	31,31,31,31	0
56	MG	1a	1780	1/1	0.94	0.29	68,68,68,68	0
56	MG	1a	1772	1/1	0.94	0.23	78,78,78,78	0
56	MG	1A	3608	1/1	0.94	0.19	25,25,25,25	0
56	MG	1P	204	1/1	0.94	0.12	47,47,47,47	0
56	MG	2A	3426	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3012	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3831	1/1	0.94	0.15	70,70,70,70	0
56	MG	1A	3596	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3413	1/1	0.94	0.14	41,41,41,41	0
56	MG	1A	3787	1/1	0.94	0.14	74,74,74,74	0
56	MG	2A	3222	1/1	0.94	0.62	36,36,36,36	0
56	MG	1A	3370	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3179	1/1	0.94	0.39	44,44,44,44	0
56	MG	1A	3873	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3281	1/1	0.94	0.22	59,59,59,59	0
56	MG	1A	3411	1/1	0.94	0.30	62,62,62,62	0
56	MG	1A	3289	1/1	0.94	0.84	43,43,43,43	0
56	MG	1A	3210	1/1	0.94	0.21	43,43,43,43	0
56	MG	2F	306	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3686	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3340	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3748	1/1	0.94	0.13	37,37,37,37	0
56	MG	2Q	3005	1/1	0.94	0.53	52,52,52,52	0
56	MG	2A	3291	1/1	0.94	0.15	36,36,36,36	0
56	MG	1A	3898	1/1	0.94	0.15	25,25,25,25	0
56	MG	1a	1647	1/1	0.94	0.19	56,56,56,56	0
56	MG	2A	3133	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3795	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3801	1/1	0.94	0.16	42,42,42,42	0
56	MG	2A	3167	1/1	0.94	0.20	25,25,25,25	0
56	MG	1q	204	1/1	0.94	0.26	52,52,52,52	0
56	MG	2a	3227	1/1	0.94	0.19	66,66,66,66	0
56	MG	1A	3967	1/1	0.94	0.11	19,19,19,19	0
56	MG	1N	3005	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3237	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3081	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3850	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3090	1/1	0.94	0.43	53,53,53,53	0
56	MG	1A	3844	1/1	0.94	0.13	71,71,71,71	0
56	MG	1A	3947	1/1	0.94	0.37	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3363	1/1	0.94	0.17	61,61,61,61	0
56	MG	1A	3586	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	4003	1/1	0.94	0.90	43,43,43,43	0
56	MG	2A	3425	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3911	1/1	0.94	0.27	39,39,39,39	0
56	MG	1A	3773	1/1	0.94	0.27	80,80,80,80	0
56	MG	1A	3202	1/1	0.94	0.22	43,43,43,43	0
56	MG	1a	1767	1/1	0.94	0.15	64,64,64,64	0
56	MG	1a	1697	1/1	0.94	0.10	52,52,52,52	0
56	MG	2A	3168	1/1	0.94	0.19	47,47,47,47	0
56	MG	1a	1661	1/1	0.94	0.10	15,15,15,15	0
56	MG	2a	3129	1/1	0.95	0.14	65,65,65,65	0
56	MG	1x	104	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3565	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	3669	1/1	0.95	0.11	46,46,46,46	0
56	MG	1W	3003	1/1	0.95	0.28	35,35,35,35	0
56	MG	2A	3384	1/1	0.95	0.06	45,45,45,45	0
56	MG	1A	3184	1/1	0.95	0.21	52,52,52,52	0
56	MG	1A	3949	1/1	0.95	0.16	48,48,48,48	0
56	MG	2a	3212	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3093	1/1	0.95	0.50	47,47,47,47	0
56	MG	1A	3389	1/1	0.95	0.60	45,45,45,45	0
56	MG	2a	3209	1/1	0.95	0.14	70,70,70,70	0
56	MG	1A	3805	1/1	0.95	0.28	41,41,41,41	0
56	MG	1A	3055	1/1	0.95	0.66	59,59,59,59	0
56	MG	1A	3626	1/1	0.95	0.16	25,25,25,25	0
56	MG	1a	1834	1/1	0.95	0.20	63,63,63,63	0
56	MG	1A	3930	1/1	0.95	0.70	44,44,44,44	0
56	MG	1A	3707	1/1	0.95	0.20	70,70,70,70	0
56	MG	1A	3808	1/1	0.95	0.22	51,51,51,51	0
56	MG	1A	3695	1/1	0.95	0.24	41,41,41,41	0
56	MG	1A	3839	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3696	1/1	0.95	0.12	65,65,65,65	0
56	MG	2A	3054	1/1	0.95	0.15	49,49,49,49	0
56	MG	2A	3476	1/1	0.95	0.19	33,33,33,33	0
56	MG	1A	3678	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	3316	1/1	0.95	0.26	48,48,48,48	0
56	MG	25	502	1/1	0.95	0.30	47,47,47,47	0
56	MG	1a	1832	1/1	0.95	0.13	50,50,50,50	0
56	MG	2a	3178	1/1	0.95	0.15	59,59,59,59	0
57	ZN	26	102	1/1	0.95	0.20	56,56,56,56	0
56	MG	2a	3243	1/1	0.95	0.10	67,67,67,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4021	1/1	0.95	0.11	57,57,57,57	0
56	MG	2a	3057	1/1	0.95	0.12	96,96,96,96	0
56	MG	1A	3706	1/1	0.95	0.13	22,22,22,22	0
56	MG	1A	3919	1/1	0.95	0.30	49,49,49,49	0
56	MG	1A	3116	1/1	0.95	0.29	41,41,41,41	0
56	MG	1A	3190	1/1	0.95	0.16	44,44,44,44	0
56	MG	1A	3535	1/1	0.95	0.11	41,41,41,41	0
56	MG	1a	1804	1/1	0.95	0.11	52,52,52,52	0
56	MG	2a	3154	1/1	0.95	0.44	87,87,87,87	0
56	MG	2l	202	1/1	0.95	0.23	40,40,40,40	0
56	MG	1A	3175	1/1	0.95	0.39	35,35,35,35	0
56	MG	1a	1731	1/1	0.95	0.11	57,57,57,57	0
56	MG	2A	3062	1/1	0.95	0.10	39,39,39,39	0
56	MG	1a	1803	1/1	0.95	0.16	49,49,49,49	0
56	MG	1a	1711	1/1	0.95	0.20	49,49,49,49	0
56	MG	1A	3848	1/1	0.95	0.24	61,61,61,61	0
56	MG	2A	3349	1/1	0.95	0.24	59,59,59,59	0
56	MG	2A	3172	1/1	0.95	0.27	49,49,49,49	0
56	MG	2A	3399	1/1	0.95	0.12	31,31,31,31	0
56	MG	2a	3095	1/1	0.95	0.23	45,45,45,45	0
56	MG	2A	3275	1/1	0.95	0.12	60,60,60,60	0
56	MG	1a	1859	1/1	0.95	0.17	59,59,59,59	0
56	MG	1A	3662	1/1	0.95	0.27	44,44,44,44	0
56	MG	2a	3042	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3989	1/1	0.95	0.13	25,25,25,25	0
56	MG	2Q	3003	1/1	0.95	0.14	41,41,41,41	0
56	MG	1a	1692	1/1	0.95	0.09	57,57,57,57	0
56	MG	2A	3109	1/1	0.95	0.15	64,64,64,64	0
56	MG	1A	3199	1/1	0.95	0.20	37,37,37,37	0
56	MG	2A	3324	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3851	1/1	0.95	0.18	62,62,62,62	0
56	MG	2A	3491	1/1	0.95	0.04	47,47,47,47	0
56	MG	1A	3215	1/1	0.95	0.24	51,51,51,51	0
56	MG	1A	3584	1/1	0.95	0.17	33,33,33,33	0
56	MG	1A	3260	1/1	0.95	0.22	58,58,58,58	0
56	MG	1A	3954	1/1	0.95	0.12	51,51,51,51	0
56	MG	1B	210	1/1	0.95	0.14	49,49,49,49	0
56	MG	1W	3004	1/1	0.95	0.46	31,31,31,31	0
56	MG	2a	3179	1/1	0.95	0.12	49,49,49,49	0
56	MG	1B	218	1/1	0.95	0.12	39,39,39,39	0
56	MG	1e	3002	1/1	0.95	0.18	83,83,83,83	0
56	MG	1A	3742	1/1	0.95	0.20	35,35,35,35	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3343	1/1	0.95	0.14	56,56,56,56	0
56	MG	2A	3507	1/1	0.95	0.17	47,47,47,47	0
56	MG	16	101	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	3288	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3595	1/1	0.95	0.31	56,56,56,56	0
56	MG	2A	3463	1/1	0.95	0.04	57,57,57,57	0
56	MG	1A	3480	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3816	1/1	0.95	0.18	68,68,68,68	0
56	MG	1A	3853	1/1	0.95	0.15	46,46,46,46	0
56	MG	1a	1795	1/1	0.95	0.21	75,75,75,75	0
56	MG	1A	3293	1/1	0.95	0.13	27,27,27,27	0
56	MG	1A	3925	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3476	1/1	0.95	0.23	53,53,53,53	0
56	MG	1T	201	1/1	0.95	0.18	41,41,41,41	0
56	MG	1A	3817	1/1	0.95	0.23	51,51,51,51	0
56	MG	2A	3205	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3673	1/1	0.95	0.27	65,65,65,65	0
56	MG	1a	1779	1/1	0.95	0.11	82,82,82,82	0
56	MG	1A	3383	1/1	0.95	0.21	56,56,56,56	0
56	MG	2A	3552	1/1	0.95	0.11	22,22,22,22	0
56	MG	1a	1746	1/1	0.95	0.23	55,55,55,55	0
56	MG	1A	3727	1/1	0.95	0.19	26,26,26,26	0
56	MG	2A	3377	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3285	1/1	0.95	0.21	54,54,54,54	0
56	MG	2A	3286	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3861	1/1	0.95	0.18	48,48,48,48	0
56	MG	1A	3691	1/1	0.95	0.09	51,51,51,51	0
56	MG	2a	3197	1/1	0.95	0.13	58,58,58,58	0
56	MG	1a	1866	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	3307	1/1	0.95	0.30	59,59,59,59	0
56	MG	2A	3146	1/1	0.95	0.14	64,64,64,64	0
56	MG	2a	3249	1/1	0.95	0.12	61,61,61,61	0
56	MG	2a	3208	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3679	1/1	0.95	0.13	25,25,25,25	0
56	MG	2A	3263	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3643	1/1	0.95	0.13	19,19,19,19	0
56	MG	2A	3423	1/1	0.95	0.06	66,66,66,66	0
56	MG	1B	215	1/1	0.95	0.16	31,31,31,31	0
56	MG	2A	3100	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3191	1/1	0.95	0.16	37,37,37,37	0
56	MG	2a	3101	1/1	0.95	0.17	53,53,53,53	0
56	MG	2A	3129	1/1	0.95	0.16	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3004	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3030	1/1	0.95	0.25	49,49,49,49	0
56	MG	2z	101	1/1	0.95	0.67	54,54,54,54	0
56	MG	2A	3385	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	4004	1/1	0.95	0.22	49,49,49,49	0
56	MG	1A	3321	1/1	0.95	0.24	37,37,37,37	0
56	MG	1a	1738	1/1	0.95	0.12	64,64,64,64	0
56	MG	2A	3237	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3531	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3471	1/1	0.95	0.14	34,34,34,34	0
56	MG	1a	1818	1/1	0.95	0.17	63,63,63,63	0
56	MG	1A	4006	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3797	1/1	0.95	0.80	40,40,40,40	0
56	MG	1a	1603	1/1	0.95	0.09	57,57,57,57	0
56	MG	2A	3494	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3011	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	3080	1/1	0.95	0.32	50,50,50,50	0
56	MG	1A	3638	1/1	0.95	0.30	41,41,41,41	0
56	MG	2A	3095	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3834	1/1	0.95	0.14	46,46,46,46	0
56	MG	1W	3001	1/1	0.95	0.33	34,34,34,34	0
56	MG	1a	1645	1/1	0.95	0.11	67,67,67,67	0
56	MG	1A	3829	1/1	0.95	0.27	55,55,55,55	0
56	MG	2a	3211	1/1	0.95	0.12	61,61,61,61	0
56	MG	2a	3112	1/1	0.95	0.13	45,45,45,45	0
56	MG	1a	1840	1/1	0.95	0.20	41,41,41,41	0
56	MG	2A	3538	1/1	0.95	0.19	22,22,22,22	0
56	MG	2a	3109	1/1	0.95	0.12	47,47,47,47	0
56	MG	1D	307	1/1	0.95	0.14	15,15,15,15	0
56	MG	1a	1655	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3554	1/1	0.95	0.14	80,80,80,80	0
56	MG	2a	3147	1/1	0.95	0.08	73,73,73,73	0
56	MG	1A	3538	1/1	0.95	0.22	57,57,57,57	0
56	MG	2A	3079	1/1	0.95	0.34	52,52,52,52	0
56	MG	1A	3713	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3298	1/1	0.95	0.28	50,50,50,50	0
56	MG	2A	3060	1/1	0.95	0.14	43,43,43,43	0
56	MG	1A	3824	1/1	0.95	0.18	33,33,33,33	0
56	MG	1A	3650	1/1	0.95	0.18	19,19,19,19	0
56	MG	1A	3173	1/1	0.95	0.19	62,62,62,62	0
56	MG	1a	1863	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3057	1/1	0.95	0.23	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3245	1/1	0.95	0.23	62,62,62,62	0
56	MG	1a	1850	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3537	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3987	1/1	0.95	0.27	38,38,38,38	0
56	MG	2Q	3004	1/1	0.95	0.27	42,42,42,42	0
56	MG	1a	1810	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3222	1/1	0.95	0.23	50,50,50,50	0
56	MG	1a	1696	1/1	0.95	0.17	70,70,70,70	0
56	MG	1A	3292	1/1	0.95	0.27	17,17,17,17	0
56	MG	2a	3062	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3251	1/1	0.95	0.09	53,53,53,53	0
56	MG	2a	3253	1/1	0.95	0.31	56,56,56,56	0
56	MG	2A	3378	1/1	0.95	0.18	66,66,66,66	0
56	MG	1A	3843	1/1	0.95	0.18	50,50,50,50	0
56	MG	2a	3143	1/1	0.95	0.20	88,88,88,88	0
56	MG	2A	3063	1/1	0.95	0.45	45,45,45,45	0
56	MG	1A	3424	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	3506	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3708	1/1	0.95	0.18	63,63,63,63	0
56	MG	28	8001	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	4011	1/1	0.95	0.95	47,47,47,47	0
56	MG	1O	3002	1/1	0.95	0.22	46,46,46,46	0
56	MG	1a	1648	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3312	1/1	0.95	0.27	38,38,38,38	0
56	MG	1A	3501	1/1	0.95	0.18	56,56,56,56	0
56	MG	1A	3317	1/1	0.95	0.18	34,34,34,34	0
56	MG	1a	1814	1/1	0.95	0.30	67,67,67,67	0
56	MG	1A	3978	1/1	0.95	0.12	29,29,29,29	0
56	MG	1o	3002	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3258	1/1	0.95	0.24	36,36,36,36	0
56	MG	2A	3248	1/1	0.95	0.22	56,56,56,56	0
56	MG	1A	3551	1/1	0.95	0.21	33,33,33,33	0
56	MG	1A	3856	1/1	0.95	0.09	69,69,69,69	0
56	MG	1A	3752	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3108	1/1	0.95	0.30	56,56,56,56	0
56	MG	2A	3439	1/1	0.95	0.08	68,68,68,68	0
56	MG	1A	3914	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3347	1/1	0.95	0.16	60,60,60,60	0
56	MG	1a	1808	1/1	0.95	0.11	52,52,52,52	0
56	MG	1a	1870	1/1	0.95	0.30	88,88,88,88	0
56	MG	1R	202	1/1	0.96	0.29	52,52,52,52	0
56	MG	2x	3004	1/1	0.96	0.13	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3200	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	3329	1/1	0.96	0.26	52,52,52,52	0
56	MG	1A	3885	1/1	0.96	0.17	53,53,53,53	0
56	MG	1A	3204	1/1	0.96	0.27	37,37,37,37	0
56	MG	2A	3259	1/1	0.96	0.16	72,72,72,72	0
56	MG	2A	3392	1/1	0.96	0.13	28,28,28,28	0
56	MG	2A	3188	1/1	0.96	0.23	35,35,35,35	0
56	MG	2A	3424	1/1	0.96	0.14	80,80,80,80	0
56	MG	1A	3893	1/1	0.96	0.18	30,30,30,30	0
56	MG	2A	3350	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3990	1/1	0.96	0.23	36,36,36,36	0
56	MG	1a	1735	1/1	0.96	0.13	66,66,66,66	0
56	MG	1A	3935	1/1	0.96	0.19	28,28,28,28	0
56	MG	1A	3091	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3736	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3072	1/1	0.96	0.16	56,56,56,56	0
56	MG	2a	3017	1/1	0.96	0.23	70,70,70,70	0
56	MG	1a	1650	1/1	0.96	0.27	57,57,57,57	0
56	MG	1A	3663	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3348	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3201	1/1	0.96	0.15	49,49,49,49	0
56	MG	1a	1830	1/1	0.96	0.25	61,61,61,61	0
56	MG	16	103	1/1	0.96	0.10	68,68,68,68	0
56	MG	1a	1605	1/1	0.96	0.13	55,55,55,55	0
56	MG	1P	203	1/1	0.96	0.11	65,65,65,65	0
56	MG	1A	3716	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3581	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3492	1/1	0.96	0.56	52,52,52,52	0
56	MG	1A	3870	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3048	1/1	0.96	0.23	45,45,45,45	0
56	MG	1A	3453	1/1	0.96	0.17	18,18,18,18	0
56	MG	2A	3434	1/1	0.96	0.23	63,63,63,63	0
56	MG	2a	3237	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3050	1/1	0.96	0.16	38,38,38,38	0
56	MG	2a	3177	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3644	1/1	0.96	0.20	19,19,19,19	0
56	MG	1A	3701	1/1	0.96	0.09	68,68,68,68	0
56	MG	1a	1768	1/1	0.96	0.18	72,72,72,72	0
56	MG	1A	3212	1/1	0.96	0.08	39,39,39,39	0
56	MG	1B	212	1/1	0.96	0.20	54,54,54,54	0
56	MG	2a	3144	1/1	0.96	0.09	56,56,56,56	0
56	MG	2A	3136	1/1	0.96	0.09	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1853	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3487	1/1	0.96	0.32	63,63,63,63	0
56	MG	2N	8001	1/1	0.96	0.15	53,53,53,53	0
56	MG	2a	3142	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3864	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3327	1/1	0.96	0.19	36,36,36,36	0
56	MG	2A	3208	1/1	0.96	0.14	40,40,40,40	0
56	MG	1a	1749	1/1	0.96	0.89	57,57,57,57	0
56	MG	1A	3593	1/1	0.96	0.22	35,35,35,35	0
56	MG	2A	3417	1/1	0.96	0.13	70,70,70,70	0
56	MG	1A	3589	1/1	0.96	0.21	29,29,29,29	0
56	MG	1A	3674	1/1	0.96	0.15	52,52,52,52	0
56	MG	2A	3285	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3753	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3214	1/1	0.96	0.26	60,60,60,60	0
56	MG	1A	3590	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3073	1/1	0.96	0.25	51,51,51,51	0
56	MG	2B	3008	1/1	0.96	0.19	47,47,47,47	0
56	MG	2A	3262	1/1	0.96	0.18	54,54,54,54	0
56	MG	1A	3866	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3975	1/1	0.96	0.89	45,45,45,45	0
56	MG	1A	3342	1/1	0.96	0.35	52,52,52,52	0
56	MG	2A	3532	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3789	1/1	0.96	0.09	26,26,26,26	0
56	MG	1A	3326	1/1	0.96	0.09	53,53,53,53	0
56	MG	1a	1693	1/1	0.96	0.14	52,52,52,52	0
56	MG	2A	3042	1/1	0.96	0.51	43,43,43,43	0
56	MG	1A	3192	1/1	0.96	0.19	35,35,35,35	0
56	MG	1a	1829	1/1	0.96	0.25	47,47,47,47	0
56	MG	2A	3387	1/1	0.96	0.21	63,63,63,63	0
56	MG	1A	3802	1/1	0.96	0.11	77,77,77,77	0
56	MG	2a	3061	1/1	0.96	0.10	73,73,73,73	0
56	MG	1A	3335	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3051	1/1	0.96	0.62	50,50,50,50	0
56	MG	2a	3252	1/1	0.96	0.12	70,70,70,70	0
56	MG	1A	3469	1/1	0.96	0.13	49,49,49,49	0
56	MG	2E	303	1/1	0.96	0.20	26,26,26,26	0
56	MG	1A	3244	1/1	0.96	0.12	67,67,67,67	0
56	MG	1A	3265	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3166	1/1	0.96	0.26	49,49,49,49	0
56	MG	2d	502	1/1	0.96	0.24	40,40,40,40	0
56	MG	2A	3253	1/1	0.96	0.24	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3137	1/1	0.96	0.11	51,51,51,51	0
56	MG	1P	205	1/1	0.96	0.53	31,31,31,31	0
56	MG	1A	3016	1/1	0.96	0.22	61,61,61,61	0
56	MG	2A	3541	1/1	0.96	0.34	42,42,42,42	0
56	MG	1a	1856	1/1	0.96	0.16	43,43,43,43	0
56	MG	2A	3454	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3743	1/1	0.96	0.38	57,57,57,57	0
56	MG	1A	3945	1/1	0.96	0.21	60,60,60,60	0
56	MG	1B	224	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3964	1/1	0.96	0.30	29,29,29,29	0
56	MG	1A	3517	1/1	0.96	0.65	43,43,43,43	0
56	MG	2a	3169	1/1	0.96	0.69	99,99,99,99	0
56	MG	1A	3934	1/1	0.96	0.12	33,33,33,33	0
56	MG	2A	3529	1/1	0.96	0.10	68,68,68,68	0
56	MG	2A	3108	1/1	0.96	0.12	46,46,46,46	0
56	MG	2f	3001	1/1	0.96	0.09	59,59,59,59	0
56	MG	1A	3859	1/1	0.96	0.12	24,24,24,24	0
56	MG	2a	3132	1/1	0.96	0.10	65,65,65,65	0
56	MG	1a	1831	1/1	0.96	0.12	54,54,54,54	0
56	MG	1x	103	1/1	0.96	0.14	70,70,70,70	0
56	MG	2a	3088	1/1	0.96	0.22	54,54,54,54	0
56	MG	1A	3899	1/1	0.96	0.24	47,47,47,47	0
56	MG	2A	3409	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3969	1/1	0.96	0.11	18,18,18,18	0
56	MG	1Q	3002	1/1	0.96	0.12	44,44,44,44	0
56	MG	2a	3078	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3149	1/1	0.96	0.23	43,43,43,43	0
56	MG	1A	3582	1/1	0.96	0.17	45,45,45,45	0
56	MG	2A	3199	1/1	0.96	0.23	39,39,39,39	0
56	MG	2A	3561	1/1	0.96	0.95	41,41,41,41	0
56	MG	2a	3263	1/1	0.96	0.22	71,71,71,71	0
56	MG	1A	3176	1/1	0.96	0.84	40,40,40,40	0
56	MG	1A	3825	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3636	1/1	0.96	0.16	43,43,43,43	0
56	MG	2A	3482	1/1	0.96	0.27	60,60,60,60	0
56	MG	1a	1656	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3464	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3558	1/1	0.96	0.10	61,61,61,61	0
56	MG	1A	3566	1/1	0.96	0.17	23,23,23,23	0
56	MG	1A	3496	1/1	0.96	0.13	88,88,88,88	0
56	MG	2A	3155	1/1	0.96	0.23	33,33,33,33	0
56	MG	1A	3803	1/1	0.96	0.08	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3213	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3592	1/1	0.96	0.26	47,47,47,47	0
56	MG	2A	3154	1/1	0.96	0.16	32,32,32,32	0
56	MG	2P	201	1/1	0.96	0.56	41,41,41,41	0
56	MG	1A	3366	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3376	1/1	0.96	0.19	53,53,53,53	0
56	MG	1A	3841	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3153	1/1	0.96	0.12	24,24,24,24	0
56	MG	2A	3223	1/1	0.96	0.42	50,50,50,50	0
56	MG	2a	3172	1/1	0.96	0.15	60,60,60,60	0
56	MG	1A	3938	1/1	0.96	0.18	44,44,44,44	0
56	MG	2a	3200	1/1	0.96	0.11	49,49,49,49	0
56	MG	1A	3950	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3659	1/1	0.96	0.09	23,23,23,23	0
56	MG	1A	3594	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3510	1/1	0.96	0.25	55,55,55,55	0
56	MG	1D	314	1/1	0.96	0.34	63,63,63,63	0
56	MG	2A	3478	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3812	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3814	1/1	0.96	0.24	56,56,56,56	0
56	MG	2A	3181	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3112	1/1	0.96	0.27	40,40,40,40	0
56	MG	1A	3313	1/1	0.96	0.38	53,53,53,53	0
56	MG	2a	3222	1/1	0.96	0.17	46,46,46,46	0
56	MG	1A	3782	1/1	0.96	0.18	34,34,34,34	0
56	MG	2A	3566	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3972	1/1	0.96	0.65	42,42,42,42	0
56	MG	2A	3007	1/1	0.96	0.60	46,46,46,46	0
56	MG	2a	3148	1/1	0.96	0.07	72,72,72,72	0
56	MG	1F	302	1/1	0.96	0.16	51,51,51,51	0
56	MG	2A	3121	1/1	0.96	0.18	32,32,32,32	0
56	MG	2a	3126	1/1	0.96	0.21	41,41,41,41	0
56	MG	1a	1664	1/1	0.96	0.12	61,61,61,61	0
56	MG	2A	3202	1/1	0.96	0.17	46,46,46,46	0
56	MG	2U	201	1/1	0.96	0.69	48,48,48,48	0
56	MG	2A	3518	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3904	1/1	0.96	0.12	27,27,27,27	0
56	MG	1a	1817	1/1	0.96	0.30	52,52,52,52	0
56	MG	2a	3119	1/1	0.96	0.29	56,56,56,56	0
56	MG	1A	3069	1/1	0.96	0.28	39,39,39,39	0
56	MG	1A	3319	1/1	0.96	0.11	57,57,57,57	0
56	MG	1A	3401	1/1	0.96	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
56	MG	2a	3131	1/1	0.96	0.18	44,44,44,44	0
56	MG	1X	101	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	3504	1/1	0.96	0.11	60,60,60,60	0
56	MG	1A	3667	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	3739	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3374	1/1	0.96	0.26	37,37,37,37	0
56	MG	2A	3296	1/1	0.96	0.18	45,45,45,45	0
56	MG	2A	3406	1/1	0.96	0.07	41,41,41,41	0
56	MG	2a	3195	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3151	1/1	0.96	0.28	47,47,47,47	0
56	MG	1A	3247	1/1	0.97	0.61	43,43,43,43	0
56	MG	1a	1625	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3155	1/1	0.97	0.19	37,37,37,37	0
56	MG	1A	3456	1/1	0.97	0.53	39,39,39,39	0
56	MG	1A	3373	1/1	0.97	0.06	48,48,48,48	0
56	MG	1a	1613	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3720	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3774	1/1	0.97	0.12	20,20,20,20	0
56	MG	1A	3271	1/1	0.97	0.09	17,17,17,17	0
56	MG	1a	1728	1/1	0.97	0.13	53,53,53,53	0
56	MG	1A	3907	1/1	0.97	0.16	15,15,15,15	0
56	MG	1A	3559	1/1	0.97	0.14	51,51,51,51	0
56	MG	2A	3391	1/1	0.97	0.18	48,48,48,48	0
56	MG	1a	1752	1/1	0.97	0.06	72,72,72,72	0
56	MG	1D	309	1/1	0.97	0.80	41,41,41,41	0
56	MG	1P	206	1/1	0.97	0.78	54,54,54,54	0
56	MG	1A	3791	1/1	0.97	0.17	20,20,20,20	0
56	MG	1A	3728	1/1	0.97	0.21	52,52,52,52	0
56	MG	1a	1641	1/1	0.97	0.08	55,55,55,55	0
56	MG	1a	1833	1/1	0.97	0.14	59,59,59,59	0
56	MG	1A	3572	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3550	1/1	0.97	0.17	33,33,33,33	0
56	MG	2A	3394	1/1	0.97	0.22	54,54,54,54	0
56	MG	1A	3660	1/1	0.97	0.10	11,11,11,11	0
56	MG	1A	3463	1/1	0.97	0.08	80,80,80,80	0
56	MG	1A	3196	1/1	0.97	0.21	25,25,25,25	0
56	MG	1A	3754	1/1	0.97	0.19	18,18,18,18	0
56	MG	1a	1826	1/1	0.97	0.15	36,36,36,36	0
56	MG	1A	4012	1/1	0.97	0.45	36,36,36,36	0
56	MG	1A	3994	1/1	0.97	0.61	47,47,47,47	0
56	MG	2A	3467	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3790	1/1	0.97	0.18	48,48,48,48	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3208	1/1	0.97	0.29	34,34,34,34	0
56	MG	1A	3587	1/1	0.97	0.11	40,40,40,40	0
56	MG	1a	1747	1/1	0.97	0.08	56,56,56,56	0
56	MG	1a	1845	1/1	0.97	0.11	46,46,46,46	0
56	MG	2A	3099	1/1	0.97	0.11	30,30,30,30	0
56	MG	2A	3330	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3623	1/1	0.97	0.26	25,25,25,25	0
56	MG	1A	3585	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3580	1/1	0.97	0.23	46,46,46,46	0
56	MG	1A	3546	1/1	0.97	0.19	36,36,36,36	0
56	MG	1F	303	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3532	1/1	0.97	0.10	62,62,62,62	0
56	MG	1a	1839	1/1	0.97	0.12	56,56,56,56	0
56	MG	2A	3335	1/1	0.97	0.17	40,40,40,40	0
56	MG	1A	3158	1/1	0.97	0.14	24,24,24,24	0
57	ZN	14	501	1/1	0.97	0.14	106,106,106,106	0
56	MG	2A	3480	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3879	1/1	0.97	0.22	31,31,31,31	0
56	MG	1a	1825	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3630	1/1	0.97	0.14	32,32,32,32	0
56	MG	2A	3090	1/1	0.97	0.15	45,45,45,45	0
56	MG	2a	3107	1/1	0.97	0.07	57,57,57,57	0
56	MG	2A	3382	1/1	0.97	0.11	42,42,42,42	0
56	MG	1R	204	1/1	0.97	0.21	36,36,36,36	0
56	MG	2A	3520	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3882	1/1	0.97	0.23	49,49,49,49	0
56	MG	2A	3517	1/1	0.97	0.15	56,56,56,56	0
56	MG	1a	1636	1/1	0.97	0.20	44,44,44,44	0
56	MG	2A	3344	1/1	0.97	0.15	39,39,39,39	0
56	MG	2a	3218	1/1	0.97	0.14	62,62,62,62	0
56	MG	1A	3588	1/1	0.97	0.22	33,33,33,33	0
56	MG	1A	4009	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3574	1/1	0.97	0.21	48,48,48,48	0
56	MG	1A	3182	1/1	0.97	0.46	42,42,42,42	0
56	MG	2a	3239	1/1	0.97	0.05	76,76,76,76	0
56	MG	2A	3362	1/1	0.97	0.17	57,57,57,57	0
56	MG	2A	3438	1/1	0.97	0.17	62,62,62,62	0
56	MG	1a	1680	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3422	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3435	1/1	0.97	0.13	56,56,56,56	0
56	MG	1A	3015	1/1	0.97	0.10	52,52,52,52	0
56	MG	2A	3481	1/1	0.97	0.15	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3764	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3218	1/1	0.97	0.16	21,21,21,21	0
56	MG	1A	3892	1/1	0.97	0.15	43,43,43,43	0
56	MG	1A	3719	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	3356	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3086	1/1	0.97	0.53	44,44,44,44	0
56	MG	1A	3438	1/1	0.97	0.30	58,58,58,58	0
56	MG	2A	3161	1/1	0.97	0.24	32,32,32,32	0
56	MG	1a	1712	1/1	0.97	0.17	25,25,25,25	0
56	MG	1A	3548	1/1	0.97	0.20	38,38,38,38	0
56	MG	1A	3604	1/1	0.97	0.14	27,27,27,27	0
56	MG	1A	3922	1/1	0.97	0.14	19,19,19,19	0
56	MG	1A	3156	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3348	1/1	0.97	0.14	47,47,47,47	0
56	MG	2a	3193	1/1	0.97	0.12	47,47,47,47	0
56	MG	2a	3182	1/1	0.97	0.15	51,51,51,51	0
56	MG	2A	3152	1/1	0.97	0.11	58,58,58,58	0
56	MG	2A	3245	1/1	0.97	0.18	48,48,48,48	0
56	MG	1A	3025	1/1	0.97	0.16	57,57,57,57	0
56	MG	2A	3451	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3970	1/1	0.97	1.05	30,30,30,30	0
56	MG	1A	3993	1/1	0.97	0.19	73,73,73,73	0
57	ZN	1Y	201	1/1	0.97	0.19	61,61,61,61	0
56	MG	2a	3226	1/1	0.97	0.07	58,58,58,58	0
56	MG	2A	3372	1/1	0.97	0.19	45,45,45,45	0
56	MG	1A	3770	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3379	1/1	0.97	0.09	42,42,42,42	0
56	MG	2A	3459	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3304	1/1	0.97	0.28	41,41,41,41	0
56	MG	2A	3537	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3535	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3760	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3216	1/1	0.97	0.14	37,37,37,37	0
56	MG	2A	3331	1/1	0.97	0.16	48,48,48,48	0
56	MG	1A	3071	1/1	0.97	0.19	44,44,44,44	0
56	MG	1a	1789	1/1	0.97	0.08	66,66,66,66	0
56	MG	1A	3159	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3242	1/1	0.97	0.15	52,52,52,52	0
56	MG	1A	3963	1/1	0.97	0.17	14,14,14,14	0
56	MG	1A	3880	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3432	1/1	0.97	0.17	61,61,61,61	0
56	MG	1a	1819	1/1	0.97	0.14	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3622	1/1	0.97	0.14	22,22,22,22	0
56	MG	2a	3133	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3768	1/1	0.97	0.15	10,10,10,10	0
56	MG	1A	3181	1/1	0.97	0.16	24,24,24,24	0
56	MG	1A	3781	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3948	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3561	1/1	0.97	0.10	44,44,44,44	0
56	MG	2a	3106	1/1	0.97	0.22	63,63,63,63	0
56	MG	2a	3009	1/1	0.97	0.23	65,65,65,65	0
56	MG	2a	3150	1/1	0.97	0.19	51,51,51,51	0
56	MG	1A	3223	1/1	0.97	0.24	33,33,33,33	0
56	MG	2A	3345	1/1	0.97	0.11	35,35,35,35	0
56	MG	1A	3946	1/1	0.97	0.24	41,41,41,41	0
56	MG	2A	3312	1/1	0.97	0.20	28,28,28,28	0
56	MG	1a	1816	1/1	0.97	0.13	40,40,40,40	0
56	MG	2a	3194	1/1	0.97	0.22	72,72,72,72	0
56	MG	1B	217	1/1	0.97	0.19	50,50,50,50	0
56	MG	1A	3369	1/1	0.97	0.50	40,40,40,40	0
56	MG	2a	3076	1/1	0.97	0.16	83,83,83,83	0
56	MG	1a	1851	1/1	0.97	0.11	74,74,74,74	0
56	MG	2a	3084	1/1	0.97	0.23	56,56,56,56	0
56	MG	1A	3395	1/1	0.97	0.50	37,37,37,37	0
56	MG	1a	1718	1/1	0.97	0.15	48,48,48,48	0
56	MG	2k	8001	1/1	0.97	0.06	83,83,83,83	0
56	MG	1A	3250	1/1	0.97	0.20	34,34,34,34	0
56	MG	1A	3304	1/1	0.97	0.18	34,34,34,34	0
56	MG	1A	3058	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3519	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3074	1/1	0.97	0.71	51,51,51,51	0
56	MG	2A	3020	1/1	0.97	0.15	48,48,48,48	0
56	MG	1A	3161	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3746	1/1	0.97	0.18	7,7,7,7	0
56	MG	1a	1619	1/1	0.97	0.22	54,54,54,54	0
56	MG	1A	3001	1/1	0.97	0.84	42,42,42,42	0
56	MG	1A	3601	1/1	0.97	0.23	44,44,44,44	0
56	MG	2A	3549	1/1	0.97	0.27	43,43,43,43	0
56	MG	1a	1743	1/1	0.97	0.12	56,56,56,56	0
56	MG	1a	1631	1/1	0.97	0.12	36,36,36,36	0
56	MG	1a	1730	1/1	0.97	0.24	70,70,70,70	0
56	MG	1A	3897	1/1	0.97	0.18	29,29,29,29	0
56	MG	1a	1844	1/1	0.97	0.10	43,43,43,43	0
56	MG	2a	3233	1/1	0.97	0.10	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3800	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3206	1/1	0.97	0.17	21,21,21,21	0
56	MG	2a	3122	1/1	0.97	0.18	72,72,72,72	0
56	MG	1A	3717	1/1	0.97	0.17	59,59,59,59	0
56	MG	1D	306	1/1	0.97	0.48	31,31,31,31	0
56	MG	1A	3578	1/1	0.97	0.17	64,64,64,64	0
56	MG	1a	1806	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3577	1/1	0.97	0.23	60,60,60,60	0
56	MG	2Q	3002	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3528	1/1	0.97	0.20	54,54,54,54	0
56	MG	1A	3710	1/1	0.97	0.24	39,39,39,39	0
56	MG	1a	1632	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3860	1/1	0.97	0.23	29,29,29,29	0
56	MG	1A	3635	1/1	0.98	0.11	46,46,46,46	0
56	MG	1A	3063	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3828	1/1	0.98	0.08	67,67,67,67	0
56	MG	1A	3088	1/1	0.98	0.44	60,60,60,60	0
56	MG	1A	3203	1/1	0.98	0.28	32,32,32,32	0
56	MG	1A	3267	1/1	0.98	0.72	27,27,27,27	0
57	ZN	25	501	1/1	0.98	0.21	54,54,54,54	0
56	MG	2A	3366	1/1	0.98	0.21	69,69,69,69	0
58	SF4	1d	501	8/8	0.98	0.18	66,73,85,85	0
56	MG	1A	3680	1/1	0.98	0.11	42,42,42,42	0
56	MG	1a	1824	1/1	0.98	0.16	52,52,52,52	0
56	MG	1A	3229	1/1	0.98	0.12	50,50,50,50	0
56	MG	1A	3629	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	3702	1/1	0.98	0.14	44,44,44,44	0
56	MG	2A	3150	1/1	0.98	0.15	30,30,30,30	0
56	MG	2a	3059	1/1	0.98	0.11	83,83,83,83	0
56	MG	1A	3169	1/1	0.98	0.18	21,21,21,21	0
56	MG	1a	1663	1/1	0.98	0.08	76,76,76,76	0
56	MG	2A	3421	1/1	0.98	0.09	59,59,59,59	0
56	MG	1A	3259	1/1	0.98	0.16	38,38,38,38	0
56	MG	1Q	3004	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3714	1/1	0.98	0.21	46,46,46,46	0
56	MG	2a	3080	1/1	0.98	0.08	40,40,40,40	0
56	MG	1a	1622	1/1	0.98	0.18	90,90,90,90	0
56	MG	1A	3693	1/1	0.98	0.17	21,21,21,21	0
56	MG	2A	3422	1/1	0.98	0.29	57,57,57,57	0
56	MG	2Z	3001	1/1	0.98	0.12	68,68,68,68	0
56	MG	19	101	1/1	0.98	0.27	65,65,65,65	0
56	MG	2A	3192	1/1	0.98	0.14	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3681	1/1	0.98	0.14	14,14,14,14	0
56	MG	2A	3458	1/1	0.98	0.09	54,54,54,54	0
56	MG	1a	1740	1/1	0.98	0.07	47,47,47,47	0
56	MG	2A	3431	1/1	0.98	0.18	68,68,68,68	0
56	MG	1A	3310	1/1	0.98	0.31	44,44,44,44	0
56	MG	1A	3085	1/1	0.98	0.60	47,47,47,47	0
56	MG	1A	3484	1/1	0.98	0.17	48,48,48,48	0
56	MG	1a	1683	1/1	0.98	0.12	68,68,68,68	0
56	MG	2A	3558	1/1	0.98	0.31	34,34,34,34	0
56	MG	1A	3799	1/1	0.98	0.33	42,42,42,42	0
56	MG	1A	3835	1/1	0.98	0.10	66,66,66,66	0
56	MG	1A	3690	1/1	0.98	0.15	48,48,48,48	0
56	MG	2A	3500	1/1	0.98	0.12	49,49,49,49	0
56	MG	1A	3620	1/1	0.98	0.12	38,38,38,38	0
56	MG	2A	3196	1/1	0.98	0.17	35,35,35,35	0
56	MG	2A	3470	1/1	0.98	0.27	44,44,44,44	0
56	MG	1A	3286	1/1	0.98	0.39	36,36,36,36	0
56	MG	1A	3309	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3253	1/1	0.98	0.26	31,31,31,31	0
56	MG	2A	3215	1/1	0.98	0.18	39,39,39,39	0
56	MG	2a	3111	1/1	0.98	0.25	56,56,56,56	0
56	MG	1A	3666	1/1	0.98	0.12	37,37,37,37	0
56	MG	1A	3651	1/1	0.98	0.16	21,21,21,21	0
56	MG	1A	3916	1/1	0.98	0.17	52,52,52,52	0
56	MG	1a	1835	1/1	0.98	0.07	73,73,73,73	0
56	MG	2a	3136	1/1	0.98	0.09	51,51,51,51	0
56	MG	1A	3529	1/1	0.98	0.24	48,48,48,48	0
56	MG	2A	3125	1/1	0.98	0.21	56,56,56,56	0
56	MG	1A	3756	1/1	0.98	0.15	51,51,51,51	0
56	MG	1A	3576	1/1	0.98	0.12	19,19,19,19	0
56	MG	1A	3688	1/1	0.98	0.16	41,41,41,41	0
56	MG	2a	3033	1/1	0.98	0.41	53,53,53,53	0
56	MG	1D	312	1/1	0.98	0.44	47,47,47,47	0
56	MG	2A	3462	1/1	0.98	0.22	60,60,60,60	0
56	MG	2a	3183	1/1	0.98	0.14	37,37,37,37	0
56	MG	1A	3672	1/1	0.98	0.12	13,13,13,13	0
56	MG	1A	3232	1/1	0.98	0.61	43,43,43,43	0
56	MG	2D	305	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3163	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3420	1/1	0.98	0.12	53,53,53,53	0
56	MG	2A	3457	1/1	0.98	0.12	45,45,45,45	0
56	MG	1a	1652	1/1	0.98	0.21	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3019	1/1	0.98	0.30	46,46,46,46	0
56	MG	1A	3269	1/1	0.98	0.12	36,36,36,36	0
56	MG	2A	3526	1/1	0.98	0.09	49,49,49,49	0
56	MG	1B	206	1/1	0.98	0.26	46,46,46,46	0
56	MG	1A	3652	1/1	0.98	0.10	36,36,36,36	0
56	MG	2A	3534	1/1	0.98	0.10	64,64,64,64	0
56	MG	2A	3545	1/1	0.98	0.19	39,39,39,39	0
56	MG	2a	3085	1/1	0.98	0.08	40,40,40,40	0
56	MG	2a	3232	1/1	0.98	0.13	66,66,66,66	0
56	MG	1A	3171	1/1	0.98	0.25	38,38,38,38	0
56	MG	1a	1713	1/1	0.98	0.13	63,63,63,63	0
56	MG	1A	3272	1/1	0.98	0.22	29,29,29,29	0
56	MG	2A	3316	1/1	0.98	0.21	57,57,57,57	0
56	MG	1x	101	1/1	0.98	0.30	51,51,51,51	0
56	MG	1A	3382	1/1	0.98	0.08	40,40,40,40	0
56	MG	1A	3809	1/1	0.98	0.22	45,45,45,45	0
56	MG	2A	3370	1/1	0.98	0.16	44,44,44,44	0
56	MG	2A	3303	1/1	0.98	0.23	55,55,55,55	0
56	MG	1A	3194	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	3256	1/1	0.98	0.17	43,43,43,43	0
56	MG	19	104	1/1	0.98	0.13	31,31,31,31	0
56	MG	1A	3656	1/1	0.98	0.21	33,33,33,33	0
56	MG	1A	3174	1/1	0.98	0.65	37,37,37,37	0
56	MG	2A	3276	1/1	0.98	0.15	42,42,42,42	0
56	MG	2a	3223	1/1	0.98	0.11	49,49,49,49	0
56	MG	1A	3646	1/1	0.98	0.14	10,10,10,10	0
56	MG	2a	3130	1/1	0.98	0.08	43,43,43,43	0
56	MG	2a	3007	1/1	0.98	0.21	46,46,46,46	0
56	MG	1A	3540	1/1	0.98	0.32	45,45,45,45	0
56	MG	1A	3677	1/1	0.98	0.16	51,51,51,51	0
56	MG	2A	3413	1/1	0.98	0.23	62,62,62,62	0
56	MG	1a	1714	1/1	0.98	0.09	68,68,68,68	0
56	MG	1A	3157	1/1	0.98	0.16	28,28,28,28	0
56	MG	2O	202	1/1	0.99	0.16	42,42,42,42	0
56	MG	2A	3052	1/1	0.99	0.14	43,43,43,43	0
56	MG	2A	3043	1/1	0.99	0.20	49,49,49,49	0
56	MG	1a	1716	1/1	0.99	0.08	53,53,53,53	0
56	MG	1A	3775	1/1	0.99	0.17	14,14,14,14	0
56	MG	1A	3908	1/1	0.99	0.16	40,40,40,40	0
56	MG	1a	1837	1/1	0.99	0.16	37,37,37,37	0
56	MG	1B	216	1/1	0.99	0.23	54,54,54,54	0
56	MG	1a	1815	1/1	0.99	0.10	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3762	1/1	0.99	0.16	45,45,45,45	0
56	MG	1A	3926	1/1	0.99	0.31	38,38,38,38	0
57	ZN	19	103	1/1	0.99	0.22	45,45,45,45	0
56	MG	2A	3466	1/1	0.99	0.15	69,69,69,69	0
56	MG	1d	503	1/1	0.99	0.11	52,52,52,52	0
56	MG	1A	3571	1/1	0.99	0.22	25,25,25,25	0
56	MG	2A	3444	1/1	0.99	0.22	29,29,29,29	0
56	MG	2A	3123	1/1	0.99	0.20	41,41,41,41	0
56	MG	1A	3687	1/1	0.99	0.13	48,48,48,48	0
56	MG	2a	3199	1/1	0.99	0.16	62,62,62,62	0
56	MG	1a	1719	1/1	0.99	0.14	53,53,53,53	0
56	MG	1a	1847	1/1	0.99	0.10	53,53,53,53	0
56	MG	1a	1729	1/1	0.99	0.23	35,35,35,35	0
56	MG	1A	3858	1/1	0.99	0.24	46,46,46,46	0
56	MG	2a	3028	1/1	0.99	0.23	76,76,76,76	0
56	MG	1A	3225	1/1	0.99	0.55	34,34,34,34	0
56	MG	2a	3074	1/1	0.99	0.18	74,74,74,74	0
57	ZN	16	102	1/1	0.99	0.19	29,29,29,29	0
56	MG	1A	3796	1/1	0.99	0.12	16,16,16,16	0
56	MG	1A	3553	1/1	0.99	0.14	44,44,44,44	0
56	MG	2A	3351	1/1	0.99	0.11	37,37,37,37	0
56	MG	1A	4020	1/1	0.99	0.30	32,32,32,32	0
56	MG	1A	3694	1/1	0.99	0.13	16,16,16,16	0
56	MG	1A	3195	1/1	0.99	0.18	33,33,33,33	0
57	ZN	15	103	1/1	0.99	0.18	43,43,43,43	0
56	MG	1A	4014	1/1	0.99	0.16	43,43,43,43	0
56	MG	2A	3120	1/1	0.99	0.26	45,45,45,45	0
58	SF4	2d	501	8/8	0.99	0.17	56,76,90,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.