



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 11:24 AM UTC

PDB ID : 9D0G / pdb\_00009d0g  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with O-cresomycin, mRNA, deacylated A-site tRNA<sup>phe</sup>, aminoacylated P-site fMet-tRNA<sup>met</sup>, and deacylated E-site tRNA<sup>phe</sup> at 2.50Å resolution  
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Robinson, P.J.; Benedetto, A.E.; Yu, M.; Tresco, B.I.C.; See, D.N.Y.; Jiang, T.; Ramkisson, A.; Dunand, C.F.; Svetlov, M.S.; Lee, J.; Myers, A.G.; Polikanov, Y.S.  
Deposited on : 2024-08-07  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

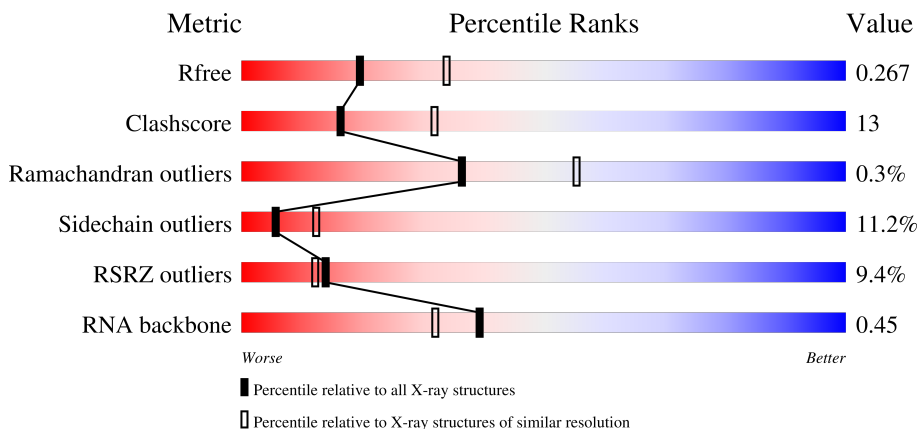
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>4%</div> <div>59% 31% 8%</div> </div>
1	2A	2915	<div> <div>4%</div> <div>49% 37% 10%</div> </div>

*Continued on next page...*

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
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	











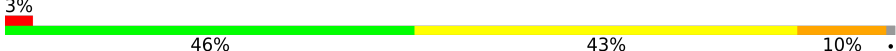
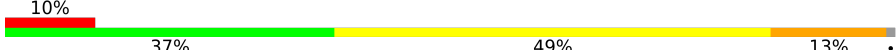
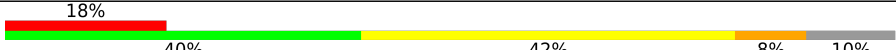
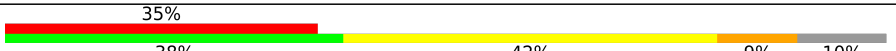

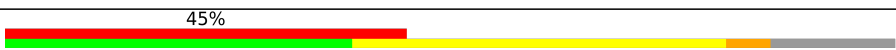




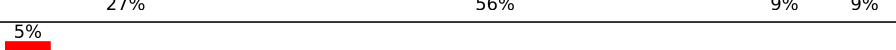
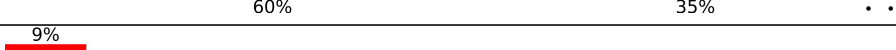

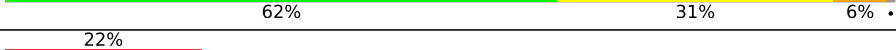
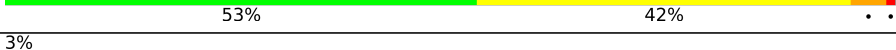
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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	1U	211	-	-	-	X
56	MG	1a	1642	-	-	-	X
56	MG	2A	3394	-	-	-	X
56	MG	2A	3491	-	-	-	X
60	SF4	2d	302	-	-	X	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	79	Total	C	N	O	S	0	0	0
			620	383	131	105	1			

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0	0
			1530	685	274	498	71	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1108	Total	Mg	0	0
			1108	1108		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	16	Total	Mg	0	0
			16	16		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	5	Total 5	Mg 5	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	6	Total 6	Mg 6	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	5	Total 5	Mg 5	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	11	Total 11	Mg 11	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1X	7	Total 7	Mg 7	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	10	8	Total 8	Mg 8	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	4	Total 4	Mg 4	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	6	Total 6	Mg 6	0	0
56	16	1	Total 1	Mg 1	0	0
56	17	5	Total 5	Mg 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	18	8	Total 8	Mg 8	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	211	Total 211	Mg 211	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1h	1	Total 1	Mg 1	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	2	Total 2	Mg 2	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	2	Total 2	Mg 2	0	0
56	1w	8	Total 8	Mg 8	0	0
56	1x	12	Total 12	Mg 12	0	0
56	1y	2	Total 2	Mg 2	0	0
56	2A	873	Total 873	Mg 873	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2E	10	Total 10	Mg 10	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2F	6	Total 6	Mg 6	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	2	Total 2	Mg 2	0	0
56	21	3	Total 3	Mg 3	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	5	Total 5	Mg 5	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	3	Total 3	Mg 3	0	0
56	28	5	Total 5	Mg 5	0	0
56	29	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2a	240	Total 240	Mg 240	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2l	5	Total 5	Mg 5	0	0
56	2q	3	Total 3	Mg 3	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	3	Total 3	Mg 3	0	0
56	2w	7	Total 7	Mg 7	0	0
56	2x	7	Total 7	Mg 7	0	0
56	2y	7	Total 7	Mg 7	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

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

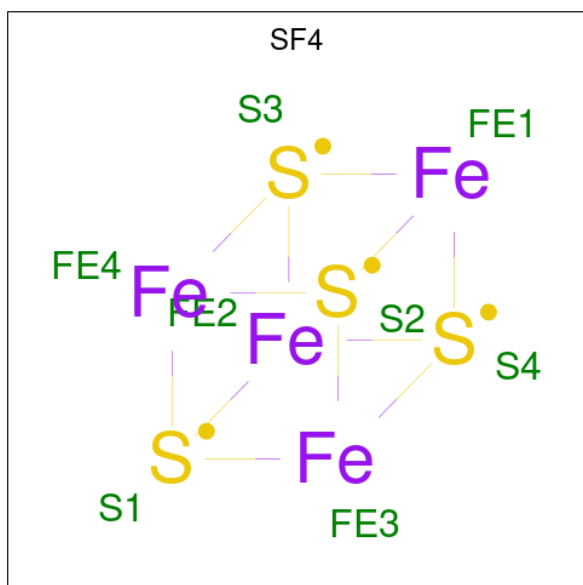
- Molecule 58 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1S,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-2,13-dioxabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: A1A1F) (formula: C<sub>25</sub>H<sub>42</sub>N<sub>2</sub>O<sub>7</sub>).



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2002	Total	O	0	0
			2002	2002		
61	1B	63	Total	O	0	0
			63	63		
61	1D	28	Total	O	0	0
			28	28		
61	1E	30	Total	O	0	0
			30	30		
61	1F	19	Total	O	0	0
			19	19		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	3	Total 3	O 3	0	0
61	1H	2	Total 2	O 2	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	7	Total 7	O 7	0	0
61	1O	7	Total 7	O 7	0	0
61	1P	19	Total 19	O 19	0	0
61	1Q	9	Total 9	O 9	0	0
61	1R	13	Total 13	O 13	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	8	Total 8	O 8	0	0
61	1U	15	Total 15	O 15	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	7	Total 7	O 7	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	13	Total 13	O 13	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	14	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	6	Total 6	O 6	0	0
61	16	2	Total 2	O 2	0	0
61	17	11	Total 11	O 11	0	0
61	18	10	Total 10	O 10	0	0
61	1a	374	Total 374	O 374	0	0
61	1b	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	8	Total 8	O 8	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	3	Total 3	O 3	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	4	Total 4	O 4	0	0
61	1w	11	Total 11	O 11	0	0
61	1x	13	Total 13	O 13	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1175	Total 1175	O 1175	0	0
61	2B	24	Total 24	O 24	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2D	20	Total 20	O 20	0	0
61	2E	12	Total 12	O 12	0	0
61	2F	13	Total 13	O 13	0	0
61	2I	3	Total 3	O 3	0	0
61	2N	1	Total 1	O 1	0	0
61	2P	13	Total 13	O 13	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	5	Total 5	O 5	0	0
61	2U	3	Total 3	O 3	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	2	Total 2	O 2	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	4	Total 4	O 4	0	0
61	21	11	Total 11	O 11	0	0
61	23	2	Total 2	O 2	0	0
61	25	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	268	Total 268	O 268	0	0

*Continued on next page...*

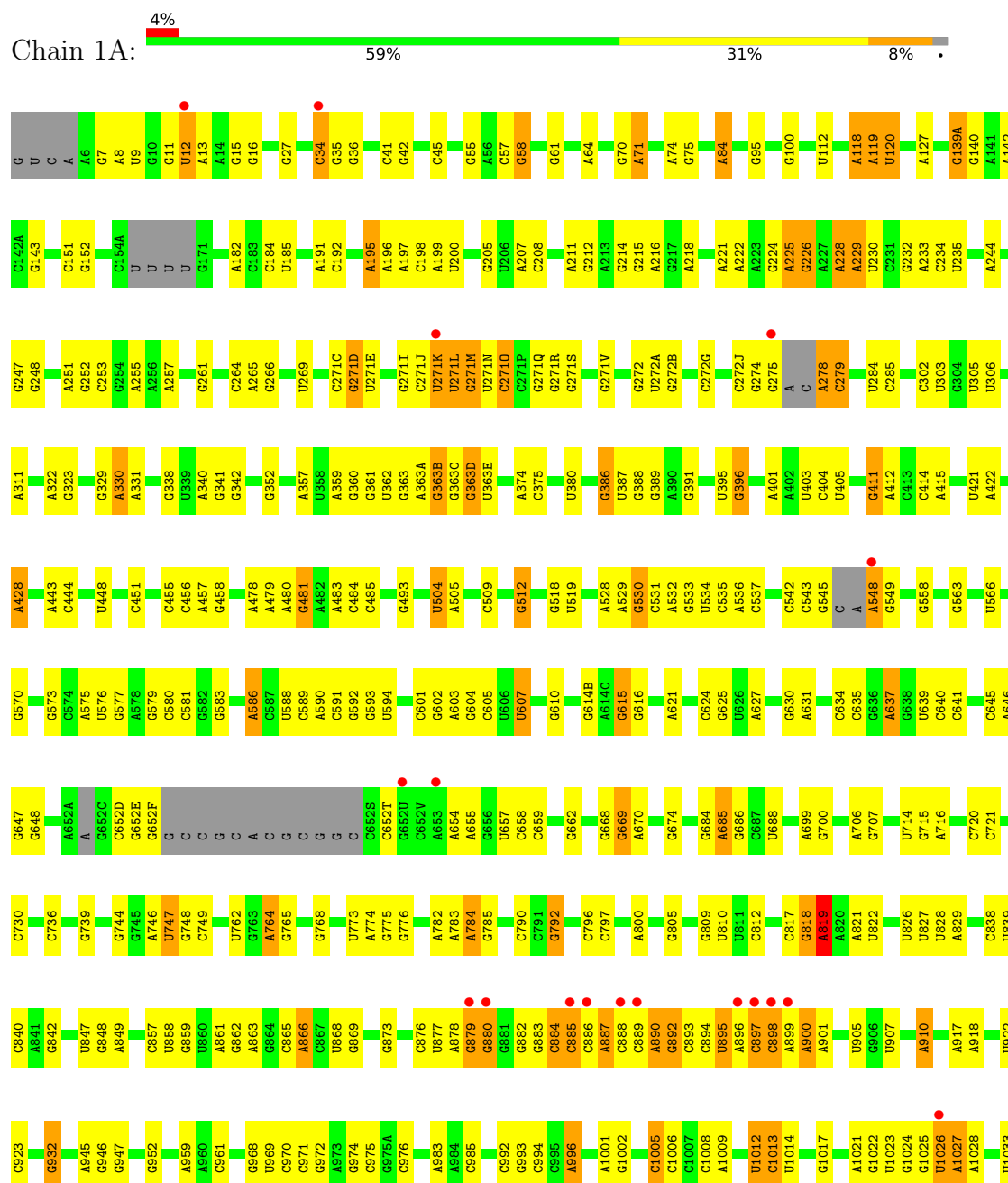
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2c	1	Total	O	0	0
			1	1		
61	2d	1	Total	O	0	0
			1	1		
61	2e	1	Total	O	0	0
			1	1		
61	2j	3	Total	O	0	0
			3	3		
61	2l	6	Total	O	0	0
			6	6		
61	2o	1	Total	O	0	0
			1	1		
61	2p	1	Total	O	0	0
			1	1		
61	2q	1	Total	O	0	0
			1	1		
61	2r	1	Total	O	0	0
			1	1		
61	2t	2	Total	O	0	0
			2	2		
61	2v	2	Total	O	0	0
			2	2		
61	2w	1	Total	O	0	0
			1	1		
61	2x	5	Total	O	0	0
			5	5		
61	2y	7	Total	O	0	0
			7	7		

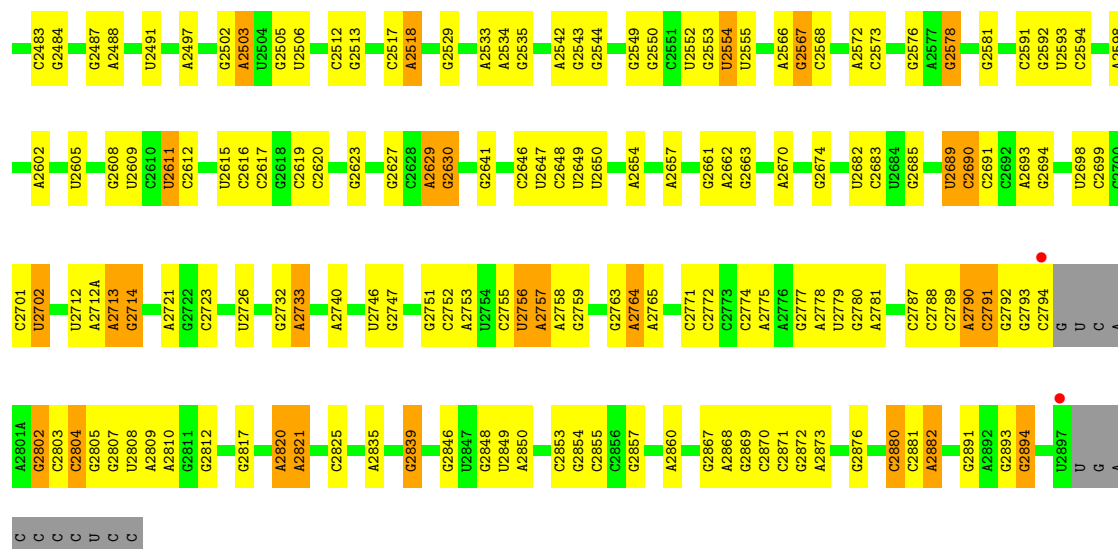
### 3 Residue-property plots

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

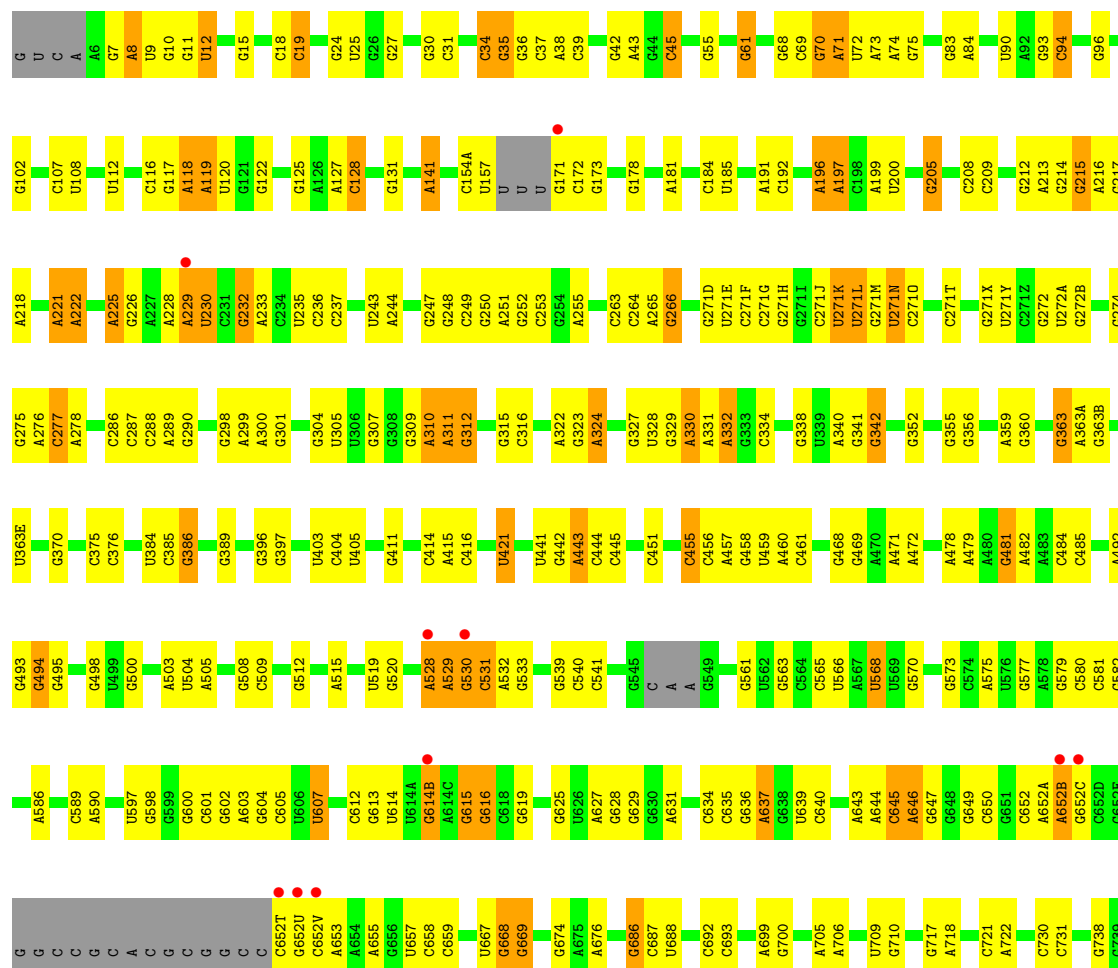
#### • Molecule 1: 23S Ribosomal RNA





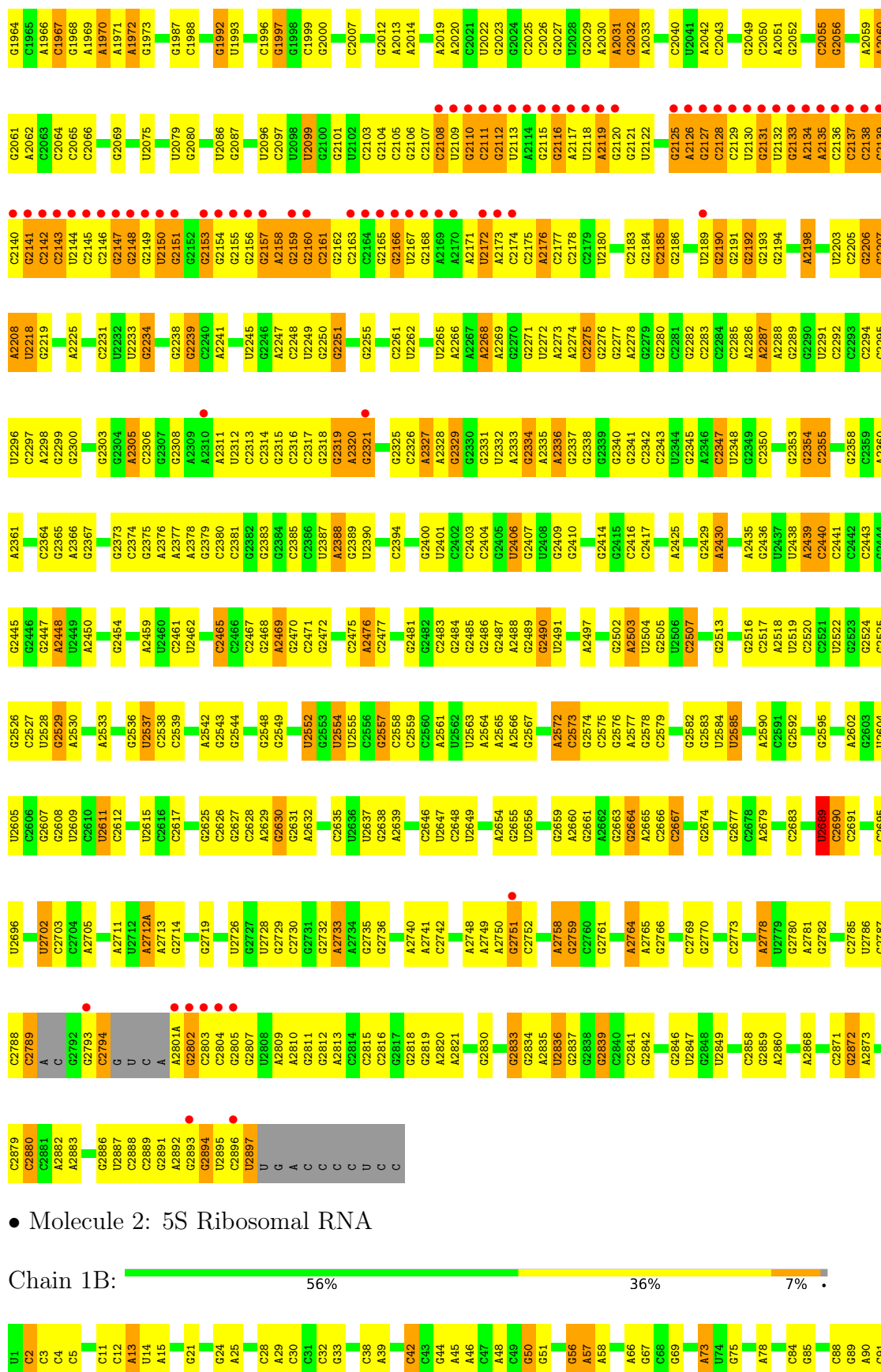


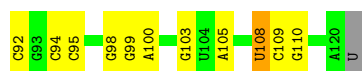
### • Molecule 1: 23S Ribosomal RNA



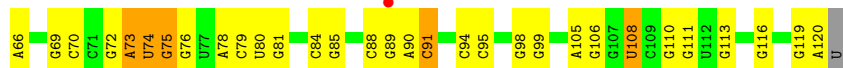
A1853	C1767	G1651	G1538	C1464	A1373	U1263	G	C	G1042	A973	C897	U828	U740
G1857	U1768	A1652	G1539	G1465	G1374	G1264	A	A	C1043	G974	C896	A829	G741
G1858	G1769	G1653	U1540	G1466	C1375	A1265	C	C	G	C975	A899	G832	U747
A1877	A1773	A1654	G1541	C1467	G1376	G1266	U	U	A	G976	A900	G832	G748
G1878	C1774	A1664	A1542	C1468	A1378	U1267	G	G	A	G977	C901	U839	A752
A1885	U1777	A1665	C1543	G1470	G1380	A1268	U	U	A	A981	C902	C840	C753
A1889	U1778	G1666	C1546	A1471	A1384	C1270	C	C	A	C982	C903	A841	C754
A1890	U1779	A1668	C1547	G1473	G1385	U1271	G	A	G	A983	A909	C844	C755
A1899	A1780	A1669	A1554	C1474	G1386	A1272	C	C	C	A983	A910	C845	G759
G1899	G1781	C1670	C1557	G1475	U1394	U1273	A	A	C	C986	A911	C846	G760
A1900	U1782	U1671	A1558	C1476	U1405	A1274	U	U	G	A990	C912	U847	A761
A1901	A1784	G1674	A1566	A1477	U1406	U1278	G	G	G	C991	U913	C848	
G1902	U1785	A1674	A1567	G1478	C1407	U1288	A	A	G	C992	G916	A849	A764
G1903	A1786	C1685	G1568	A1479	C1408	G1288	G	G	A	C993	A917	U851	G765
G1904	A1791	C1686	A1569	G1482	U1409	G1297	U	U	G	C994	G920	G852	A774
G1905	U1796	A1689	C1577	A1490	A1411	C1298	U	U	C	C995	G921	G853	G775
U1911	C1797	U1693	A1578	G1491	A1412	G1299	U	U	G	A996	G922	G854	G776
A1912	U1798	C1694	A1579	C1492	G1416	U1300	G	G	A	C997	G923	G855	A777
A1913	G1799	G1695	A1580	A1493	C1417	A1301	C	C	C	C998	G924	C856	
C1914	C1800	G1696	G1581	A1494	G1418	A1302	U	U	C	U999	G925	C857	
U1915	G1801	G1697	C1582	A1495	G1419	G1303	U	U	C	A1000	G926	U858	A782
A1916	A1802	A1698	A1583	U1497	U1420	C1314	A	A	C	A1001	U930	G859	A783
A1917	G1804	G1699	C1584	G1421	G1422	G1324	G	G	A	G1002	G931	U860	A784
A1918	U1700	A1586	A1586	G1423	G1423	G1325	A	A	G	C1003	G932	A861	G785
A1919	G1707	C1589	C1589	A1427	A1427	A1331	C	C	G	C1004	U937	G862	
C1920	U1708	U1708	A1507	C1428	G1429	U1331	A	A	C	C1005	G938	C865	A788
U1926	A1811	U1709	A1508	G1429	C1429	G1334	C	C	C	C1006	G939	A866	G792
A1927	G1813	G1593	G1593	A1509	A1429	U1335	G	G	A	G1011	G940	C867	A793
A1928	C1711	G1594	C1430	A1509A	G1430	G1336	C	C	C	U1012	A941	U868	G794
G1929	A1815	C1712	A1509B	U1431	A1431	G1337	A	A	C	C1013	G942	G869	C795
U1930	G1816	C1599	G1510	A1434	G1435	U1340	U	U	C	U1014	U943	C796	A870
A1931	G1817	C1604	C1511	G1436	C1437	G1341	C	C	C	G1015	G944	G873	C797
A1932	U1818	C1607	C1512	G1437	G1437	U1341	C	C	C	G1016	U945	G874	A802
C1933	A1819	A1608	C1513	G1437	G1437	G1345	U	U	C	C1017	G947	G875	U803
G1934	G1826	U1739	G1514	G1442	G1442	U1345	U	U	C	U1018	G948	C876	A804
G1935	C1827	A1609	G1515	G1443	G1443	U1352	A	A	C	A1020	G952	U877	G805
A1936	G1828	A1610	C1516	G1444	G1444	A1353	A	A	C	A1021	C953	C884	C806
A1937	A1829	G1745A	U1517	A1445	A1445	G1354	A	A	C	U1022	G954	C885	U807
A1938	C1830	A1616	G1519	C1445A	C1446	G1355	G	G	C	U1023	C955	C886	
U1939	G1750	G1627	G1520	G1446	G1446	G1356	A	A	C	G1024	C956	C887	U811
C1942	G1835	C1751	C1521	A1449	A1449	G1358	A	A	C	U1025	C957	C888	C812
U1943	C1836	G1752	G1522	G1450	G1450	A1359	A	A	C	G1026	U958	C889	U813
G1945	G1837	G1753	G1527	G1451	G1451	A1360	U	U	C	A1027	U959	C890	C817
C1947	C1838	G1756	G1529	A1452	A1452	G1361	C	C	C	U1028	A960	C891	G818
U1955	C1843	U1757	C1530	U1453	U1453	G1364	G	G	C	G1029	C961	C892	A819
U1956	A1847	G1758	C1531	G1455	G1455	A1365	U	U	C	U1030	G962	C893	A820
C1958	U1762	G1642	G1532	G1459	G1459	A1365	A	A	C	A1032	U963	C894	A821
A1843	A1763	G1643	G1533	A1460	A1460	G1368	U	U	C	U1033	C964	C895	U822
U1851	G1764	C1647	U	A1461	A1461	G1369	A	A	C	C1038	C965	G892	G823
C1962	C1765	C1648	A	G1462	G1462	G1371	C	C	C	G1039	G966	C893	A824
U1963	U1766	C1536	G1537	C1463	C1463	U1372	G	G	C	U1040	C971	C894	U825
							U	U	C	C1041	G972	A896	U827



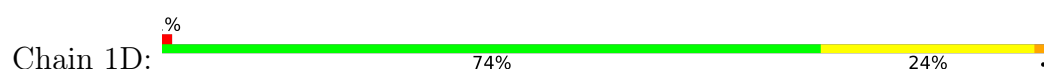




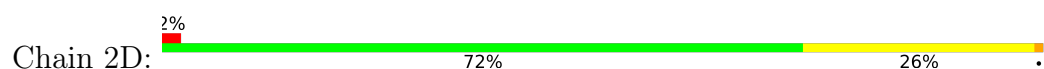
- Molecule 2: 5S Ribosomal RNA



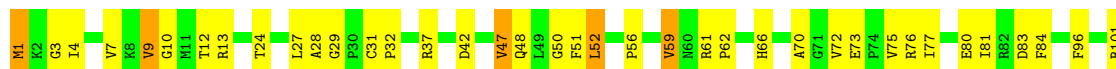
- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



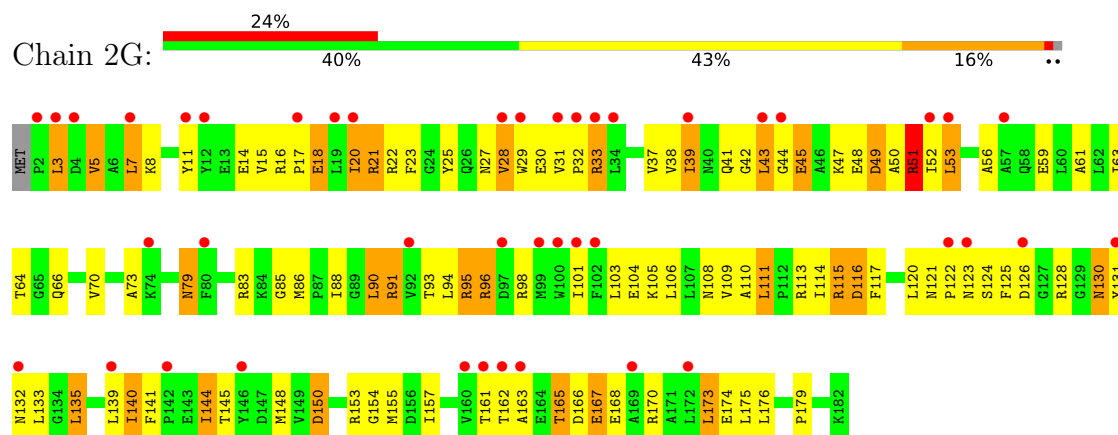
- Molecule 4: 50S ribosomal protein L3



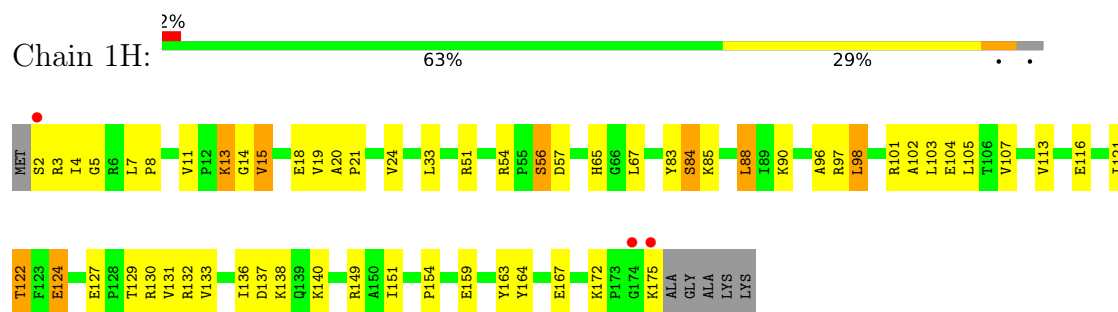


F180  
R181  
K182

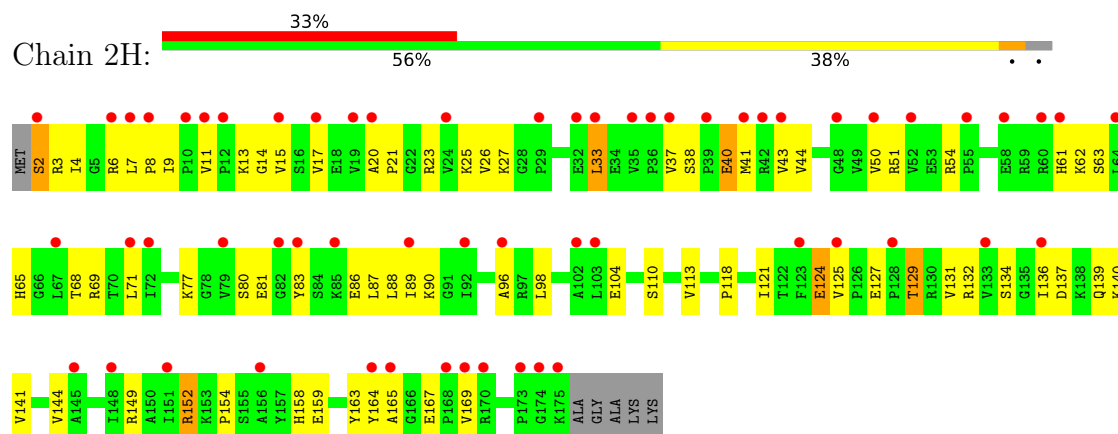
• Molecule 6: 50S ribosomal protein L5



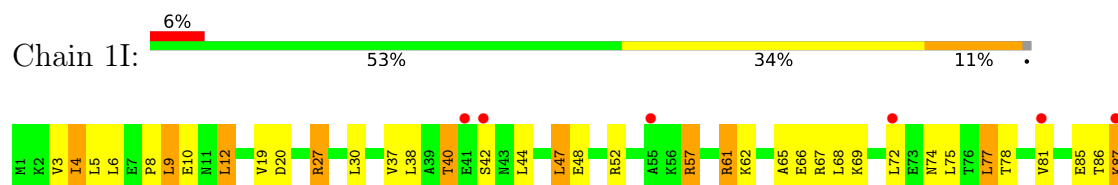
• Molecule 7: 50S ribosomal protein L6

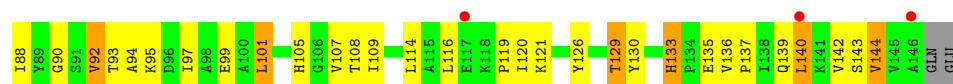


• Molecule 7: 50S ribosomal protein L6

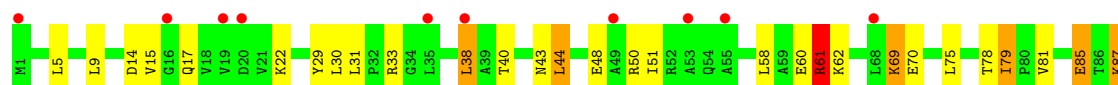


• Molecule 8: 50S ribosomal protein L9

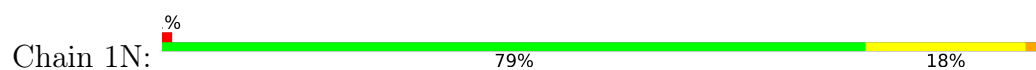




• Molecule 8: 50S ribosomal protein L9



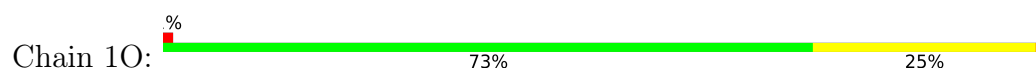
• Molecule 9: 50S ribosomal protein L13



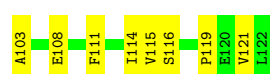
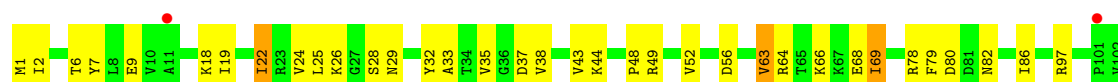
• Molecule 9: 50S ribosomal protein L13



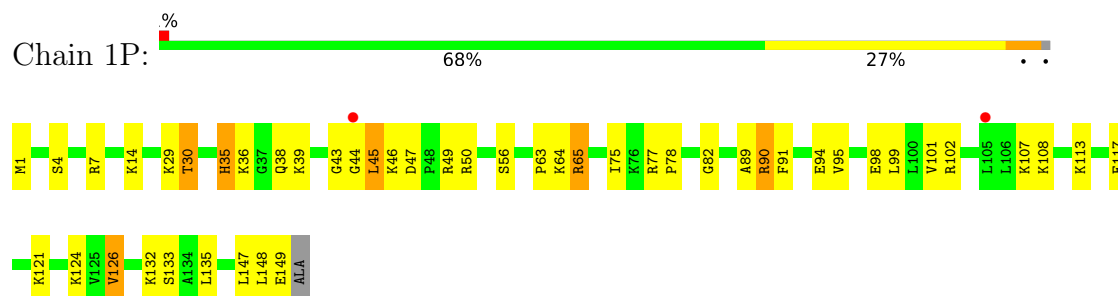
• Molecule 10: 50S ribosomal protein L14



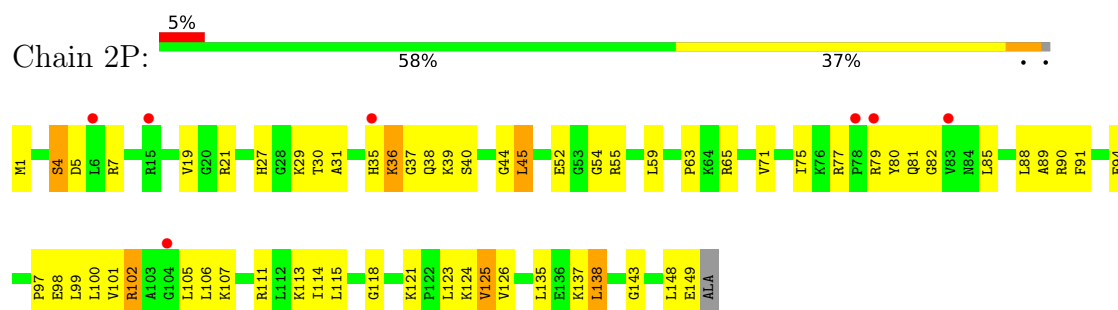
• Molecule 10: 50S ribosomal protein L14



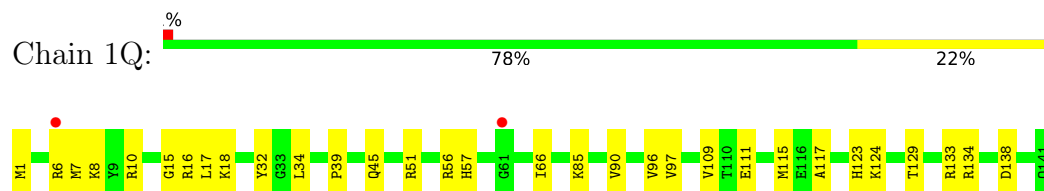
## • Molecule 11: 50S ribosomal protein L15



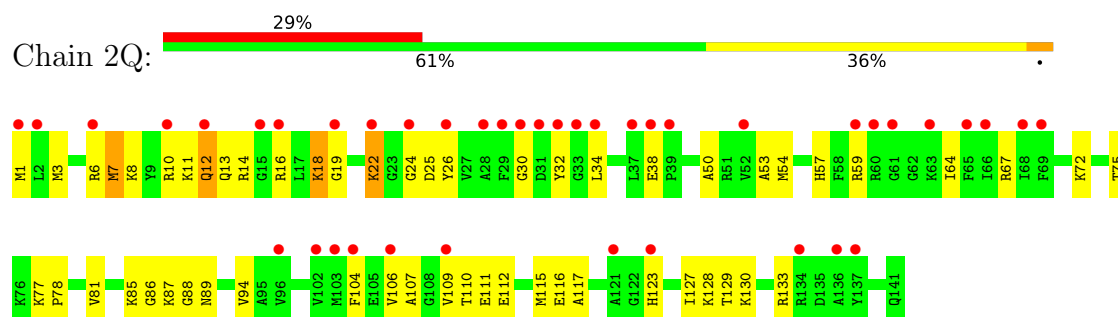
## • Molecule 11: 50S ribosomal protein L15



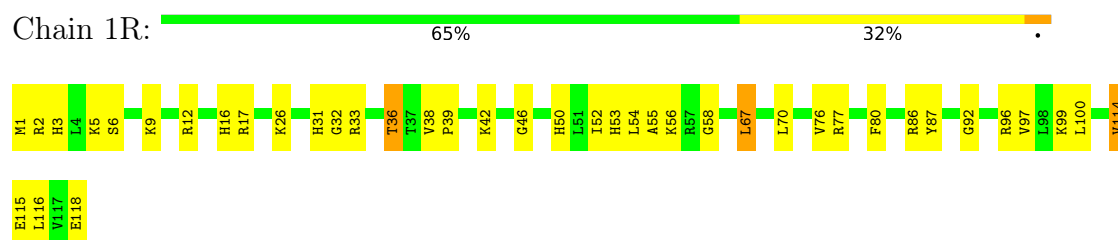
## • Molecule 12: 50S ribosomal protein L16




## • Molecule 12: 50S ribosomal protein L16



## • Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  76% 20%



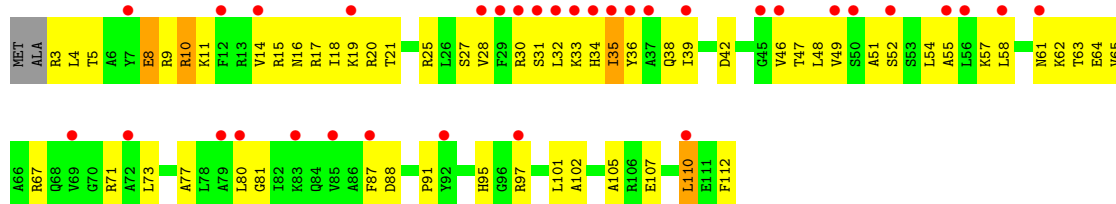
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  71% 24%



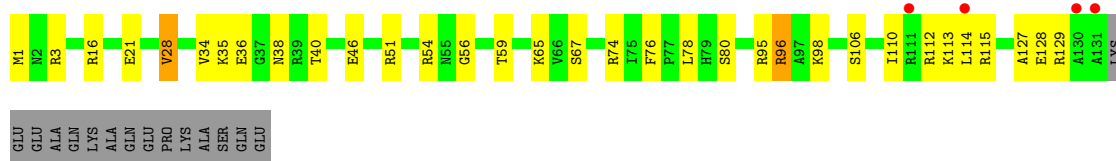
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  30% 45% 50%



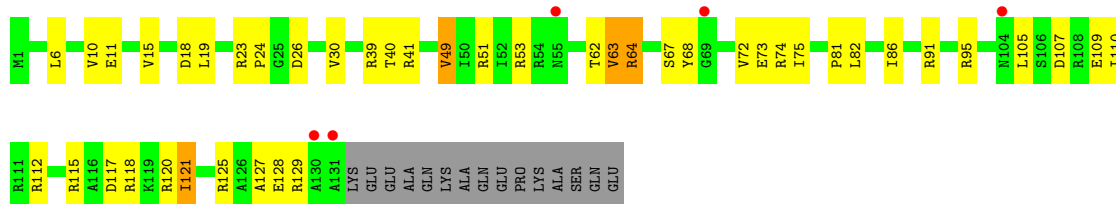
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  3% 67% 21% 10%




- Molecule 15: 50S ribosomal protein L19

Chain 2T:  3% 60% 27% 10%

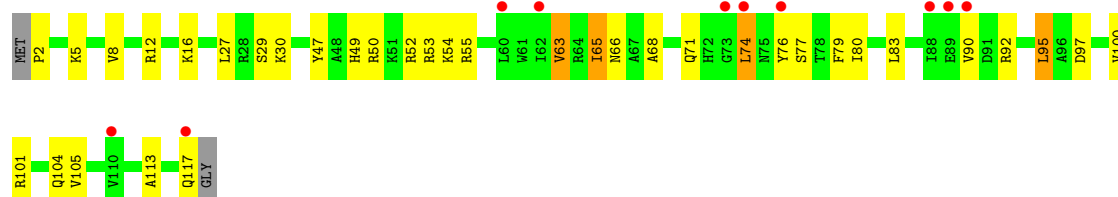


- Molecule 16: 50S ribosomal protein L20

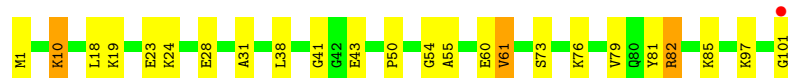
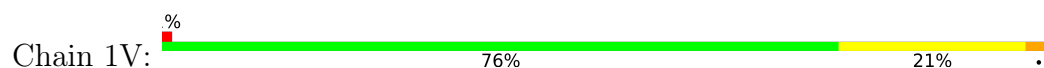
Chain 1U:  75% 21%



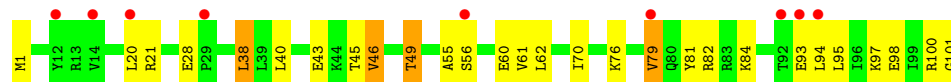
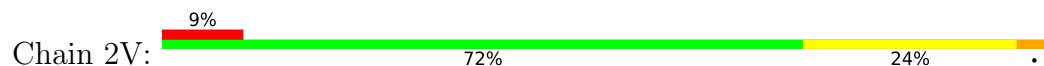
- Molecule 16: 50S ribosomal protein L20



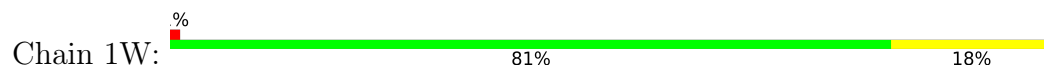
- Molecule 17: 50S ribosomal protein L21



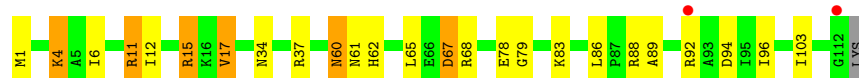
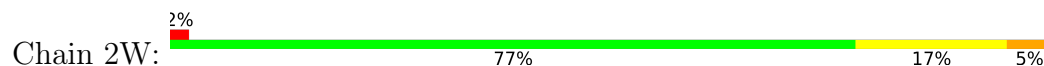
- Molecule 17: 50S ribosomal protein L21



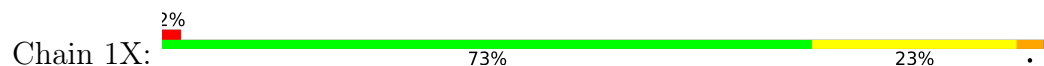
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22

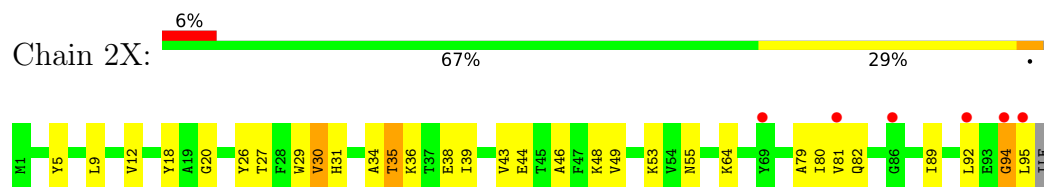


- Molecule 19: 50S ribosomal protein L23

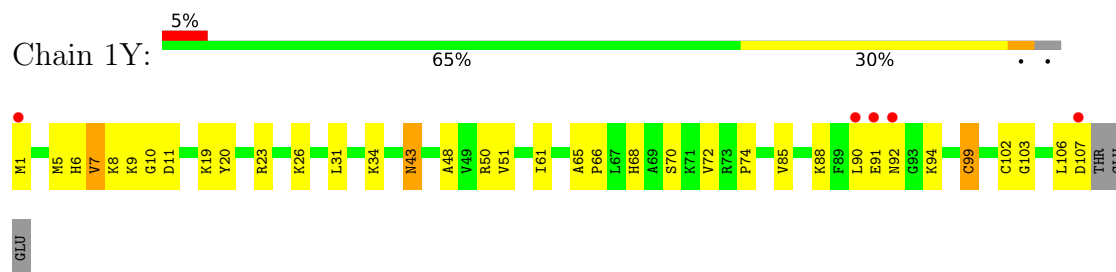




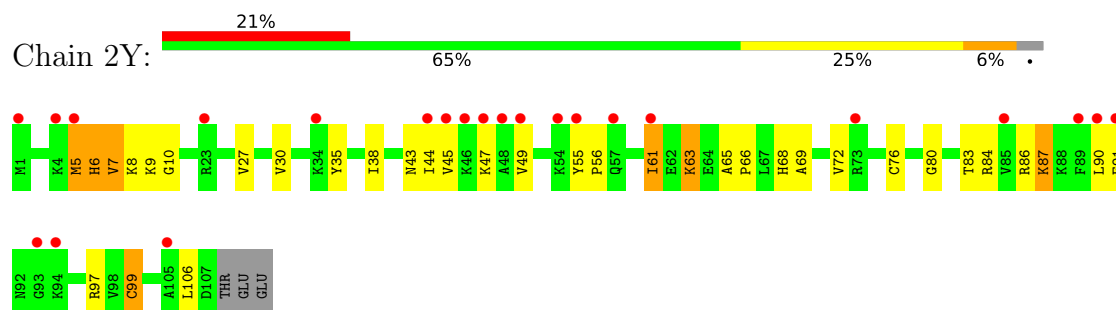
- Molecule 19: 50S ribosomal protein L23



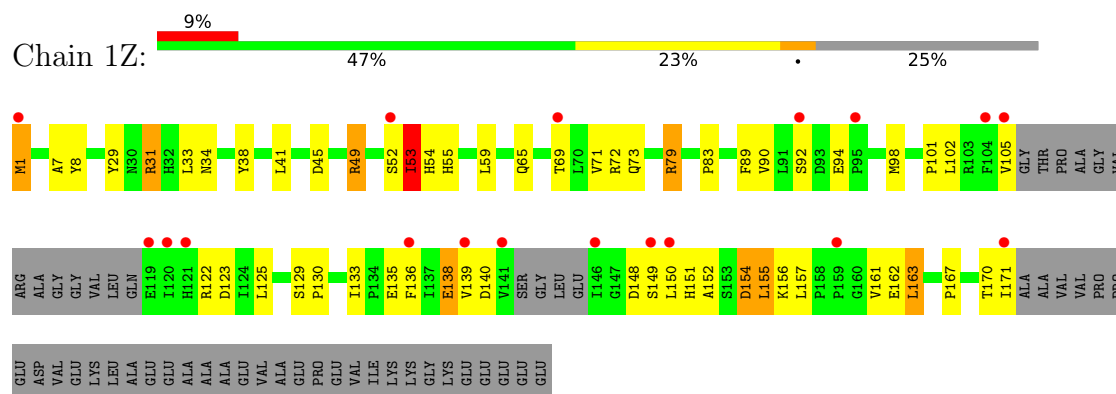
- Molecule 20: 50S ribosomal protein L24



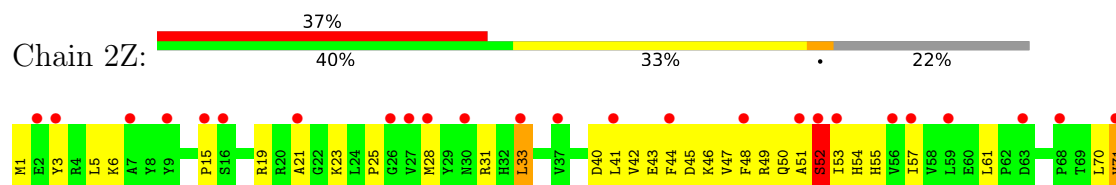
- Molecule 20: 50S ribosomal protein L24

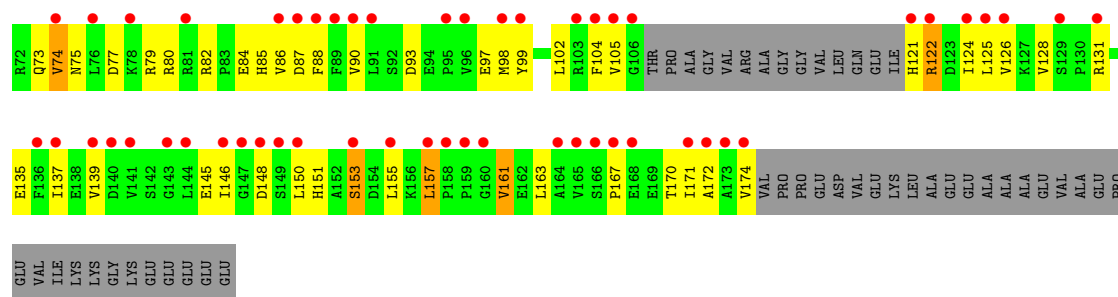


- Molecule 21: 50S ribosomal protein L25

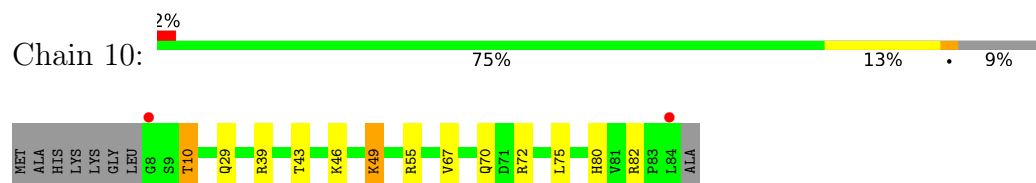


- Molecule 21: 50S ribosomal protein L25

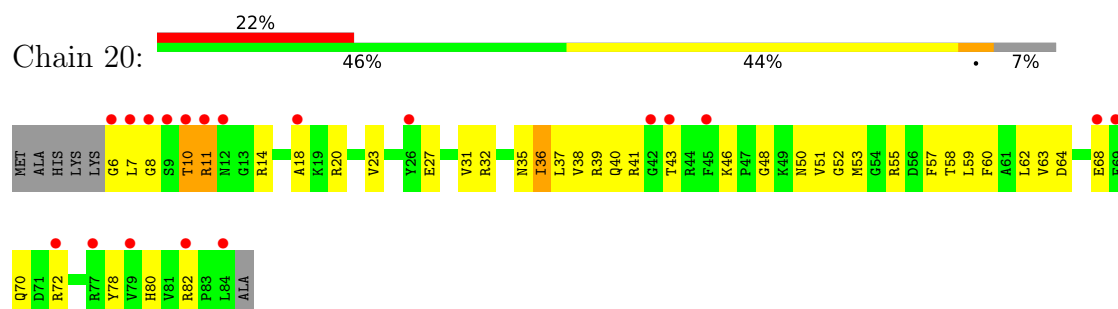




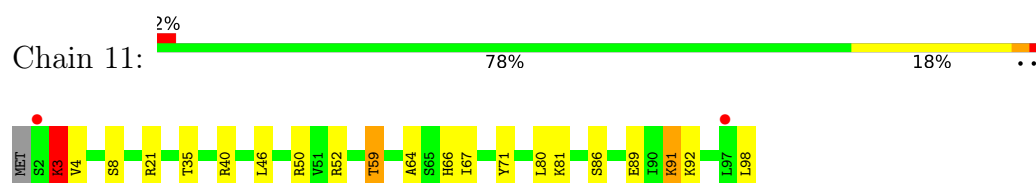
- Molecule 22: 50S ribosomal protein L27



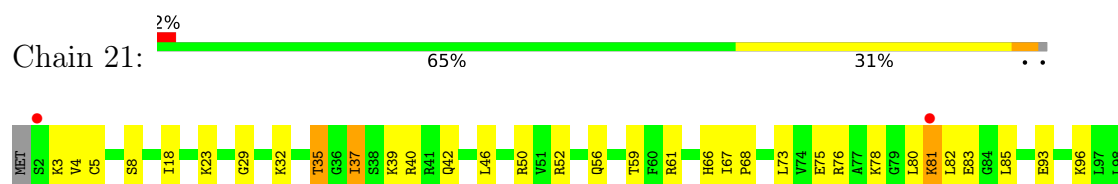
- Molecule 22: 50S ribosomal protein L27



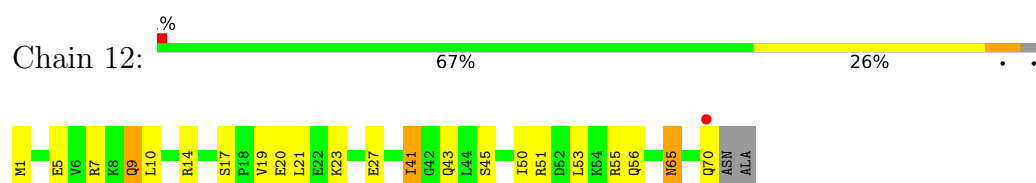
- Molecule 23: 50S ribosomal protein L28



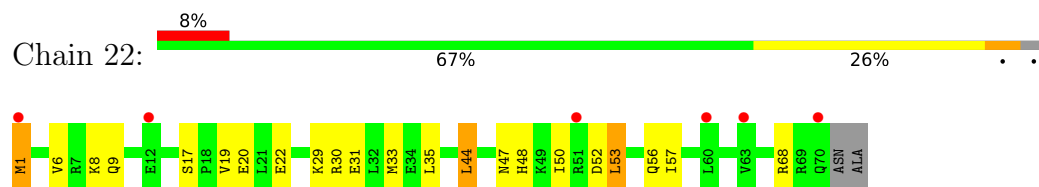
- Molecule 23: 50S ribosomal protein L28



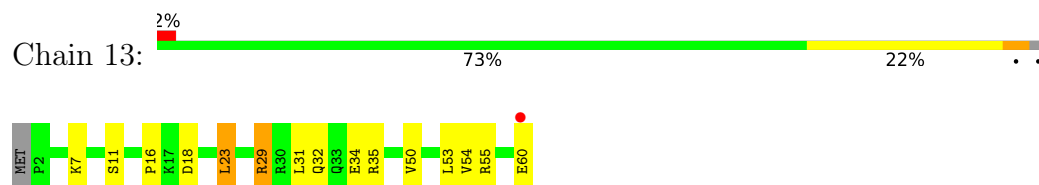
- Molecule 24: 50S ribosomal protein L29



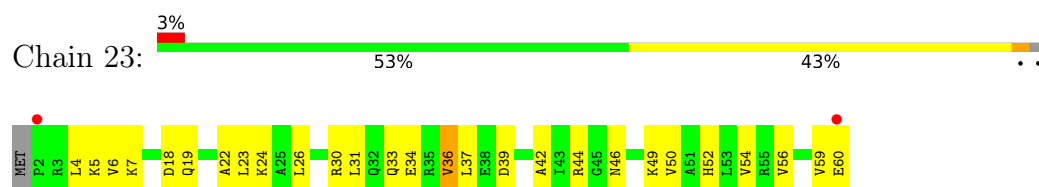
- Molecule 24: 50S ribosomal protein L29



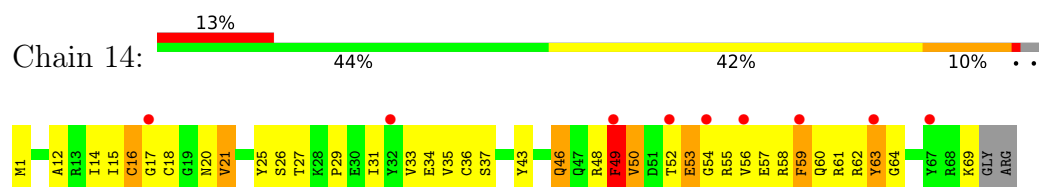
- Molecule 25: 50S ribosomal protein L30



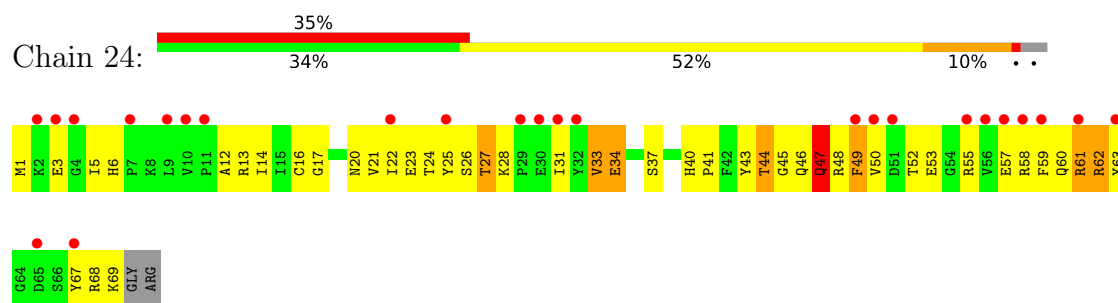
- Molecule 25: 50S ribosomal protein L30



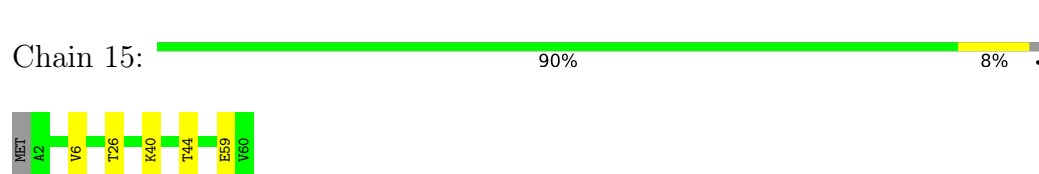
- Molecule 26: 50S ribosomal protein L31



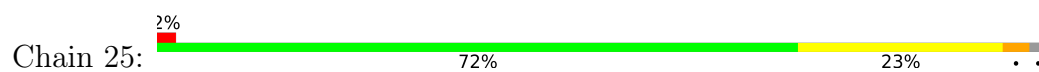
- Molecule 26: 50S ribosomal protein L31



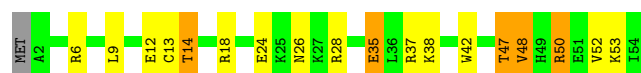
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



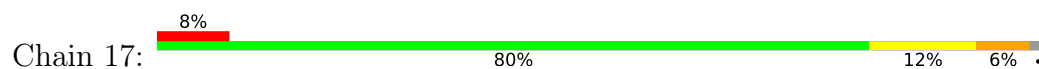
- Molecule 28: 50S ribosomal protein L33



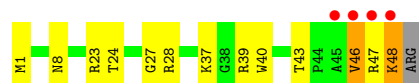
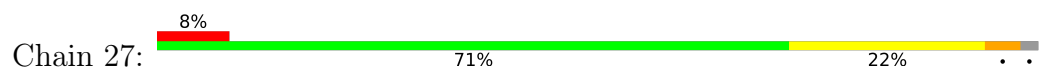
- Molecule 28: 50S ribosomal protein L33



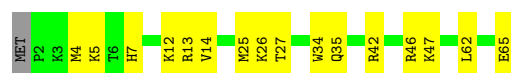
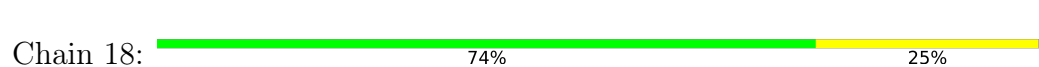
- Molecule 29: 50S ribosomal protein L34



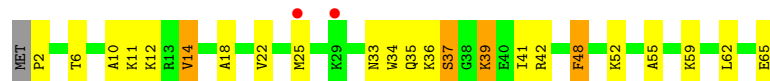
- Molecule 29: 50S ribosomal protein L34




- Molecule 30: 50S ribosomal protein L35

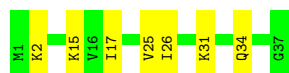


- Molecule 30: 50S ribosomal protein L35



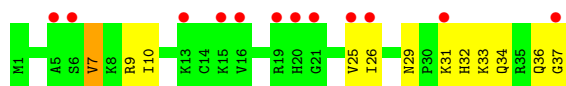
- Molecule 31: 50S ribosomal protein L36

Chain 19:  81% 19%



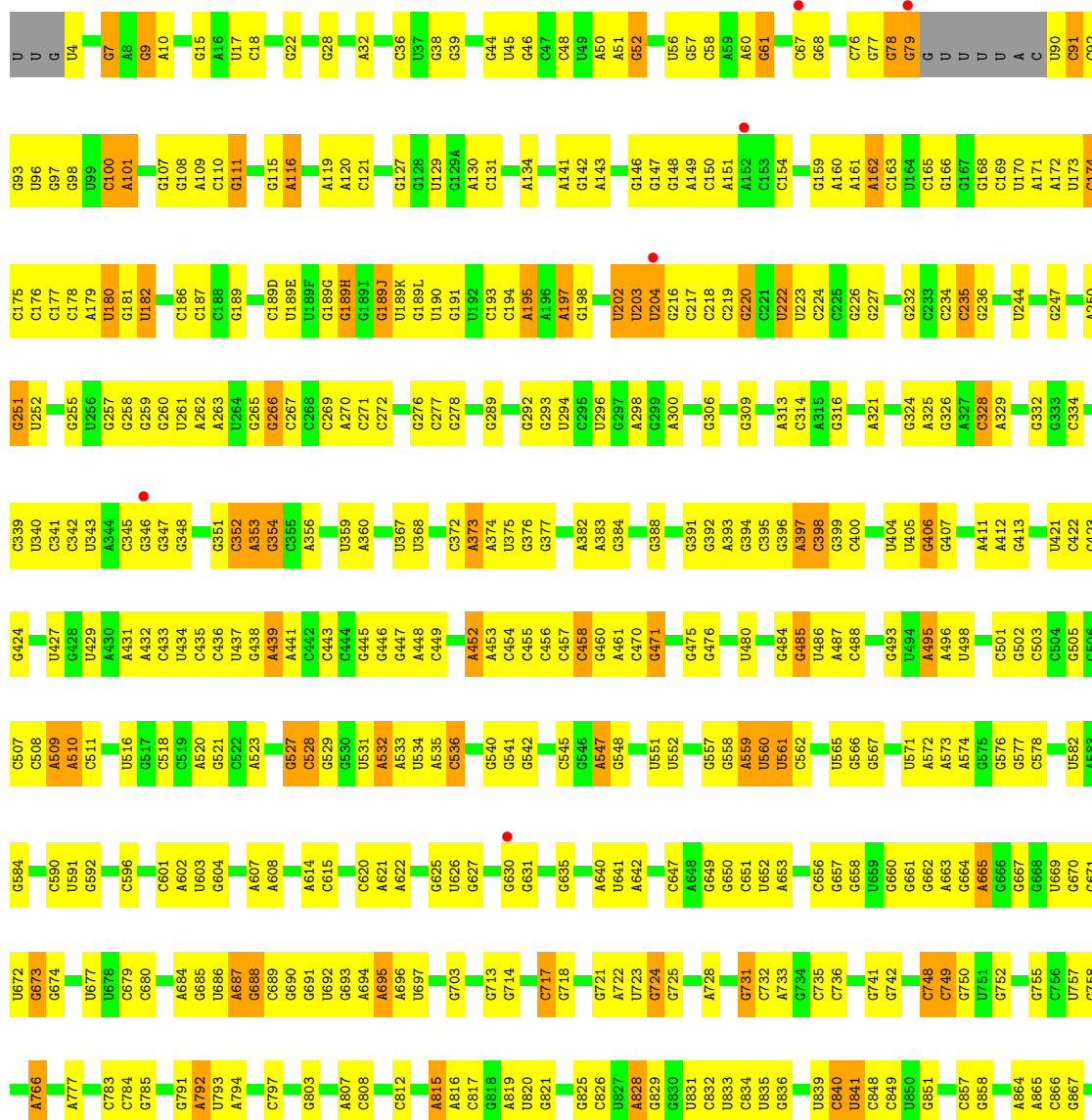
- Molecule 31: 50S ribosomal protein L36

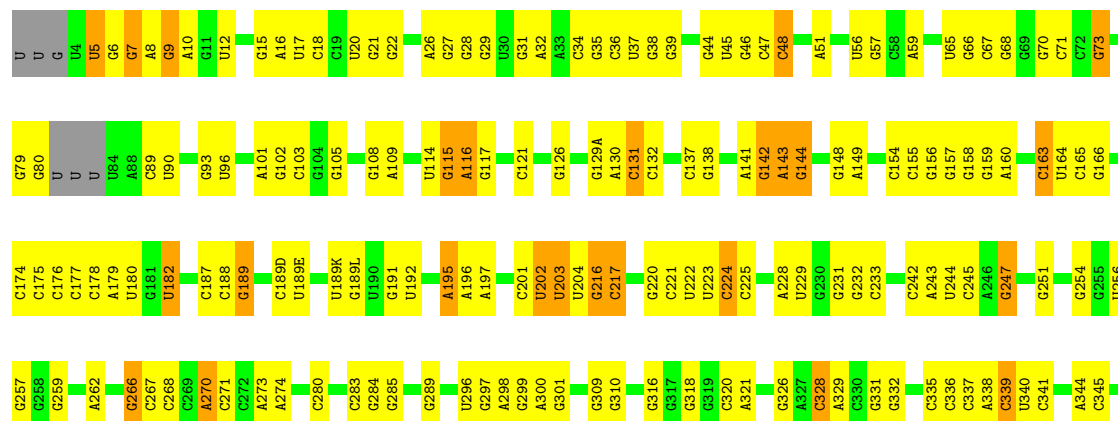
Chain 29:  32% 68% 30%



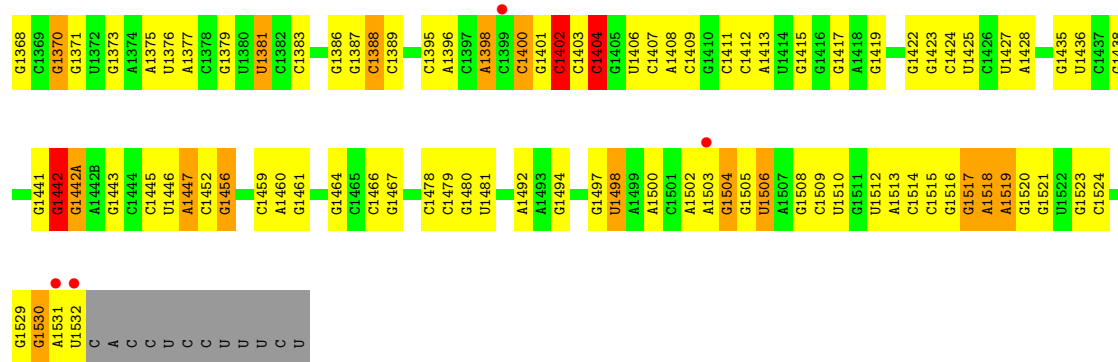
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  3% 46% 43% 10%

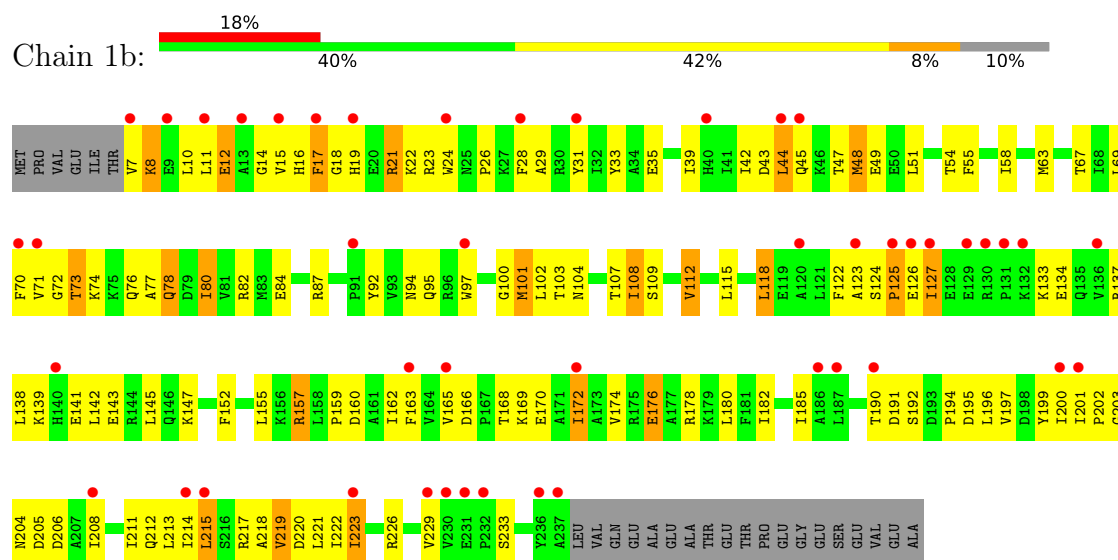




A1306	U1307	A1308	G1309	G1310	G1311	G1312	A1313	G1314	G1315	G1316	G1317	A1318	A1319	G1320	G1321	G1322	G1323	G1324	G1325	A1326	G1327	G1328	A1329	G1330	G1331	A1332	A1333	G1334	G1338	A1339	G1342	G1343	G1344	U1345	A1346	G1347	A1348	A1349	A1350	C1351	C1352	C1353	G1354	G1355	G1356	G1357	G1358	G1359	A1360	G1361	C1362	C1363	A1364	G1365	G1366	G1367										
C1242		A1245	C1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	G1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	A1269	C1270	G1271	G1272	G1273	A1274	A1275	C1276	C1277	U1278	A1279	A1280	U1281		C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293		C1297	C1298	A1299	G1300	A1301	A1302	C1303	A1304	C1305							
G1181	G1182	A1183	G1184	G1185	G1186	G1187	A1188	G1189	G1190	A1191	C1192	G1193	U1194	G1195	G1196	G1197	G1198	U1199	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	C1208	C1209	G1210	U1211	U1212	A1213	C1214	G1215	G1216	G1217	C1218	U1219	G1220	G1221	G1222	C1223	G1224	A1225	C1226	A1227	C1228	A1229		U1232	G1233	G1234	U1235	A1236	C1237	A1238	A1239	U1240	G1241							
C1119	G1120	U1121	U1122	A1123	G1124	U1125	U1126	G1127	C1128	G1129	A1130	G1131	C1132	G1133	G1134	U1135	U1136	G1137	G1138	G1139	C1140	C1141	G1142	G1143	G1144	C1145	A1146	C1147	U1148	C1149	U1150	A1151	C1152	G1153	G1154	U1155	G1156	A1157	C1158	U1159	G1160	C1161	C1162	G1163	G1164	C1165	G1166	A1168	A1169	U1170	G1171	C1172	G1173		A1176	G1177	G1178	A1179	A1180							
G1058	C1059	C1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	C1073	G1074	G1075	C1076	G1077		A1080	G1081	G1082	U1083	G1084	U1085	U1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	C1096	C1097	G1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	G1113	G1114	C1115	G1116	G1117	C1118							
G1002	G1003	A1004	A1005	C1006	C1007	G1008	G1009	G1010	G1011	U1012	G1013	A1014	A1015	A1016	U1017	C1018	C1019	U1020	G1021	G1022	G1023	G1024	U1025	G1026	C1027	C1028	C1029	C1030	G1031	G1032	G1033	G1034	A1035	G1036	C1037	C1038	C1039	U1040	A1041	G1042	C1043	C1044	U1045	U1046	G1047	U1048	G1049	A1110	A1111	C1112	G1113	G1114	C1115	G1116	C1117	G1118										
U943	G944	G945	A946	G947	G948	A949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961	G962	G963	A964	A965	G966	A968	A969	C970	G971	G972	G973	A974	A975	G976	A977	A978	G979	C980	U981	U982	A983	C984	C985	A986	G987	G988	C989	C990	U991	U992	G993	A994	C995	C996	A997	A998	C999	U1000	G1001A									
A865	C866	G867	C868		A872	A873	G874	C875	G876	C877	G878		G881	C882	U883	U884	G885	G890	U891	A892		A900	A901	G902		G906	G907	G908	A909	C910	A914	A915	A916	G917	A918	A919	U920	U921	G922	A923	C924	G925	G926	G927	G928		C931	C932	G933	C934	A935	C936	A937	A938	G939	C940	G941	G942								
	A777	G778	G779	A780	A781	A782	G783	G784	G785		A790	G791	A792	G793	A794	G795	G796	G797	G798	G799	G800		A814	A815	A816	C817	G818	A819	U820	G821		C826	U827	A828	G829		U833	C834	U835	G836		C840	U841		U850	G851	G852	G853	C854	G855	C856	G857	A768	G769	C770	G771	U772	G773	G774							
U605	G606	A607	G608	A609	G610		G618	U619	A620	A621	G622	A623	C624	G625	U626		G629	G630	G631	A632	G633	C634	G635		A640	U641		U646	A647	C648	A649	A650	G651	G652	U653	C654	U655	G656	G657		U657	A658	A659	A660	A661	G662	A663	G664	A665		G668		G671	U672	G673	G674	A675	A676	U677	U678	C679	G682	G683	A684	G685	U686
G428	U429	A430	G431	A432	C433	A434	C435	G436	U437	G438	A439	A441	C442	C443	G444	G445	G446	G447	A448		A452		C457	C458	G460	A461	C470	G471	A472	G473	G474		G485		A496	U498	A499	G500	C501	G502	C503	G504	C505	G506	C507	C508	A509	A510	C511		U516	G517	C518		G521	G522	A523	G524	C525							
C526	G527	C528	G529	A530	U531	A532	A533		A539	G540	G541	A542	C543	C544	G545	G546	G547	G548		A553	C554	C555		G558	A559	U560	U561	C562	A563	C564	U565	G566	G567		U571	A572	A573	G574	G575	G576	G577	C578	G579	U580	G581	U582		C586	G587	U588		G594	C595	G597	U598		G604									

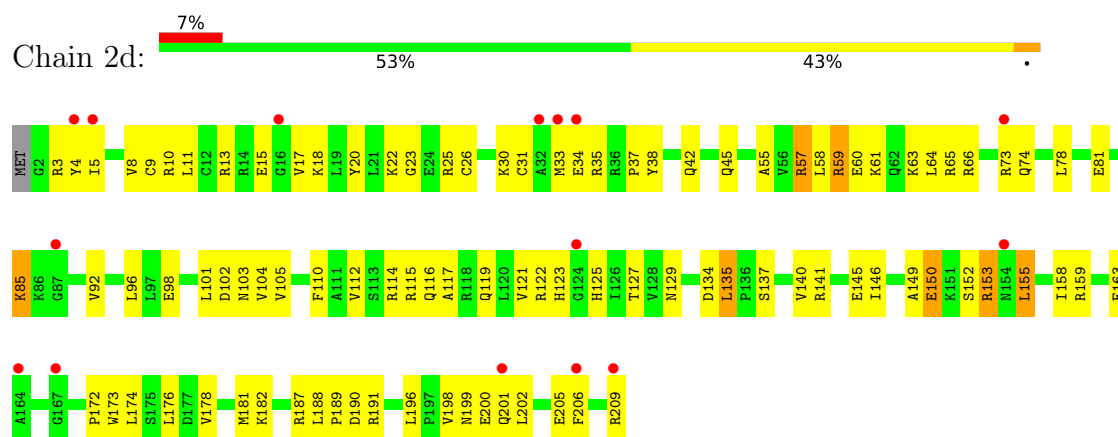


• Molecule 33: 30S ribosomal protein S2

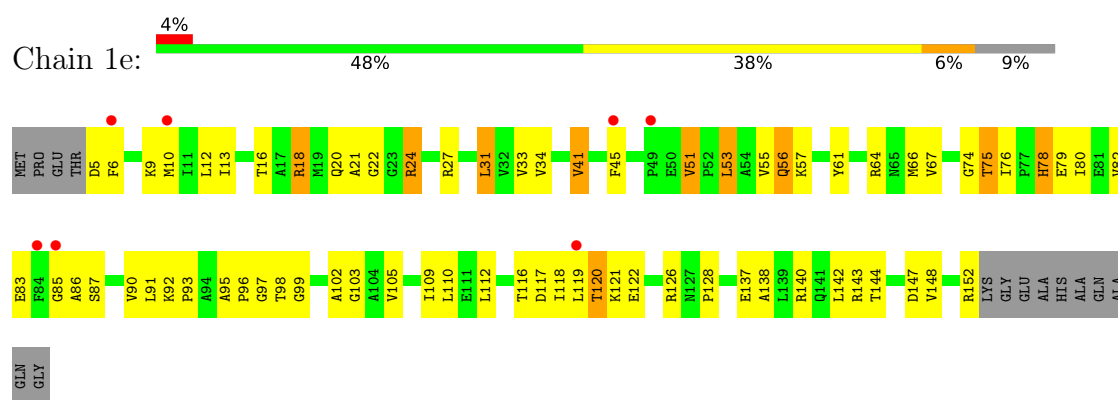




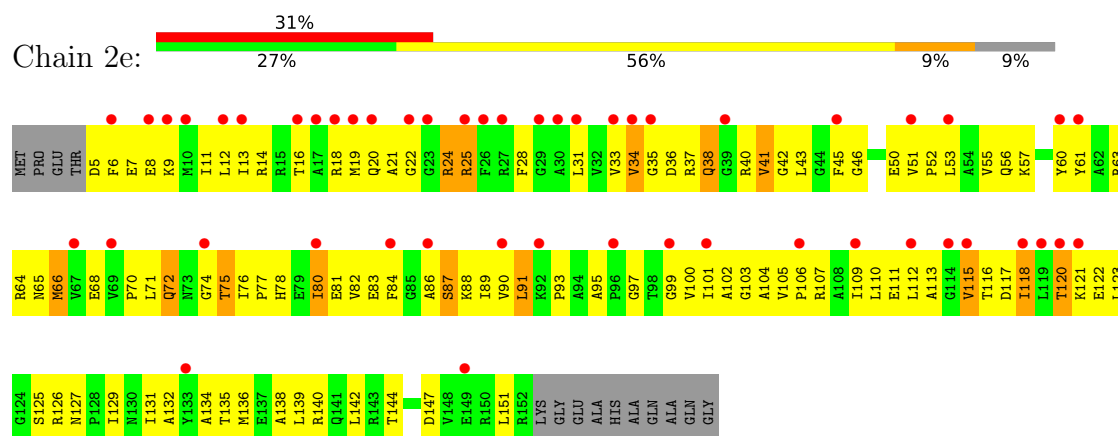




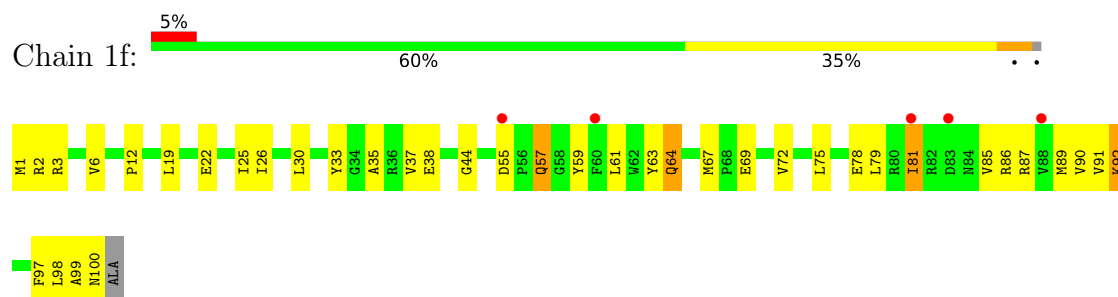
• Molecule 36: 30S ribosomal protein S5



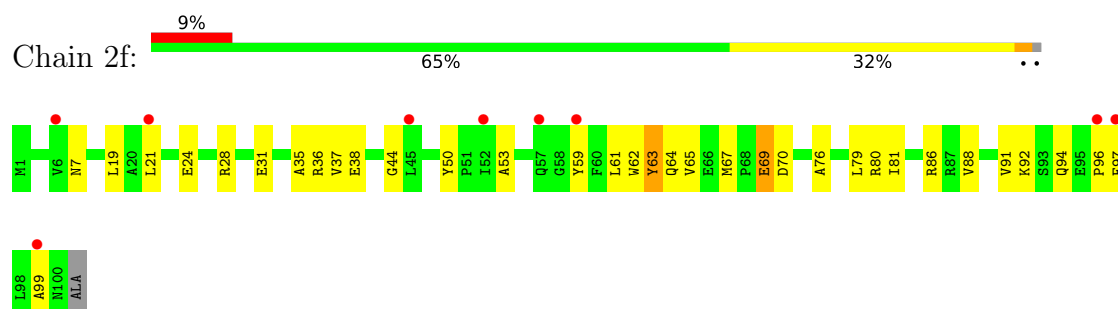
• Molecule 36: 30S ribosomal protein S5



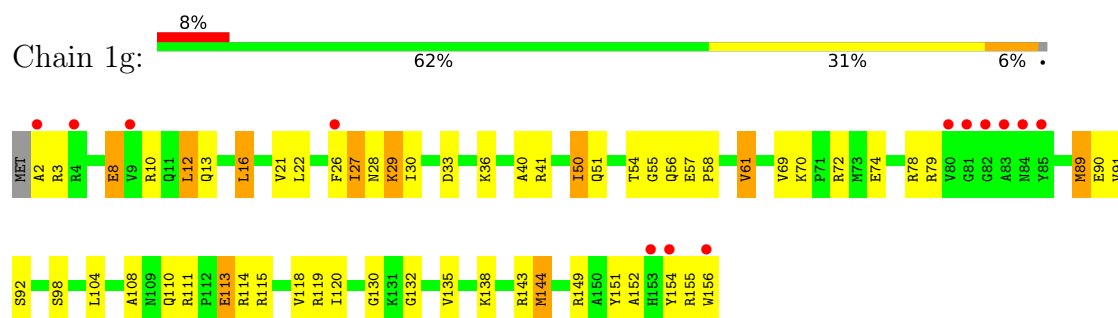
• Molecule 37: 30S ribosomal protein S6



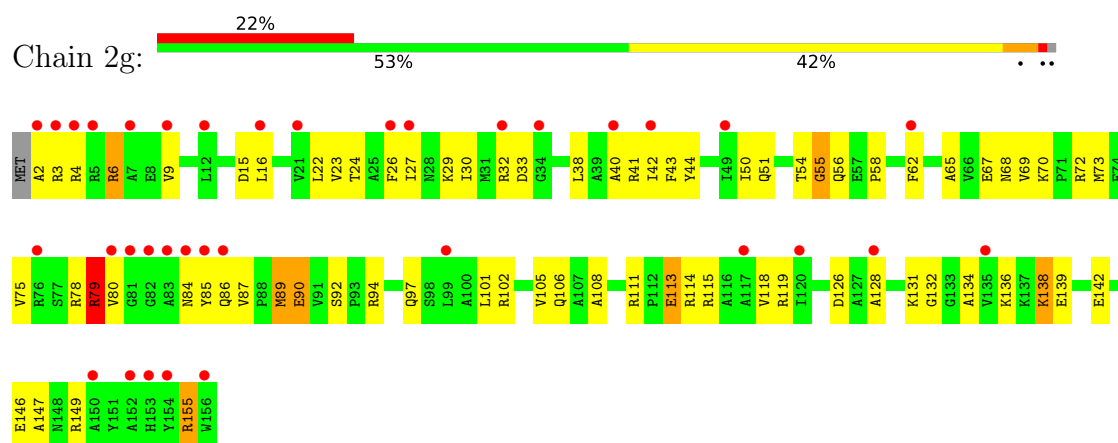
- Molecule 37: 30S ribosomal protein S6



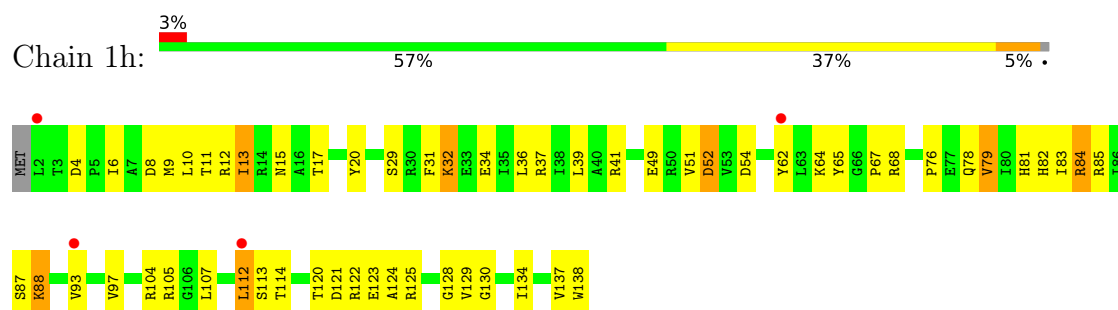
- Molecule 38: 30S ribosomal protein S7



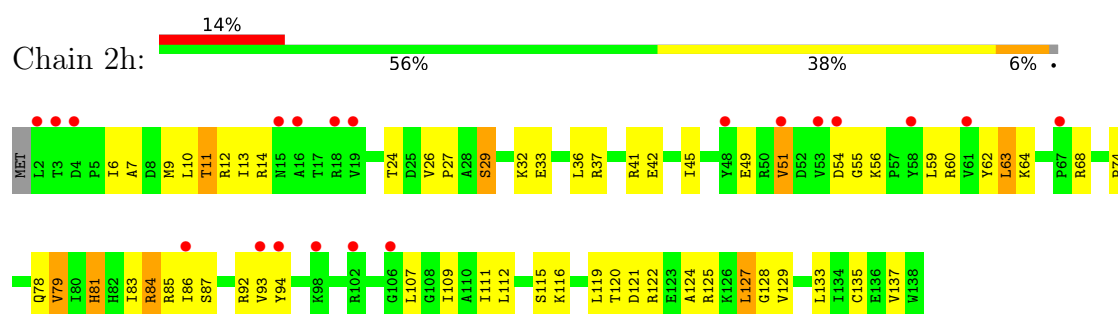
- Molecule 38: 30S ribosomal protein S7



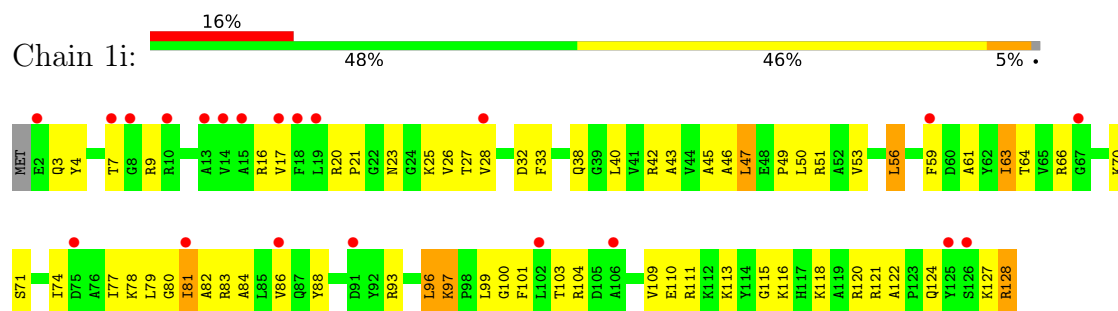
- Molecule 39: 30S ribosomal protein S8



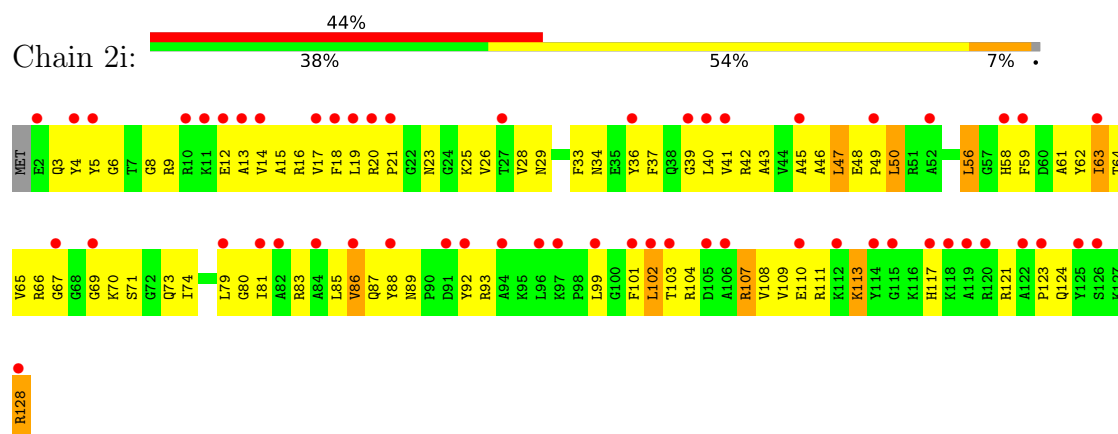
- Molecule 39: 30S ribosomal protein S8



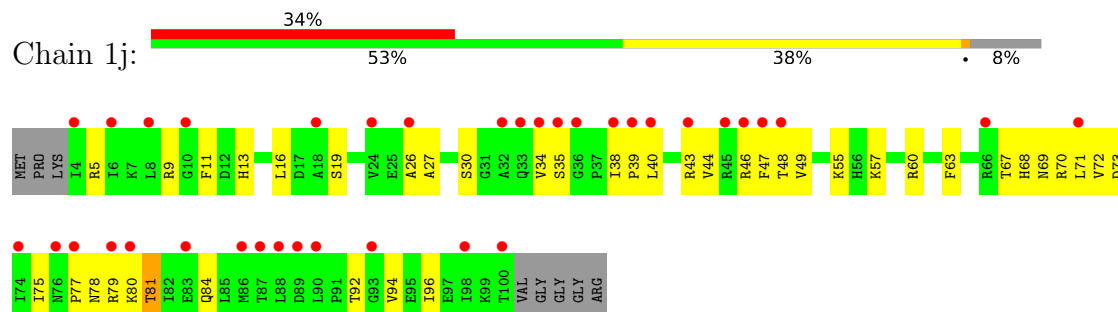
- Molecule 40: 30S ribosomal protein S9



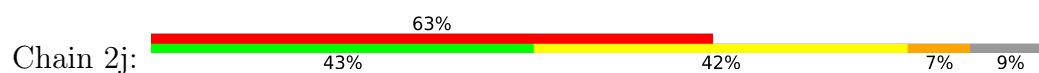
- Molecule 40: 30S ribosomal protein S9

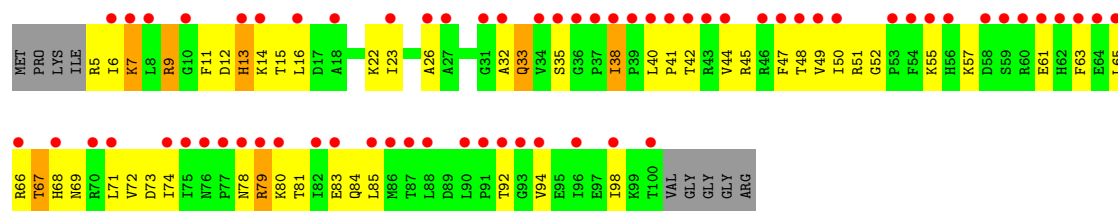


- Molecule 41: 30S ribosomal protein S10

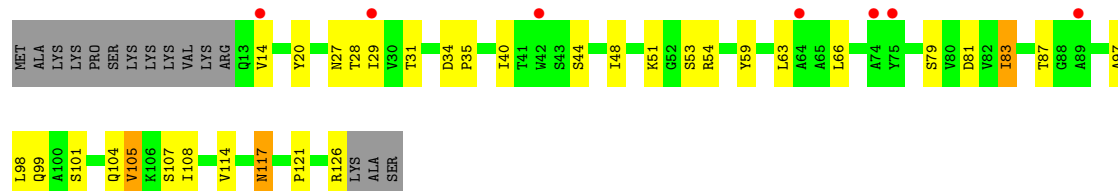


- Molecule 41: 30S ribosomal protein S10

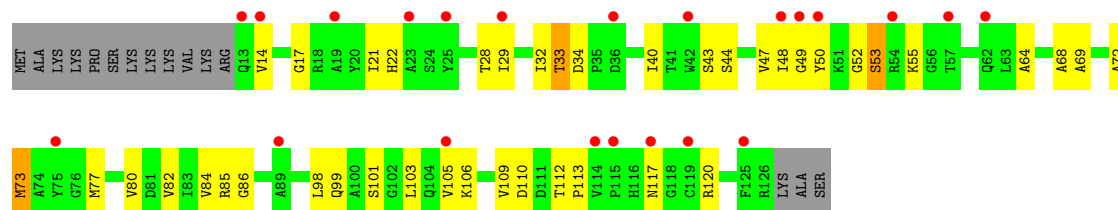




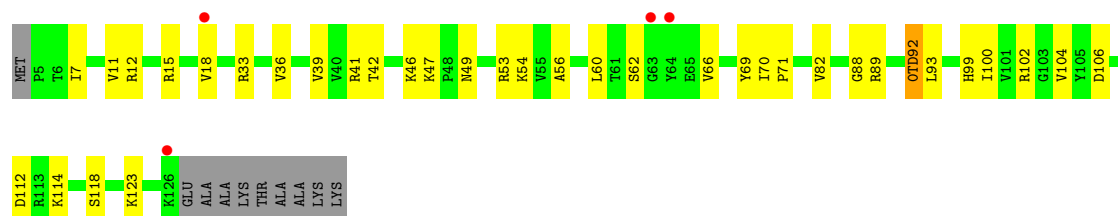
• Molecule 42: 30S ribosomal protein S11



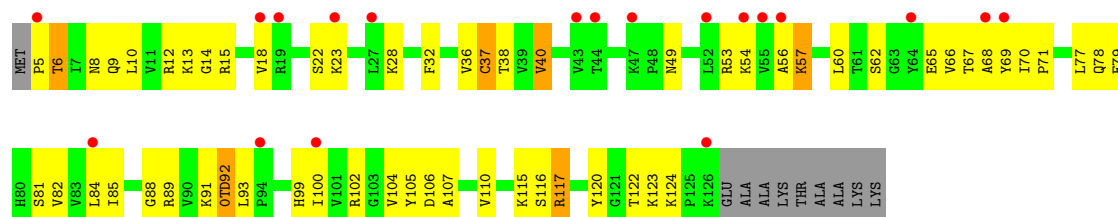
• Molecule 42: 30S ribosomal protein S11



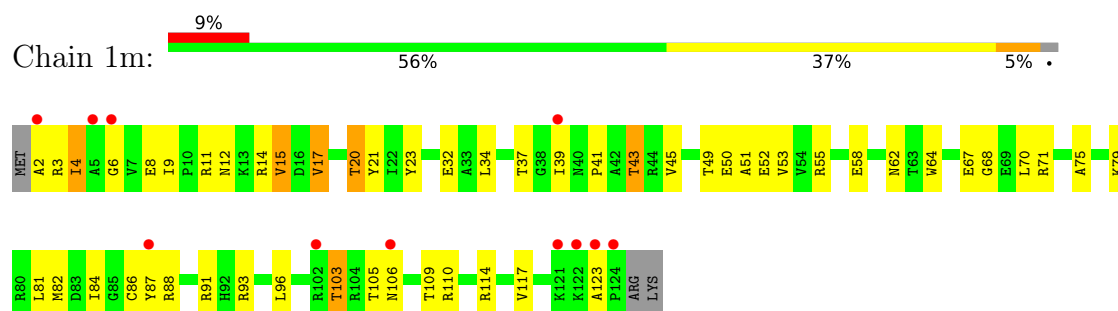
• Molecule 43: 30S ribosomal protein S12



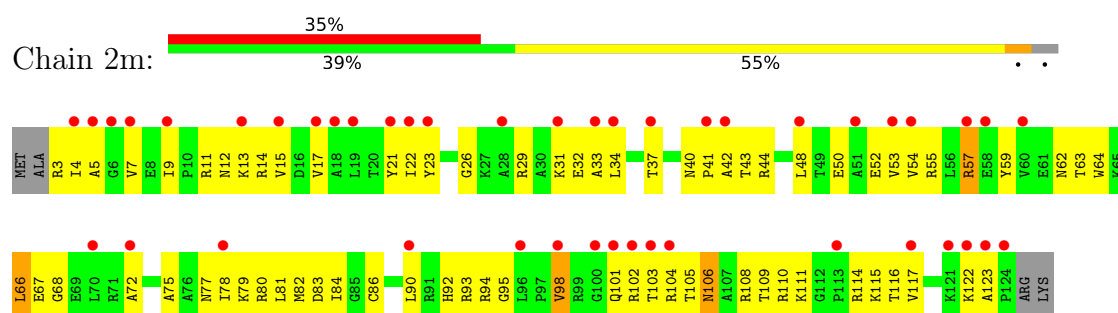
• Molecule 43: 30S ribosomal protein S12



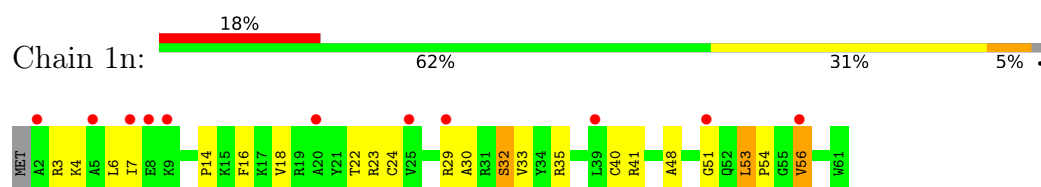
## • Molecule 44: 30S ribosomal protein S13



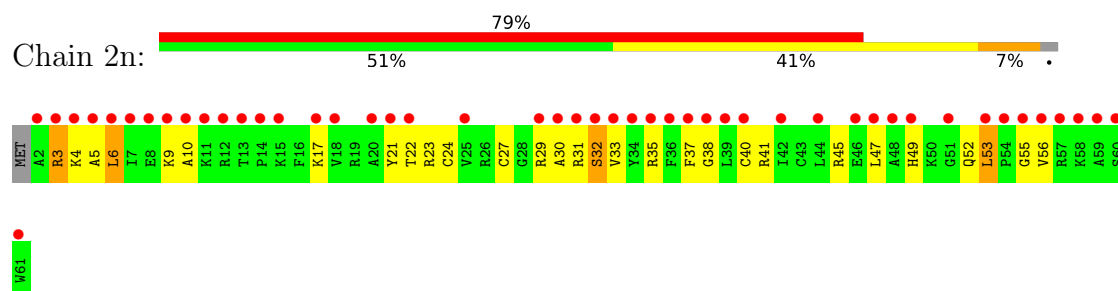
## • Molecule 44: 30S ribosomal protein S13



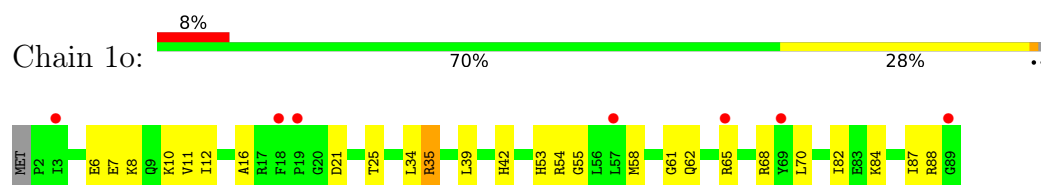
## • Molecule 45: 30S ribosomal protein S14 type Z



## • Molecule 45: 30S ribosomal protein S14 type Z

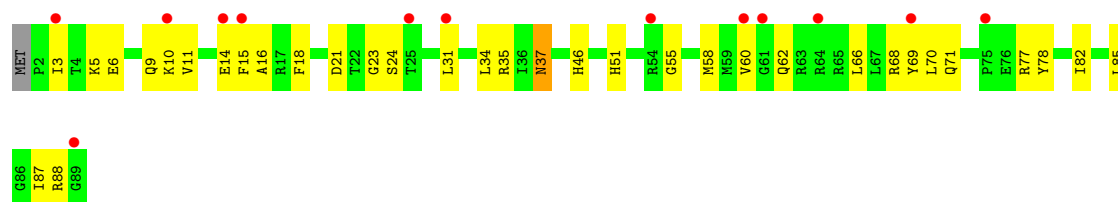


## • Molecule 46: 30S ribosomal protein S15

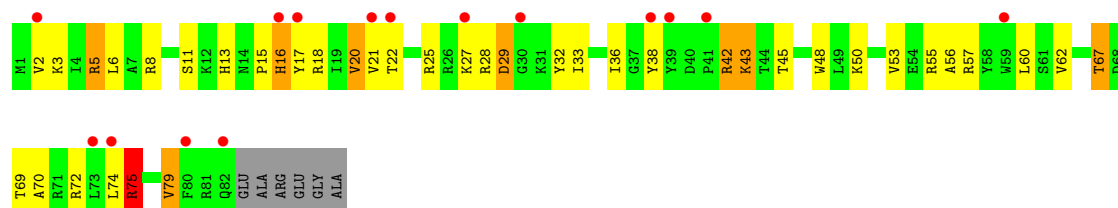


## • Molecule 46: 30S ribosomal protein S15

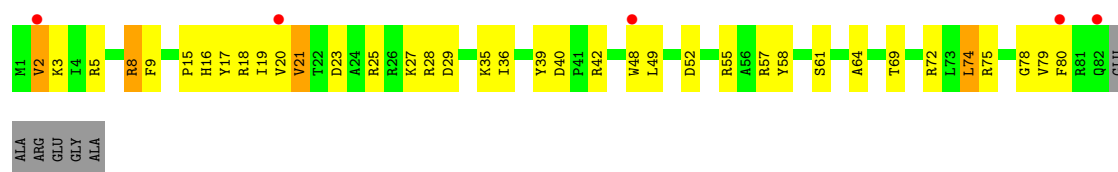




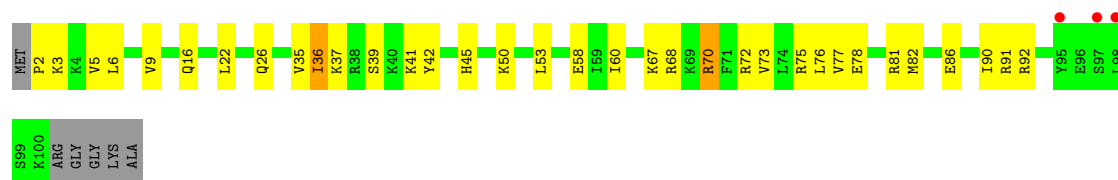
• Molecule 47: 30S ribosomal protein S16



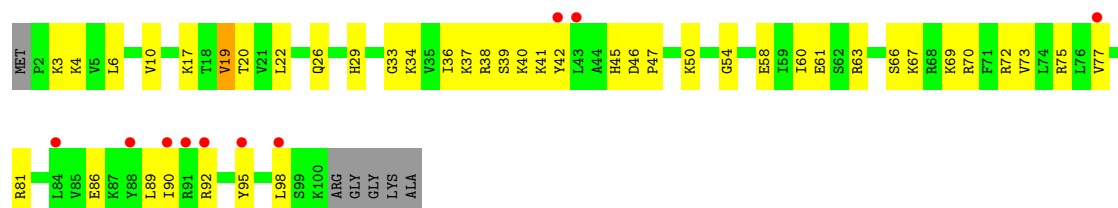
• Molecule 47: 30S ribosomal protein S16



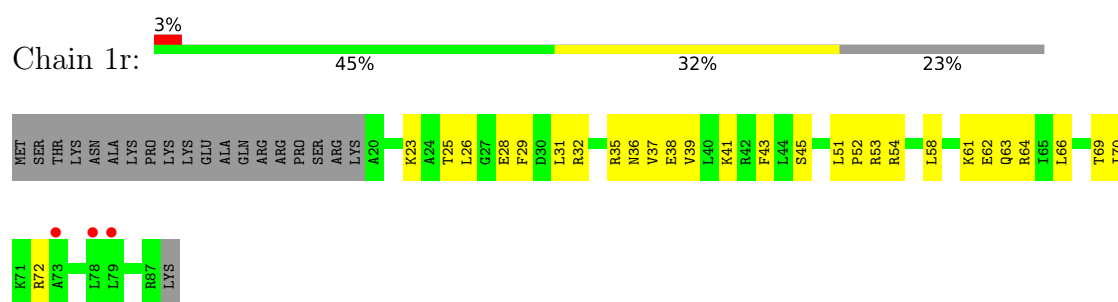
• Molecule 48: 30S ribosomal protein S17



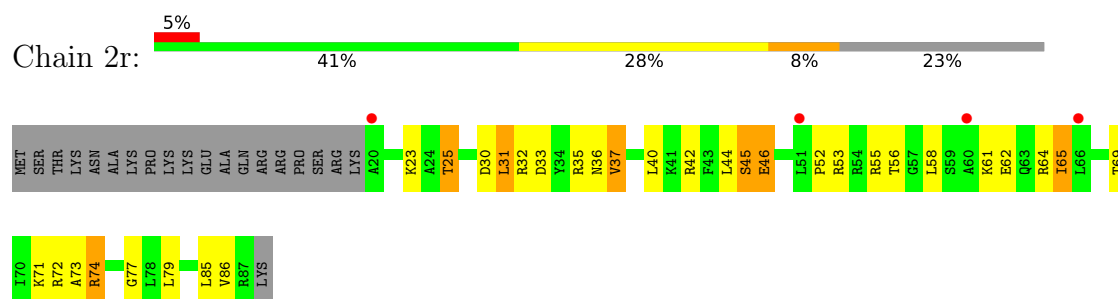
• Molecule 48: 30S ribosomal protein S17



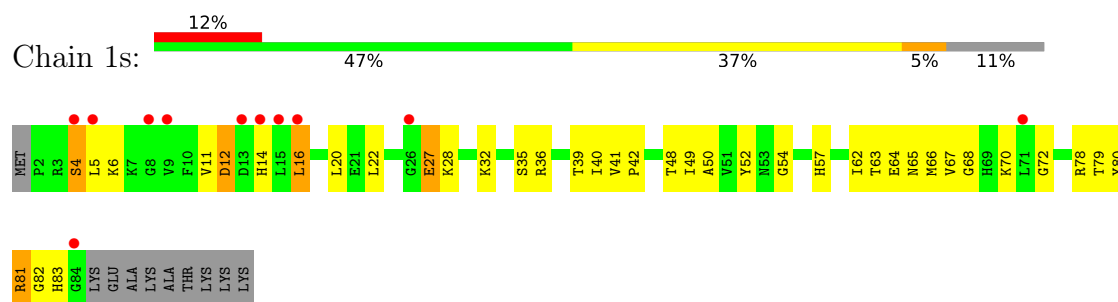
• Molecule 49: 30S ribosomal protein S18



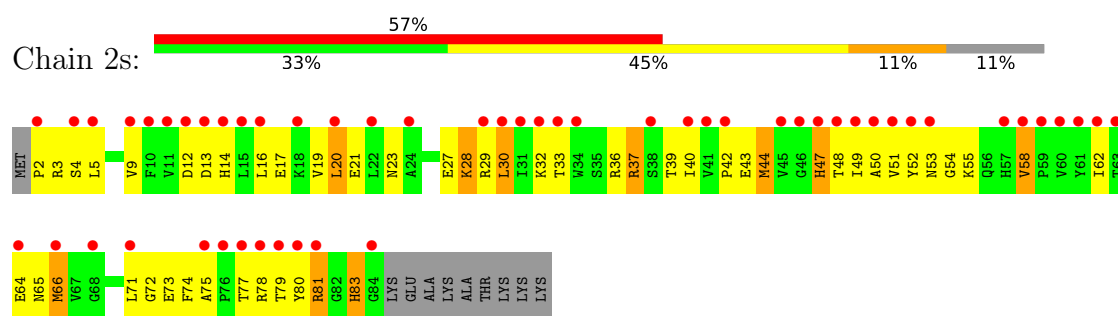
• Molecule 49: 30S ribosomal protein S18



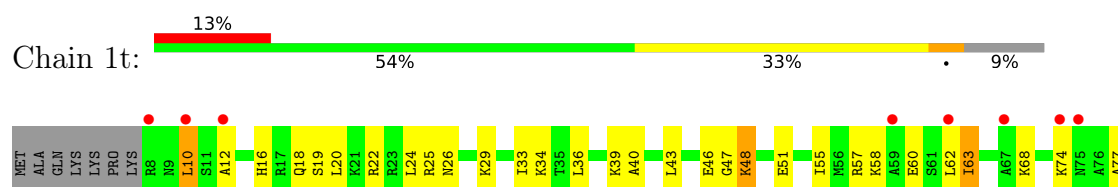
• Molecule 50: 30S ribosomal protein S19



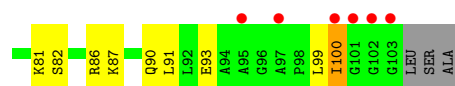
• Molecule 50: 30S ribosomal protein S19



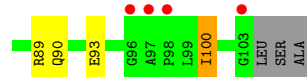
• Molecule 51: 30S ribosomal protein S20







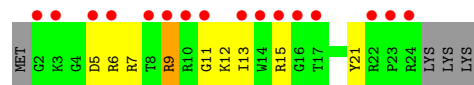
• Molecule 51: 30S ribosomal protein S20



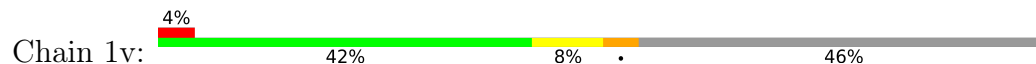
• Molecule 52: 30S ribosomal protein Thx



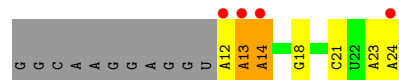
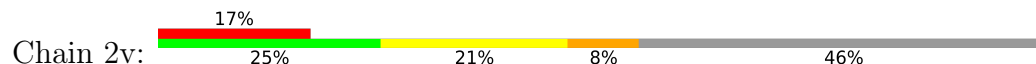
• Molecule 52: 30S ribosomal protein Thx



• Molecule 53: MF-mRNA



• Molecule 53: MF-mRNA

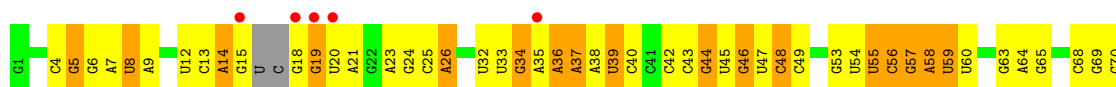


• Molecule 54: A-site and E-site Deacylated tRNAphe

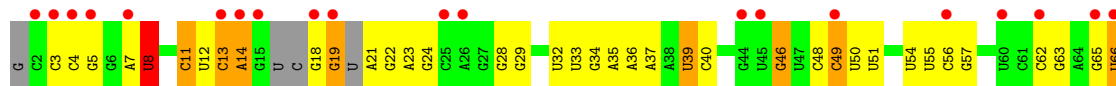




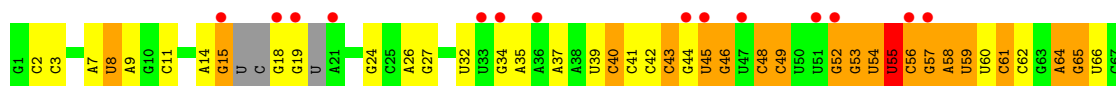
- Molecule 54: A-site and E-site Deacylated tRNA<sup>phe</sup>



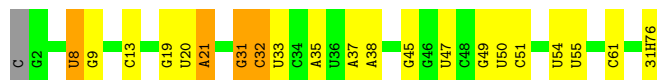
- Molecule 54: A-site and E-site Deacylated tRNA<sup>phe</sup>



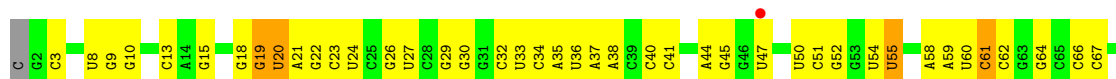
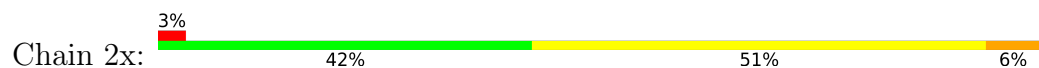
- Molecule 54: A-site and E-site Deacylated tRNA<sup>phe</sup>



- Molecule 55: P-site Aminoacylated fMet-tRNA<sup>met</sup>



- Molecule 55: P-site Aminoacylated fMet-tRNA<sup>met</sup>





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.40Å 449.82Å 621.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.22 – 2.50 147.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (147.22-2.50) 99.6 (147.22-2.50)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.217 , 0.265 0.219 , 0.267	Depositor DCC
$R_{free}$ test set	99599 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	300040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: M2G, UR3, OMG, 2MA, OMU, 31H, OMC, ZN, PSU, 2MG, MG, 4OC, SF4, MA6, MIA, G7M, 0TD, 4SU, 5MC, A1A1F, 5MU, K

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	0.64	0/69011	0.80	18/107720 (0.0%)
1	2A	0.45	1/67295 (0.0%)	0.66	7/105042 (0.0%)
2	1B	0.52	0/2882	0.75	0/4494
2	2B	0.42	0/2879	0.62	0/4487
3	1D	0.61	0/2186	0.80	1/2944 (0.0%)
3	2D	0.47	0/2186	0.68	0/2944
4	1E	0.59	0/1592	0.82	0/2149
4	2E	0.41	0/1592	0.66	0/2149
5	1F	0.59	0/1619	0.80	4/2193 (0.2%)
5	2F	0.43	0/1615	0.66	0/2188
6	1G	0.45	0/1448	0.70	0/1957
6	2G	0.41	0/1453	0.62	0/1963
7	1H	0.47	0/1356	0.67	0/1834
7	2H	0.40	0/1356	0.55	0/1834
8	1I	0.40	0/1112	0.64	0/1514
8	2I	0.37	0/1079	0.60	0/1475
9	1N	0.62	0/1144	0.78	0/1543
9	2N	0.41	0/1144	0.60	0/1543
10	1O	0.58	0/943	0.73	0/1269
10	2O	0.42	0/943	0.63	0/1269
11	1P	0.63	0/1152	0.86	1/1533 (0.1%)
11	2P	0.44	0/1152	0.71	2/1533 (0.1%)
12	1Q	0.60	0/1143	0.77	0/1527
12	2Q	0.41	0/1143	0.64	2/1527 (0.1%)
13	1R	0.68	0/982	0.88	2/1312 (0.2%)
13	2R	0.42	0/982	0.67	0/1312
14	1S	0.52	0/883	0.77	0/1176
14	2S	0.44	0/880	0.62	0/1172
15	1T	0.55	0/1105	0.75	0/1477
15	2T	0.43	0/1097	0.64	0/1468
16	1U	0.65	0/977	0.85	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.42	0/977	0.62	0/1301
17	1V	0.63	0/782	0.85	1/1049 (0.1%)
17	2V	0.39	0/782	0.60	0/1049
18	1W	0.68	0/897	0.81	0/1205
18	2W	0.48	0/897	0.65	0/1205
19	1X	0.61	0/764	0.82	2/1025 (0.2%)
19	2X	0.44	0/764	0.74	2/1025 (0.2%)
20	1Y	0.54	0/819	0.78	0/1095
20	2Y	0.41	0/819	0.65	0/1095
21	1Z	0.49	0/1267	0.75	1/1717 (0.1%)
21	2Z	0.46	0/1299	0.64	0/1763
22	10	0.63	0/616	0.81	0/821
22	20	0.43	0/628	0.62	0/837
23	11	0.57	0/762	0.78	0/1014
23	21	0.50	0/762	0.67	0/1014
24	12	0.56	0/590	0.71	0/781
24	22	0.40	0/590	0.62	0/781
25	13	0.66	0/474	0.81	0/635
25	23	0.39	0/469	0.60	0/630
26	14	0.45	0/565	0.81	0/761
26	24	0.48	0/545	0.73	0/737
27	15	0.63	0/469	0.84	0/635
27	25	0.46	0/469	0.65	0/635
28	16	0.57	0/460	0.83	0/613
28	26	0.42	0/456	0.64	0/608
29	17	0.69	0/426	0.83	0/561
29	27	0.53	0/426	0.72	0/561
30	18	0.62	0/525	0.82	0/691
30	28	0.40	0/525	0.61	0/691
31	19	0.61	0/310	0.76	0/407
31	29	0.39	0/310	0.64	0/407
32	1a	0.43	1/35795 (0.0%)	0.63	2/55864 (0.0%)
32	2a	0.42	0/35886	0.62	2/56005 (0.0%)
33	1b	0.46	0/1881	0.79	3/2542 (0.1%)
33	2b	0.50	0/1860	0.71	0/2518
34	1c	0.42	0/1572	0.68	2/2126 (0.1%)
34	2c	0.48	0/1566	0.66	0/2119
35	1d	0.40	0/1685	0.64	1/2262 (0.0%)
35	2d	0.41	0/1704	0.66	1/2284 (0.0%)
36	1e	0.40	0/1145	0.67	1/1543 (0.1%)
36	2e	0.46	0/1149	0.68	0/1548
37	1f	0.40	0/823	0.58	0/1115
37	2f	0.40	0/829	0.56	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.38	0/1250	0.59	0/1679
38	2g	0.40	0/1254	0.60	0/1683
39	1h	0.39	0/1108	0.65	0/1494
39	2h	0.38	0/1108	0.63	0/1494
40	1i	0.40	0/1002	0.64	0/1346
40	2i	0.46	0/997	0.62	0/1343
41	1j	0.45	0/722	0.62	0/982
41	2j	0.48	0/727	0.67	0/988
42	1k	0.41	0/844	0.68	0/1145
42	2k	0.39	0/848	0.58	0/1149
43	1l	0.43	0/937	0.69	2/1260 (0.2%)
43	2l	0.42	0/937	0.69	0/1260
44	1m	0.41	0/969	0.63	0/1302
44	2m	0.45	0/961	0.68	0/1291
45	1n	0.40	0/501	0.66	0/664
45	2n	0.48	0/501	0.70	0/664
46	1o	0.41	0/739	0.60	0/985
46	2o	0.37	0/739	0.56	0/985
47	1p	0.41	0/697	0.70	1/939 (0.1%)
47	2p	0.40	0/693	0.69	0/935
48	1q	0.40	0/836	0.63	0/1117
48	2q	0.39	0/836	0.59	0/1117
49	1r	0.41	0/560	0.65	0/746
49	2r	0.37	0/560	0.59	0/746
50	1s	0.36	0/667	0.66	0/900
50	2s	0.52	0/661	0.77	0/893
51	1t	0.41	0/730	0.63	0/965
51	2t	0.41	0/729	0.64	0/965
52	1u	0.38	0/203	0.58	0/266
52	2u	0.44	0/203	0.63	0/266
53	1v	0.47	0/310	0.51	0/480
53	2v	0.45	0/310	0.52	0/480
54	1w	0.53	2/1537 (0.1%)	0.60	0/2390
54	1y	0.48	1/1606 (0.1%)	0.57	0/2497
54	2w	0.60	2/1487 (0.1%)	0.58	0/2311
54	2y	0.53	2/1583 (0.1%)	0.56	0/2459
55	1x	0.50	1/1700 (0.1%)	0.68	0/2650
55	2x	0.44	1/1700 (0.1%)	0.61	0/2650
All	All	0.50	11/316422 (0.0%)	0.69	58/473733 (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
4	2E	0	1
5	2F	0	1
6	1G	0	3
6	2G	0	1
8	2I	0	1
11	1P	0	2
12	1Q	0	1
15	2T	0	1
17	1V	0	1
21	1Z	0	2
21	2Z	0	1
26	24	0	1
30	18	0	1
33	1b	0	2
33	2b	0	2
34	1c	0	1
38	2g	0	1
40	1i	0	1
41	2j	0	1
44	1m	0	1
44	2m	0	1
50	1s	0	1
50	2s	0	1
51	1t	0	1
All	All	0	30

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	8	4SU	O3'-P	6.07	1.62	1.56
55	2x	8	4SU	O3'-P	5.93	1.62	1.56
54	2y	46	G7M	O3'-P	5.82	1.62	1.56
54	1y	46	G7M	O3'-P	5.71	1.61	1.56
54	1w	46	G7M	O3'-P	5.60	1.61	1.56

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	9.85	124.28	109.50
33	1b	123	ALA	N-CA-C	-8.88	102.54	112.57
1	2A	1992	G	C2'-C3'-O3'	8.23	121.85	109.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2689	U	C2'-C3'-O3'	7.80	121.20	109.50
1	1A	819	A	P-O5'-C5'	6.90	131.25	120.90

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1G	126	ASP	Peptide
6	1G	49	ASP	Peptide
6	1G	95	ARG	Peptide
11	1P	35	HIS	Peptide
11	1P	43	GLY	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	61852	0	31195	762	0
1	2A	60322	0	30426	1034	0
2	1B	2577	0	1305	42	0
2	2B	2575	0	1303	76	0
3	1D	2136	0	2218	50	0
3	2D	2136	0	2218	55	0
4	1E	1559	0	1618	43	0
4	2E	1559	0	1618	52	0
5	1F	1584	0	1625	34	0
5	2F	1580	0	1619	62	0
6	1G	1423	0	1436	55	0
6	2G	1428	0	1438	110	0
7	1H	1330	0	1407	36	0
7	2H	1330	0	1407	51	0
8	1I	1097	0	1140	45	0
8	2I	1064	0	1082	31	0
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	38	0
10	1O	933	0	996	26	0
10	2O	933	0	996	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	1P	1135	0	1212	41	0
11	2P	1135	0	1212	51	0
12	1Q	1122	0	1179	22	0
12	2Q	1122	0	1179	41	0
13	1R	968	0	1033	35	0
13	2R	968	0	1033	21	0
14	1S	873	0	927	22	0
14	2S	870	0	923	56	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	27	0
17	1V	771	0	830	14	0
17	2V	771	0	830	20	0
18	1W	886	0	940	12	0
18	2W	886	0	940	17	0
19	1X	750	0	814	19	0
19	2X	750	0	814	20	0
20	1Y	806	0	881	23	0
20	2Y	806	0	881	22	0
21	1Z	1240	0	1240	36	0
21	2Z	1271	0	1273	74	0
22	10	608	0	622	13	0
22	20	620	0	636	31	0
23	11	755	0	826	12	0
23	21	755	0	826	22	0
24	12	588	0	643	13	0
24	22	588	0	643	16	0
25	13	469	0	518	6	0
25	23	464	0	514	19	0
26	14	552	0	533	35	0
26	24	532	0	503	37	0
27	15	455	0	465	1	0
27	25	455	0	465	10	0
28	16	453	0	473	9	0
28	26	449	0	469	18	0
29	17	418	0	467	7	0
29	27	418	0	467	12	0
30	18	517	0	582	12	0
30	28	517	0	582	18	0
31	19	307	0	335	4	0
31	29	307	0	335	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	1a	32246	0	16294	622	0
32	2a	32327	0	16337	872	0
33	1b	1846	0	1867	111	0
33	2b	1825	0	1828	117	0
34	1c	1548	0	1535	63	0
34	2c	1542	0	1517	103	0
35	1d	1655	0	1672	76	0
35	2d	1674	0	1714	75	0
36	1e	1129	0	1185	46	0
36	2e	1133	0	1191	75	0
37	1f	810	0	804	30	0
37	2f	816	0	808	28	0
38	1g	1231	0	1238	46	0
38	2g	1235	0	1249	60	0
39	1h	1088	0	1126	43	0
39	2h	1088	0	1126	43	0
40	1i	983	0	986	52	0
40	2i	978	0	966	85	0
41	1j	709	0	650	36	0
41	2j	714	0	672	47	0
42	1k	829	0	825	17	0
42	2k	833	0	836	27	0
43	1l	932	0	981	20	0
43	2l	932	0	981	36	0
44	1m	958	0	1002	33	0
44	2m	950	0	988	66	0
45	1n	492	0	529	20	0
45	2n	492	0	529	36	0
46	1o	728	0	760	19	0
46	2o	728	0	760	24	0
47	1p	681	0	697	34	0
47	2p	677	0	686	32	0
48	1q	823	0	891	25	0
48	2q	823	0	891	29	0
49	1r	555	0	618	21	0
49	2r	555	0	618	31	0
50	1s	652	0	662	36	0
50	2s	646	0	644	47	0
51	1t	728	0	798	29	0
51	2t	727	0	796	26	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	1v	277	0	140	5	0
53	2v	277	0	140	6	0
54	1w	1530	0	785	42	0
54	1y	1585	0	803	35	0
54	2w	1482	0	754	26	0
54	2y	1565	0	794	35	0
55	1x	1635	0	838	10	0
55	2x	1635	0	839	27	0
56	10	8	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	6	0	0	0	0
56	16	1	0	0	0	0
56	17	5	0	0	0	0
56	18	8	0	0	0	0
56	19	1	0	0	0	0
56	1A	1108	0	0	0	0
56	1B	36	0	0	0	0
56	1D	13	0	0	0	0
56	1E	16	0	0	0	0
56	1F	13	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	6	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	11	0	0	0	0
56	1V	6	0	0	0	0
56	1W	5	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	211	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	2	0	0	0	0
56	1t	1	0	0	0	0
56	1v	2	0	0	0	0
56	1w	8	0	0	0	0
56	1x	12	0	0	0	0
56	1y	2	0	0	0	0
56	20	2	0	0	0	0
56	21	3	0	0	0	0
56	23	1	0	0	0	0
56	25	5	0	0	0	0
56	26	1	0	0	0	0
56	27	3	0	0	0	0
56	28	5	0	0	0	0
56	29	1	0	0	0	0
56	2A	873	0	0	0	0
56	2B	20	0	0	0	0
56	2D	6	0	0	0	0
56	2E	10	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	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	3	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	240	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	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	2l	5	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	7	0	0	0	0
56	2x	7	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	34	0	0	1	0
58	2A	34	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	2	0
61	10	10	0	0	1	0
61	11	13	0	0	0	0
61	12	4	0	0	0	0
61	13	4	0	0	0	0
61	14	1	0	0	0	0
61	15	6	0	0	0	0
61	16	2	0	0	0	0
61	17	11	0	0	1	0
61	18	10	0	0	0	0
61	1A	2002	0	0	78	0
61	1B	63	0	0	5	0
61	1D	28	0	0	0	0
61	1E	30	0	0	3	0
61	1F	19	0	0	0	0
61	1G	3	0	0	3	0
61	1H	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1I	2	0	0	0	0
61	1N	7	0	0	0	0
61	1O	7	0	0	0	0
61	1P	19	0	0	1	0
61	1Q	9	0	0	0	0
61	1R	13	0	0	6	0
61	1S	5	0	0	1	0
61	1T	8	0	0	1	0
61	1U	15	0	0	0	0
61	1V	8	0	0	1	0
61	1W	7	0	0	0	0
61	1X	6	0	0	0	0
61	1Y	2	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	374	0	0	24	0
61	1b	1	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	0	0
61	1i	1	0	0	0	0
61	1l	8	0	0	0	0
61	1n	1	0	0	0	0
61	1o	3	0	0	0	0
61	1p	1	0	0	0	0
61	1q	2	0	0	0	0
61	1u	1	0	0	0	0
61	1v	4	0	0	0	0
61	1w	11	0	0	0	0
61	1x	13	0	0	0	0
61	1y	2	0	0	0	0
61	20	4	0	0	0	0
61	21	11	0	0	2	0
61	23	2	0	0	0	0
61	25	1	0	0	0	0
61	27	4	0	0	0	0
61	28	3	0	0	0	0
61	29	1	0	0	0	0
61	2A	1175	0	0	92	0
61	2B	24	0	0	1	0
61	2D	20	0	0	0	0
61	2E	12	0	0	0	0
61	2F	13	0	0	0	0
61	2I	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2N	1	0	0	0	0
61	2P	13	0	0	5	0
61	2Q	1	0	0	0	0
61	2R	4	0	0	0	0
61	2T	5	0	0	0	0
61	2U	3	0	0	0	0
61	2W	2	0	0	0	0
61	2X	2	0	0	0	0
61	2Z	1	0	0	1	0
61	2a	268	0	0	27	0
61	2c	1	0	0	0	0
61	2d	1	0	0	0	0
61	2e	1	0	0	0	0
61	2j	3	0	0	2	0
61	2l	6	0	0	0	0
61	2o	1	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	1	0
61	2t	2	0	0	0	0
61	2v	2	0	0	0	0
61	2w	1	0	0	0	0
61	2x	5	0	0	0	0
61	2y	7	0	0	1	0
All	All	300040	0	196551	6188	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 13.

The worst 5 of 6188 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.35	1.23
1:1A:1054:A:N6	1:1A:1105:U:H3	1.46	1.13
1:2A:2711:A:OP2	61:2A:3901:HOH:O	1.79	1.00
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.44	0.98
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.11	0.97

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%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	43
4	2E	202/206 (98%)	192 (95%)	10 (5%)	0	100	100
5	1F	201/210 (96%)	196 (98%)	5 (2%)	0	100	100
5	2F	201/210 (96%)	186 (92%)	15 (8%)	0	100	100
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	21	38
6	2G	179/182 (98%)	153 (86%)	24 (13%)	2 (1%)	11	22
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	16 (9%)	0	100	100
8	1I	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	18 (12%)	0	100	100
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
10	1O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
11	1P	147/150 (98%)	135 (92%)	11 (8%)	1 (1%)	18	34
11	2P	147/150 (98%)	126 (86%)	20 (14%)	1 (1%)	18	34
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	27
14	2S	108/112 (96%)	97 (90%)	11 (10%)	0	100	100
15	1T	129/146 (88%)	120 (93%)	9 (7%)	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%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
17	2V	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	22
19	2X	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	148/206 (72%)	132 (89%)	15 (10%)	1 (1%)	18	34
21	2Z	156/206 (76%)	127 (81%)	27 (17%)	2 (1%)	9	18
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	22
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	53 (79%)	12 (18%)	2 (3%)	3	5
26	24	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	8	16
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	57 (100%)	0	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	58 (94%)	4 (6%)	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%)	31 (89%)	4 (11%)	0	100	100
33	1b	229/256 (90%)	187 (82%)	38 (17%)	4 (2%)	7	13
33	2b	229/256 (90%)	179 (78%)	48 (21%)	2 (1%)	14	27
34	1c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	8	16
34	2c	204/239 (85%)	159 (78%)	45 (22%)	0	100	100
35	1d	206/209 (99%)	180 (87%)	26 (13%)	0	100	100
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
36	1e	146/162 (90%)	127 (87%)	18 (12%)	1 (1%)	18	34
36	2e	146/162 (90%)	122 (84%)	24 (16%)	0	100	100
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
38	2g	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	18	34
39	1h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	11	22
41	2j	94/105 (90%)	78 (83%)	15 (16%)	1 (1%)	11	22
42	1k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
42	2k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	14	27
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	107 (90%)	11 (9%)	1 (1%)	16	31
44	1m	121/126 (96%)	105 (87%)	16 (13%)	0	100	100
44	2m	120/126 (95%)	100 (83%)	20 (17%)	0	100	100
45	1n	58/61 (95%)	46 (79%)	12 (21%)	0	100	100
45	2n	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
49	1r	66/88 (75%)	56 (85%)	10 (15%)	0	100	100
49	2r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	20
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10	20
51	1t	94/106 (89%)	79 (84%)	15 (16%)	0	100	100
51	2t	94/106 (89%)	83 (88%)	11 (12%)	0	100	100
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11360/12128 (94%)	10287 (91%)	1041 (9%)	32 (0%)	36	55

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	36	LYS
21	1Z	53	ILE
33	1b	17	PHE
34	1c	66	VAL
41	1j	79	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	199 (93%)	16 (7%)	13	27
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	43
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19	40
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	27
5	1F	160/166 (96%)	138 (86%)	22 (14%)	3	7

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	148 (93%)	11 (7%)	14	30
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	11
6	2G	143/156 (92%)	111 (78%)	32 (22%)	1	2
7	1H	144/148 (97%)	128 (89%)	16 (11%)	6	12
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	14
8	1I	113/124 (91%)	90 (80%)	23 (20%)	1	2
8	2I	105/124 (85%)	83 (79%)	22 (21%)	1	2
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7	15
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	18
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	44
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14	29
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	17
11	2P	115/116 (99%)	102 (89%)	13 (11%)	5	12
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	41
12	2Q	111/111 (100%)	99 (89%)	12 (11%)	6	13
13	1R	101/101 (100%)	97 (96%)	4 (4%)	28	54
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	44
14	1S	86/88 (98%)	76 (88%)	10 (12%)	5	11
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	4
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	29
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	17
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	21
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	41
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	26
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	9
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	61
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	24
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	32
19	2X	77/78 (99%)	73 (95%)	4 (5%)	21	42
20	1Y	85/91 (93%)	72 (85%)	13 (15%)	3	5
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	116 (86%)	19 (14%)	3	7
21	2Z	137/179 (76%)	126 (92%)	11 (8%)	11	24
22	10	61/67 (91%)	58 (95%)	3 (5%)	22	45
22	20	62/67 (92%)	57 (92%)	5 (8%)	11	23
23	11	80/83 (96%)	71 (89%)	9 (11%)	5	12
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	15
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	13
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	24
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	4
26	24	53/63 (84%)	42 (79%)	11 (21%)	1	2
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	36
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	7
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	7
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	16
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	16
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	27
30	28	54/55 (98%)	49 (91%)	5 (9%)	8	18
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	11
33	1b	192/220 (87%)	162 (84%)	30 (16%)	2	5
33	2b	187/220 (85%)	150 (80%)	37 (20%)	1	2
34	1c	142/188 (76%)	119 (84%)	23 (16%)	2	4
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	9
35	1d	169/181 (93%)	141 (83%)	28 (17%)	2	4
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19
36	1e	113/123 (92%)	94 (83%)	19 (17%)	2	4
36	2e	114/123 (93%)	92 (81%)	22 (19%)	1	2
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	23
38	1g	119/127 (94%)	99 (83%)	20 (17%)	2	4
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	11
39	1h	114/119 (96%)	102 (90%)	12 (10%)	6	14
39	2h	114/119 (96%)	96 (84%)	18 (16%)	2	5
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2	5
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	5
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	5
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	11
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	10
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	28
43	1l	96/108 (89%)	87 (91%)	9 (9%)	8	18
43	2l	96/108 (89%)	79 (82%)	17 (18%)	2	3
44	1m	93/101 (92%)	80 (86%)	13 (14%)	3	7
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	10
45	1n	49/50 (98%)	42 (86%)	7 (14%)	3	6
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	6
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	56
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	43
47	1p	69/74 (93%)	54 (78%)	15 (22%)	1	2
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	20
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	27
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	33
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	22
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	8
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	8
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	2
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	21
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	21
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	39
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9296/10064 (92%)	8257 (89%)	1039 (11%)	<b>6</b> <b>12</b>

5 of 1039 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	2h	115	SER
42	2k	14	VAL
39	2h	112	LEU
38	1g	92	SER
38	1g	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
33	2b	40	HIS
43	2l	99	HIS
33	2b	135	GLN
36	2e	130	ASN
50	2s	23	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	463 (16%)	38 (1%)
1	2A	2791/2915 (95%)	499 (17%)	36 (1%)
2	1B	119/121 (98%)	17 (14%)	0
2	2B	118/121 (97%)	26 (22%)	0
32	1a	1497/1521 (98%)	256 (17%)	0
32	2a	1501/1521 (98%)	300 (19%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	69/76 (90%)	24 (34%)	0
54	1y	72/76 (94%)	26 (36%)	0
54	2w	66/76 (86%)	19 (28%)	0
54	2y	70/76 (92%)	27 (38%)	0
55	1x	74/77 (96%)	8 (10%)	0
55	2x	74/77 (96%)	9 (12%)	0
All	All	9339/9620 (97%)	1677 (17%)	74 (0%)

5 of 1677 RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	36	G
1	1A	45	C

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1249	U
1	2A	2439	A
1	2A	1379	A
1	2A	1653	G
1	1A	1762	A

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

86 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
43	0TD	1l	92	43	8,9,10	4.23	3 (37%)	6,11,13	8.05	2 (33%)
32	2MG	1a	1207	32,56	23,26,27	1.20	3 (13%)	33,38,41	2.19	8 (24%)
32	UR3	1a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.80	6 (23%)
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.70	5 (18%)
55	5MC	1x	32	55,56	19,22,23	1.71	2 (10%)	26,32,35	1.56	5 (19%)
54	PSU	2w	55	54	18,21,22	1.56	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	2A	2605	1	18,21,22	1.27	2 (11%)	21,30,33	2.48	5 (23%)
55	4SU	2x	8	55	18,21,22	1.94	6 (33%)	25,30,33	1.54	5 (20%)
32	5MC	2a	1404	32	19,22,23	1.95	3 (15%)	26,32,35	1.48	4 (15%)
54	MIA	1w	37	54	28,31,32	2.35	6 (21%)	38,44,47	2.87	11 (28%)
32	5MC	1a	1407	32	19,22,23	1.64	3 (15%)	26,32,35	1.32	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.90	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	PSU	1w	32	54	18,21,22	1.30	2 (11%)	21,30,33	1.90	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.51	0	33,38,41	1.97	10 (30%)
32	PSU	2a	516	32	18,21,22	1.27	1 (5%)	21,30,33	1.96	4 (19%)
32	UR3	2a	1498	32,56	19,22,23	1.13	2 (10%)	26,32,35	1.82	4 (15%)
54	PSU	1y	32	54	18,21,22	1.56	2 (11%)	21,30,33	1.97	4 (19%)
1	5MC	1A	1962	1,56	19,22,23	1.60	2 (10%)	26,32,35	1.43	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.36	1 (5%)	21,30,33	1.76	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.48	0	33,38,41	2.11	9 (27%)
55	5MU	1x	54	55,56	19,22,23	1.52	5 (26%)	27,32,35	1.85	6 (22%)
32	G7M	2a	527	32,56	23,26,27	1.44	4 (17%)	34,39,42	1.70	4 (11%)
54	PSU	2w	32	54	18,21,22	1.37	3 (16%)	21,30,33	1.85	4 (19%)
54	5MU	1w	54	54	19,22,23	1.38	5 (26%)	27,32,35	1.95	6 (22%)
1	5MU	1A	1915	1	19,22,23	1.63	4 (21%)	27,32,35	2.16	7 (25%)
54	PSU	2y	32	54	18,21,22	1.45	2 (11%)	21,30,33	1.92	4 (19%)
55	31H	1x	76	55,56	31,34,35	1.22	4 (12%)	35,47,50	2.39	13 (37%)
54	5MU	1y	54	54	19,22,23	1.61	5 (26%)	27,32,35	1.68	7 (25%)
1	2MA	1A	2503	1,56	22,25,26	1.51	5 (22%)	32,37,40	2.59	8 (25%)
54	MIA	2y	37	54	21,24,32	1.68	3 (14%)	30,35,47	2.17	10 (33%)
32	5MC	2a	1400	32	19,22,23	1.77	3 (15%)	26,32,35	1.40	4 (15%)
1	OMG	2A	2251	55,1,56	23,26,27	1.34	3 (13%)	32,38,41	2.08	7 (21%)
1	OMG	1A	2251	55,1,56	23,26,27	1.47	4 (17%)	32,38,41	1.74	6 (18%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.03	10 (30%)
32	G7M	1a	527	32	23,26,27	1.61	4 (17%)	34,39,42	1.66	5 (14%)
54	PSU	2y	55	54	18,21,22	1.42	2 (11%)	21,30,33	1.87	5 (23%)
54	G7M	1y	46	54	23,26,27	1.51	3 (13%)	34,39,42	1.55	4 (11%)
54	G7M	1w	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.56	5 (14%)
1	5MC	2A	1962	1,56	19,22,23	1.38	3 (15%)	26,32,35	1.37	4 (15%)
54	PSU	1y	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.98	3 (14%)
54	4SU	1w	8	54	18,21,22	1.62	5 (27%)	25,30,33	1.98	6 (24%)
54	MIA	2w	37	54	24,27,32	2.00	8 (33%)	32,39,47	2.53	9 (28%)
54	G7M	2w	46	54	23,26,27	1.44	4 (17%)	34,39,42	1.51	4 (11%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
32	PSU	1a	516	32,56	18,21,22	1.51	3 (16%)	21,30,33	1.83	4 (19%)
43	0TD	2l	92	43	8,9,10	4.59	2 (25%)	6,11,13	1.13	0
54	4SU	2y	8	54	18,21,22	1.67	4 (22%)	25,30,33	2.41	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	1A	2552	1,56	19,22,23	1.28	4 (21%)	25,31,34	2.63	7 (28%)
32	5MC	1a	967	32	19,22,23	1.83	2 (10%)	26,32,35	1.24	3 (11%)
55	31H	2x	76	55,56	31,34,35	1.48	3 (9%)	35,47,50	2.00	8 (22%)
32	M2G	1a	966	32	24,27,28	1.41	4 (16%)	33,40,43	1.91	7 (21%)
55	4SU	1x	8	55	18,21,22	2.46	5 (27%)	25,30,33	2.22	7 (28%)
32	5MC	1a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.42	4 (15%)
55	5MC	2x	32	55	19,22,23	1.67	2 (10%)	26,32,35	1.30	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.82	1 (5%)	25,31,34	0.98	1 (4%)
1	5MU	1A	1939	1,56	19,22,23	1.66	4 (21%)	27,32,35	2.66	7 (25%)
32	5MC	1a	1400	32	19,22,23	1.77	3 (15%)	26,32,35	1.18	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.52	3 (16%)	21,30,33	1.93	5 (23%)
54	PSU	1w	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.69	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.53	5 (26%)	27,32,35	2.23	5 (18%)
54	PSU	2y	39	54	18,21,22	1.29	1 (5%)	21,30,33	1.96	3 (14%)
32	4OC	1a	1402	32	20,23,24	0.82	0	25,32,35	1.12	3 (12%)
54	4SU	2w	8	54	18,21,22	1.49	3 (16%)	25,30,33	2.28	5 (20%)
54	PSU	1y	39	54	18,21,22	1.47	2 (11%)	21,30,33	1.80	5 (23%)
54	5MU	2y	54	54	19,22,23	1.52	4 (21%)	27,32,35	2.24	9 (33%)
32	MA6	1a	1519	32	23,26,27	0.47	0	33,38,41	2.04	10 (30%)
55	5MU	2x	54	55	19,22,23	1.50	5 (26%)	27,32,35	2.09	8 (29%)
1	5MU	2A	1939	1,56	19,22,23	1.42	4 (21%)	27,32,35	2.65	6 (22%)
54	G7M	2y	46	54	23,26,27	1.66	3 (13%)	34,39,42	1.83	4 (11%)
32	2MG	2a	1207	32,56	23,26,27	1.25	3 (13%)	33,38,41	2.22	7 (21%)
55	PSU	1x	55	55	18,21,22	1.31	2 (11%)	21,30,33	1.89	4 (19%)
54	MIA	1y	37	54	21,24,32	1.68	3 (14%)	30,35,47	2.13	10 (33%)
1	2MA	2A	2503	1,56	22,25,26	1.35	2 (9%)	32,37,40	2.64	10 (31%)
32	5MC	2a	967	32	19,22,23	1.97	2 (10%)	26,32,35	1.18	4 (15%)
32	5MC	2a	1407	32,56	19,22,23	1.37	3 (15%)	26,32,35	1.43	4 (15%)
55	PSU	2x	55	55	18,21,22	1.44	2 (11%)	21,30,33	1.98	5 (23%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
1	OMU	2A	2552	1,56	19,22,23	1.19	4 (21%)	25,31,34	1.92	5 (20%)
1	PSU	1A	2605	1,56	18,21,22	1.52	3 (16%)	21,30,33	2.25	5 (23%)
1	OMC	2A	1920	1	19,22,23	0.80	1 (5%)	25,31,34	0.92	0
1	5MC	2A	1942	1	19,22,23	1.51	3 (15%)	26,32,35	1.10	2 (7%)
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.98	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	2a	1402	32,56	20,23,24	0.83	0	25,32,35	1.00	2 (8%)
1	5MC	1A	1942	1	19,22,23	1.19	3 (15%)	26,32,35	1.67	5 (19%)
54	4SU	1y	8	54	18,21,22	1.59	4 (22%)	25,30,33	1.65	5 (20%)
54	PSU	1w	55	54	18,21,22	1.43	2 (11%)	21,30,33	2.08	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	0TD	1l	92	43	-	3/7/12/14	-
32	2MG	1a	1207	32,56	-	2/9/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55,56	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,56	-	6/22/40/41	0/3/3/3
54	5MU	1y	54	54	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	0/7/25/26	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MIA	2y	37	54	-	1/7/25/34	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1,56	-	0/9/27/28	0/3/3/3
1	OMG	1A	2251	55,1,56	-	1/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	G7M	1a	527	32	-	2/7/25/26	0/3/3/3
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	5MC	2A	1962	1,56	-	2/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
55	31H	2x	76	55,56	-	4/22/40/41	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	1/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
54	4SU	2w	8	54	-	2/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	1/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
32	2MG	2a	1207	32,56	-	2/9/27/28	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	1/7/25/34	0/3/3/3
1	2MA	2A	2503	1,56	-	2/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2

The worst 5 of 248 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.42	1.69	1.82
43	1l	92	0TD	CB-SB	-11.04	1.71	1.82
32	2a	967	5MC	C5-C4	7.54	1.49	1.44
32	2a	1404	5MC	C5-C4	7.36	1.49	1.44
54	1w	37	MIA	C2-S10	-7.23	1.69	1.75

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-19.51	67.30	102.36
54	1w	37	MIA	C12-C13-C14	-10.89	107.47	127.01
54	2w	37	MIA	C5-C4-N3	-8.75	117.96	127.18
1	2A	2503	2MA	C5-C4-N3	-8.51	118.21	127.18
1	2A	2503	2MA	N3-C4-N9	8.18	137.38	126.99

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB

There are no ring outliers.

42 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	2	0
55	1x	32	5MC	1	0
32	2a	1404	5MC	1	0
32	2a	1518	MA6	5	0
32	2a	1498	UR3	1	0
32	2a	1519	MA6	4	0
54	1w	54	5MU	1	0
1	1A	2503	2MA	1	0
32	2a	1400	5MC	2	0
1	2A	2251	OMG	1	0
1	1A	2251	OMG	1	0
32	1a	1518	MA6	2	0
32	1a	527	G7M	1	0
54	2y	55	PSU	4	0
54	1w	46	G7M	1	0
54	1y	55	PSU	2	0
54	1w	8	4SU	1	0
1	1A	1917	PSU	1	0
43	2l	92	0TD	3	0
54	2y	8	4SU	3	0
55	2x	76	31H	1	0
55	1x	8	4SU	2	0
1	1A	1920	OMC	1	0
1	1A	1911	PSU	1	0
54	1w	39	PSU	2	0
1	2A	1915	5MU	1	0
32	1a	1402	4OC	2	0
54	2w	8	4SU	4	0
54	1y	39	PSU	1	0
32	1a	1519	MA6	1	0
1	2A	1939	5MU	2	0
54	2y	46	G7M	1	0
32	2a	1207	2MG	5	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1y	37	MIA	1	0
1	2A	2503	2MA	1	0
32	2a	967	5MC	4	0
55	2x	55	PSU	1	0
54	2w	39	PSU	3	0
1	2A	2552	OMU	1	0
32	2a	966	M2G	1	0
32	2a	1402	4OC	4	0
54	1y	8	4SU	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2810 ligands modelled in this entry, 2806 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
60	SF4	2d	302	35	0,12,12	-	-	-		
58	A1A1F	1A	4110	56	34,37,37	1.74	9 (26%)	33,53,53	1.29	5 (15%)
58	A1A1F	2A	3875	-	34,37,37	1.33	2 (5%)	33,53,53	1.22	3 (9%)
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	302	35	-	-	0/6/5/5
58	A1A1F	1A	4110	56	-	3/28/71/71	0/3/4/4

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	A1A1F	2A	3875	-	-	3/28/71/71	0/3/4/4
60	SF4	1d	302	35	-	-	0/6/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4110	A1A1F	CAM-CBF	-4.66	1.40	1.51
58	2A	3875	A1A1F	CAM-CBF	-4.63	1.40	1.51
58	1A	4110	A1A1F	CD2-CAZ	-3.40	1.50	1.53
58	1A	4110	A1A1F	CAF-CAE	-3.12	1.43	1.52
58	1A	4110	A1A1F	CD2-CG	2.63	1.58	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4110	A1A1F	CBC-CBB-CAZ	-3.69	109.53	116.68
58	2A	3875	A1A1F	CD2-CAZ-CAY	-3.52	108.53	113.78
58	1A	4110	A1A1F	OAA-CAF-CAE	-2.94	104.33	110.37
58	1A	4110	A1A1F	OAG-CAF-CAE	2.76	112.47	108.27
58	2A	3875	A1A1F	OAG-CAF-CAE	2.76	112.47	108.27

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4110	A1A1F	CBH-CAO-OAG-CAF
58	2A	3875	A1A1F	CBH-CAO-OAG-CAF
58	1A	4110	A1A1F	O-C-CA-CB
58	2A	3875	A1A1F	O-C-CA-CB
58	1A	4110	A1A1F	NAL-C-CA-CB

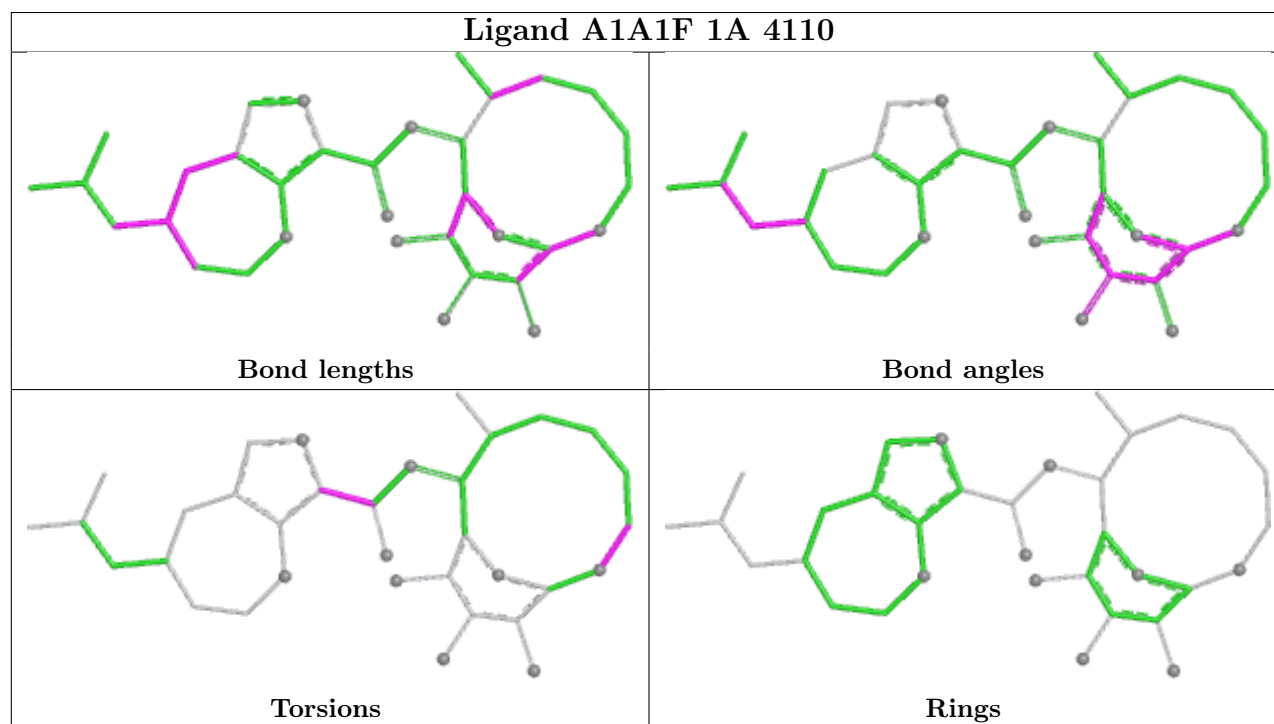
There are no ring outliers.

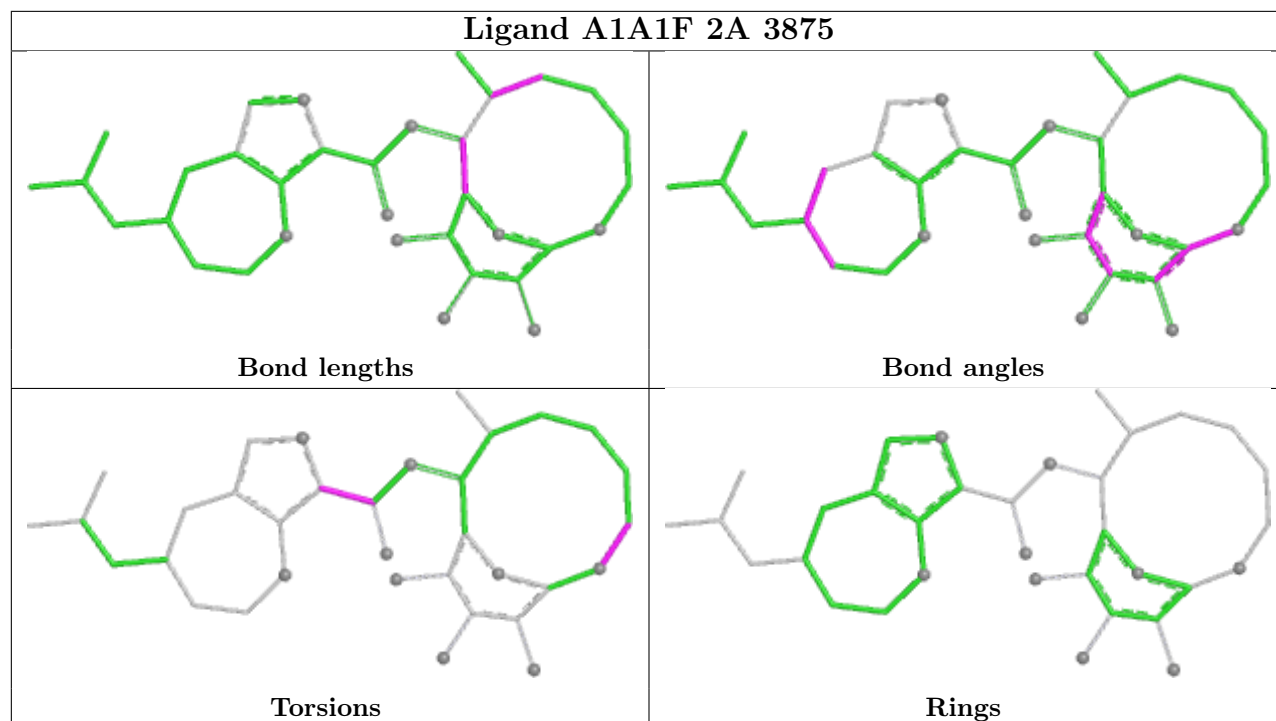
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2d	302	SF4	2	0
58	1A	4110	A1A1F	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	1V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1V	34:GLU	C	35:LEU	N	1.19

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	-0.53	115 (4%)	42	38	23, 40, 94, 106	0
1	2A	2789/2915 (95%)	0.08	104 (3%)	45	40	41, 65, 94, 105	0
2	1B	120/121 (99%)	-0.37	0	100	100	32, 54, 68, 89	0
2	2B	120/121 (99%)	0.93	1 (0%)	82	80	68, 84, 90, 97	0
3	1D	275/276 (99%)	-0.06	3 (1%)	78	75	22, 41, 54, 83	0
3	2D	275/276 (99%)	0.47	6 (2%)	62	58	39, 58, 69, 85	0
4	1E	204/206 (99%)	-0.17	1 (0%)	87	85	22, 43, 61, 75	0
4	2E	204/206 (99%)	0.63	9 (4%)	39	34	45, 66, 77, 87	0
5	1F	203/210 (96%)	-0.05	2 (0%)	79	76	24, 46, 71, 87	0
5	2F	203/210 (96%)	0.66	9 (4%)	39	34	43, 72, 82, 86	0
6	1G	181/182 (99%)	0.64	12 (6%)	24	21	43, 63, 76, 87	0
6	2G	181/182 (99%)	1.52	43 (23%)	2	1	72, 83, 89, 94	0
7	1H	174/180 (96%)	0.30	3 (1%)	69	65	44, 57, 69, 73	0
7	2H	174/180 (96%)	1.71	59 (33%)	1	1	77, 86, 94, 97	0
8	1I	146/148 (98%)	0.91	9 (6%)	26	23	51, 76, 84, 87	0
8	2I	146/148 (98%)	1.00	13 (8%)	15	13	56, 76, 84, 88	0
9	1N	140/140 (100%)	-0.04	2 (1%)	73	70	27, 41, 61, 73	0
9	2N	140/140 (100%)	1.06	9 (6%)	25	22	56, 72, 83, 91	0
10	1O	122/122 (100%)	0.11	1 (0%)	82	80	32, 45, 62, 68	0
10	2O	122/122 (100%)	0.61	2 (1%)	70	67	55, 65, 76, 80	0
11	1P	149/150 (99%)	0.09	2 (1%)	75	71	23, 50, 71, 79	0
11	2P	149/150 (99%)	0.88	7 (4%)	36	32	48, 71, 86, 92	0
12	1Q	141/141 (100%)	0.04	2 (1%)	73	70	32, 44, 60, 75	0
12	2Q	141/141 (100%)	1.63	41 (29%)	1	1	61, 76, 84, 87	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%)	-0.18	0 100 100	28, 38, 49, 58	0
13	2R	118/118 (100%)	0.17	0 100 100	47, 58, 69, 75	0
14	1S	110/112 (98%)	0.27	0 100 100	40, 54, 66, 71	0
14	2S	110/112 (98%)	1.66	34 (30%) 1 1	67, 79, 85, 90	0
15	1T	131/146 (89%)	0.20	4 (3%) 51 47	38, 49, 69, 75	0
15	2T	131/146 (89%)	0.72	5 (3%) 44 39	57, 67, 77, 83	0
16	1U	116/118 (98%)	-0.41	0 100 100	24, 33, 49, 71	0
16	2U	116/118 (98%)	0.89	10 (8%) 16 14	51, 71, 81, 86	0
17	1V	101/101 (100%)	-0.17	1 (0%) 79 76	24, 41, 58, 70	0
17	2V	101/101 (100%)	1.09	9 (8%) 15 13	48, 78, 84, 90	0
18	1W	112/113 (99%)	-0.31	1 (0%) 81 78	25, 34, 55, 79	0
18	2W	112/113 (99%)	0.43	2 (1%) 67 64	45, 57, 72, 89	0
19	1X	95/96 (98%)	0.11	2 (2%) 63 59	32, 42, 65, 81	0
19	2X	95/96 (98%)	0.93	6 (6%) 26 23	49, 64, 77, 86	0
20	1Y	107/110 (97%)	0.55	5 (4%) 36 32	43, 54, 72, 80	0
20	2Y	107/110 (97%)	1.51	23 (21%) 2 2	63, 77, 85, 94	0
21	1Z	154/206 (74%)	0.83	18 (11%) 9 7	42, 66, 85, 88	0
21	2Z	160/206 (77%)	2.12	77 (48%) 0 0	75, 85, 91, 93	0
22	10	77/85 (90%)	0.13	2 (2%) 57 52	31, 41, 58, 64	0
22	20	79/85 (92%)	1.52	19 (24%) 2 1	60, 72, 79, 83	0
23	11	97/98 (98%)	0.26	2 (2%) 63 59	31, 48, 71, 78	0
23	21	97/98 (98%)	0.61	2 (2%) 63 59	46, 60, 76, 81	0
24	12	70/72 (97%)	0.37	1 (1%) 73 70	39, 54, 64, 75	0
24	22	70/72 (97%)	0.92	6 (8%) 16 14	62, 73, 79, 86	0
25	13	59/60 (98%)	-0.06	1 (1%) 69 65	27, 38, 63, 80	0
25	23	59/60 (98%)	0.96	2 (3%) 48 43	64, 72, 82, 85	0
26	14	69/71 (97%)	0.90	9 (13%) 7 6	61, 78, 88, 94	0
26	24	69/71 (97%)	1.81	25 (36%) 1 1	80, 88, 94, 102	0
27	15	59/60 (98%)	-0.32	0 100 100	24, 35, 51, 61	0
27	25	59/60 (98%)	0.36	1 (1%) 69 65	44, 58, 68, 82	0
28	16	53/54 (98%)	-0.02	0 100 100	36, 47, 61, 67	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%)	0.93	5 (9%) 14 12	59, 68, 76, 80	0
29	17	48/49 (97%)	0.02	4 (8%) 17 15	26, 32, 62, 70	0
29	27	48/49 (97%)	0.53	4 (8%) 17 15	41, 47, 72, 75	0
30	18	64/65 (98%)	-0.24	0 100 100	30, 38, 44, 57	0
30	28	64/65 (98%)	0.86	2 (3%) 51 47	55, 63, 71, 77	0
31	19	37/37 (100%)	0.20	0 100 100	36, 43, 62, 67	0
31	29	37/37 (100%)	1.74	12 (32%) 1 1	67, 76, 84, 87	0
32	1a	1488/1521 (97%)	0.29	45 (3%) 52 48	41, 73, 95, 108	0
32	2a	1491/1521 (98%)	0.81	155 (10%) 11 10	56, 80, 97, 108	0
33	1b	231/256 (90%)	1.36	46 (19%) 3 2	68, 80, 89, 93	0
33	2b	231/256 (90%)	1.80	89 (38%) 1 0	76, 87, 91, 93	0
34	1c	206/239 (86%)	1.12	19 (9%) 14 13	68, 78, 86, 90	0
34	2c	206/239 (86%)	2.15	108 (52%) 0 0	76, 86, 90, 95	0
35	1d	208/209 (99%)	1.19	24 (11%) 9 8	61, 76, 83, 89	0
35	2d	208/209 (99%)	0.85	15 (7%) 21 19	63, 72, 79, 84	0
36	1e	148/162 (91%)	0.79	7 (4%) 36 32	57, 70, 78, 82	0
36	2e	148/162 (91%)	1.61	50 (33%) 1 1	69, 80, 86, 90	0
37	1f	100/101 (99%)	0.91	5 (5%) 34 30	62, 72, 80, 82	0
37	2f	100/101 (99%)	1.09	9 (9%) 15 13	67, 77, 83, 84	0
38	1g	155/156 (99%)	0.79	13 (8%) 17 15	63, 74, 85, 88	0
38	2g	155/156 (99%)	1.49	35 (22%) 2 2	73, 83, 88, 95	0
39	1h	137/138 (99%)	0.80	4 (2%) 53 49	60, 71, 77, 79	0
39	2h	137/138 (99%)	1.42	20 (14%) 6 4	72, 81, 86, 90	0
40	1i	127/128 (99%)	1.36	21 (16%) 4 3	64, 81, 86, 89	0
40	2i	127/128 (99%)	1.88	56 (44%) 0 0	74, 87, 92, 93	0
41	1j	97/105 (92%)	1.82	36 (37%) 1 1	66, 82, 88, 90	0
41	2j	96/105 (91%)	2.51	66 (68%) 0 0	82, 88, 93, 95	0
42	1k	114/129 (88%)	0.77	7 (6%) 27 23	51, 68, 80, 83	0
42	2k	114/129 (88%)	1.25	22 (19%) 3 2	63, 77, 86, 88	0
43	1l	121/132 (91%)	0.59	4 (3%) 49 45	48, 64, 74, 82	0
43	2l	121/132 (91%)	1.27	19 (15%) 5 4	63, 76, 82, 90	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	1.00	11 (8%) 15 13	60, 74, 80, 84	0
44	2m	122/126 (96%)	1.80	44 (36%) 1 1	76, 85, 89, 91	0
45	1n	60/61 (98%)	1.50	11 (18%) 3 3	68, 76, 82, 89	0
45	2n	60/61 (98%)	3.21	48 (80%) 0 0	81, 88, 92, 94	0
46	1o	88/89 (98%)	0.71	7 (7%) 18 16	53, 70, 77, 80	0
46	2o	88/89 (98%)	1.28	13 (14%) 5 4	66, 78, 85, 90	0
47	1p	82/88 (93%)	1.28	15 (18%) 3 3	63, 75, 82, 85	0
47	2p	82/88 (93%)	0.99	5 (6%) 27 23	61, 70, 78, 82	0
48	1q	99/105 (94%)	0.88	3 (3%) 52 48	57, 70, 79, 80	0
48	2q	99/105 (94%)	1.14	10 (10%) 12 10	66, 77, 84, 87	0
49	1r	68/88 (77%)	0.62	3 (4%) 39 34	59, 69, 77, 80	0
49	2r	68/88 (77%)	1.11	4 (5%) 28 24	70, 77, 84, 85	0
50	1s	83/93 (89%)	1.04	11 (13%) 7 6	71, 78, 83, 87	0
50	2s	83/93 (89%)	2.30	53 (63%) 0 0	80, 89, 94, 97	0
51	1t	96/106 (90%)	1.10	14 (14%) 6 4	65, 74, 81, 83	0
51	2t	96/106 (90%)	1.01	6 (6%) 26 23	63, 74, 83, 87	0
52	1u	23/27 (85%)	1.38	4 (17%) 4 3	67, 73, 77, 79	0
52	2u	23/27 (85%)	2.81	16 (69%) 0 0	80, 85, 90, 91	0
53	1v	13/24 (54%)	0.80	1 (7%) 19 17	55, 74, 90, 97	0
53	2v	13/24 (54%)	1.52	4 (30%) 1 1	77, 87, 98, 101	0
54	1w	64/76 (84%)	1.47	13 (20%) 3 2	72, 95, 101, 105	0
54	1y	67/76 (88%)	0.86	5 (7%) 20 18	43, 92, 99, 104	0
54	2w	62/76 (81%)	1.90	25 (40%) 0 0	84, 100, 104, 108	0
54	2y	66/76 (86%)	1.36	14 (21%) 2 2	62, 99, 103, 104	0
55	1x	71/77 (92%)	0.01	0 100 100	33, 65, 83, 89	0
55	2x	71/77 (92%)	0.70	2 (2%) 55 50	57, 85, 93, 102	0
All	All	20857/21748 (95%)	0.53	1966 (9%) 14 12	22, 69, 91, 108	0

The worst 5 of 1966 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	8.3
45	2n	34	TYR	7.4

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
45	2n	38	GLY	7.1
54	1w	73	A	6.4
45	1n	2	ALA	6.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	G7M	2w	46	24/25	0.46	0.17	87,99,104,114	0
54	PSU	2y	55	20/21	0.48	0.16	94,100,112,112	0
54	G7M	1w	46	24/25	0.51	0.17	90,96,109,126	0
54	4SU	2w	8	20/21	0.58	0.17	93,101,113,121	0
54	5MU	2y	54	21/22	0.59	0.18	90,98,105,120	0
54	G7M	2y	46	24/25	0.60	0.16	88,95,102,119	0
54	5MU	2w	54	21/22	0.62	0.16	86,91,99,102	0
54	G7M	1y	46	24/25	0.62	0.15	87,95,104,112	0
54	PSU	2y	32	20/21	0.63	0.16	86,91,100,106	0
54	PSU	2w	55	20/21	0.65	0.15	93,97,107,111	0
54	5MU	1y	54	21/22	0.65	0.14	89,93,101,112	0
54	MIA	2y	37	22/30	0.65	0.15	82,90,98,109	0
54	4SU	2y	8	20/21	0.67	0.14	93,97,109,117	0
54	4SU	1y	8	20/21	0.73	0.12	90,93,102,111	0
54	PSU	1y	55	20/21	0.73	0.13	91,96,105,109	0
54	4SU	1w	8	20/21	0.78	0.13	87,94,103,106	0
55	PSU	2x	55	20/21	0.79	0.13	75,85,93,94	0
32	2MG	2a	1207	24/25	0.82	0.13	86,91,96,101	0
54	PSU	1y	32	20/21	0.82	0.13	85,89,92,94	0
54	PSU	1w	55	20/21	0.82	0.11	83,90,97,97	0
55	4SU	2x	8	20/21	0.83	0.13	89,91,95,98	0
54	PSU	2y	39	20/21	0.84	0.13	85,90,99,105	0
55	5MU	2x	54	21/22	0.85	0.13	81,86,91,99	0
54	MIA	1y	37	22/30	0.85	0.12	79,84,90,96	0
32	PSU	2a	516	20/21	0.85	0.13	74,84,88,90	0
54	PSU	2w	32	20/21	0.86	0.11	82,89,99,103	0
1	5MU	2A	1915	21/22	0.86	0.12	75,80,84,88	0
54	PSU	1y	39	20/21	0.88	0.10	80,85,91,92	0
54	MIA	2w	37	25/30	0.88	0.11	74,83,91,103	0
54	PSU	1w	32	20/21	0.88	0.14	75,81,86,92	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	M2G	2a	966	25/26	0.89	0.16	70,76,88,92	0
1	PSU	2A	1917	20/21	0.89	0.11	61,77,81,82	0
55	5MC	2x	32	21/22	0.90	0.13	76,81,84,89	0
32	4OC	2a	1402	22/23	0.90	0.15	63,74,79,82	0
32	5MC	2a	967	21/22	0.90	0.12	73,76,83,93	0
32	G7M	2a	527	24/25	0.90	0.14	68,76,81,83	0
32	5MC	2a	1400	21/22	0.90	0.15	79,83,87,94	0
54	5MU	1w	54	21/22	0.91	0.10	69,81,87,90	0
1	PSU	2A	1911	20/21	0.91	0.10	61,71,76,79	0
32	5MC	2a	1404	21/22	0.91	0.12	59,67,72,73	0
55	PSU	1x	55	20/21	0.91	0.10	60,69,78,86	0
32	MA6	2a	1518	24/25	0.92	0.14	65,76,81,82	0
54	PSU	2w	39	20/21	0.92	0.09	78,87,91,93	0
55	5MU	1x	54	21/22	0.92	0.10	65,70,74,77	0
32	UR3	2a	1498	21/22	0.92	0.14	62,66,72,73	0
54	PSU	1w	39	20/21	0.93	0.10	70,77,81,83	0
1	OMC	2A	1920	21/22	0.93	0.11	64,71,74,80	0
32	2MG	1a	1207	24/25	0.93	0.10	74,79,83,83	0
54	MIA	1w	37	29/30	0.93	0.12	62,72,77,78	0
32	MA6	2a	1519	24/25	0.93	0.14	63,74,79,82	0
43	0TD	2l	92	10/11	0.93	0.10	73,77,82,86	0
32	PSU	1a	516	20/21	0.94	0.10	64,70,75,75	0
32	5MC	1a	967	21/22	0.94	0.10	55,60,69,71	0
1	5MC	2A	1942	21/22	0.94	0.12	57,65,68,69	0
1	5MU	1A	1915	21/22	0.94	0.10	50,62,65,67	0
55	5MC	1x	32	21/22	0.94	0.11	59,64,69,78	0
32	5MC	2a	1407	21/22	0.94	0.11	60,65,73,76	0
43	0TD	1l	92	10/11	0.94	0.09	58,64,69,80	0
32	G7M	1a	527	24/25	0.95	0.09	51,61,67,68	0
55	31H	2x	76	32/33	0.95	0.10	51,57,66,86	0
32	M2G	1a	966	25/26	0.95	0.11	52,60,65,70	0
55	4SU	1x	8	20/21	0.96	0.08	51,67,71,72	0
1	5MU	2A	1939	21/22	0.96	0.08	40,47,52,59	0
1	PSU	1A	1917	20/21	0.96	0.07	52,60,64,64	0
1	OMG	2A	2251	24/25	0.96	0.09	45,51,56,60	0
32	4OC	1a	1402	22/23	0.97	0.08	49,52,56,58	0
1	2MA	2A	2503	23/24	0.97	0.08	39,45,49,50	0
1	OMU	2A	2552	21/22	0.97	0.09	45,54,59,65	0
1	PSU	2A	2605	20/21	0.97	0.08	37,46,52,57	0
32	5MC	1a	1404	21/22	0.97	0.07	41,47,53,54	0
55	31H	1x	76	32/33	0.97	0.09	24,32,41,64	10
32	5MC	1a	1407	21/22	0.97	0.09	41,49,51,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MA6	1a	1519	24/25	0.97	0.10	43,48,53,56	0
1	5MC	1A	1942	21/22	0.97	0.09	34,41,47,48	0
1	PSU	1A	1911	20/21	0.97	0.07	37,51,61,62	0
32	5MC	1a	1400	21/22	0.97	0.09	52,60,64,66	0
1	5MC	2A	1962	21/22	0.97	0.08	35,54,62,66	0
1	OMG	1A	2251	24/25	0.98	0.05	25,28,30,32	0
1	OMU	1A	2552	21/22	0.98	0.06	29,33,39,41	0
1	PSU	1A	2605	20/21	0.98	0.07	26,29,35,37	0
1	5MU	1A	1939	21/22	0.98	0.07	25,33,36,37	0
1	OMC	1A	1920	21/22	0.98	0.08	44,50,55,57	0
1	5MC	1A	1962	21/22	0.98	0.07	35,40,45,48	0
32	UR3	1a	1498	21/22	0.98	0.07	42,48,52,55	0
32	MA6	1a	1518	24/25	0.98	0.08	35,46,49,50	0
1	2MA	1A	2503	23/24	0.99	0.05	20,25,28,29	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	229	1/1	0.32	0.29	96,96,96,96	0
56	MG	1w	102	1/1	0.51	0.23	93,93,93,93	0
56	MG	2w	105	1/1	0.52	0.13	94,94,94,94	0
56	MG	2a	1750	1/1	0.53	0.20	85,85,85,85	0
56	MG	1A	4097	1/1	0.55	0.25	87,87,87,87	0
56	MG	2a	1731	1/1	0.56	0.22	96,96,96,96	0
56	MG	2w	107	1/1	0.56	0.35	88,88,88,88	0
56	MG	2w	102	1/1	0.57	0.14	96,96,96,96	0
56	MG	2A	3298	1/1	0.58	0.26	88,88,88,88	0
56	MG	2A	3652	1/1	0.60	0.24	86,86,86,86	0
56	MG	2A	3284	1/1	0.60	0.24	87,87,87,87	0
56	MG	2A	3293	1/1	0.61	0.18	84,84,84,84	0
56	MG	1a	1713	1/1	0.62	0.34	81,81,81,81	0
56	MG	2A	3346	1/1	0.62	0.25	82,82,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4013	1/1	0.63	0.22	82,82,82,82	0
56	MG	1a	1754	1/1	0.63	0.16	83,83,83,83	0
56	MG	2A	3801	1/1	0.63	0.20	88,88,88,88	0
56	MG	2A	3858	1/1	0.63	0.18	83,83,83,83	0
56	MG	2a	1658	1/1	0.63	0.27	81,81,81,81	0
56	MG	2A	3250	1/1	0.64	0.25	94,94,94,94	0
56	MG	2A	3212	1/1	0.64	0.18	74,74,74,74	0
56	MG	1w	105	1/1	0.65	0.24	92,92,92,92	0
56	MG	2A	3269	1/1	0.65	0.17	88,88,88,88	0
56	MG	1A	4043	1/1	0.65	0.14	67,67,67,67	0
56	MG	2a	1657	1/1	0.65	0.29	81,81,81,81	0
56	MG	2A	3455	1/1	0.65	0.33	88,88,88,88	0
56	MG	2A	3354	1/1	0.66	0.24	85,85,85,85	0
56	MG	1A	3799	1/1	0.66	0.32	90,90,90,90	0
56	MG	2A	3640	1/1	0.66	0.26	72,72,72,72	0
56	MG	1V	206	1/1	0.66	0.22	65,65,65,65	0
56	MG	2a	1811	1/1	0.66	0.20	90,90,90,90	0
56	MG	2A	3337	1/1	0.66	0.23	80,80,80,80	0
56	MG	1a	1788	1/1	0.66	0.12	73,73,73,73	0
56	MG	2a	1604	1/1	0.66	0.15	88,88,88,88	0
56	MG	2A	3602	1/1	0.67	0.23	83,83,83,83	0
56	MG	2l	202	1/1	0.67	0.26	88,88,88,88	0
56	MG	2A	3841	1/1	0.67	0.19	86,86,86,86	0
56	MG	1U	211	1/1	0.67	0.48	65,65,65,65	0
56	MG	2A	3194	1/1	0.67	0.18	91,91,91,91	0
56	MG	1A	4099	1/1	0.68	0.23	62,62,62,62	0
56	MG	1B	221	1/1	0.68	0.23	72,72,72,72	0
56	MG	2A	3394	1/1	0.68	0.43	82,82,82,82	0
56	MG	1a	1715	1/1	0.68	0.23	68,68,68,68	0
56	MG	2A	3471	1/1	0.68	0.19	81,81,81,81	0
56	MG	2A	3866	1/1	0.68	0.19	86,86,86,86	0
56	MG	2A	3551	1/1	0.68	0.20	83,83,83,83	0
56	MG	1a	1738	1/1	0.68	0.25	93,93,93,93	0
56	MG	2A	3277	1/1	0.69	0.20	79,79,79,79	0
56	MG	2A	3744	1/1	0.69	0.25	76,76,76,76	0
56	MG	2y	105	1/1	0.69	0.19	96,96,96,96	0
56	MG	2A	3321	1/1	0.70	0.18	78,78,78,78	0
56	MG	20	101	1/1	0.70	0.27	83,83,83,83	0
56	MG	2A	3209	1/1	0.70	0.22	81,81,81,81	0
56	MG	1w	104	1/1	0.70	0.11	74,74,74,74	0
56	MG	2a	1815	1/1	0.70	0.16	88,88,88,88	0
56	MG	2A	3241	1/1	0.71	0.37	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3991	1/1	0.71	0.16	71,71,71,71	0
56	MG	2A	3663	1/1	0.71	0.19	72,72,72,72	0
56	MG	2a	1659	1/1	0.72	0.18	83,83,83,83	0
56	MG	2w	101	1/1	0.72	0.22	88,88,88,88	0
56	MG	2A	3249	1/1	0.72	0.36	90,90,90,90	0
56	MG	2A	3391	1/1	0.72	0.15	74,74,74,74	0
56	MG	1A	3560	1/1	0.72	0.21	77,77,77,77	0
56	MG	2y	101	1/1	0.72	0.17	91,91,91,91	0
56	MG	2B	220	1/1	0.72	0.28	82,82,82,82	0
56	MG	2a	1617	1/1	0.73	0.24	82,82,82,82	0
56	MG	2A	3066	1/1	0.73	0.28	74,74,74,74	0
56	MG	1a	1808	1/1	0.73	0.21	89,89,89,89	0
56	MG	2A	3306	1/1	0.73	0.26	75,75,75,75	0
56	MG	2a	1727	1/1	0.73	0.32	84,84,84,84	0
56	MG	1a	1685	1/1	0.73	0.18	74,74,74,74	0
56	MG	1A	4026	1/1	0.73	0.15	67,67,67,67	0
56	MG	1A	3818	1/1	0.73	0.21	53,53,53,53	0
56	MG	1a	1712	1/1	0.74	0.26	84,84,84,84	0
56	MG	2a	1700	1/1	0.74	0.33	76,76,76,76	0
56	MG	2a	1708	1/1	0.74	0.24	78,78,78,78	0
56	MG	2a	1724	1/1	0.74	0.34	88,88,88,88	0
56	MG	2A	3399	1/1	0.74	0.11	82,82,82,82	0
56	MG	2A	3315	1/1	0.74	0.23	88,88,88,88	0
56	MG	2A	3466	1/1	0.74	0.14	76,76,76,76	0
56	MG	2A	3273	1/1	0.74	0.36	74,74,74,74	0
56	MG	1A	3852	1/1	0.74	0.13	68,68,68,68	0
56	MG	2G	201	1/1	0.74	0.26	76,76,76,76	0
56	MG	1Z	3702	1/1	0.74	0.13	78,78,78,78	0
56	MG	2A	3351	1/1	0.74	0.29	86,86,86,86	0
56	MG	2A	3176	1/1	0.74	0.33	81,81,81,81	0
56	MG	2a	1637	1/1	0.74	0.30	86,86,86,86	0
56	MG	1A	3267	1/1	0.74	0.33	79,79,79,79	0
56	MG	2A	3697	1/1	0.74	0.22	82,82,82,82	0
56	MG	2y	106	1/1	0.74	0.32	84,84,84,84	0
56	MG	1A	3811	1/1	0.75	0.16	60,60,60,60	0
56	MG	2a	1749	1/1	0.75	0.27	79,79,79,79	0
56	MG	1a	1743	1/1	0.75	0.22	73,73,73,73	0
56	MG	2A	3669	1/1	0.75	0.23	71,71,71,71	0
56	MG	2A	3681	1/1	0.75	0.21	67,67,67,67	0
56	MG	1w	106	1/1	0.75	0.12	96,96,96,96	0
56	MG	2A	3054	1/1	0.75	0.24	70,70,70,70	0
56	MG	1a	1642	1/1	0.75	0.47	88,88,88,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3287	1/1	0.75	0.16	79,79,79,79	0
56	MG	2A	3290	1/1	0.75	0.39	83,83,83,83	0
56	MG	2A	3127	1/1	0.75	0.23	82,82,82,82	0
56	MG	2B	202	1/1	0.75	0.19	74,74,74,74	0
56	MG	2A	3371	1/1	0.75	0.18	91,91,91,91	0
56	MG	2A	3733	1/1	0.76	0.21	74,74,74,74	0
56	MG	1A	4038	1/1	0.76	0.13	41,41,41,41	0
56	MG	1A	3854	1/1	0.76	0.23	62,62,62,62	0
56	MG	2A	3332	1/1	0.76	0.34	82,82,82,82	0
56	MG	2A	3413	1/1	0.76	0.23	71,71,71,71	0
56	MG	1A	3457	1/1	0.76	0.29	85,85,85,85	0
56	MG	2a	1646	1/1	0.76	0.37	82,82,82,82	0
56	MG	2A	3699	1/1	0.76	0.15	80,80,80,80	0
56	MG	2B	208	1/1	0.76	0.26	75,75,75,75	0
56	MG	1A	3635	1/1	0.77	0.25	63,63,63,63	0
56	MG	1A	3690	1/1	0.77	0.22	72,72,72,72	0
56	MG	1A	3743	1/1	0.77	0.18	61,61,61,61	0
56	MG	1A	4079	1/1	0.77	0.13	59,59,59,59	0
56	MG	1a	1716	1/1	0.77	0.25	67,67,67,67	0
56	MG	1A	3531	1/1	0.77	0.20	87,87,87,87	0
56	MG	1A	3298	1/1	0.77	0.17	57,57,57,57	0
56	MG	2A	3863	1/1	0.77	0.22	79,79,79,79	0
56	MG	2A	3475	1/1	0.77	0.26	80,80,80,80	0
56	MG	2A	3869	1/1	0.77	0.18	70,70,70,70	0
56	MG	2A	3496	1/1	0.77	0.18	75,75,75,75	0
56	MG	1a	1646	1/1	0.77	0.35	78,78,78,78	0
56	MG	2A	3263	1/1	0.77	0.17	81,81,81,81	0
56	MG	2E	308	1/1	0.77	0.24	79,79,79,79	0
56	MG	2A	3616	1/1	0.77	0.19	77,77,77,77	0
56	MG	2A	3075	1/1	0.77	0.20	82,82,82,82	0
56	MG	2A	3090	1/1	0.77	0.20	78,78,78,78	0
56	MG	2A	3091	1/1	0.77	0.18	75,75,75,75	0
56	MG	2A	3357	1/1	0.77	0.17	76,76,76,76	0
56	MG	2A	3122	1/1	0.77	0.24	77,77,77,77	0
56	MG	2y	107	1/1	0.77	0.26	88,88,88,88	0
56	MG	2A	3666	1/1	0.78	0.18	77,77,77,77	0
56	MG	1A	3694	1/1	0.78	0.18	68,68,68,68	0
56	MG	2a	1711	1/1	0.78	0.24	91,91,91,91	0
56	MG	2a	1718	1/1	0.78	0.37	80,80,80,80	0
56	MG	1B	233	1/1	0.78	0.17	61,61,61,61	0
56	MG	2a	1725	1/1	0.78	0.27	75,75,75,75	0
56	MG	1A	4098	1/1	0.78	0.21	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1761	1/1	0.78	0.21	79,79,79,79	0
56	MG	2a	1733	1/1	0.78	0.28	81,81,81,81	0
56	MG	2A	3727	1/1	0.78	0.21	76,76,76,76	0
56	MG	2A	3529	1/1	0.78	0.12	63,63,63,63	0
56	MG	2a	1808	1/1	0.78	0.24	74,74,74,74	0
56	MG	1A	3982	1/1	0.78	0.17	83,83,83,83	0
56	MG	2A	3753	1/1	0.78	0.21	62,62,62,62	0
56	MG	2a	1825	1/1	0.78	0.26	82,82,82,82	0
56	MG	2a	1621	1/1	0.78	0.25	79,79,79,79	0
56	MG	2a	1624	1/1	0.78	0.16	88,88,88,88	0
56	MG	2a	1629	1/1	0.78	0.26	80,80,80,80	0
56	MG	2a	1632	1/1	0.78	0.29	78,78,78,78	0
56	MG	1A	4086	1/1	0.78	0.16	62,62,62,62	0
56	MG	2A	3102	1/1	0.78	0.35	90,90,90,90	0
56	MG	14	101	1/1	0.78	0.13	86,86,86,86	0
56	MG	1a	1632	1/1	0.78	0.20	71,71,71,71	0
56	MG	1a	1721	1/1	0.78	0.34	78,78,78,78	0
56	MG	2A	3262	1/1	0.79	0.30	80,80,80,80	0
56	MG	2A	3314	1/1	0.79	0.17	78,78,78,78	0
56	MG	1A	3756	1/1	0.79	0.16	51,51,51,51	0
56	MG	2A	3406	1/1	0.79	0.20	79,79,79,79	0
56	MG	2A	3409	1/1	0.79	0.14	73,73,73,73	0
56	MG	2A	3172	1/1	0.79	0.27	84,84,84,84	0
56	MG	2A	3445	1/1	0.79	0.38	70,70,70,70	0
56	MG	28	101	1/1	0.79	0.33	86,86,86,86	0
56	MG	1A	3304	1/1	0.79	0.32	70,70,70,70	0
56	MG	2a	1616	1/1	0.79	0.17	74,74,74,74	0
56	MG	2a	1759	1/1	0.79	0.11	86,86,86,86	0
56	MG	1A	3498	1/1	0.79	0.23	73,73,73,73	0
56	MG	1A	3388	1/1	0.79	0.17	75,75,75,75	0
56	MG	1A	3732	1/1	0.79	0.20	57,57,57,57	0
56	MG	2A	3491	1/1	0.79	0.43	72,72,72,72	0
56	MG	2A	3353	1/1	0.79	0.17	72,72,72,72	0
56	MG	2A	3501	1/1	0.79	0.24	72,72,72,72	0
56	MG	2A	3823	1/1	0.79	0.12	78,78,78,78	0
56	MG	2w	103	1/1	0.79	0.13	85,85,85,85	0
56	MG	1A	3436	1/1	0.79	0.21	67,67,67,67	0
56	MG	1a	1637	1/1	0.79	0.25	79,79,79,79	0
56	MG	2A	3576	1/1	0.79	0.15	68,68,68,68	0
56	MG	2a	1670	1/1	0.79	0.28	76,76,76,76	0
56	MG	2a	1685	1/1	0.79	0.26	79,79,79,79	0
56	MG	1A	4067	1/1	0.79	0.23	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	1735	1/1	0.80	0.16	75,75,75,75	0
56	MG	2a	1666	1/1	0.80	0.15	82,82,82,82	0
56	MG	2A	3272	1/1	0.80	0.18	73,73,73,73	0
56	MG	2A	3154	1/1	0.80	0.20	87,87,87,87	0
56	MG	2A	3166	1/1	0.80	0.42	79,79,79,79	0
56	MG	2A	3537	1/1	0.80	0.18	74,74,74,74	0
56	MG	1A	3938	1/1	0.80	0.13	50,50,50,50	0
56	MG	2a	1717	1/1	0.80	0.38	82,82,82,82	0
56	MG	2A	3554	1/1	0.80	0.21	57,57,57,57	0
56	MG	2A	3868	1/1	0.80	0.23	66,66,66,66	0
56	MG	1x	111	1/1	0.80	0.18	72,72,72,72	0
56	MG	2A	3873	1/1	0.80	0.20	70,70,70,70	0
56	MG	2A	3389	1/1	0.80	0.23	79,79,79,79	0
56	MG	2A	3051	1/1	0.80	0.21	75,75,75,75	0
56	MG	1a	1682	1/1	0.80	0.25	81,81,81,81	0
56	MG	1A	3416	1/1	0.80	0.17	76,76,76,76	0
56	MG	2A	3222	1/1	0.80	0.20	69,69,69,69	0
56	MG	2a	1786	1/1	0.80	0.20	69,69,69,69	0
56	MG	2A	3664	1/1	0.80	0.21	78,78,78,78	0
56	MG	1A	3356	1/1	0.80	0.19	71,71,71,71	0
56	MG	2A	3668	1/1	0.80	0.14	75,75,75,75	0
56	MG	2a	1823	1/1	0.80	0.21	72,72,72,72	0
56	MG	1a	1611	1/1	0.80	0.29	74,74,74,74	0
56	MG	2f	202	1/1	0.80	0.17	87,87,87,87	0
56	MG	1A	4008	1/1	0.80	0.32	39,39,39,39	0
56	MG	2a	1619	1/1	0.80	0.15	74,74,74,74	0
56	MG	1A	3062	1/1	0.80	0.21	59,59,59,59	0
56	MG	2A	3333	1/1	0.80	0.23	62,62,62,62	0
56	MG	2A	3703	1/1	0.80	0.19	78,78,78,78	0
56	MG	2A	3713	1/1	0.80	0.15	66,66,66,66	0
56	MG	1A	3717	1/1	0.80	0.17	49,49,49,49	0
56	MG	2A	3341	1/1	0.80	0.32	81,81,81,81	0
56	MG	2A	3484	1/1	0.80	0.18	72,72,72,72	0
56	MG	2A	3751	1/1	0.80	0.15	64,64,64,64	0
56	MG	2A	3452	1/1	0.81	0.18	66,66,66,66	0
56	MG	2A	3192	1/1	0.81	0.17	81,81,81,81	0
56	MG	2a	1757	1/1	0.81	0.14	77,77,77,77	0
56	MG	1A	3210	1/1	0.81	0.16	58,58,58,58	0
56	MG	2A	3204	1/1	0.81	0.25	77,77,77,77	0
56	MG	2a	1796	1/1	0.81	0.26	83,83,83,83	0
56	MG	2a	1800	1/1	0.81	0.53	83,83,83,83	0
56	MG	1a	1640	1/1	0.81	0.28	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	2A	3355	1/1	0.81	0.16	69,69,69,69	0
56	MG	1A	3517	1/1	0.81	0.23	61,61,61,61	0
56	MG	1A	4037	1/1	0.81	0.19	61,61,61,61	0
56	MG	2A	3384	1/1	0.81	0.23	78,78,78,78	0
56	MG	1a	1662	1/1	0.81	0.20	72,72,72,72	0
56	MG	1a	1669	1/1	0.81	0.29	68,68,68,68	0
56	MG	1a	1680	1/1	0.81	0.26	76,76,76,76	0
56	MG	2A	3398	1/1	0.81	0.17	69,69,69,69	0
56	MG	2A	3146	1/1	0.81	0.32	79,79,79,79	0
56	MG	2w	104	1/1	0.81	0.19	83,83,83,83	0
56	MG	2A	3577	1/1	0.81	0.26	80,80,80,80	0
56	MG	2w	106	1/1	0.81	0.14	94,94,94,94	0
56	MG	1A	3272	1/1	0.81	0.19	66,66,66,66	0
56	MG	1a	1748	1/1	0.81	0.20	84,84,84,84	0
56	MG	2y	102	1/1	0.81	0.16	86,86,86,86	0
56	MG	2y	103	1/1	0.81	0.10	84,84,84,84	0
56	MG	2y	104	1/1	0.81	0.10	85,85,85,85	0
56	MG	1A	3250	1/1	0.81	0.23	81,81,81,81	0
56	MG	2A	3059	1/1	0.81	0.17	70,70,70,70	0
56	MG	2a	1737	1/1	0.81	0.32	74,74,74,74	0
56	MG	1a	1676	1/1	0.82	0.30	79,79,79,79	0
56	MG	2A	3206	1/1	0.82	0.17	77,77,77,77	0
56	MG	2A	3343	1/1	0.82	0.16	83,83,83,83	0
56	MG	1A	3862	1/1	0.82	0.17	77,77,77,77	0
56	MG	1E	310	1/1	0.82	0.19	70,70,70,70	0
56	MG	1A	3869	1/1	0.82	0.16	54,54,54,54	0
56	MG	2a	1660	1/1	0.82	0.21	93,93,93,93	0
56	MG	2A	3228	1/1	0.82	0.17	64,64,64,64	0
56	MG	2a	1669	1/1	0.82	0.15	87,87,87,87	0
56	MG	1a	1699	1/1	0.82	0.37	81,81,81,81	0
56	MG	2a	1672	1/1	0.82	0.19	80,80,80,80	0
56	MG	2A	3247	1/1	0.82	0.26	62,62,62,62	0
56	MG	2a	1689	1/1	0.82	0.17	80,80,80,80	0
56	MG	2A	3358	1/1	0.82	0.25	70,70,70,70	0
56	MG	2a	1702	1/1	0.82	0.34	81,81,81,81	0
56	MG	1A	3024	1/1	0.82	0.13	61,61,61,61	0
56	MG	2A	3373	1/1	0.82	0.26	80,80,80,80	0
56	MG	1W	205	1/1	0.82	0.23	44,44,44,44	0
56	MG	2A	3388	1/1	0.82	0.19	79,79,79,79	0
56	MG	2A	3254	1/1	0.82	0.26	71,71,71,71	0
56	MG	2A	3261	1/1	0.82	0.30	72,72,72,72	0
56	MG	2A	3065	1/1	0.82	0.18	83,83,83,83	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4075	1/1	0.82	0.11	38,38,38,38	0
56	MG	2A	3265	1/1	0.82	0.29	80,80,80,80	0
56	MG	2A	3405	1/1	0.82	0.13	74,74,74,74	0
56	MG	1A	3480	1/1	0.82	0.17	64,64,64,64	0
56	MG	2A	3829	1/1	0.82	0.16	48,48,48,48	0
56	MG	2A	3836	1/1	0.82	0.14	72,72,72,72	0
56	MG	1A	3095	1/1	0.82	0.34	71,71,71,71	0
56	MG	2A	3844	1/1	0.82	0.16	68,68,68,68	0
56	MG	2A	3852	1/1	0.82	0.17	65,65,65,65	0
56	MG	1a	1630	1/1	0.82	0.15	73,73,73,73	0
56	MG	2A	3441	1/1	0.82	0.31	71,71,71,71	0
56	MG	1A	3101	1/1	0.82	0.16	70,70,70,70	0
56	MG	2A	3103	1/1	0.82	0.21	66,66,66,66	0
56	MG	2A	3106	1/1	0.82	0.24	87,87,87,87	0
56	MG	2A	3463	1/1	0.82	0.12	68,68,68,68	0
56	MG	1A	3847	1/1	0.82	0.18	53,53,53,53	0
56	MG	2A	3291	1/1	0.82	0.26	74,74,74,74	0
56	MG	1A	3165	1/1	0.82	0.25	68,68,68,68	0
56	MG	2A	3294	1/1	0.82	0.20	68,68,68,68	0
56	MG	1A	4100	1/1	0.82	0.12	69,69,69,69	0
56	MG	2A	3301	1/1	0.82	0.22	82,82,82,82	0
56	MG	26	101	1/1	0.82	0.25	73,73,73,73	0
56	MG	1A	4033	1/1	0.82	0.13	84,84,84,84	0
56	MG	1a	1661	1/1	0.82	0.22	67,67,67,67	0
56	MG	1B	228	1/1	0.82	0.15	70,70,70,70	0
56	MG	2A	3317	1/1	0.82	0.20	74,74,74,74	0
56	MG	1f	202	1/1	0.82	0.25	82,82,82,82	0
56	MG	1n	101	1/1	0.82	0.21	68,68,68,68	0
56	MG	1A	3198	1/1	0.82	0.21	58,58,58,58	0
56	MG	2a	1628	1/1	0.82	0.12	80,80,80,80	0
56	MG	2A	3596	1/1	0.82	0.21	70,70,70,70	0
56	MG	2A	3153	1/1	0.83	0.25	68,68,68,68	0
56	MG	2A	3765	1/1	0.83	0.24	53,53,53,53	0
56	MG	2A	3352	1/1	0.83	0.13	66,66,66,66	0
56	MG	2A	3810	1/1	0.83	0.10	90,90,90,90	0
56	MG	1a	1625	1/1	0.83	0.14	64,64,64,64	0
56	MG	1A	3258	1/1	0.83	0.11	63,63,63,63	0
56	MG	1x	105	1/1	0.83	0.21	75,75,75,75	0
56	MG	1A	3414	1/1	0.83	0.21	42,42,42,42	0
56	MG	2a	1704	1/1	0.83	0.19	84,84,84,84	0
56	MG	2A	3520	1/1	0.83	0.23	78,78,78,78	0
56	MG	2A	3521	1/1	0.83	0.13	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3499	1/1	0.83	0.39	68,68,68,68	0
56	MG	1A	3353	1/1	0.83	0.21	65,65,65,65	0
56	MG	2a	1722	1/1	0.83	0.30	83,83,83,83	0
56	MG	2A	3544	1/1	0.83	0.19	60,60,60,60	0
56	MG	2A	3199	1/1	0.83	0.20	64,64,64,64	0
56	MG	2a	1726	1/1	0.83	0.42	80,80,80,80	0
56	MG	2A	3379	1/1	0.83	0.26	75,75,75,75	0
56	MG	2A	3058	1/1	0.83	0.34	75,75,75,75	0
56	MG	1A	3420	1/1	0.83	0.33	80,80,80,80	0
56	MG	2a	1736	1/1	0.83	0.21	85,85,85,85	0
56	MG	2A	3063	1/1	0.83	0.21	66,66,66,66	0
56	MG	2a	1741	1/1	0.83	0.25	69,69,69,69	0
56	MG	2B	217	1/1	0.83	0.14	72,72,72,72	0
56	MG	1A	4046	1/1	0.83	0.16	48,48,48,48	0
56	MG	2A	3607	1/1	0.83	0.16	71,71,71,71	0
56	MG	2A	3219	1/1	0.83	0.19	75,75,75,75	0
56	MG	2a	1763	1/1	0.83	0.10	96,96,96,96	0
56	MG	1A	4065	1/1	0.83	0.15	58,58,58,58	0
56	MG	1G	203	1/1	0.83	0.13	82,82,82,82	0
56	MG	1O	206	1/1	0.83	0.29	66,66,66,66	0
56	MG	28	105	1/1	0.83	0.30	70,70,70,70	0
56	MG	2A	3316	1/1	0.83	0.12	70,70,70,70	0
56	MG	2a	1607	1/1	0.83	0.29	76,76,76,76	0
56	MG	2A	3407	1/1	0.83	0.12	70,70,70,70	0
56	MG	1A	3545	1/1	0.83	0.24	55,55,55,55	0
56	MG	1A	3962	1/1	0.83	0.19	61,61,61,61	0
56	MG	2A	3676	1/1	0.83	0.15	69,69,69,69	0
56	MG	2t	201	1/1	0.83	0.21	63,63,63,63	0
56	MG	2A	3425	1/1	0.83	0.31	66,66,66,66	0
56	MG	2a	1627	1/1	0.83	0.11	77,77,77,77	0
56	MG	2A	3440	1/1	0.83	0.39	73,73,73,73	0
56	MG	1A	3208	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3252	1/1	0.83	0.27	90,90,90,90	0
56	MG	2a	1634	1/1	0.83	0.18	87,87,87,87	0
56	MG	2a	1635	1/1	0.83	0.18	85,85,85,85	0
56	MG	2x	101	1/1	0.83	0.12	74,74,74,74	0
56	MG	1A	3357	1/1	0.83	0.14	58,58,58,58	0
56	MG	2A	3717	1/1	0.83	0.14	57,57,57,57	0
56	MG	1w	101	1/1	0.83	0.12	73,73,73,73	0
56	MG	1A	3648	1/1	0.83	0.14	60,60,60,60	0
56	MG	1A	3841	1/1	0.83	0.24	68,68,68,68	0
56	MG	2A	3470	1/1	0.83	0.13	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	1663	1/1	0.83	0.29	69,69,69,69	0
56	MG	2A	3182	1/1	0.84	0.12	61,61,61,61	0
56	MG	2A	3737	1/1	0.84	0.19	67,67,67,67	0
56	MG	1w	107	1/1	0.84	0.22	78,78,78,78	0
56	MG	2a	1662	1/1	0.84	0.17	80,80,80,80	0
56	MG	2A	3453	1/1	0.84	0.28	67,67,67,67	0
56	MG	1A	3855	1/1	0.84	0.12	58,58,58,58	0
56	MG	2A	3759	1/1	0.84	0.20	70,70,70,70	0
56	MG	1x	110	1/1	0.84	0.18	82,82,82,82	0
56	MG	2A	3785	1/1	0.84	0.14	77,77,77,77	0
56	MG	2a	1676	1/1	0.84	0.14	69,69,69,69	0
56	MG	1A	3522	1/1	0.84	0.22	67,67,67,67	0
56	MG	2A	3469	1/1	0.84	0.33	76,76,76,76	0
56	MG	2A	3008	1/1	0.84	0.14	58,58,58,58	0
56	MG	1A	3472	1/1	0.84	0.14	67,67,67,67	0
56	MG	1A	3916	1/1	0.84	0.12	51,51,51,51	0
56	MG	2A	3339	1/1	0.84	0.19	75,75,75,75	0
56	MG	1a	1606	1/1	0.84	0.10	77,77,77,77	0
56	MG	1A	3932	1/1	0.84	0.11	64,64,64,64	0
56	MG	1A	3731	1/1	0.84	0.20	69,69,69,69	0
56	MG	2A	3512	1/1	0.84	0.29	64,64,64,64	0
56	MG	2A	3064	1/1	0.84	0.19	78,78,78,78	0
56	MG	1A	3538	1/1	0.84	0.18	60,60,60,60	0
56	MG	1a	1742	1/1	0.84	0.19	77,77,77,77	0
56	MG	2A	3068	1/1	0.84	0.35	80,80,80,80	0
56	MG	2B	201	1/1	0.84	0.23	86,86,86,86	0
56	MG	2A	3074	1/1	0.84	0.14	69,69,69,69	0
56	MG	2B	206	1/1	0.84	0.24	74,74,74,74	0
56	MG	1A	3542	1/1	0.84	0.16	77,77,77,77	0
56	MG	2B	213	1/1	0.84	0.30	77,77,77,77	0
56	MG	2a	1742	1/1	0.84	0.19	80,80,80,80	0
56	MG	2a	1747	1/1	0.84	0.38	69,69,69,69	0
56	MG	1A	3316	1/1	0.84	0.32	63,63,63,63	0
56	MG	1A	4001	1/1	0.84	0.15	70,70,70,70	0
56	MG	2A	3092	1/1	0.84	0.29	73,73,73,73	0
56	MG	1A	3482	1/1	0.84	0.22	72,72,72,72	0
56	MG	2V	201	1/1	0.84	0.39	59,59,59,59	0
56	MG	1A	3590	1/1	0.84	0.13	61,61,61,61	0
56	MG	2a	1795	1/1	0.84	0.21	65,65,65,65	0
56	MG	25	105	1/1	0.84	0.18	81,81,81,81	0
56	MG	2A	3385	1/1	0.84	0.30	78,78,78,78	0
56	MG	2a	1805	1/1	0.84	0.28	76,76,76,76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1806	1/1	0.84	0.17	72,72,72,72	0
56	MG	2A	3611	1/1	0.84	0.14	60,60,60,60	0
56	MG	2a	1809	1/1	0.84	0.20	78,78,78,78	0
56	MG	1a	1659	1/1	0.84	0.21	82,82,82,82	0
56	MG	2A	3108	1/1	0.84	0.41	61,61,61,61	0
56	MG	2A	3111	1/1	0.84	0.36	77,77,77,77	0
56	MG	2a	1612	1/1	0.84	0.22	80,80,80,80	0
56	MG	1A	4020	1/1	0.84	0.09	56,56,56,56	0
56	MG	1l	202	1/1	0.84	0.14	71,71,71,71	0
56	MG	2a	1618	1/1	0.84	0.20	76,76,76,76	0
56	MG	2v	101	1/1	0.84	0.13	81,81,81,81	0
56	MG	2v	102	1/1	0.84	0.24	80,80,80,80	0
56	MG	2A	3289	1/1	0.84	0.16	79,79,79,79	0
56	MG	2A	3135	1/1	0.84	0.27	63,63,63,63	0
56	MG	1A	3597	1/1	0.84	0.13	54,54,54,54	0
56	MG	2a	1626	1/1	0.84	0.20	68,68,68,68	0
56	MG	1A	3259	1/1	0.84	0.11	83,83,83,83	0
56	MG	1E	311	1/1	0.84	0.16	79,79,79,79	0
56	MG	1A	3379	1/1	0.84	0.22	69,69,69,69	0
56	MG	2a	1630	1/1	0.84	0.18	74,74,74,74	0
56	MG	1A	3671	1/1	0.84	0.12	54,54,54,54	0
56	MG	2A	3439	1/1	0.84	0.30	75,75,75,75	0
56	MG	1A	3463	1/1	0.84	0.20	64,64,64,64	0
56	MG	2A	3309	1/1	0.84	0.32	79,79,79,79	0
56	MG	2a	1642	1/1	0.84	0.25	72,72,72,72	0
56	MG	2A	3442	1/1	0.84	0.27	68,68,68,68	0
56	MG	2A	3729	1/1	0.84	0.21	83,83,83,83	0
56	MG	1A	4012	1/1	0.85	0.09	79,79,79,79	0
56	MG	1A	3430	1/1	0.85	0.29	64,64,64,64	0
56	MG	2A	3142	1/1	0.85	0.20	66,66,66,66	0
56	MG	2A	3325	1/1	0.85	0.21	76,76,76,76	0
56	MG	2A	3558	1/1	0.85	0.13	74,74,74,74	0
56	MG	2A	3794	1/1	0.85	0.18	59,59,59,59	0
56	MG	2A	3258	1/1	0.85	0.12	57,57,57,57	0
56	MG	10	102	1/1	0.85	0.25	66,66,66,66	0
56	MG	2A	3336	1/1	0.85	0.20	77,77,77,77	0
56	MG	1A	3561	1/1	0.85	0.20	78,78,78,78	0
56	MG	1a	1604	1/1	0.85	0.13	72,72,72,72	0
56	MG	1A	3342	1/1	0.85	0.11	59,59,59,59	0
56	MG	1A	3735	1/1	0.85	0.18	54,54,54,54	0
56	MG	2A	3270	1/1	0.85	0.12	62,62,62,62	0
56	MG	2a	1771	1/1	0.85	0.09	81,81,81,81	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	3446	1/1	0.85	0.15	68,68,68,68	0
56	MG	1A	3345	1/1	0.85	0.11	59,59,59,59	0
56	MG	1A	3391	1/1	0.85	0.16	55,55,55,55	0
56	MG	2a	1797	1/1	0.85	0.16	81,81,81,81	0
56	MG	2a	1643	1/1	0.85	0.25	77,77,77,77	0
56	MG	1A	3809	1/1	0.85	0.12	63,63,63,63	0
56	MG	2a	1650	1/1	0.85	0.32	73,73,73,73	0
56	MG	2a	1653	1/1	0.85	0.29	78,78,78,78	0
56	MG	1A	3050	1/1	0.85	0.35	46,46,46,46	0
56	MG	1x	101	1/1	0.85	0.20	68,68,68,68	0
56	MG	2a	1814	1/1	0.85	0.28	65,65,65,65	0
56	MG	1A	3103	1/1	0.85	0.23	73,73,73,73	0
56	MG	2a	1818	1/1	0.85	0.31	73,73,73,73	0
56	MG	2A	3367	1/1	0.85	0.09	82,82,82,82	0
56	MG	2A	3695	1/1	0.85	0.18	66,66,66,66	0
56	MG	1A	3823	1/1	0.85	0.18	60,60,60,60	0
56	MG	2j	201	1/1	0.85	0.17	80,80,80,80	0
56	MG	2B	209	1/1	0.85	0.24	75,75,75,75	0
56	MG	2l	203	1/1	0.85	0.22	80,80,80,80	0
56	MG	1T	201	1/1	0.85	0.16	68,68,68,68	0
56	MG	2B	214	1/1	0.85	0.17	76,76,76,76	0
56	MG	2a	1671	1/1	0.85	0.26	61,61,61,61	0
56	MG	2A	3377	1/1	0.85	0.25	73,73,73,73	0
56	MG	1A	3140	1/1	0.85	0.22	49,49,49,49	0
56	MG	2E	305	1/1	0.85	0.25	77,77,77,77	0
56	MG	2A	3715	1/1	0.85	0.16	70,70,70,70	0
56	MG	2a	1699	1/1	0.85	0.22	83,83,83,83	0
56	MG	2F	304	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3110	1/1	0.85	0.19	86,86,86,86	0
56	MG	2A	3723	1/1	0.85	0.17	61,61,61,61	0
56	MG	2A	3023	1/1	0.85	0.18	75,75,75,75	0
56	MG	2A	3234	1/1	0.85	0.24	65,65,65,65	0
56	MG	2A	3113	1/1	0.85	0.20	68,68,68,68	0
56	MG	2A	3115	1/1	0.85	0.24	73,73,73,73	0
56	MG	2A	3738	1/1	0.85	0.18	66,66,66,66	0
56	MG	1A	3708	1/1	0.85	0.14	53,53,53,53	0
56	MG	2A	3745	1/1	0.85	0.12	82,82,82,82	0
56	MG	2A	3845	1/1	0.86	0.18	79,79,79,79	0
56	MG	2A	3280	1/1	0.86	0.27	74,74,74,74	0
56	MG	2A	3282	1/1	0.86	0.21	67,67,67,67	0
56	MG	1e	201	1/1	0.86	0.39	74,74,74,74	0
56	MG	1e	202	1/1	0.86	0.12	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1693	1/1	0.86	0.26	73,73,73,73	0
56	MG	1A	4072	1/1	0.86	0.10	43,43,43,43	0
56	MG	1A	4073	1/1	0.86	0.12	59,59,59,59	0
56	MG	2A	3872	1/1	0.86	0.09	60,60,60,60	0
56	MG	2a	1703	1/1	0.86	0.14	79,79,79,79	0
56	MG	1A	3843	1/1	0.86	0.14	44,44,44,44	0
56	MG	2A	3292	1/1	0.86	0.27	70,70,70,70	0
56	MG	2A	3202	1/1	0.86	0.18	62,62,62,62	0
56	MG	2B	204	1/1	0.86	0.19	81,81,81,81	0
56	MG	2B	205	1/1	0.86	0.25	73,73,73,73	0
56	MG	2A	3203	1/1	0.86	0.36	72,72,72,72	0
56	MG	2A	3637	1/1	0.86	0.23	79,79,79,79	0
56	MG	1A	3845	1/1	0.86	0.12	57,57,57,57	0
56	MG	1A	3418	1/1	0.86	0.18	61,61,61,61	0
56	MG	2A	3653	1/1	0.86	0.19	61,61,61,61	0
56	MG	2A	3659	1/1	0.86	0.12	71,71,71,71	0
56	MG	1A	4095	1/1	0.86	0.16	70,70,70,70	0
56	MG	2A	3097	1/1	0.86	0.24	72,72,72,72	0
56	MG	2A	3665	1/1	0.86	0.16	75,75,75,75	0
56	MG	2a	1738	1/1	0.86	0.36	67,67,67,67	0
56	MG	2a	1740	1/1	0.86	0.28	71,71,71,71	0
56	MG	2A	3214	1/1	0.86	0.32	76,76,76,76	0
56	MG	2A	3411	1/1	0.86	0.11	74,74,74,74	0
56	MG	2P	201	1/1	0.86	0.16	75,75,75,75	0
56	MG	2A	3098	1/1	0.86	0.21	79,79,79,79	0
56	MG	2Z	301	1/1	0.86	0.27	73,73,73,73	0
56	MG	2A	3220	1/1	0.86	0.23	69,69,69,69	0
56	MG	2I	101	1/1	0.86	0.14	78,78,78,78	0
56	MG	2A	3427	1/1	0.86	0.33	64,64,64,64	0
56	MG	1A	3658	1/1	0.86	0.15	71,71,71,71	0
56	MG	1A	3484	1/1	0.86	0.37	59,59,59,59	0
56	MG	1A	3765	1/1	0.86	0.22	58,58,58,58	0
56	MG	2A	3331	1/1	0.86	0.23	78,78,78,78	0
56	MG	2A	3711	1/1	0.86	0.12	57,57,57,57	0
56	MG	2a	1798	1/1	0.86	0.19	80,80,80,80	0
56	MG	2a	1609	1/1	0.86	0.35	73,73,73,73	0
56	MG	1A	3494	1/1	0.86	0.17	58,58,58,58	0
56	MG	2A	3447	1/1	0.86	0.11	55,55,55,55	0
56	MG	1B	212	1/1	0.86	0.30	69,69,69,69	0
56	MG	1A	3063	1/1	0.86	0.40	72,72,72,72	0
56	MG	1a	1626	1/1	0.86	0.29	70,70,70,70	0
56	MG	2A	3457	1/1	0.86	0.29	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1y	102	1/1	0.86	0.08	84,84,84,84	0
56	MG	2A	3340	1/1	0.86	0.32	84,84,84,84	0
56	MG	2a	1822	1/1	0.86	0.12	73,73,73,73	0
56	MG	1A	3458	1/1	0.86	0.32	69,69,69,69	0
56	MG	2A	3342	1/1	0.86	0.28	84,84,84,84	0
56	MG	2A	3257	1/1	0.86	0.28	74,74,74,74	0
56	MG	2A	3747	1/1	0.86	0.17	48,48,48,48	0
56	MG	2A	3474	1/1	0.86	0.11	62,62,62,62	0
56	MG	1A	3422	1/1	0.86	0.14	67,67,67,67	0
56	MG	2A	3132	1/1	0.86	0.16	75,75,75,75	0
56	MG	2A	3032	1/1	0.86	0.14	70,70,70,70	0
56	MG	2a	1638	1/1	0.86	0.27	70,70,70,70	0
56	MG	1B	232	1/1	0.86	0.15	57,57,57,57	0
56	MG	2A	3792	1/1	0.86	0.11	68,68,68,68	0
56	MG	1A	3081	1/1	0.86	0.19	73,73,73,73	0
56	MG	2A	3797	1/1	0.86	0.11	70,70,70,70	0
56	MG	2A	3507	1/1	0.86	0.26	65,65,65,65	0
56	MG	2A	3802	1/1	0.86	0.14	76,76,76,76	0
56	MG	2A	3805	1/1	0.86	0.14	58,58,58,58	0
56	MG	1A	3835	1/1	0.86	0.11	53,53,53,53	0
56	MG	2A	3813	1/1	0.86	0.12	53,53,53,53	0
56	MG	1A	3968	1/1	0.86	0.09	54,54,54,54	0
56	MG	2A	3161	1/1	0.86	0.14	70,70,70,70	0
56	MG	1A	3300	1/1	0.86	0.19	61,61,61,61	0
56	MG	2a	1668	1/1	0.86	0.18	73,73,73,73	0
56	MG	1O	201	1/1	0.86	0.16	72,72,72,72	0
56	MG	2A	3372	1/1	0.86	0.21	57,57,57,57	0
56	MG	2a	1661	1/1	0.87	0.14	82,82,82,82	0
56	MG	1A	3475	1/1	0.87	0.10	51,51,51,51	0
56	MG	1x	109	1/1	0.87	0.22	76,76,76,76	0
56	MG	2A	3478	1/1	0.87	0.20	70,70,70,70	0
56	MG	2a	1667	1/1	0.87	0.21	88,88,88,88	0
56	MG	2A	3327	1/1	0.87	0.16	63,63,63,63	0
56	MG	2A	3487	1/1	0.87	0.19	65,65,65,65	0
56	MG	2A	3828	1/1	0.87	0.16	71,71,71,71	0
56	MG	1A	3526	1/1	0.87	0.19	61,61,61,61	0
56	MG	1A	3476	1/1	0.87	0.10	52,52,52,52	0
56	MG	2A	3498	1/1	0.87	0.12	63,63,63,63	0
56	MG	1a	1668	1/1	0.87	0.20	67,67,67,67	0
56	MG	1A	3478	1/1	0.87	0.12	67,67,67,67	0
56	MG	2A	3201	1/1	0.87	0.24	73,73,73,73	0
56	MG	2A	3855	1/1	0.87	0.13	68,68,68,68	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3266	1/1	0.87	0.15	67,67,67,67	0
56	MG	2A	3028	1/1	0.87	0.32	64,64,64,64	0
56	MG	1A	3719	1/1	0.87	0.10	58,58,58,58	0
56	MG	2A	3034	1/1	0.87	0.09	54,54,54,54	0
56	MG	2a	1705	1/1	0.87	0.32	73,73,73,73	0
56	MG	2a	1706	1/1	0.87	0.20	65,65,65,65	0
56	MG	1A	3848	1/1	0.87	0.14	52,52,52,52	0
56	MG	2a	1710	1/1	0.87	0.17	74,74,74,74	0
56	MG	1a	1684	1/1	0.87	0.22	74,74,74,74	0
56	MG	2a	1714	1/1	0.87	0.13	71,71,71,71	0
56	MG	1A	3729	1/1	0.87	0.13	51,51,51,51	0
56	MG	1a	1687	1/1	0.87	0.27	74,74,74,74	0
56	MG	2a	1720	1/1	0.87	0.18	78,78,78,78	0
56	MG	2A	3570	1/1	0.87	0.14	68,68,68,68	0
56	MG	2a	1723	1/1	0.87	0.20	89,89,89,89	0
56	MG	1I	201	1/1	0.87	0.15	74,74,74,74	0
56	MG	1N	202	1/1	0.87	0.10	52,52,52,52	0
56	MG	1A	3438	1/1	0.87	0.16	59,59,59,59	0
56	MG	2B	207	1/1	0.87	0.16	75,75,75,75	0
56	MG	1A	3378	1/1	0.87	0.42	63,63,63,63	0
56	MG	1A	3856	1/1	0.87	0.11	67,67,67,67	0
56	MG	1A	4048	1/1	0.87	0.14	60,60,60,60	0
56	MG	1A	4059	1/1	0.87	0.12	57,57,57,57	0
56	MG	2A	3624	1/1	0.87	0.17	69,69,69,69	0
56	MG	2A	3085	1/1	0.87	0.14	60,60,60,60	0
56	MG	2D	305	1/1	0.87	0.35	65,65,65,65	0
56	MG	1A	3349	1/1	0.87	0.24	60,60,60,60	0
56	MG	2a	1743	1/1	0.87	0.17	76,76,76,76	0
56	MG	2a	1745	1/1	0.87	0.28	80,80,80,80	0
56	MG	1A	3335	1/1	0.87	0.11	63,63,63,63	0
56	MG	2F	303	1/1	0.87	0.13	59,59,59,59	0
56	MG	1A	3900	1/1	0.87	0.11	40,40,40,40	0
56	MG	1A	3913	1/1	0.87	0.18	57,57,57,57	0
56	MG	19	101	1/1	0.87	0.22	63,63,63,63	0
56	MG	2R	201	1/1	0.87	0.25	66,66,66,66	0
56	MG	2R	202	1/1	0.87	0.14	63,63,63,63	0
56	MG	2A	3099	1/1	0.87	0.18	66,66,66,66	0
56	MG	1a	1603	1/1	0.87	0.16	74,74,74,74	0
56	MG	1A	3255	1/1	0.87	0.14	65,65,65,65	0
56	MG	1a	1605	1/1	0.87	0.14	71,71,71,71	0
56	MG	1d	301	1/1	0.87	0.38	70,70,70,70	0
56	MG	2a	1799	1/1	0.87	0.24	81,81,81,81	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	3609	1/1	0.87	0.19	54,54,54,54	0
56	MG	1A	3788	1/1	0.87	0.12	42,42,42,42	0
56	MG	2A	3685	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3688	1/1	0.87	0.29	73,73,73,73	0
56	MG	2A	3274	1/1	0.87	0.11	59,59,59,59	0
56	MG	1a	1616	1/1	0.87	0.12	83,83,83,83	0
56	MG	1l	201	1/1	0.87	0.11	91,91,91,91	0
56	MG	1A	3501	1/1	0.87	0.22	55,55,55,55	0
56	MG	2A	3126	1/1	0.87	0.09	59,59,59,59	0
56	MG	2a	1821	1/1	0.87	0.12	71,71,71,71	0
56	MG	2A	3418	1/1	0.87	0.25	57,57,57,57	0
56	MG	2A	3419	1/1	0.87	0.23	53,53,53,53	0
56	MG	1A	3511	1/1	0.87	0.25	77,77,77,77	0
56	MG	2A	3129	1/1	0.87	0.27	72,72,72,72	0
56	MG	2a	1625	1/1	0.87	0.16	77,77,77,77	0
56	MG	2A	3431	1/1	0.87	0.14	70,70,70,70	0
56	MG	2A	3435	1/1	0.87	0.29	70,70,70,70	0
56	MG	1v	101	1/1	0.87	0.25	76,76,76,76	0
56	MG	1A	3652	1/1	0.87	0.17	73,73,73,73	0
56	MG	2A	3137	1/1	0.87	0.18	62,62,62,62	0
56	MG	1A	3983	1/1	0.87	0.20	75,75,75,75	0
56	MG	2a	1633	1/1	0.87	0.38	78,78,78,78	0
56	MG	2A	3143	1/1	0.87	0.20	51,51,51,51	0
56	MG	2A	3297	1/1	0.87	0.27	81,81,81,81	0
56	MG	1A	3986	1/1	0.87	0.12	69,69,69,69	0
56	MG	2A	3300	1/1	0.87	0.37	62,62,62,62	0
56	MG	2A	3756	1/1	0.87	0.14	67,67,67,67	0
56	MG	2A	3758	1/1	0.87	0.19	75,75,75,75	0
56	MG	2x	106	1/1	0.87	0.14	65,65,65,65	0
56	MG	2A	3152	1/1	0.87	0.24	68,68,68,68	0
56	MG	1B	207	1/1	0.87	0.26	76,76,76,76	0
56	MG	1A	3408	1/1	0.87	0.14	64,64,64,64	0
56	MG	1B	215	1/1	0.87	0.12	56,56,56,56	0
56	MG	2A	3164	1/1	0.87	0.17	64,64,64,64	0
56	MG	1a	1649	1/1	0.87	0.25	67,67,67,67	0
56	MG	2A	3167	1/1	0.87	0.23	69,69,69,69	0
56	MG	1A	3836	1/1	0.88	0.18	59,59,59,59	0
56	MG	2A	3803	1/1	0.88	0.10	73,73,73,73	0
56	MG	2A	3804	1/1	0.88	0.09	70,70,70,70	0
56	MG	1A	4077	1/1	0.88	0.08	50,50,50,50	0
56	MG	1A	3427	1/1	0.88	0.20	64,64,64,64	0
56	MG	2A	3350	1/1	0.88	0.09	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	2A	3817	1/1	0.88	0.14	55,55,55,55	0
56	MG	1a	1681	1/1	0.88	0.19	69,69,69,69	0
56	MG	2A	3826	1/1	0.88	0.14	56,56,56,56	0
56	MG	1A	4085	1/1	0.88	0.15	66,66,66,66	0
56	MG	1Y	201	1/1	0.88	0.11	65,65,65,65	0
56	MG	2a	1679	1/1	0.88	0.29	80,80,80,80	0
56	MG	2a	1682	1/1	0.88	0.18	74,74,74,74	0
56	MG	2A	3116	1/1	0.88	0.47	80,80,80,80	0
56	MG	1A	3562	1/1	0.88	0.22	70,70,70,70	0
56	MG	2a	1690	1/1	0.88	0.21	77,77,77,77	0
56	MG	2a	1692	1/1	0.88	0.20	66,66,66,66	0
56	MG	1A	4093	1/1	0.88	0.24	68,68,68,68	0
56	MG	10	107	1/1	0.88	0.17	70,70,70,70	0
56	MG	2A	3847	1/1	0.88	0.11	63,63,63,63	0
56	MG	2A	3532	1/1	0.88	0.25	67,67,67,67	0
56	MG	2A	3854	1/1	0.88	0.11	47,47,47,47	0
56	MG	1a	1708	1/1	0.88	0.13	77,77,77,77	0
56	MG	1A	3724	1/1	0.88	0.12	57,57,57,57	0
56	MG	2A	3268	1/1	0.88	0.21	74,74,74,74	0
56	MG	2a	1707	1/1	0.88	0.26	72,72,72,72	0
56	MG	2A	3001	1/1	0.88	0.56	76,76,76,76	0
56	MG	2A	3376	1/1	0.88	0.45	77,77,77,77	0
56	MG	2A	3003	1/1	0.88	0.40	68,68,68,68	0
56	MG	2A	3005	1/1	0.88	0.42	81,81,81,81	0
56	MG	1A	3182	1/1	0.88	0.28	61,61,61,61	0
56	MG	2A	3594	1/1	0.88	0.11	63,63,63,63	0
56	MG	1A	3596	1/1	0.88	0.16	47,47,47,47	0
56	MG	2a	1721	1/1	0.88	0.19	76,76,76,76	0
56	MG	2A	3600	1/1	0.88	0.18	65,65,65,65	0
56	MG	2A	3275	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	3512	1/1	0.88	0.11	51,51,51,51	0
56	MG	2A	3390	1/1	0.88	0.19	72,72,72,72	0
56	MG	1A	3434	1/1	0.88	0.13	61,61,61,61	0
56	MG	2A	3393	1/1	0.88	0.21	64,64,64,64	0
56	MG	2a	1728	1/1	0.88	0.15	75,75,75,75	0
56	MG	2B	211	1/1	0.88	0.20	65,65,65,65	0
56	MG	1A	3610	1/1	0.88	0.12	56,56,56,56	0
56	MG	2A	3041	1/1	0.88	0.26	68,68,68,68	0
56	MG	2A	3648	1/1	0.88	0.26	64,64,64,64	0
56	MG	2A	3286	1/1	0.88	0.26	82,82,82,82	0
56	MG	2a	1739	1/1	0.88	0.31	68,68,68,68	0
56	MG	2A	3401	1/1	0.88	0.12	82,82,82,82	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2E	302	1/1	0.88	0.17	66,66,66,66	0
56	MG	2A	3657	1/1	0.88	0.20	74,74,74,74	0
56	MG	2A	3163	1/1	0.88	0.33	78,78,78,78	0
56	MG	2a	1744	1/1	0.88	0.36	59,59,59,59	0
56	MG	1A	3754	1/1	0.88	0.31	65,65,65,65	0
56	MG	1A	3297	1/1	0.88	0.11	43,43,43,43	0
56	MG	1A	3241	1/1	0.88	0.13	52,52,52,52	0
56	MG	2A	3410	1/1	0.88	0.22	70,70,70,70	0
56	MG	1a	1744	1/1	0.88	0.12	79,79,79,79	0
56	MG	1A	3885	1/1	0.88	0.16	54,54,54,54	0
56	MG	2A	3416	1/1	0.88	0.25	64,64,64,64	0
56	MG	2A	3180	1/1	0.88	0.17	65,65,65,65	0
56	MG	2a	1777	1/1	0.88	0.18	81,81,81,81	0
56	MG	1A	3372	1/1	0.88	0.28	49,49,49,49	0
56	MG	1A	4045	1/1	0.88	0.12	59,59,59,59	0
56	MG	2A	3193	1/1	0.88	0.27	74,74,74,74	0
56	MG	1a	1782	1/1	0.88	0.15	62,62,62,62	0
56	MG	27	103	1/1	0.88	0.13	59,59,59,59	0
56	MG	2A	3433	1/1	0.88	0.26	63,63,63,63	0
56	MG	2A	3434	1/1	0.88	0.36	79,79,79,79	0
56	MG	2a	1601	1/1	0.88	0.13	72,72,72,72	0
56	MG	2A	3704	1/1	0.88	0.18	61,61,61,61	0
56	MG	1A	3002	1/1	0.88	0.19	57,57,57,57	0
56	MG	2a	1608	1/1	0.88	0.17	72,72,72,72	0
56	MG	2A	3438	1/1	0.88	0.18	61,61,61,61	0
56	MG	1B	234	1/1	0.88	0.12	71,71,71,71	0
56	MG	2A	3311	1/1	0.88	0.11	81,81,81,81	0
56	MG	2a	1816	1/1	0.88	0.14	80,80,80,80	0
56	MG	2a	1817	1/1	0.88	0.25	61,61,61,61	0
56	MG	1A	3348	1/1	0.88	0.15	69,69,69,69	0
56	MG	2a	1820	1/1	0.88	0.28	68,68,68,68	0
56	MG	1A	4050	1/1	0.88	0.12	52,52,52,52	0
56	MG	2A	3728	1/1	0.88	0.17	61,61,61,61	0
56	MG	2A	3444	1/1	0.88	0.18	80,80,80,80	0
56	MG	2a	1622	1/1	0.88	0.18	78,78,78,78	0
56	MG	2a	1836	1/1	0.88	0.34	74,74,74,74	0
56	MG	2A	3088	1/1	0.88	0.17	68,68,68,68	0
56	MG	2A	3736	1/1	0.88	0.11	72,72,72,72	0
56	MG	1A	3687	1/1	0.88	0.14	52,52,52,52	0
56	MG	2A	3320	1/1	0.88	0.20	72,72,72,72	0
56	MG	2l	205	1/1	0.88	0.14	80,80,80,80	0
56	MG	2r	101	1/1	0.88	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	2A	3740	1/1	0.88	0.12	74,74,74,74	0
56	MG	2A	3741	1/1	0.88	0.11	74,74,74,74	0
56	MG	1a	1650	1/1	0.88	0.22	73,73,73,73	0
56	MG	2A	3211	1/1	0.88	0.10	63,63,63,63	0
56	MG	1A	3020	1/1	0.88	0.18	50,50,50,50	0
56	MG	2A	3458	1/1	0.88	0.16	58,58,58,58	0
56	MG	2A	3462	1/1	0.88	0.21	68,68,68,68	0
56	MG	1A	3547	1/1	0.88	0.25	52,52,52,52	0
56	MG	2A	3464	1/1	0.88	0.36	59,59,59,59	0
56	MG	1A	3965	1/1	0.88	0.14	56,56,56,56	0
56	MG	2A	3761	1/1	0.88	0.24	73,73,73,73	0
56	MG	2a	1645	1/1	0.88	0.31	66,66,66,66	0
56	MG	1t	201	1/1	0.88	0.24	69,69,69,69	0
56	MG	2A	3101	1/1	0.88	0.29	74,74,74,74	0
56	MG	2A	3791	1/1	0.88	0.11	68,68,68,68	0
56	MG	2A	3225	1/1	0.88	0.15	57,57,57,57	0
56	MG	1a	1667	1/1	0.88	0.16	71,71,71,71	0
56	MG	2A	3230	1/1	0.88	0.40	59,59,59,59	0
56	MG	1A	3470	1/1	0.88	0.18	66,66,66,66	0
56	MG	2A	3790	1/1	0.89	0.12	80,80,80,80	0
56	MG	1A	3235	1/1	0.89	0.12	50,50,50,50	0
56	MG	1A	3440	1/1	0.89	0.13	61,61,61,61	0
56	MG	2A	3173	1/1	0.89	0.23	69,69,69,69	0
56	MG	2A	3174	1/1	0.89	0.23	82,82,82,82	0
56	MG	2A	3319	1/1	0.89	0.13	75,75,75,75	0
56	MG	2A	3175	1/1	0.89	0.22	60,60,60,60	0
56	MG	1a	1658	1/1	0.89	0.25	76,76,76,76	0
56	MG	1B	217	1/1	0.89	0.10	56,56,56,56	0
56	MG	1a	1660	1/1	0.89	0.13	72,72,72,72	0
56	MG	2A	3481	1/1	0.89	0.20	60,60,60,60	0
56	MG	2A	3329	1/1	0.89	0.38	72,72,72,72	0
56	MG	2A	3485	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3190	1/1	0.89	0.11	79,79,79,79	0
56	MG	2A	3489	1/1	0.89	0.10	63,63,63,63	0
56	MG	1A	3618	1/1	0.89	0.12	61,61,61,61	0
56	MG	1A	3401	1/1	0.89	0.29	71,71,71,71	0
56	MG	2A	3832	1/1	0.89	0.12	69,69,69,69	0
56	MG	1A	3817	1/1	0.89	0.20	68,68,68,68	0
56	MG	1A	3513	1/1	0.89	0.14	60,60,60,60	0
56	MG	2a	1695	1/1	0.89	0.28	73,73,73,73	0
56	MG	2a	1696	1/1	0.89	0.13	74,74,74,74	0
56	MG	1A	3268	1/1	0.89	0.10	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	3029	1/1	0.89	0.11	72,72,72,72	0
56	MG	2A	3518	1/1	0.89	0.16	83,83,83,83	0
56	MG	1a	1673	1/1	0.89	0.18	62,62,62,62	0
56	MG	1A	3411	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3039	1/1	0.89	0.23	71,71,71,71	0
56	MG	1D	311	1/1	0.89	0.31	68,68,68,68	0
56	MG	2A	3862	1/1	0.89	0.10	58,58,58,58	0
56	MG	1D	313	1/1	0.89	0.17	44,44,44,44	0
56	MG	2a	1709	1/1	0.89	0.17	63,63,63,63	0
56	MG	2A	3864	1/1	0.89	0.15	66,66,66,66	0
56	MG	1E	308	1/1	0.89	0.21	58,58,58,58	0
56	MG	2a	1712	1/1	0.89	0.26	78,78,78,78	0
56	MG	2A	3867	1/1	0.89	0.20	63,63,63,63	0
56	MG	2a	1715	1/1	0.89	0.11	76,76,76,76	0
56	MG	2A	3056	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3308	1/1	0.89	0.11	44,44,44,44	0
56	MG	1A	4024	1/1	0.89	0.14	50,50,50,50	0
56	MG	2A	3559	1/1	0.89	0.11	65,65,65,65	0
56	MG	1F	313	1/1	0.89	0.19	60,60,60,60	0
56	MG	1a	1691	1/1	0.89	0.31	61,61,61,61	0
56	MG	1a	1696	1/1	0.89	0.33	63,63,63,63	0
56	MG	1A	3415	1/1	0.89	0.21	61,61,61,61	0
56	MG	2A	3368	1/1	0.89	0.32	60,60,60,60	0
56	MG	2A	3370	1/1	0.89	0.11	77,77,77,77	0
56	MG	2A	3232	1/1	0.89	0.21	76,76,76,76	0
56	MG	1G	205	1/1	0.89	0.15	66,66,66,66	0
56	MG	1A	3532	1/1	0.89	0.16	79,79,79,79	0
56	MG	2B	212	1/1	0.89	0.17	75,75,75,75	0
56	MG	2A	3242	1/1	0.89	0.14	70,70,70,70	0
56	MG	2A	3244	1/1	0.89	0.30	80,80,80,80	0
56	MG	2B	215	1/1	0.89	0.21	70,70,70,70	0
56	MG	1A	3534	1/1	0.89	0.10	60,60,60,60	0
56	MG	1A	3313	1/1	0.89	0.28	55,55,55,55	0
56	MG	1A	4041	1/1	0.89	0.41	67,67,67,67	0
56	MG	2A	3651	1/1	0.89	0.14	88,88,88,88	0
56	MG	1R	205	1/1	0.89	0.19	49,49,49,49	0
56	MG	2E	307	1/1	0.89	0.14	71,71,71,71	0
56	MG	1a	1723	1/1	0.89	0.18	74,74,74,74	0
56	MG	2A	3655	1/1	0.89	0.11	67,67,67,67	0
56	MG	2A	3255	1/1	0.89	0.19	66,66,66,66	0
56	MG	2a	1754	1/1	0.89	0.10	93,93,93,93	0
56	MG	1A	3417	1/1	0.89	0.17	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	3090	1/1	0.89	0.13	56,56,56,56	0
56	MG	2A	3259	1/1	0.89	0.16	69,69,69,69	0
56	MG	1A	3363	1/1	0.89	0.25	79,79,79,79	0
56	MG	2a	1776	1/1	0.89	0.09	89,89,89,89	0
56	MG	1A	3554	1/1	0.89	0.16	58,58,58,58	0
56	MG	2A	3400	1/1	0.89	0.12	68,68,68,68	0
56	MG	2a	1794	1/1	0.89	0.11	82,82,82,82	0
56	MG	1A	3371	1/1	0.89	0.11	63,63,63,63	0
56	MG	2A	3673	1/1	0.89	0.09	54,54,54,54	0
56	MG	1A	3328	1/1	0.89	0.27	65,65,65,65	0
56	MG	1A	3734	1/1	0.89	0.16	64,64,64,64	0
56	MG	2A	3684	1/1	0.89	0.23	75,75,75,75	0
56	MG	1A	3873	1/1	0.89	0.12	49,49,49,49	0
56	MG	2a	1804	1/1	0.89	0.25	76,76,76,76	0
56	MG	1a	1781	1/1	0.89	0.10	74,74,74,74	0
56	MG	1A	4070	1/1	0.89	0.06	27,27,27,27	0
56	MG	2a	1603	1/1	0.89	0.11	83,83,83,83	0
56	MG	18	108	1/1	0.89	0.17	64,64,64,64	0
56	MG	2a	1810	1/1	0.89	0.24	80,80,80,80	0
56	MG	1a	1796	1/1	0.89	0.13	88,88,88,88	0
56	MG	1a	1797	1/1	0.89	0.15	69,69,69,69	0
56	MG	1A	3877	1/1	0.89	0.09	45,45,45,45	0
56	MG	2a	1611	1/1	0.89	0.30	80,80,80,80	0
56	MG	2A	3705	1/1	0.89	0.34	74,74,74,74	0
56	MG	2A	3278	1/1	0.89	0.26	73,73,73,73	0
56	MG	2A	3423	1/1	0.89	0.39	70,70,70,70	0
56	MG	1a	1602	1/1	0.89	0.28	68,68,68,68	0
56	MG	2A	3426	1/1	0.89	0.21	68,68,68,68	0
56	MG	1A	3429	1/1	0.89	0.14	52,52,52,52	0
56	MG	1A	3886	1/1	0.89	0.14	39,39,39,39	0
56	MG	1A	3742	1/1	0.89	0.12	66,66,66,66	0
56	MG	2a	1838	1/1	0.89	0.14	62,62,62,62	0
56	MG	2a	1839	1/1	0.89	0.20	72,72,72,72	0
56	MG	2d	301	1/1	0.89	0.26	65,65,65,65	0
56	MG	1A	3905	1/1	0.89	0.14	53,53,53,53	0
56	MG	2g	201	1/1	0.89	0.19	71,71,71,71	0
56	MG	2A	3133	1/1	0.89	0.15	82,82,82,82	0
56	MG	1A	3274	1/1	0.89	0.36	72,72,72,72	0
56	MG	1A	3915	1/1	0.89	0.19	65,65,65,65	0
56	MG	1a	1618	1/1	0.89	0.12	69,69,69,69	0
56	MG	2q	202	1/1	0.89	0.17	83,83,83,83	0
56	MG	1A	4090	1/1	0.89	0.16	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3746	1/1	0.89	0.07	47,47,47,47	0
56	MG	2A	3743	1/1	0.89	0.14	71,71,71,71	0
56	MG	2A	3295	1/1	0.89	0.30	78,78,78,78	0
56	MG	1a	1628	1/1	0.89	0.18	69,69,69,69	0
56	MG	1A	3751	1/1	0.89	0.12	36,36,36,36	0
56	MG	2A	3748	1/1	0.89	0.12	69,69,69,69	0
56	MG	2a	1640	1/1	0.89	0.28	66,66,66,66	0
56	MG	2A	3449	1/1	0.89	0.25	74,74,74,74	0
56	MG	2A	3451	1/1	0.89	0.20	62,62,62,62	0
56	MG	2a	1644	1/1	0.89	0.16	73,73,73,73	0
56	MG	1A	3592	1/1	0.89	0.35	69,69,69,69	0
56	MG	1A	3227	1/1	0.89	0.12	48,48,48,48	0
56	MG	2a	1647	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3305	1/1	0.89	0.14	70,70,70,70	0
56	MG	2a	1651	1/1	0.89	0.17	67,67,67,67	0
56	MG	1A	3764	1/1	0.89	0.09	56,56,56,56	0
56	MG	2a	1656	1/1	0.89	0.13	77,77,77,77	0
56	MG	1A	3253	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3971	1/1	0.89	0.09	57,57,57,57	0
57	K	1A	3575	1/1	0.89	0.25	73,73,73,73	0
56	MG	1A	3089	1/1	0.90	0.13	38,38,38,38	0
56	MG	1N	205	1/1	0.90	0.29	54,54,54,54	0
56	MG	2A	3414	1/1	0.90	0.25	58,58,58,58	0
56	MG	2A	3415	1/1	0.90	0.23	52,52,52,52	0
56	MG	1a	1709	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3264	1/1	0.90	0.16	60,60,60,60	0
56	MG	2a	1655	1/1	0.90	0.16	75,75,75,75	0
56	MG	1A	3110	1/1	0.90	0.33	37,37,37,37	0
56	MG	2A	3267	1/1	0.90	0.21	73,73,73,73	0
56	MG	2A	3089	1/1	0.90	0.23	76,76,76,76	0
56	MG	1A	3837	1/1	0.90	0.16	48,48,48,48	0
56	MG	1A	3118	1/1	0.90	0.09	42,42,42,42	0
56	MG	2A	3271	1/1	0.90	0.24	73,73,73,73	0
56	MG	1S	203	1/1	0.90	0.08	67,67,67,67	0
56	MG	1A	3629	1/1	0.90	0.13	69,69,69,69	0
56	MG	1a	1722	1/1	0.90	0.17	71,71,71,71	0
56	MG	2A	3755	1/1	0.90	0.23	67,67,67,67	0
56	MG	2A	3437	1/1	0.90	0.28	63,63,63,63	0
56	MG	1A	3633	1/1	0.90	0.11	51,51,51,51	0
56	MG	1A	3125	1/1	0.90	0.19	58,58,58,58	0
56	MG	1A	3352	1/1	0.90	0.17	45,45,45,45	0
56	MG	1A	3075	1/1	0.90	0.41	74,74,74,74	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3784	1/1	0.90	0.12	70,70,70,70	0
56	MG	1Z	3700	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	4052	1/1	0.90	0.14	39,39,39,39	0
56	MG	2a	1683	1/1	0.90	0.22	63,63,63,63	0
56	MG	1A	3510	1/1	0.90	0.10	45,45,45,45	0
56	MG	10	105	1/1	0.90	0.20	65,65,65,65	0
56	MG	2A	3448	1/1	0.90	0.41	65,65,65,65	0
56	MG	1A	4061	1/1	0.90	0.06	21,21,21,21	0
56	MG	10	108	1/1	0.90	0.09	55,55,55,55	0
56	MG	1A	3661	1/1	0.90	0.11	45,45,45,45	0
56	MG	2A	3118	1/1	0.90	0.16	59,59,59,59	0
56	MG	16	101	1/1	0.90	0.09	62,62,62,62	0
56	MG	1a	1795	1/1	0.90	0.09	87,87,87,87	0
56	MG	18	104	1/1	0.90	0.25	51,51,51,51	0
56	MG	2A	3296	1/1	0.90	0.28	67,67,67,67	0
56	MG	1A	3153	1/1	0.90	0.14	52,52,52,52	0
56	MG	1a	1805	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3465	1/1	0.90	0.50	59,59,59,59	0
56	MG	1a	1807	1/1	0.90	0.16	70,70,70,70	0
56	MG	1A	3303	1/1	0.90	0.33	60,60,60,60	0
56	MG	2A	3302	1/1	0.90	0.21	71,71,71,71	0
56	MG	2A	3304	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3837	1/1	0.90	0.10	62,62,62,62	0
56	MG	1a	1811	1/1	0.90	0.12	67,67,67,67	0
56	MG	2A	3140	1/1	0.90	0.12	71,71,71,71	0
56	MG	1b	301	1/1	0.90	0.17	79,79,79,79	0
56	MG	2A	3479	1/1	0.90	0.17	71,71,71,71	0
56	MG	1A	3358	1/1	0.90	0.10	45,45,45,45	0
56	MG	2a	1719	1/1	0.90	0.15	76,76,76,76	0
56	MG	1A	3158	1/1	0.90	0.11	43,43,43,43	0
56	MG	2A	3147	1/1	0.90	0.19	60,60,60,60	0
56	MG	2A	3148	1/1	0.90	0.23	64,64,64,64	0
56	MG	1A	3367	1/1	0.90	0.22	52,52,52,52	0
56	MG	1A	3368	1/1	0.90	0.12	56,56,56,56	0
56	MG	1A	3370	1/1	0.90	0.17	52,52,52,52	0
56	MG	1A	3720	1/1	0.90	0.25	60,60,60,60	0
56	MG	2A	3323	1/1	0.90	0.16	69,69,69,69	0
56	MG	1A	3025	1/1	0.90	0.20	46,46,46,46	0
56	MG	1A	3442	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3535	1/1	0.90	0.10	73,73,73,73	0
56	MG	1A	3169	1/1	0.90	0.18	40,40,40,40	0
56	MG	2A	3874	1/1	0.90	0.15	97,97,97,97	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	3918	1/1	0.90	0.13	55,55,55,55	0
56	MG	1w	103	1/1	0.90	0.15	86,86,86,86	0
56	MG	2B	203	1/1	0.90	0.24	81,81,81,81	0
56	MG	1A	3925	1/1	0.90	0.13	37,37,37,37	0
56	MG	2A	3533	1/1	0.90	0.14	58,58,58,58	0
56	MG	1A	3450	1/1	0.90	0.17	46,46,46,46	0
56	MG	1A	3096	1/1	0.90	0.09	68,68,68,68	0
56	MG	1A	4104	1/1	0.90	0.10	59,59,59,59	0
56	MG	2a	1746	1/1	0.90	0.15	70,70,70,70	0
56	MG	1A	3940	1/1	0.90	0.10	64,64,64,64	0
56	MG	1x	104	1/1	0.90	0.17	76,76,76,76	0
56	MG	1A	3957	1/1	0.90	0.09	79,79,79,79	0
56	MG	2A	3567	1/1	0.90	0.18	64,64,64,64	0
56	MG	1x	108	1/1	0.90	0.20	71,71,71,71	0
56	MG	2A	3349	1/1	0.90	0.31	68,68,68,68	0
56	MG	2a	1762	1/1	0.90	0.14	84,84,84,84	0
56	MG	2B	216	1/1	0.90	0.18	83,83,83,83	0
56	MG	1B	214	1/1	0.90	0.11	57,57,57,57	0
56	MG	2a	1774	1/1	0.90	0.09	97,97,97,97	0
56	MG	2B	219	1/1	0.90	0.19	78,78,78,78	0
56	MG	2A	3585	1/1	0.90	0.18	73,73,73,73	0
56	MG	2A	3588	1/1	0.90	0.09	61,61,61,61	0
56	MG	2a	1789	1/1	0.90	0.25	71,71,71,71	0
56	MG	2a	1792	1/1	0.90	0.22	83,83,83,83	0
56	MG	2E	301	1/1	0.90	0.20	68,68,68,68	0
56	MG	1A	3318	1/1	0.90	0.23	61,61,61,61	0
56	MG	2A	3595	1/1	0.90	0.19	74,74,74,74	0
56	MG	1a	1657	1/1	0.90	0.31	73,73,73,73	0
56	MG	1x	112	1/1	0.90	0.21	67,67,67,67	0
56	MG	2F	302	1/1	0.90	0.22	69,69,69,69	0
56	MG	2A	3601	1/1	0.90	0.15	66,66,66,66	0
56	MG	2a	1801	1/1	0.90	0.12	75,75,75,75	0
56	MG	1A	3963	1/1	0.90	0.15	57,57,57,57	0
56	MG	1A	3549	1/1	0.90	0.25	62,62,62,62	0
56	MG	2A	3356	1/1	0.90	0.08	63,63,63,63	0
56	MG	2a	1807	1/1	0.90	0.14	67,67,67,67	0
56	MG	2A	3612	1/1	0.90	0.14	52,52,52,52	0
56	MG	2A	3205	1/1	0.90	0.16	83,83,83,83	0
56	MG	1A	3197	1/1	0.90	0.19	43,43,43,43	0
56	MG	2W	201	1/1	0.90	0.23	72,72,72,72	0
56	MG	2a	1813	1/1	0.90	0.18	70,70,70,70	0
56	MG	2A	3625	1/1	0.90	0.22	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3360	1/1	0.90	0.19	69,69,69,69	0
56	MG	2A	3364	1/1	0.90	0.29	74,74,74,74	0
56	MG	2A	3642	1/1	0.90	0.20	72,72,72,72	0
56	MG	2A	3647	1/1	0.90	0.17	62,62,62,62	0
56	MG	2A	3207	1/1	0.90	0.14	66,66,66,66	0
56	MG	2A	3649	1/1	0.90	0.30	75,75,75,75	0
56	MG	1A	3970	1/1	0.90	0.11	55,55,55,55	0
56	MG	1B	230	1/1	0.90	0.09	69,69,69,69	0
56	MG	1A	3469	1/1	0.90	0.12	69,69,69,69	0
56	MG	2a	1827	1/1	0.90	0.12	86,86,86,86	0
56	MG	2a	1828	1/1	0.90	0.26	71,71,71,71	0
56	MG	2a	1834	1/1	0.90	0.18	58,58,58,58	0
56	MG	1A	3329	1/1	0.90	0.22	53,53,53,53	0
56	MG	2a	1605	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	3396	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3375	1/1	0.90	0.25	86,86,86,86	0
56	MG	1A	3568	1/1	0.90	0.16	42,42,42,42	0
56	MG	2a	1610	1/1	0.90	0.27	73,73,73,73	0
56	MG	1A	3574	1/1	0.90	0.27	59,59,59,59	0
56	MG	2l	201	1/1	0.90	0.16	79,79,79,79	0
56	MG	1A	3398	1/1	0.90	0.26	49,49,49,49	0
56	MG	2a	1613	1/1	0.90	0.38	82,82,82,82	0
56	MG	2A	3381	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3382	1/1	0.90	0.23	54,54,54,54	0
56	MG	1A	3085	1/1	0.90	0.11	41,41,41,41	0
56	MG	2A	3042	1/1	0.90	0.37	64,64,64,64	0
56	MG	2A	3045	1/1	0.90	0.13	69,69,69,69	0
56	MG	2A	3050	1/1	0.90	0.20	51,51,51,51	0
56	MG	1A	3336	1/1	0.90	0.24	61,61,61,61	0
56	MG	2A	3052	1/1	0.90	0.10	58,58,58,58	0
56	MG	1a	1683	1/1	0.90	0.30	73,73,73,73	0
56	MG	1F	309	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3057	1/1	0.90	0.23	74,74,74,74	0
56	MG	1A	3339	1/1	0.90	0.28	63,63,63,63	0
56	MG	1A	3598	1/1	0.90	0.17	72,72,72,72	0
56	MG	2A	3253	1/1	0.90	0.14	78,78,78,78	0
56	MG	2A	3402	1/1	0.90	0.12	76,76,76,76	0
56	MG	1a	1688	1/1	0.90	0.36	72,72,72,72	0
56	MG	1A	3600	1/1	0.90	0.28	59,59,59,59	0
56	MG	1a	1692	1/1	0.90	0.26	60,60,60,60	0
56	MG	2A	3408	1/1	0.90	0.08	62,62,62,62	0
56	MG	2A	3718	1/1	0.90	0.16	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1695	1/1	0.90	0.31	60,60,60,60	0
56	MG	2A	3724	1/1	0.90	0.09	60,60,60,60	0
56	MG	1A	3603	1/1	0.90	0.18	63,63,63,63	0
56	MG	2A	3047	1/1	0.91	0.21	60,60,60,60	0
56	MG	2A	3798	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	3524	1/1	0.91	0.39	47,47,47,47	0
56	MG	2A	3486	1/1	0.91	0.13	68,68,68,68	0
56	MG	1A	3973	1/1	0.91	0.11	46,46,46,46	0
56	MG	2A	3488	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3164	1/1	0.91	0.26	60,60,60,60	0
56	MG	2a	1681	1/1	0.91	0.27	70,70,70,70	0
56	MG	1B	202	1/1	0.91	0.25	61,61,61,61	0
56	MG	2A	3492	1/1	0.91	0.24	69,69,69,69	0
56	MG	2a	1684	1/1	0.91	0.23	66,66,66,66	0
56	MG	1A	3529	1/1	0.91	0.27	68,68,68,68	0
56	MG	2A	3819	1/1	0.91	0.11	60,60,60,60	0
56	MG	1a	1724	1/1	0.91	0.13	60,60,60,60	0
56	MG	1a	1727	1/1	0.91	0.15	63,63,63,63	0
56	MG	1a	1601	1/1	0.91	0.35	70,70,70,70	0
56	MG	2A	3508	1/1	0.91	0.18	79,79,79,79	0
56	MG	2A	3830	1/1	0.91	0.14	72,72,72,72	0
56	MG	2A	3218	1/1	0.91	0.14	65,65,65,65	0
56	MG	1a	1736	1/1	0.91	0.18	64,64,64,64	0
56	MG	2a	1701	1/1	0.91	0.17	61,61,61,61	0
56	MG	1B	208	1/1	0.91	0.32	70,70,70,70	0
56	MG	2A	3221	1/1	0.91	0.21	75,75,75,75	0
56	MG	2A	3843	1/1	0.91	0.13	48,48,48,48	0
56	MG	1B	211	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3651	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3466	1/1	0.91	0.24	71,71,71,71	0
56	MG	2A	3851	1/1	0.91	0.09	73,73,73,73	0
56	MG	1A	3468	1/1	0.91	0.15	63,63,63,63	0
56	MG	2A	3231	1/1	0.91	0.24	56,56,56,56	0
56	MG	1A	3533	1/1	0.91	0.21	78,78,78,78	0
56	MG	2A	3363	1/1	0.91	0.14	72,72,72,72	0
56	MG	2a	1713	1/1	0.91	0.09	89,89,89,89	0
56	MG	2A	3083	1/1	0.91	0.29	65,65,65,65	0
56	MG	2A	3238	1/1	0.91	0.29	61,61,61,61	0
56	MG	1B	218	1/1	0.91	0.20	55,55,55,55	0
56	MG	2A	3369	1/1	0.91	0.16	61,61,61,61	0
56	MG	1a	1763	1/1	0.91	0.09	70,70,70,70	0
56	MG	2A	3243	1/1	0.91	0.13	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	1772	1/1	0.91	0.08	77,77,77,77	0
56	MG	2A	3246	1/1	0.91	0.25	78,78,78,78	0
56	MG	1B	220	1/1	0.91	0.07	49,49,49,49	0
56	MG	1a	1621	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	3338	1/1	0.91	0.21	60,60,60,60	0
56	MG	2A	3598	1/1	0.91	0.18	80,80,80,80	0
56	MG	2A	3599	1/1	0.91	0.14	74,74,74,74	0
56	MG	2A	3096	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3205	1/1	0.91	0.08	55,55,55,55	0
56	MG	1a	1627	1/1	0.91	0.19	68,68,68,68	0
56	MG	2a	1734	1/1	0.91	0.16	68,68,68,68	0
56	MG	2A	3603	1/1	0.91	0.14	64,64,64,64	0
56	MG	1A	4014	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3608	1/1	0.91	0.15	73,73,73,73	0
56	MG	1A	3106	1/1	0.91	0.30	48,48,48,48	0
56	MG	1A	3474	1/1	0.91	0.25	56,56,56,56	0
56	MG	1A	3344	1/1	0.91	0.23	64,64,64,64	0
56	MG	2A	3618	1/1	0.91	0.17	72,72,72,72	0
56	MG	2A	3260	1/1	0.91	0.12	69,69,69,69	0
56	MG	2A	3105	1/1	0.91	0.12	67,67,67,67	0
56	MG	2A	3626	1/1	0.91	0.13	73,73,73,73	0
56	MG	2A	3392	1/1	0.91	0.15	72,72,72,72	0
56	MG	1A	4031	1/1	0.91	0.07	55,55,55,55	0
56	MG	2a	1748	1/1	0.91	0.20	70,70,70,70	0
56	MG	1A	3145	1/1	0.91	0.20	42,42,42,42	0
56	MG	2A	3643	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3644	1/1	0.91	0.08	57,57,57,57	0
56	MG	2A	3645	1/1	0.91	0.14	76,76,76,76	0
56	MG	2A	3397	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3211	1/1	0.91	0.21	76,76,76,76	0
56	MG	2F	301	1/1	0.91	0.11	73,73,73,73	0
56	MG	2a	1767	1/1	0.91	0.12	74,74,74,74	0
56	MG	1a	1648	1/1	0.91	0.12	61,61,61,61	0
56	MG	1E	301	1/1	0.91	0.18	34,34,34,34	0
56	MG	2A	3114	1/1	0.91	0.13	71,71,71,71	0
56	MG	1E	303	1/1	0.91	0.23	56,56,56,56	0
56	MG	2a	1785	1/1	0.91	0.15	64,64,64,64	0
56	MG	2A	3403	1/1	0.91	0.10	67,67,67,67	0
56	MG	1h	201	1/1	0.91	0.08	74,74,74,74	0
56	MG	1a	1651	1/1	0.91	0.19	72,72,72,72	0
56	MG	2A	3119	1/1	0.91	0.17	74,74,74,74	0
56	MG	1A	3479	1/1	0.91	0.16	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3217	1/1	0.91	0.09	53,53,53,53	0
56	MG	1n	102	1/1	0.91	0.22	62,62,62,62	0
56	MG	1A	3868	1/1	0.91	0.22	35,35,35,35	0
56	MG	1A	3026	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3186	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3876	1/1	0.91	0.14	59,59,59,59	0
56	MG	2a	1803	1/1	0.91	0.14	71,71,71,71	0
56	MG	2A	3677	1/1	0.91	0.25	71,71,71,71	0
56	MG	1a	1663	1/1	0.91	0.13	70,70,70,70	0
56	MG	2A	3682	1/1	0.91	0.10	47,47,47,47	0
56	MG	2A	3417	1/1	0.91	0.26	65,65,65,65	0
56	MG	2A	3285	1/1	0.91	0.12	77,77,77,77	0
56	MG	1A	3491	1/1	0.91	0.15	53,53,53,53	0
56	MG	1A	3189	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3399	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3281	1/1	0.91	0.17	42,42,42,42	0
56	MG	1a	1675	1/1	0.91	0.37	82,82,82,82	0
56	MG	2A	3429	1/1	0.91	0.32	71,71,71,71	0
56	MG	1A	3402	1/1	0.91	0.14	67,67,67,67	0
56	MG	1A	3330	1/1	0.91	0.16	61,61,61,61	0
56	MG	2a	1615	1/1	0.91	0.30	71,71,71,71	0
56	MG	2A	3712	1/1	0.91	0.13	63,63,63,63	0
56	MG	1Q	206	1/1	0.91	0.16	47,47,47,47	0
56	MG	1A	3748	1/1	0.91	0.09	55,55,55,55	0
56	MG	2A	3159	1/1	0.91	0.19	69,69,69,69	0
56	MG	2a	1824	1/1	0.91	0.09	80,80,80,80	0
56	MG	1S	201	1/1	0.91	0.22	53,53,53,53	0
56	MG	1A	3447	1/1	0.91	0.22	46,46,46,46	0
56	MG	2A	3299	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3362	1/1	0.91	0.14	65,65,65,65	0
56	MG	1a	1686	1/1	0.91	0.31	65,65,65,65	0
56	MG	2A	3443	1/1	0.91	0.20	60,60,60,60	0
56	MG	2A	3730	1/1	0.91	0.08	57,57,57,57	0
56	MG	2a	1840	1/1	0.91	0.21	72,72,72,72	0
56	MG	1T	202	1/1	0.91	0.17	55,55,55,55	0
56	MG	2e	201	1/1	0.91	0.09	77,77,77,77	0
56	MG	1A	3413	1/1	0.91	0.11	43,43,43,43	0
56	MG	1A	3516	1/1	0.91	0.14	58,58,58,58	0
56	MG	1A	3136	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3308	1/1	0.91	0.34	67,67,67,67	0
56	MG	2A	3011	1/1	0.91	0.12	64,64,64,64	0
56	MG	2a	1636	1/1	0.91	0.10	88,88,88,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3310	1/1	0.91	0.23	74,74,74,74	0
56	MG	1A	3766	1/1	0.91	0.11	53,53,53,53	0
56	MG	2A	3177	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3746	1/1	0.91	0.12	64,64,64,64	0
56	MG	1A	3775	1/1	0.91	0.14	38,38,38,38	0
56	MG	2A	3181	1/1	0.91	0.19	61,61,61,61	0
56	MG	1a	1698	1/1	0.91	0.27	58,58,58,58	0
56	MG	1A	3521	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3191	1/1	0.91	0.14	69,69,69,69	0
56	MG	1A	3619	1/1	0.91	0.09	29,29,29,29	0
56	MG	1A	3801	1/1	0.91	0.16	61,61,61,61	0
56	MG	1a	1710	1/1	0.91	0.09	54,54,54,54	0
56	MG	2A	3326	1/1	0.91	0.23	63,63,63,63	0
56	MG	2A	3196	1/1	0.91	0.14	58,58,58,58	0
56	MG	2x	102	1/1	0.91	0.28	77,77,77,77	0
56	MG	2A	3780	1/1	0.91	0.08	77,77,77,77	0
56	MG	2A	3197	1/1	0.91	0.21	66,66,66,66	0
56	MG	1A	3621	1/1	0.91	0.09	40,40,40,40	0
56	MG	2A	3788	1/1	0.91	0.12	73,73,73,73	0
56	MG	2A	3043	1/1	0.91	0.21	74,74,74,74	0
56	MG	1A	3461	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3335	1/1	0.91	0.12	70,70,70,70	0
56	MG	2A	3482	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3796	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3497	1/1	0.92	0.10	62,62,62,62	0
56	MG	2a	1639	1/1	0.92	0.32	64,64,64,64	0
56	MG	1A	3758	1/1	0.92	0.09	40,40,40,40	0
56	MG	2A	3424	1/1	0.92	0.21	47,47,47,47	0
56	MG	2A	3060	1/1	0.92	0.14	56,56,56,56	0
56	MG	2A	3062	1/1	0.92	0.08	58,58,58,58	0
56	MG	1B	235	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3428	1/1	0.92	0.53	74,74,74,74	0
56	MG	1A	3594	1/1	0.92	0.09	43,43,43,43	0
56	MG	2a	1649	1/1	0.92	0.31	76,76,76,76	0
56	MG	1D	312	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3387	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3976	1/1	0.92	0.07	49,49,49,49	0
56	MG	1a	1690	1/1	0.92	0.25	64,64,64,64	0
56	MG	2A	3436	1/1	0.92	0.26	69,69,69,69	0
56	MG	2A	3742	1/1	0.92	0.32	61,61,61,61	0
56	MG	1A	3977	1/1	0.92	0.20	62,62,62,62	0
56	MG	1A	3173	1/1	0.92	0.10	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1694	1/1	0.92	0.38	62,62,62,62	0
56	MG	1A	3444	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3985	1/1	0.92	0.08	70,70,70,70	0
56	MG	1E	314	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3780	1/1	0.92	0.10	71,71,71,71	0
56	MG	1a	1701	1/1	0.92	0.42	75,75,75,75	0
56	MG	1a	1702	1/1	0.92	0.23	63,63,63,63	0
56	MG	2A	3446	1/1	0.92	0.16	52,52,52,52	0
56	MG	1a	1705	1/1	0.92	0.25	66,66,66,66	0
56	MG	1a	1707	1/1	0.92	0.11	67,67,67,67	0
56	MG	1A	3989	1/1	0.92	0.10	72,72,72,72	0
56	MG	2a	1674	1/1	0.92	0.31	71,71,71,71	0
56	MG	1A	3784	1/1	0.92	0.12	67,67,67,67	0
56	MG	2A	3770	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3776	1/1	0.92	0.13	71,71,71,71	0
56	MG	1A	4000	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3782	1/1	0.92	0.08	45,45,45,45	0
56	MG	1A	3115	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3792	1/1	0.92	0.07	76,76,76,76	0
56	MG	2a	1688	1/1	0.92	0.24	62,62,62,62	0
56	MG	1A	3602	1/1	0.92	0.27	65,65,65,65	0
56	MG	1A	3294	1/1	0.92	0.17	61,61,61,61	0
56	MG	2a	1691	1/1	0.92	0.22	64,64,64,64	0
56	MG	2A	3109	1/1	0.92	0.12	49,49,49,49	0
56	MG	1A	3604	1/1	0.92	0.22	56,56,56,56	0
56	MG	1A	3810	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3606	1/1	0.92	0.18	61,61,61,61	0
56	MG	2a	1698	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	3237	1/1	0.92	0.30	49,49,49,49	0
56	MG	1S	202	1/1	0.92	0.16	56,56,56,56	0
56	MG	1A	4027	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	4030	1/1	0.92	0.13	74,74,74,74	0
56	MG	2A	3472	1/1	0.92	0.22	58,58,58,58	0
56	MG	1A	3456	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3346	1/1	0.92	0.22	45,45,45,45	0
56	MG	1A	3831	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3238	1/1	0.92	0.11	63,63,63,63	0
56	MG	2A	3816	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3128	1/1	0.92	0.13	65,65,65,65	0
56	MG	1a	1745	1/1	0.92	0.09	66,66,66,66	0
56	MG	1A	3620	1/1	0.92	0.12	52,52,52,52	0
56	MG	1a	1753	1/1	0.92	0.15	73,73,73,73	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3519	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3313	1/1	0.92	0.16	81,81,81,81	0
56	MG	2A	3136	1/1	0.92	0.10	58,58,58,58	0
56	MG	1a	1757	1/1	0.92	0.24	72,72,72,72	0
56	MG	1a	1758	1/1	0.92	0.10	74,74,74,74	0
56	MG	1Z	3701	1/1	0.92	0.15	66,66,66,66	0
56	MG	2A	3495	1/1	0.92	0.20	50,50,50,50	0
56	MG	1A	3838	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3184	1/1	0.92	0.11	65,65,65,65	0
56	MG	1a	1773	1/1	0.92	0.10	70,70,70,70	0
56	MG	2A	3504	1/1	0.92	0.10	60,60,60,60	0
56	MG	2A	3850	1/1	0.92	0.22	68,68,68,68	0
56	MG	2A	3505	1/1	0.92	0.12	64,64,64,64	0
56	MG	10	103	1/1	0.92	0.08	47,47,47,47	0
56	MG	1A	3630	1/1	0.92	0.09	35,35,35,35	0
56	MG	2a	1730	1/1	0.92	0.20	75,75,75,75	0
56	MG	1A	3243	1/1	0.92	0.12	39,39,39,39	0
56	MG	1A	3149	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3861	1/1	0.92	0.15	70,70,70,70	0
56	MG	2A	3157	1/1	0.92	0.18	59,59,59,59	0
56	MG	2A	3330	1/1	0.92	0.10	60,60,60,60	0
56	MG	11	105	1/1	0.92	0.11	56,56,56,56	0
56	MG	2A	3530	1/1	0.92	0.09	42,42,42,42	0
56	MG	13	104	1/1	0.92	0.11	57,57,57,57	0
56	MG	2A	3162	1/1	0.92	0.14	76,76,76,76	0
56	MG	1A	4057	1/1	0.92	0.08	58,58,58,58	0
56	MG	15	102	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3305	1/1	0.92	0.14	51,51,51,51	0
56	MG	1A	3850	1/1	0.92	0.25	60,60,60,60	0
56	MG	18	105	1/1	0.92	0.25	68,68,68,68	0
56	MG	1A	3064	1/1	0.92	0.26	56,56,56,56	0
56	MG	2A	3561	1/1	0.92	0.14	62,62,62,62	0
56	MG	1A	3059	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	4068	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3131	1/1	0.92	0.11	72,72,72,72	0
56	MG	2A	3347	1/1	0.92	0.26	64,64,64,64	0
56	MG	2A	3348	1/1	0.92	0.15	67,67,67,67	0
56	MG	1A	3019	1/1	0.92	0.19	51,51,51,51	0
56	MG	2B	210	1/1	0.92	0.15	73,73,73,73	0
56	MG	2a	1766	1/1	0.92	0.11	83,83,83,83	0
56	MG	2A	3179	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3858	1/1	0.92	0.11	58,58,58,58	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1772	1/1	0.92	0.08	79,79,79,79	0
56	MG	1A	3262	1/1	0.92	0.09	37,37,37,37	0
56	MG	1A	3866	1/1	0.92	0.09	48,48,48,48	0
56	MG	1a	1608	1/1	0.92	0.23	70,70,70,70	0
56	MG	2a	1778	1/1	0.92	0.09	73,73,73,73	0
56	MG	2a	1779	1/1	0.92	0.10	81,81,81,81	0
56	MG	1A	3867	1/1	0.92	0.13	55,55,55,55	0
56	MG	1a	1614	1/1	0.92	0.11	71,71,71,71	0
56	MG	2a	1787	1/1	0.92	0.12	71,71,71,71	0
56	MG	1A	4081	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	3263	1/1	0.92	0.18	53,53,53,53	0
56	MG	2D	304	1/1	0.92	0.29	46,46,46,46	0
56	MG	2A	3359	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	3536	1/1	0.92	0.10	63,63,63,63	0
56	MG	2A	3362	1/1	0.92	0.13	67,67,67,67	0
56	MG	1A	3477	1/1	0.92	0.09	59,59,59,59	0
56	MG	1A	4091	1/1	0.92	0.14	48,48,48,48	0
56	MG	2A	3617	1/1	0.92	0.13	61,61,61,61	0
56	MG	2A	3200	1/1	0.92	0.43	64,64,64,64	0
56	MG	2A	3622	1/1	0.92	0.18	58,58,58,58	0
56	MG	1A	3539	1/1	0.92	0.22	41,41,41,41	0
56	MG	1A	4094	1/1	0.92	0.14	43,43,43,43	0
56	MG	1a	1629	1/1	0.92	0.22	58,58,58,58	0
56	MG	1A	3166	1/1	0.92	0.17	39,39,39,39	0
56	MG	2Q	201	1/1	0.92	0.14	74,74,74,74	0
56	MG	1A	3879	1/1	0.92	0.09	37,37,37,37	0
56	MG	1a	1634	1/1	0.92	0.15	72,72,72,72	0
56	MG	2T	201	1/1	0.92	0.11	64,64,64,64	0
56	MG	2T	202	1/1	0.92	0.17	74,74,74,74	0
56	MG	2T	203	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3544	1/1	0.92	0.21	53,53,53,53	0
56	MG	2A	3208	1/1	0.92	0.11	50,50,50,50	0
56	MG	2W	203	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3333	1/1	0.92	0.27	55,55,55,55	0
56	MG	1a	1641	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3721	1/1	0.92	0.08	71,71,71,71	0
56	MG	21	103	1/1	0.92	0.15	60,60,60,60	0
56	MG	23	101	1/1	0.92	0.11	62,62,62,62	0
56	MG	25	103	1/1	0.92	0.18	62,62,62,62	0
56	MG	1a	1644	1/1	0.92	0.21	75,75,75,75	0
56	MG	1A	4101	1/1	0.92	0.10	57,57,57,57	0
56	MG	27	102	1/1	0.92	0.22	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1830	1/1	0.92	0.11	71,71,71,71	0
56	MG	2a	1831	1/1	0.92	0.29	77,77,77,77	0
56	MG	1A	3167	1/1	0.92	0.28	42,42,42,42	0
56	MG	2a	1835	1/1	0.92	0.26	68,68,68,68	0
56	MG	1A	4105	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	3909	1/1	0.92	0.08	57,57,57,57	0
56	MG	29	101	1/1	0.92	0.25	77,77,77,77	0
56	MG	1A	3377	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3016	1/1	0.92	0.18	76,76,76,76	0
56	MG	2A	3226	1/1	0.92	0.11	68,68,68,68	0
56	MG	2f	201	1/1	0.92	0.11	60,60,60,60	0
56	MG	2A	3022	1/1	0.92	0.16	55,55,55,55	0
56	MG	1a	1655	1/1	0.92	0.10	60,60,60,60	0
56	MG	2A	3395	1/1	0.92	0.07	72,72,72,72	0
56	MG	2A	3024	1/1	0.92	0.15	65,65,65,65	0
56	MG	1A	3552	1/1	0.92	0.22	52,52,52,52	0
56	MG	2A	3233	1/1	0.92	0.12	62,62,62,62	0
56	MG	2A	3675	1/1	0.92	0.13	76,76,76,76	0
56	MG	1B	210	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3483	1/1	0.92	0.13	58,58,58,58	0
56	MG	2A	3680	1/1	0.92	0.17	70,70,70,70	0
56	MG	1A	3733	1/1	0.92	0.15	69,69,69,69	0
56	MG	1B	213	1/1	0.92	0.28	69,69,69,69	0
56	MG	2A	3404	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3022	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3489	1/1	0.92	0.15	44,44,44,44	0
56	MG	2a	1623	1/1	0.92	0.08	62,62,62,62	0
56	MG	1A	3170	1/1	0.92	0.20	61,61,61,61	0
56	MG	2A	3696	1/1	0.92	0.08	62,62,62,62	0
56	MG	1A	3493	1/1	0.92	0.13	57,57,57,57	0
56	MG	2A	3248	1/1	0.92	0.12	74,74,74,74	0
56	MG	1A	3948	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3953	1/1	0.92	0.13	70,70,70,70	0
56	MG	1A	3380	1/1	0.92	0.31	49,49,49,49	0
56	MG	2a	1631	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	3576	1/1	0.92	0.12	57,57,57,57	0
56	MG	2A	3053	1/1	0.92	0.13	75,75,75,75	0
56	MG	1a	1679	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3714	1/1	0.92	0.11	61,61,61,61	0
56	MG	1A	3589	1/1	0.92	0.18	27,27,27,27	0
56	MG	1A	3496	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3289	1/1	0.93	0.16	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	3291	1/1	0.93	0.09	57,57,57,57	0
56	MG	1x	103	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	4103	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3454	1/1	0.93	0.15	35,35,35,35	0
56	MG	1x	107	1/1	0.93	0.22	70,70,70,70	0
56	MG	1A	3455	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	4108	1/1	0.93	0.25	63,63,63,63	0
56	MG	1a	1638	1/1	0.93	0.13	53,53,53,53	0
56	MG	1B	201	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3216	1/1	0.93	0.07	51,51,51,51	0
56	MG	1B	203	1/1	0.93	0.08	43,43,43,43	0
56	MG	1a	1643	1/1	0.93	0.28	78,78,78,78	0
56	MG	1A	3927	1/1	0.93	0.20	60,60,60,60	0
56	MG	1A	3929	1/1	0.93	0.12	64,64,64,64	0
56	MG	2A	3007	1/1	0.93	0.11	61,61,61,61	0
56	MG	2A	3709	1/1	0.93	0.10	42,42,42,42	0
56	MG	1B	209	1/1	0.93	0.11	50,50,50,50	0
56	MG	2a	1641	1/1	0.93	0.13	91,91,91,91	0
56	MG	1A	3055	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3122	1/1	0.93	0.09	37,37,37,37	0
56	MG	2A	3018	1/1	0.93	0.07	58,58,58,58	0
56	MG	2A	3019	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3020	1/1	0.93	0.13	67,67,67,67	0
56	MG	1A	3299	1/1	0.93	0.35	70,70,70,70	0
56	MG	2A	3719	1/1	0.93	0.10	74,74,74,74	0
56	MG	1A	3945	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3240	1/1	0.93	0.15	69,69,69,69	0
56	MG	1A	3546	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3741	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3229	1/1	0.93	0.14	63,63,63,63	0
56	MG	2A	3420	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3731	1/1	0.93	0.09	64,64,64,64	0
56	MG	2A	3421	1/1	0.93	0.24	53,53,53,53	0
56	MG	2A	3734	1/1	0.93	0.11	60,60,60,60	0
56	MG	1A	3233	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3467	1/1	0.93	0.20	45,45,45,45	0
56	MG	1A	3964	1/1	0.93	0.10	56,56,56,56	0
56	MG	2a	1665	1/1	0.93	0.07	68,68,68,68	0
56	MG	1B	222	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3124	1/1	0.93	0.25	54,54,54,54	0
56	MG	1A	3555	1/1	0.93	0.19	59,59,59,59	0
56	MG	2A	3251	1/1	0.93	0.10	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3044	1/1	0.93	0.16	62,62,62,62	0
56	MG	2A	3432	1/1	0.93	0.28	69,69,69,69	0
56	MG	1A	3556	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3046	1/1	0.93	0.12	67,67,67,67	0
56	MG	2a	1675	1/1	0.93	0.23	67,67,67,67	0
56	MG	1a	1672	1/1	0.93	0.13	60,60,60,60	0
56	MG	2a	1678	1/1	0.93	0.13	61,61,61,61	0
56	MG	2A	3256	1/1	0.93	0.11	71,71,71,71	0
56	MG	1A	3558	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3754	1/1	0.93	0.13	72,72,72,72	0
56	MG	1a	1674	1/1	0.93	0.24	61,61,61,61	0
56	MG	1A	3972	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3559	1/1	0.93	0.12	65,65,65,65	0
56	MG	1a	1678	1/1	0.93	0.33	67,67,67,67	0
56	MG	2A	3760	1/1	0.93	0.15	61,61,61,61	0
56	MG	2A	3055	1/1	0.93	0.19	69,69,69,69	0
56	MG	1A	3036	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3766	1/1	0.93	0.09	64,64,64,64	0
56	MG	1D	309	1/1	0.93	0.14	53,53,53,53	0
56	MG	2A	3775	1/1	0.93	0.08	76,76,76,76	0
56	MG	1A	3171	1/1	0.93	0.13	56,56,56,56	0
56	MG	2a	1697	1/1	0.93	0.12	67,67,67,67	0
56	MG	1A	3979	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3383	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3783	1/1	0.93	0.09	71,71,71,71	0
56	MG	1A	3565	1/1	0.93	0.17	59,59,59,59	0
56	MG	1A	3384	1/1	0.93	0.10	55,55,55,55	0
56	MG	1E	304	1/1	0.93	0.21	42,42,42,42	0
56	MG	2A	3789	1/1	0.93	0.16	66,66,66,66	0
56	MG	1A	3385	1/1	0.93	0.15	49,49,49,49	0
56	MG	1A	3172	1/1	0.93	0.17	57,57,57,57	0
56	MG	1A	3128	1/1	0.93	0.28	38,38,38,38	0
56	MG	2A	3456	1/1	0.93	0.31	60,60,60,60	0
56	MG	2A	3795	1/1	0.93	0.13	65,65,65,65	0
56	MG	1A	3998	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3317	1/1	0.93	0.22	55,55,55,55	0
56	MG	2A	3459	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3461	1/1	0.93	0.33	53,53,53,53	0
56	MG	1F	310	1/1	0.93	0.08	50,50,50,50	0
56	MG	2A	3279	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3246	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3281	1/1	0.93	0.14	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	202	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	4005	1/1	0.93	0.11	56,56,56,56	0
56	MG	1A	4006	1/1	0.93	0.12	33,33,33,33	0
56	MG	1a	1700	1/1	0.93	0.18	68,68,68,68	0
56	MG	1A	3247	1/1	0.93	0.14	56,56,56,56	0
56	MG	2A	3288	1/1	0.93	0.13	67,67,67,67	0
56	MG	2A	3094	1/1	0.93	0.20	66,66,66,66	0
56	MG	2A	3827	1/1	0.93	0.08	80,80,80,80	0
56	MG	2A	3477	1/1	0.93	0.28	72,72,72,72	0
56	MG	1A	4011	1/1	0.93	0.09	68,68,68,68	0
56	MG	1A	3249	1/1	0.93	0.22	57,57,57,57	0
56	MG	1A	3181	1/1	0.93	0.08	45,45,45,45	0
56	MG	2a	1732	1/1	0.93	0.19	76,76,76,76	0
56	MG	2A	3835	1/1	0.93	0.11	82,82,82,82	0
56	MG	1O	204	1/1	0.93	0.10	52,52,52,52	0
56	MG	2a	1735	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3483	1/1	0.93	0.20	76,76,76,76	0
56	MG	2A	3100	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3842	1/1	0.93	0.10	73,73,73,73	0
56	MG	1O	205	1/1	0.93	0.09	63,63,63,63	0
56	MG	1A	3816	1/1	0.93	0.28	29,29,29,29	0
56	MG	1a	1711	1/1	0.93	0.23	66,66,66,66	0
56	MG	1A	3331	1/1	0.93	0.26	67,67,67,67	0
56	MG	1A	3486	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3490	1/1	0.93	0.17	69,69,69,69	0
56	MG	1A	3819	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3403	1/1	0.93	0.22	41,41,41,41	0
56	MG	2A	3493	1/1	0.93	0.19	71,71,71,71	0
56	MG	1A	3040	1/1	0.93	0.21	62,62,62,62	0
56	MG	1A	3832	1/1	0.93	0.09	36,36,36,36	0
56	MG	1A	3041	1/1	0.93	0.09	41,41,41,41	0
56	MG	2A	3500	1/1	0.93	0.25	73,73,73,73	0
56	MG	1U	202	1/1	0.93	0.28	42,42,42,42	0
56	MG	1U	205	1/1	0.93	0.18	46,46,46,46	0
56	MG	1A	3257	1/1	0.93	0.14	33,33,33,33	0
56	MG	1V	205	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3608	1/1	0.93	0.14	56,56,56,56	0
56	MG	2A	3312	1/1	0.93	0.07	67,67,67,67	0
56	MG	2a	1768	1/1	0.93	0.08	56,56,56,56	0
56	MG	2A	3121	1/1	0.93	0.11	48,48,48,48	0
56	MG	1W	202	1/1	0.93	0.07	43,43,43,43	0
56	MG	2a	1773	1/1	0.93	0.07	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3125	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3337	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3839	1/1	0.93	0.26	71,71,71,71	0
56	MG	1A	3185	1/1	0.93	0.13	75,75,75,75	0
56	MG	1A	3611	1/1	0.93	0.13	55,55,55,55	0
56	MG	2A	3535	1/1	0.93	0.10	58,58,58,58	0
56	MG	2A	3130	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3542	1/1	0.93	0.11	55,55,55,55	0
56	MG	2a	1788	1/1	0.93	0.16	64,64,64,64	0
56	MG	1a	1752	1/1	0.93	0.07	68,68,68,68	0
56	MG	2a	1790	1/1	0.93	0.18	78,78,78,78	0
56	MG	1A	3139	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3134	1/1	0.93	0.12	55,55,55,55	0
56	MG	1Z	3703	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3328	1/1	0.93	0.17	64,64,64,64	0
56	MG	1A	3341	1/1	0.93	0.22	61,61,61,61	0
56	MG	1A	3260	1/1	0.93	0.27	32,32,32,32	0
56	MG	1a	1759	1/1	0.93	0.16	63,63,63,63	0
56	MG	2A	3571	1/1	0.93	0.10	57,57,57,57	0
56	MG	2B	218	1/1	0.93	0.12	80,80,80,80	0
56	MG	2A	3572	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3849	1/1	0.93	0.07	40,40,40,40	0
56	MG	10	106	1/1	0.93	0.11	61,61,61,61	0
56	MG	2A	3579	1/1	0.93	0.10	68,68,68,68	0
56	MG	2A	3145	1/1	0.93	0.25	55,55,55,55	0
56	MG	2A	3587	1/1	0.93	0.09	71,71,71,71	0
56	MG	2E	303	1/1	0.93	0.27	66,66,66,66	0
56	MG	1a	1764	1/1	0.93	0.20	68,68,68,68	0
56	MG	2A	3592	1/1	0.93	0.09	71,71,71,71	0
56	MG	1A	3504	1/1	0.93	0.17	57,57,57,57	0
56	MG	1A	4060	1/1	0.93	0.17	77,77,77,77	0
56	MG	2A	3149	1/1	0.93	0.20	47,47,47,47	0
56	MG	2A	3151	1/1	0.93	0.15	59,59,59,59	0
56	MG	1a	1778	1/1	0.93	0.15	55,55,55,55	0
56	MG	1a	1779	1/1	0.93	0.09	68,68,68,68	0
56	MG	2a	1819	1/1	0.93	0.18	72,72,72,72	0
56	MG	1A	3625	1/1	0.93	0.06	35,35,35,35	0
56	MG	13	103	1/1	0.93	0.26	59,59,59,59	0
56	MG	2Q	203	1/1	0.93	0.07	63,63,63,63	0
56	MG	1A	4063	1/1	0.93	0.11	56,56,56,56	0
56	MG	1A	4064	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3343	1/1	0.93	0.10	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3610	1/1	0.93	0.12	38,38,38,38	0
56	MG	15	105	1/1	0.93	0.21	49,49,49,49	0
56	MG	2U	201	1/1	0.93	0.13	61,61,61,61	0
56	MG	1A	3046	1/1	0.93	0.06	33,33,33,33	0
56	MG	2A	3613	1/1	0.93	0.19	54,54,54,54	0
56	MG	1a	1806	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	3423	1/1	0.93	0.07	51,51,51,51	0
56	MG	2A	3168	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3621	1/1	0.93	0.14	59,59,59,59	0
56	MG	2I	102	1/1	0.93	0.41	59,59,59,59	0
56	MG	2A	3171	1/1	0.93	0.14	66,66,66,66	0
56	MG	1A	3190	1/1	0.93	0.19	41,41,41,41	0
56	MG	25	101	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3004	1/1	0.93	0.08	31,31,31,31	0
56	MG	1A	3105	1/1	0.93	0.21	42,42,42,42	0
56	MG	2A	3633	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3432	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3051	1/1	0.93	0.15	29,29,29,29	0
56	MG	1A	3350	1/1	0.93	0.32	52,52,52,52	0
56	MG	28	102	1/1	0.93	0.14	63,63,63,63	0
56	MG	1e	203	1/1	0.93	0.21	67,67,67,67	0
56	MG	1A	4080	1/1	0.93	0.07	20,20,20,20	0
56	MG	1A	3437	1/1	0.93	0.25	65,65,65,65	0
56	MG	1A	3875	1/1	0.93	0.07	30,30,30,30	0
56	MG	2A	3183	1/1	0.93	0.24	62,62,62,62	0
56	MG	2A	3184	1/1	0.93	0.19	64,64,64,64	0
56	MG	2a	1606	1/1	0.93	0.22	70,70,70,70	0
56	MG	1A	3269	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3527	1/1	0.93	0.19	38,38,38,38	0
56	MG	1A	3084	1/1	0.93	0.31	46,46,46,46	0
56	MG	1a	1615	1/1	0.93	0.26	67,67,67,67	0
56	MG	1A	3273	1/1	0.93	0.32	58,58,58,58	0
56	MG	1a	1617	1/1	0.93	0.17	64,64,64,64	0
56	MG	1A	3714	1/1	0.93	0.09	35,35,35,35	0
56	MG	2a	1614	1/1	0.93	0.19	68,68,68,68	0
56	MG	2A	3198	1/1	0.93	0.19	72,72,72,72	0
56	MG	2A	3383	1/1	0.93	0.35	62,62,62,62	0
56	MG	1A	3716	1/1	0.93	0.12	36,36,36,36	0
56	MG	1A	3054	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3117	1/1	0.93	0.24	44,44,44,44	0
56	MG	2a	1620	1/1	0.93	0.12	81,81,81,81	0
56	MG	2A	3672	1/1	0.93	0.23	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	3910	1/1	0.93	0.10	58,58,58,58	0
56	MG	2A	3683	1/1	0.94	0.12	59,59,59,59	0
56	MG	1y	101	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3553	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3686	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3687	1/1	0.94	0.15	81,81,81,81	0
56	MG	1A	3394	1/1	0.94	0.20	30,30,30,30	0
56	MG	2A	3689	1/1	0.94	0.06	72,72,72,72	0
56	MG	1A	3736	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3004	1/1	0.94	0.45	67,67,67,67	0
56	MG	1A	3215	1/1	0.94	0.06	42,42,42,42	0
56	MG	2A	3698	1/1	0.94	0.09	80,80,80,80	0
56	MG	2A	3006	1/1	0.94	0.26	63,63,63,63	0
56	MG	2A	3701	1/1	0.94	0.13	67,67,67,67	0
56	MG	1A	3950	1/1	0.94	0.08	28,28,28,28	0
56	MG	1A	3951	1/1	0.94	0.10	35,35,35,35	0
56	MG	2A	3215	1/1	0.94	0.19	59,59,59,59	0
56	MG	2A	3707	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3010	1/1	0.94	0.17	63,63,63,63	0
56	MG	2A	3710	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3127	1/1	0.94	0.30	39,39,39,39	0
56	MG	1a	1656	1/1	0.94	0.07	56,56,56,56	0
56	MG	2A	3017	1/1	0.94	0.25	56,56,56,56	0
56	MG	1A	3265	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3224	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3015	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3219	1/1	0.94	0.19	40,40,40,40	0
56	MG	1A	3223	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3481	1/1	0.94	0.09	51,51,51,51	0
56	MG	1B	231	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3726	1/1	0.94	0.11	60,60,60,60	0
56	MG	2A	3025	1/1	0.94	0.14	71,71,71,71	0
56	MG	1A	3226	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3757	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3236	1/1	0.94	0.10	62,62,62,62	0
56	MG	2A	3031	1/1	0.94	0.08	66,66,66,66	0
56	MG	2a	1652	1/1	0.94	0.13	84,84,84,84	0
56	MG	2A	3732	1/1	0.94	0.16	69,69,69,69	0
56	MG	2a	1654	1/1	0.94	0.14	80,80,80,80	0
56	MG	2A	3430	1/1	0.94	0.39	68,68,68,68	0
56	MG	1A	3130	1/1	0.94	0.06	38,38,38,38	0
56	MG	2A	3735	1/1	0.94	0.14	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	2A	3033	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3569	1/1	0.94	0.35	51,51,51,51	0
56	MG	2A	3036	1/1	0.94	0.13	44,44,44,44	0
56	MG	2A	3038	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3245	1/1	0.94	0.15	78,78,78,78	0
56	MG	1a	1671	1/1	0.94	0.26	72,72,72,72	0
56	MG	2a	1664	1/1	0.94	0.21	86,86,86,86	0
56	MG	2A	3040	1/1	0.94	0.09	51,51,51,51	0
56	MG	1D	305	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3571	1/1	0.94	0.16	39,39,39,39	0
56	MG	1A	3975	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3573	1/1	0.94	0.17	58,58,58,58	0
56	MG	1A	3076	1/1	0.94	0.06	35,35,35,35	0
56	MG	2A	3749	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3779	1/1	0.94	0.08	20,20,20,20	0
56	MG	1A	3231	1/1	0.94	0.17	34,34,34,34	0
56	MG	2A	3048	1/1	0.94	0.15	58,58,58,58	0
56	MG	1A	3782	1/1	0.94	0.10	28,28,28,28	0
56	MG	1E	305	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3579	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3584	1/1	0.94	0.32	44,44,44,44	0
56	MG	1A	3791	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3586	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3992	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3134	1/1	0.94	0.09	55,55,55,55	0
56	MG	2a	1686	1/1	0.94	0.18	74,74,74,74	0
56	MG	2a	1687	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3999	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3771	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3772	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3773	1/1	0.94	0.16	74,74,74,74	0
56	MG	1A	3285	1/1	0.94	0.22	37,37,37,37	0
56	MG	2A	3266	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3779	1/1	0.94	0.14	67,67,67,67	0
56	MG	1A	3806	1/1	0.94	0.07	20,20,20,20	0
56	MG	2A	3781	1/1	0.94	0.13	67,67,67,67	0
56	MG	1A	3808	1/1	0.94	0.07	44,44,44,44	0
56	MG	1a	1693	1/1	0.94	0.39	61,61,61,61	0
56	MG	1A	3492	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3288	1/1	0.94	0.23	50,50,50,50	0
56	MG	1N	204	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3067	1/1	0.94	0.18	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	1697	1/1	0.94	0.30	59,59,59,59	0
56	MG	2A	3069	1/1	0.94	0.16	66,66,66,66	0
56	MG	2A	3276	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3073	1/1	0.94	0.09	66,66,66,66	0
56	MG	1A	3595	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3476	1/1	0.94	0.12	67,67,67,67	0
56	MG	1A	3347	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3076	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3800	1/1	0.94	0.09	81,81,81,81	0
56	MG	2A	3077	1/1	0.94	0.24	52,52,52,52	0
56	MG	2A	3081	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3283	1/1	0.94	0.12	60,60,60,60	0
56	MG	1A	3419	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3234	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3808	1/1	0.94	0.13	55,55,55,55	0
56	MG	2A	3086	1/1	0.94	0.13	64,64,64,64	0
56	MG	2A	3087	1/1	0.94	0.12	60,60,60,60	0
56	MG	1A	4018	1/1	0.94	0.08	43,43,43,43	0
56	MG	1a	1703	1/1	0.94	0.20	61,61,61,61	0
56	MG	1a	1704	1/1	0.94	0.28	69,69,69,69	0
56	MG	1P	206	1/1	0.94	0.17	48,48,48,48	0
56	MG	1Q	201	1/1	0.94	0.15	44,44,44,44	0
56	MG	1Q	205	1/1	0.94	0.13	52,52,52,52	0
56	MG	2A	3095	1/1	0.94	0.12	51,51,51,51	0
56	MG	2a	1729	1/1	0.94	0.18	70,70,70,70	0
56	MG	1A	3421	1/1	0.94	0.15	43,43,43,43	0
56	MG	1R	204	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3822	1/1	0.94	0.08	70,70,70,70	0
56	MG	2A	3833	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3601	1/1	0.94	0.24	50,50,50,50	0
56	MG	1A	3135	1/1	0.94	0.14	40,40,40,40	0
56	MG	2A	3503	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3293	1/1	0.94	0.24	69,69,69,69	0
56	MG	1A	3503	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	4032	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3236	1/1	0.94	0.14	52,52,52,52	0
56	MG	1U	204	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	4034	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3505	1/1	0.94	0.18	60,60,60,60	0
56	MG	1a	1728	1/1	0.94	0.08	60,60,60,60	0
56	MG	2A	3522	1/1	0.94	0.08	72,72,72,72	0
56	MG	2A	3528	1/1	0.94	0.20	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1734	1/1	0.94	0.14	60,60,60,60	0
56	MG	1A	3508	1/1	0.94	0.14	38,38,38,38	0
56	MG	2A	3531	1/1	0.94	0.15	76,76,76,76	0
56	MG	1A	3078	1/1	0.94	0.33	52,52,52,52	0
56	MG	1W	201	1/1	0.94	0.26	54,54,54,54	0
56	MG	2a	1756	1/1	0.94	0.07	79,79,79,79	0
56	MG	1a	1739	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3080	1/1	0.94	0.06	28,28,28,28	0
56	MG	1A	3016	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3433	1/1	0.94	0.16	59,59,59,59	0
56	MG	1Y	202	1/1	0.94	0.08	74,74,74,74	0
56	MG	2A	3871	1/1	0.94	0.08	56,56,56,56	0
56	MG	2A	3123	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3846	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	1751	1/1	0.94	0.21	66,66,66,66	0
56	MG	1A	3514	1/1	0.94	0.08	57,57,57,57	0
56	MG	2A	3564	1/1	0.94	0.09	40,40,40,40	0
56	MG	2a	1775	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3018	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3568	1/1	0.94	0.15	70,70,70,70	0
56	MG	1A	4054	1/1	0.94	0.05	38,38,38,38	0
56	MG	1A	3360	1/1	0.94	0.18	39,39,39,39	0
56	MG	2a	1781	1/1	0.94	0.07	82,82,82,82	0
56	MG	2a	1784	1/1	0.94	0.12	76,76,76,76	0
56	MG	1A	3626	1/1	0.94	0.08	13,13,13,13	0
56	MG	2A	3575	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3301	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3520	1/1	0.94	0.21	48,48,48,48	0
56	MG	1A	3187	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3112	1/1	0.94	0.12	43,43,43,43	0
56	MG	1a	1766	1/1	0.94	0.13	67,67,67,67	0
56	MG	2a	1793	1/1	0.94	0.18	68,68,68,68	0
56	MG	2A	3138	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3061	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3859	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3369	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3144	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3088	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3528	1/1	0.94	0.12	59,59,59,59	0
56	MG	2D	301	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3312	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3252	1/1	0.94	0.20	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	3871	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3872	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3674	1/1	0.94	0.10	31,31,31,31	0
56	MG	1a	1802	1/1	0.94	0.09	69,69,69,69	0
56	MG	2E	306	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3376	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3155	1/1	0.94	0.12	70,70,70,70	0
56	MG	2a	1812	1/1	0.94	0.14	57,57,57,57	0
56	MG	2E	309	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3156	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3314	1/1	0.94	0.15	62,62,62,62	0
56	MG	2A	3158	1/1	0.94	0.21	45,45,45,45	0
56	MG	1A	3159	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3701	1/1	0.94	0.12	69,69,69,69	0
56	MG	2N	201	1/1	0.94	0.06	65,65,65,65	0
56	MG	2O	201	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3882	1/1	0.94	0.15	33,33,33,33	0
56	MG	2P	202	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	4092	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3200	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3712	1/1	0.94	0.10	50,50,50,50	0
56	MG	1a	1609	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3629	1/1	0.94	0.14	64,64,64,64	0
56	MG	2A	3631	1/1	0.94	0.18	51,51,51,51	0
56	MG	1a	1610	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3887	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3888	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3890	1/1	0.94	0.10	51,51,51,51	0
56	MG	2a	1837	1/1	0.94	0.07	79,79,79,79	0
56	MG	1A	3892	1/1	0.94	0.06	19,19,19,19	0
56	MG	2X	101	1/1	0.94	0.11	72,72,72,72	0
56	MG	1A	3027	1/1	0.94	0.14	79,79,79,79	0
56	MG	1A	3381	1/1	0.94	0.07	47,47,47,47	0
56	MG	20	102	1/1	0.94	0.15	72,72,72,72	0
56	MG	2A	3646	1/1	0.94	0.17	56,56,56,56	0
56	MG	1a	1620	1/1	0.94	0.10	74,74,74,74	0
56	MG	1A	4102	1/1	0.94	0.26	55,55,55,55	0
56	MG	1a	1624	1/1	0.94	0.16	70,70,70,70	0
56	MG	2A	3650	1/1	0.94	0.22	55,55,55,55	0
56	MG	25	102	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3906	1/1	0.94	0.15	37,37,37,37	0
56	MG	2l	204	1/1	0.94	0.10	80,80,80,80	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3380	1/1	0.94	0.13	67,67,67,67	0
56	MG	1A	3382	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3718	1/1	0.94	0.14	74,74,74,74	0
56	MG	1A	3464	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3658	1/1	0.94	0.08	77,77,77,77	0
56	MG	2A	3186	1/1	0.94	0.27	69,69,69,69	0
56	MG	2v	103	1/1	0.94	0.14	76,76,76,76	0
56	MG	28	103	1/1	0.94	0.22	59,59,59,59	0
56	MG	2A	3660	1/1	0.94	0.13	72,72,72,72	0
56	MG	2A	3661	1/1	0.94	0.12	74,74,74,74	0
56	MG	2A	3188	1/1	0.94	0.20	64,64,64,64	0
56	MG	2a	1602	1/1	0.94	0.12	71,71,71,71	0
56	MG	1A	4109	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3319	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3320	1/1	0.94	0.05	31,31,31,31	0
56	MG	1a	1633	1/1	0.94	0.33	70,70,70,70	0
56	MG	2x	103	1/1	0.94	0.12	76,76,76,76	0
56	MG	2x	104	1/1	0.94	0.19	75,75,75,75	0
56	MG	2x	105	1/1	0.94	0.09	73,73,73,73	0
56	MG	1A	3327	1/1	0.94	0.08	47,47,47,47	0
56	MG	1B	204	1/1	0.94	0.24	60,60,60,60	0
56	MG	1x	106	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3029	1/1	0.94	0.10	41,41,41,41	0
56	MG	1a	1639	1/1	0.94	0.14	68,68,68,68	0
56	MG	1A	3926	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3548	1/1	0.94	0.26	53,53,53,53	0
56	MG	1A	3091	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3034	1/1	0.94	0.29	39,39,39,39	0
57	K	2A	3467	1/1	0.94	0.14	82,82,82,82	0
56	MG	1A	3891	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3583	1/1	0.95	0.18	33,33,33,33	0
56	MG	1A	3894	1/1	0.95	0.12	35,35,35,35	0
56	MG	1w	108	1/1	0.95	0.09	76,76,76,76	0
56	MG	1A	3280	1/1	0.95	0.12	51,51,51,51	0
56	MG	1x	102	1/1	0.95	0.13	62,62,62,62	0
56	MG	1A	4096	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	3904	1/1	0.95	0.10	72,72,72,72	0
56	MG	1A	3449	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3395	1/1	0.95	0.14	25,25,25,25	0
56	MG	1a	1622	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3721	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3907	1/1	0.95	0.11	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	3451	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3100	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3744	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3515	1/1	0.95	0.10	51,51,51,51	0
56	MG	2A	3213	1/1	0.95	0.08	72,72,72,72	0
56	MG	1A	3283	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3114	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3216	1/1	0.95	0.25	60,60,60,60	0
56	MG	2A	3217	1/1	0.95	0.17	63,63,63,63	0
56	MG	1a	1631	1/1	0.95	0.19	70,70,70,70	0
56	MG	1A	3322	1/1	0.95	0.22	62,62,62,62	0
56	MG	1A	3359	1/1	0.95	0.18	71,71,71,71	0
56	MG	1A	3459	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3460	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3223	1/1	0.95	0.21	53,53,53,53	0
56	MG	1A	3759	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3933	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3934	1/1	0.95	0.08	30,30,30,30	0
56	MG	2A	3227	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3761	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3229	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3014	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3763	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	3011	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3947	1/1	0.95	0.06	59,59,59,59	0
56	MG	2A	3752	1/1	0.95	0.28	52,52,52,52	0
56	MG	1a	1645	1/1	0.95	0.26	71,71,71,71	0
56	MG	2A	3235	1/1	0.95	0.12	82,82,82,82	0
56	MG	1A	3405	1/1	0.95	0.18	38,38,38,38	0
56	MG	1A	3407	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3757	1/1	0.95	0.08	65,65,65,65	0
56	MG	1A	3768	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3450	1/1	0.95	0.25	62,62,62,62	0
56	MG	1A	3605	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3954	1/1	0.95	0.09	51,51,51,51	0
56	MG	1a	1652	1/1	0.95	0.06	62,62,62,62	0
56	MG	1B	219	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3030	1/1	0.95	0.30	59,59,59,59	0
56	MG	1A	3083	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3409	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3290	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3460	1/1	0.95	0.08	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	226	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3777	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3412	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3364	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3790	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3614	1/1	0.95	0.08	50,50,50,50	0
56	MG	1a	1664	1/1	0.95	0.26	75,75,75,75	0
56	MG	1a	1665	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3365	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3794	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3797	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	3133	1/1	0.95	0.08	42,42,42,42	0
56	MG	1B	236	1/1	0.95	0.07	44,44,44,44	0
56	MG	1D	303	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3035	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3332	1/1	0.95	0.25	55,55,55,55	0
56	MG	1A	3807	1/1	0.95	0.07	43,43,43,43	0
56	MG	1a	1677	1/1	0.95	0.21	68,68,68,68	0
56	MG	1A	3980	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3230	1/1	0.95	0.21	41,41,41,41	0
56	MG	1A	3540	1/1	0.95	0.24	42,42,42,42	0
56	MG	1A	3628	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3541	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3988	1/1	0.95	0.09	66,66,66,66	0
56	MG	1A	3812	1/1	0.95	0.05	27,27,27,27	0
56	MG	1A	3990	1/1	0.95	0.11	69,69,69,69	0
56	MG	1A	3119	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3543	1/1	0.95	0.20	46,46,46,46	0
56	MG	1E	316	1/1	0.95	0.11	54,54,54,54	0
56	MG	1a	1689	1/1	0.95	0.06	61,61,61,61	0
56	MG	2A	3494	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3994	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3199	1/1	0.95	0.10	49,49,49,49	0
56	MG	1F	311	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3071	1/1	0.95	0.10	71,71,71,71	0
56	MG	2A	3072	1/1	0.95	0.19	58,58,58,58	0
56	MG	1F	312	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3639	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3820	1/1	0.95	0.13	53,53,53,53	0
56	MG	2A	3506	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3640	1/1	0.95	0.05	24,24,24,24	0
56	MG	1A	4002	1/1	0.95	0.10	39,39,39,39	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3511	1/1	0.95	0.07	31,31,31,31	0
56	MG	1A	4003	1/1	0.95	0.13	52,52,52,52	0
56	MG	2A	3516	1/1	0.95	0.11	61,61,61,61	0
56	MG	1A	3641	1/1	0.95	0.06	30,30,30,30	0
56	MG	1A	3824	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	4007	1/1	0.95	0.09	20,20,20,20	0
56	MG	1A	3826	1/1	0.95	0.30	32,32,32,32	0
56	MG	2A	3525	1/1	0.95	0.08	49,49,49,49	0
56	MG	1O	203	1/1	0.95	0.17	60,60,60,60	0
56	MG	2A	3853	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3829	1/1	0.95	0.06	21,21,21,21	0
56	MG	1A	3375	1/1	0.95	0.11	43,43,43,43	0
56	MG	2A	3857	1/1	0.95	0.15	71,71,71,71	0
56	MG	1A	3261	1/1	0.95	0.05	36,36,36,36	0
56	MG	1P	201	1/1	0.95	0.37	37,37,37,37	0
56	MG	2A	3093	1/1	0.95	0.20	51,51,51,51	0
56	MG	1P	203	1/1	0.95	0.23	35,35,35,35	0
56	MG	1P	204	1/1	0.95	0.14	34,34,34,34	0
56	MG	2a	1751	1/1	0.95	0.10	65,65,65,65	0
56	MG	2a	1753	1/1	0.95	0.06	72,72,72,72	0
56	MG	1A	3834	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	4016	1/1	0.95	0.06	27,27,27,27	0
56	MG	1A	3121	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3653	1/1	0.95	0.15	28,28,28,28	0
56	MG	2a	1760	1/1	0.95	0.15	68,68,68,68	0
56	MG	2A	3557	1/1	0.95	0.15	52,52,52,52	0
56	MG	1R	201	1/1	0.95	0.19	53,53,53,53	0
56	MG	2a	1765	1/1	0.95	0.07	82,82,82,82	0
56	MG	2A	3307	1/1	0.95	0.19	72,72,72,72	0
56	MG	1a	1718	1/1	0.95	0.28	58,58,58,58	0
56	MG	1a	1719	1/1	0.95	0.14	63,63,63,63	0
56	MG	2A	3565	1/1	0.95	0.09	60,60,60,60	0
56	MG	1A	4021	1/1	0.95	0.07	45,45,45,45	0
56	MG	2A	3104	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	3655	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	4025	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3657	1/1	0.95	0.06	31,31,31,31	0
56	MG	2A	3574	1/1	0.95	0.14	49,49,49,49	0
56	MG	1a	1725	1/1	0.95	0.17	68,68,68,68	0
56	MG	1A	3424	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	4029	1/1	0.95	0.12	55,55,55,55	0
56	MG	2a	1782	1/1	0.95	0.12	69,69,69,69	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3112	1/1	0.95	0.16	55,55,55,55	0
56	MG	2A	3581	1/1	0.95	0.09	63,63,63,63	0
56	MG	1a	1730	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3659	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3842	1/1	0.95	0.07	67,67,67,67	0
56	MG	2A	3324	1/1	0.95	0.15	64,64,64,64	0
56	MG	1U	203	1/1	0.95	0.26	34,34,34,34	0
56	MG	2a	1791	1/1	0.95	0.15	70,70,70,70	0
56	MG	1a	1737	1/1	0.95	0.11	70,70,70,70	0
56	MG	1A	3425	1/1	0.95	0.14	50,50,50,50	0
56	MG	2A	3120	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3665	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3666	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	4036	1/1	0.95	0.06	49,49,49,49	0
56	MG	2A	3124	1/1	0.95	0.21	68,68,68,68	0
56	MG	1A	3551	1/1	0.95	0.07	29,29,29,29	0
56	MG	2A	3606	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3334	1/1	0.95	0.12	66,66,66,66	0
56	MG	2a	1802	1/1	0.95	0.19	72,72,72,72	0
56	MG	1A	3485	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3682	1/1	0.95	0.05	21,21,21,21	0
56	MG	1a	1749	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3338	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	4042	1/1	0.95	0.06	55,55,55,55	0
56	MG	2A	3615	1/1	0.95	0.12	53,53,53,53	0
56	MG	1X	101	1/1	0.95	0.29	48,48,48,48	0
56	MG	1X	104	1/1	0.95	0.26	50,50,50,50	0
56	MG	1X	105	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3426	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3688	1/1	0.95	0.07	57,57,57,57	0
56	MG	1A	3487	1/1	0.95	0.11	42,42,42,42	0
56	MG	1a	1760	1/1	0.95	0.10	67,67,67,67	0
56	MG	1A	4047	1/1	0.95	0.05	34,34,34,34	0
56	MG	1A	3692	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3006	1/1	0.95	0.10	60,60,60,60	0
56	MG	1A	3697	1/1	0.95	0.10	37,37,37,37	0
56	MG	2A	3636	1/1	0.95	0.13	60,60,60,60	0
56	MG	1a	1768	1/1	0.95	0.06	76,76,76,76	0
56	MG	1a	1769	1/1	0.95	0.09	85,85,85,85	0
56	MG	1A	3698	1/1	0.95	0.13	29,29,29,29	0
56	MG	2V	202	1/1	0.95	0.09	69,69,69,69	0
56	MG	10	104	1/1	0.95	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	2a	1826	1/1	0.95	0.11	75,75,75,75	0
56	MG	1a	1776	1/1	0.95	0.08	69,69,69,69	0
56	MG	1a	1777	1/1	0.95	0.08	73,73,73,73	0
56	MG	2a	1829	1/1	0.95	0.14	68,68,68,68	0
56	MG	2A	3150	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3428	1/1	0.95	0.07	46,46,46,46	0
56	MG	2a	1832	1/1	0.95	0.24	72,72,72,72	0
56	MG	1A	3863	1/1	0.95	0.07	61,61,61,61	0
56	MG	1A	3706	1/1	0.95	0.12	27,27,27,27	0
56	MG	1A	3557	1/1	0.95	0.28	64,64,64,64	0
56	MG	2A	3365	1/1	0.95	0.14	72,72,72,72	0
56	MG	2A	3366	1/1	0.95	0.12	64,64,64,64	0
56	MG	1l	103	1/1	0.95	0.07	44,44,44,44	0
56	MG	1a	1790	1/1	0.95	0.08	81,81,81,81	0
56	MG	1a	1793	1/1	0.95	0.09	78,78,78,78	0
56	MG	1l	104	1/1	0.95	0.06	55,55,55,55	0
56	MG	1A	4062	1/1	0.95	0.11	65,65,65,65	0
56	MG	2A	3160	1/1	0.95	0.14	70,70,70,70	0
56	MG	12	101	1/1	0.95	0.08	58,58,58,58	0
56	MG	12	102	1/1	0.95	0.12	48,48,48,48	0
56	MG	1a	1804	1/1	0.95	0.06	58,58,58,58	0
56	MG	1A	3710	1/1	0.95	0.05	29,29,29,29	0
56	MG	2A	3378	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	3206	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	3123	1/1	0.95	0.29	48,48,48,48	0
56	MG	2A	3670	1/1	0.95	0.10	63,63,63,63	0
56	MG	2q	203	1/1	0.95	0.11	71,71,71,71	0
56	MG	15	101	1/1	0.95	0.13	39,39,39,39	0
56	MG	2A	3169	1/1	0.95	0.07	65,65,65,65	0
56	MG	1a	1809	1/1	0.95	0.20	72,72,72,72	0
56	MG	1a	1810	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	3107	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3678	1/1	0.95	0.16	66,66,66,66	0
56	MG	2A	3386	1/1	0.95	0.19	71,71,71,71	0
56	MG	2A	3387	1/1	0.95	0.15	66,66,66,66	0
56	MG	15	104	1/1	0.95	0.13	29,29,29,29	0
56	MG	1A	3239	1/1	0.95	0.24	37,37,37,37	0
56	MG	15	106	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3309	1/1	0.95	0.41	62,62,62,62	0
56	MG	1A	3066	1/1	0.95	0.24	63,63,63,63	0
56	MG	1A	3213	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3150	1/1	0.95	0.16	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3880	1/1	0.95	0.05	41,41,41,41	0
56	MG	2A	3694	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3722	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3884	1/1	0.95	0.26	40,40,40,40	0
56	MG	1A	3315	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	4082	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3389	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3126	1/1	0.95	0.34	40,40,40,40	0
56	MG	2A	3702	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	4088	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3393	1/1	0.95	0.33	32,32,32,32	0
56	MG	1A	3509	1/1	0.95	0.16	48,48,48,48	0
59	ZN	14	102	1/1	0.95	0.13	110,110,110,110	0
59	ZN	24	501	1/1	0.95	0.16	136,136,136,136	0
59	ZN	2n	501	1/1	0.95	0.08	108,108,108,108	0
56	MG	1A	3183	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3137	1/1	0.96	0.14	31,31,31,31	0
56	MG	2A	3422	1/1	0.96	0.31	49,49,49,49	0
56	MG	1D	306	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3984	1/1	0.96	0.10	45,45,45,45	0
56	MG	1D	310	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3821	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3410	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3005	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3116	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3663	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3827	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3292	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3142	1/1	0.96	0.06	24,24,24,24	0
56	MG	1E	309	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3667	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3144	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3237	1/1	0.96	0.14	57,57,57,57	0
56	MG	1a	1670	1/1	0.96	0.18	59,59,59,59	0
56	MG	1E	312	1/1	0.96	0.07	25,25,25,25	0
56	MG	2A	3720	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3030	1/1	0.96	0.32	32,32,32,32	0
56	MG	1E	315	1/1	0.96	0.19	41,41,41,41	0
56	MG	1A	3240	1/1	0.96	0.24	38,38,38,38	0
56	MG	1F	302	1/1	0.96	0.19	36,36,36,36	0
56	MG	1A	3191	1/1	0.96	0.28	41,41,41,41	0
56	MG	1A	3193	1/1	0.96	0.12	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	3244	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3361	1/1	0.96	0.09	58,58,58,58	0
56	MG	2a	1648	1/1	0.96	0.17	72,72,72,72	0
56	MG	1A	3069	1/1	0.96	0.17	59,59,59,59	0
56	MG	1A	3092	1/1	0.96	0.14	48,48,48,48	0
56	MG	2A	3049	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3151	1/1	0.96	0.15	41,41,41,41	0
56	MG	1G	204	1/1	0.96	0.05	67,67,67,67	0
56	MG	1A	3564	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	3705	1/1	0.96	0.08	34,34,34,34	0
56	MG	1N	201	1/1	0.96	0.17	48,48,48,48	0
56	MG	2A	3739	1/1	0.96	0.04	76,76,76,76	0
56	MG	1A	3093	1/1	0.96	0.12	59,59,59,59	0
56	MG	1N	203	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3495	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3366	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3570	1/1	0.96	0.18	36,36,36,36	0
56	MG	1O	202	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3061	1/1	0.96	0.17	69,69,69,69	0
56	MG	1A	3201	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3572	1/1	0.96	0.35	70,70,70,70	0
56	MG	1A	3204	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3750	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3254	1/1	0.96	0.16	54,54,54,54	0
56	MG	1A	3500	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	4028	1/1	0.96	0.06	58,58,58,58	0
56	MG	1A	3861	1/1	0.96	0.09	40,40,40,40	0
56	MG	2a	1673	1/1	0.96	0.07	73,73,73,73	0
56	MG	1A	3156	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	3580	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3865	1/1	0.96	0.07	25,25,25,25	0
56	MG	2a	1677	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	3502	1/1	0.96	0.05	45,45,45,45	0
56	MG	1A	3431	1/1	0.96	0.21	45,45,45,45	0
56	MG	1R	203	1/1	0.96	0.26	41,41,41,41	0
56	MG	2A	3480	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3763	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3726	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3073	1/1	0.96	0.16	35,35,35,35	0
56	MG	2A	3767	1/1	0.96	0.20	62,62,62,62	0
56	MG	2A	3768	1/1	0.96	0.07	74,74,74,74	0
56	MG	2A	3769	1/1	0.96	0.10	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3078	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	3587	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3207	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3506	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3874	1/1	0.96	0.20	62,62,62,62	0
56	MG	2a	1694	1/1	0.96	0.18	69,69,69,69	0
56	MG	1A	4044	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3507	1/1	0.96	0.15	34,34,34,34	0
56	MG	1A	3053	1/1	0.96	0.08	51,51,51,51	0
56	MG	1a	1717	1/1	0.96	0.36	54,54,54,54	0
56	MG	1A	3097	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3738	1/1	0.96	0.06	50,50,50,50	0
56	MG	1U	207	1/1	0.96	0.26	42,42,42,42	0
56	MG	1U	209	1/1	0.96	0.15	35,35,35,35	0
56	MG	1A	4049	1/1	0.96	0.05	53,53,53,53	0
56	MG	2A	3786	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3787	1/1	0.96	0.06	65,65,65,65	0
56	MG	1V	203	1/1	0.96	0.21	57,57,57,57	0
56	MG	1A	3023	1/1	0.96	0.05	22,22,22,22	0
56	MG	1a	1726	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	3881	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	4053	1/1	0.96	0.07	27,27,27,27	0
56	MG	1a	1729	1/1	0.96	0.09	69,69,69,69	0
56	MG	1A	3042	1/1	0.96	0.21	37,37,37,37	0
56	MG	1W	203	1/1	0.96	0.22	37,37,37,37	0
56	MG	1A	3439	1/1	0.96	0.06	48,48,48,48	0
56	MG	2A	3509	1/1	0.96	0.11	41,41,41,41	0
56	MG	2a	1716	1/1	0.96	0.11	75,75,75,75	0
56	MG	1A	3599	1/1	0.96	0.23	41,41,41,41	0
56	MG	2A	3303	1/1	0.96	0.11	64,64,64,64	0
56	MG	2A	3515	1/1	0.96	0.10	62,62,62,62	0
56	MG	1X	103	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3517	1/1	0.96	0.07	64,64,64,64	0
56	MG	2A	3107	1/1	0.96	0.15	52,52,52,52	0
56	MG	2A	3806	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3321	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3747	1/1	0.96	0.10	46,46,46,46	0
56	MG	1X	107	1/1	0.96	0.11	61,61,61,61	0
56	MG	2A	3524	1/1	0.96	0.12	65,65,65,65	0
56	MG	1A	3102	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3818	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3526	1/1	0.96	0.08	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	3820	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3750	1/1	0.96	0.06	21,21,21,21	0
56	MG	1A	3324	1/1	0.96	0.27	36,36,36,36	0
56	MG	1A	3753	1/1	0.96	0.06	20,20,20,20	0
56	MG	1A	4066	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3079	1/1	0.96	0.14	43,43,43,43	0
56	MG	10	101	1/1	0.96	0.15	46,46,46,46	0
56	MG	2A	3534	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3895	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3896	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3539	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3318	1/1	0.96	0.27	77,77,77,77	0
56	MG	2A	3839	1/1	0.96	0.06	65,65,65,65	0
56	MG	2A	3840	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3543	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3755	1/1	0.96	0.08	62,62,62,62	0
56	MG	2A	3547	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3550	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3056	1/1	0.96	0.05	32,32,32,32	0
56	MG	1A	3057	1/1	0.96	0.22	50,50,50,50	0
56	MG	2A	3848	1/1	0.96	0.07	55,55,55,55	0
56	MG	2a	1752	1/1	0.96	0.07	75,75,75,75	0
56	MG	2A	3555	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3220	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3222	1/1	0.96	0.17	46,46,46,46	0
56	MG	11	101	1/1	0.96	0.42	45,45,45,45	0
56	MG	2a	1758	1/1	0.96	0.07	75,75,75,75	0
56	MG	1A	3760	1/1	0.96	0.04	42,42,42,42	0
56	MG	1A	3271	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3856	1/1	0.96	0.09	70,70,70,70	0
56	MG	1a	1767	1/1	0.96	0.07	71,71,71,71	0
56	MG	2a	1764	1/1	0.96	0.06	71,71,71,71	0
56	MG	1A	3911	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3859	1/1	0.96	0.09	70,70,70,70	0
56	MG	2A	3860	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	4084	1/1	0.96	0.13	57,57,57,57	0
56	MG	2a	1769	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3045	1/1	0.96	0.13	40,40,40,40	0
56	MG	13	101	1/1	0.96	0.07	36,36,36,36	0
56	MG	1a	1774	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3914	1/1	0.96	0.19	21,21,21,21	0
56	MG	1A	4087	1/1	0.96	0.08	23,23,23,23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3525	1/1	0.96	0.26	45,45,45,45	0
56	MG	1A	3334	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3141	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3616	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3583	1/1	0.96	0.12	57,57,57,57	0
56	MG	15	103	1/1	0.96	0.28	31,31,31,31	0
56	MG	2a	1783	1/1	0.96	0.11	63,63,63,63	0
56	MG	1a	1784	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	3921	1/1	0.96	0.24	39,39,39,39	0
56	MG	2A	3589	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3924	1/1	0.96	0.08	24,24,24,24	0
56	MG	2A	3593	1/1	0.96	0.20	60,60,60,60	0
56	MG	2A	3344	1/1	0.96	0.08	67,67,67,67	0
56	MG	1a	1791	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	3767	1/1	0.96	0.07	20,20,20,20	0
56	MG	1A	3392	1/1	0.96	0.09	49,49,49,49	0
56	MG	17	102	1/1	0.96	0.15	34,34,34,34	0
56	MG	17	103	1/1	0.96	0.12	40,40,40,40	0
56	MG	1a	1799	1/1	0.96	0.06	87,87,87,87	0
56	MG	17	104	1/1	0.96	0.11	57,57,57,57	0
56	MG	1a	1803	1/1	0.96	0.11	72,72,72,72	0
56	MG	2A	3605	1/1	0.96	0.12	55,55,55,55	0
56	MG	18	101	1/1	0.96	0.28	55,55,55,55	0
56	MG	18	103	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	3770	1/1	0.96	0.09	24,24,24,24	0
56	MG	2A	3609	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3928	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3771	1/1	0.96	0.06	39,39,39,39	0
56	MG	2D	302	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3931	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3225	1/1	0.96	0.11	37,37,37,37	0
56	MG	2D	306	1/1	0.96	0.14	65,65,65,65	0
56	MG	2A	3361	1/1	0.96	0.17	67,67,67,67	0
56	MG	1A	3777	1/1	0.96	0.08	34,34,34,34	0
56	MG	1A	3001	1/1	0.96	0.17	45,45,45,45	0
56	MG	2E	304	1/1	0.96	0.26	56,56,56,56	0
56	MG	1A	3935	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3619	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3165	1/1	0.96	0.18	54,54,54,54	0
56	MG	1A	3937	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3623	1/1	0.96	0.09	51,51,51,51	0
56	MG	2E	310	1/1	0.96	0.10	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	1A	3530	1/1	0.96	0.07	48,48,48,48	0
56	MG	1a	1607	1/1	0.96	0.09	56,56,56,56	0
56	MG	1f	201	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3170	1/1	0.96	0.11	67,67,67,67	0
56	MG	2F	306	1/1	0.96	0.14	57,57,57,57	0
56	MG	1A	4107	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3632	1/1	0.96	0.19	53,53,53,53	0
56	MG	1A	3275	1/1	0.96	0.08	37,37,37,37	0
56	MG	1k	201	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3943	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3638	1/1	0.96	0.13	44,44,44,44	0
56	MG	2Q	202	1/1	0.96	0.11	55,55,55,55	0
56	MG	2A	3639	1/1	0.96	0.08	54,54,54,54	0
56	MG	2Q	204	1/1	0.96	0.09	70,70,70,70	0
56	MG	1A	3276	1/1	0.96	0.13	50,50,50,50	0
56	MG	2A	3641	1/1	0.96	0.08	50,50,50,50	0
56	MG	1m	3002	1/1	0.96	0.15	67,67,67,67	0
56	MG	1a	1613	1/1	0.96	0.10	69,69,69,69	0
56	MG	1A	3946	1/1	0.96	0.04	36,36,36,36	0
56	MG	1A	3785	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3462	1/1	0.96	0.14	45,45,45,45	0
56	MG	1v	102	1/1	0.96	0.05	63,63,63,63	0
56	MG	1A	3789	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3278	1/1	0.96	0.07	43,43,43,43	0
56	MG	1a	1619	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3340	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3189	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3465	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3956	1/1	0.96	0.06	51,51,51,51	0
56	MG	1a	1623	1/1	0.96	0.33	65,65,65,65	0
56	MG	1A	3634	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3959	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3960	1/1	0.96	0.05	51,51,51,51	0
56	MG	1A	3961	1/1	0.96	0.07	52,52,52,52	0
56	MG	1B	216	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3396	1/1	0.96	0.09	73,73,73,73	0
56	MG	1A	3537	1/1	0.96	0.09	53,53,53,53	0
56	MG	27	101	1/1	0.96	0.20	50,50,50,50	0
56	MG	1A	3637	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3667	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3800	1/1	0.96	0.18	53,53,53,53	0
56	MG	1A	3400	1/1	0.96	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	3967	1/1	0.96	0.05	36,36,36,36	0
56	MG	28	104	1/1	0.96	0.07	59,59,59,59	0
56	MG	1A	3175	1/1	0.96	0.40	36,36,36,36	0
56	MG	1B	223	1/1	0.96	0.16	57,57,57,57	0
56	MG	1B	224	1/1	0.96	0.07	51,51,51,51	0
56	MG	1B	225	1/1	0.96	0.11	60,60,60,60	0
56	MG	1A	3969	1/1	0.96	0.05	24,24,24,24	0
56	MG	1A	3179	1/1	0.96	0.09	23,23,23,23	0
56	MG	2A	3679	1/1	0.96	0.06	55,55,55,55	0
56	MG	2A	3210	1/1	0.96	0.13	57,57,57,57	0
56	MG	2A	3002	1/1	0.96	0.26	63,63,63,63	0
56	MG	1A	3643	1/1	0.96	0.14	63,63,63,63	0
56	MG	1A	3644	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3412	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3646	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3647	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3047	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1647	1/1	0.96	0.07	58,58,58,58	0
56	MG	1A	3284	1/1	0.96	0.36	44,44,44,44	0
56	MG	2A	3691	1/1	0.96	0.10	70,70,70,70	0
56	MG	1A	3406	1/1	0.96	0.28	46,46,46,46	0
56	MG	1A	3049	1/1	0.96	0.04	20,20,20,20	0
56	MG	1A	3550	1/1	0.97	0.27	52,52,52,52	0
56	MG	2A	3553	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3374	1/1	0.97	0.17	53,53,53,53	0
56	MG	1A	3899	1/1	0.97	0.07	23,23,23,23	0
56	MG	1A	3488	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3902	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3323	1/1	0.97	0.16	36,36,36,36	0
56	MG	2A	3560	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	4051	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3772	1/1	0.97	0.05	26,26,26,26	0
56	MG	1A	3774	1/1	0.97	0.08	26,26,26,26	0
56	MG	2A	3566	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3490	1/1	0.97	0.21	39,39,39,39	0
56	MG	1a	1666	1/1	0.97	0.05	73,73,73,73	0
56	MG	2A	3569	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3178	1/1	0.97	0.13	45,45,45,45	0
56	MG	1A	4055	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3776	1/1	0.97	0.09	43,43,43,43	0
56	MG	1A	4058	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3163	1/1	0.97	0.26	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	3778	1/1	0.97	0.07	35,35,35,35	0
56	MG	1Q	204	1/1	0.97	0.12	58,58,58,58	0
56	MG	2A	3578	1/1	0.97	0.07	36,36,36,36	0
56	MG	2a	1680	1/1	0.97	0.10	56,56,56,56	0
56	MG	2A	3807	1/1	0.97	0.05	60,60,60,60	0
56	MG	2A	3185	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3809	1/1	0.97	0.09	68,68,68,68	0
56	MG	2A	3580	1/1	0.97	0.14	59,59,59,59	0
56	MG	2A	3811	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3326	1/1	0.97	0.15	45,45,45,45	0
56	MG	2A	3582	1/1	0.97	0.14	64,64,64,64	0
56	MG	2A	3187	1/1	0.97	0.08	61,61,61,61	0
56	MG	1A	3132	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3007	1/1	0.97	0.05	34,34,34,34	0
56	MG	1R	202	1/1	0.97	0.21	37,37,37,37	0
56	MG	1A	3277	1/1	0.97	0.13	30,30,30,30	0
56	MG	2A	3825	1/1	0.97	0.06	55,55,55,55	0
56	MG	2A	3374	1/1	0.97	0.15	70,70,70,70	0
56	MG	1A	3094	1/1	0.97	0.07	32,32,32,32	0
56	MG	1A	3435	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3656	1/1	0.97	0.04	32,32,32,32	0
56	MG	2A	3012	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3831	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3597	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3013	1/1	0.97	0.14	55,55,55,55	0
56	MG	1A	3021	1/1	0.97	0.06	30,30,30,30	0
56	MG	2A	3015	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3563	1/1	0.97	0.24	41,41,41,41	0
56	MG	1A	3168	1/1	0.97	0.05	32,32,32,32	0
56	MG	1A	3793	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	4074	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3060	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3796	1/1	0.97	0.04	38,38,38,38	0
56	MG	1A	3662	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3798	1/1	0.97	0.04	25,25,25,25	0
56	MG	2A	3846	1/1	0.97	0.06	48,48,48,48	0
56	MG	1U	208	1/1	0.97	0.21	36,36,36,36	0
56	MG	2A	3026	1/1	0.97	0.14	49,49,49,49	0
56	MG	2A	3849	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3567	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3664	1/1	0.97	0.10	54,54,54,54	0
56	MG	2A	3614	1/1	0.97	0.07	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	3936	1/1	0.97	0.08	44,44,44,44	0
56	MG	1V	204	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3242	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3802	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3017	1/1	0.97	0.09	60,60,60,60	0
56	MG	2A	3035	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3941	1/1	0.97	0.05	68,68,68,68	0
56	MG	1A	3441	1/1	0.97	0.19	43,43,43,43	0
56	MG	1A	3669	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3287	1/1	0.97	0.28	33,33,33,33	0
56	MG	1X	102	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3628	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3672	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3443	1/1	0.97	0.27	53,53,53,53	0
56	MG	1A	3681	1/1	0.97	0.07	30,30,30,30	0
56	MG	1a	1706	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3634	1/1	0.97	0.06	61,61,61,61	0
56	MG	2A	3635	1/1	0.97	0.07	51,51,51,51	0
56	MG	1X	106	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3813	1/1	0.97	0.05	27,27,27,27	0
56	MG	1A	3952	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3138	1/1	0.97	0.28	31,31,31,31	0
56	MG	1Y	203	1/1	0.97	0.22	50,50,50,50	0
56	MG	1A	3390	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3955	1/1	0.97	0.07	46,46,46,46	0
56	MG	1a	1714	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3245	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3577	1/1	0.97	0.16	37,37,37,37	0
56	MG	1A	3958	1/1	0.97	0.08	60,60,60,60	0
56	MG	1A	3448	1/1	0.97	0.21	37,37,37,37	0
56	MG	2A	3239	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3039	1/1	0.97	0.19	34,34,34,34	0
56	MG	1a	1720	1/1	0.97	0.16	57,57,57,57	0
56	MG	1A	3209	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3248	1/1	0.97	0.25	65,65,65,65	0
56	MG	1A	3585	1/1	0.97	0.10	50,50,50,50	0
56	MG	2A	3654	1/1	0.97	0.09	63,63,63,63	0
56	MG	1A	3825	1/1	0.97	0.08	54,54,54,54	0
56	MG	2A	3656	1/1	0.97	0.10	69,69,69,69	0
56	MG	1A	3703	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3966	1/1	0.97	0.04	52,52,52,52	0
56	MG	11	102	1/1	0.97	0.05	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	2D	303	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3452	1/1	0.97	0.19	36,36,36,36	0
56	MG	1B	205	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3662	1/1	0.97	0.07	41,41,41,41	0
56	MG	1B	206	1/1	0.97	0.14	54,54,54,54	0
56	MG	2A	3070	1/1	0.97	0.09	38,38,38,38	0
56	MG	1a	1733	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3828	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3453	1/1	0.97	0.30	43,43,43,43	0
56	MG	1A	3830	1/1	0.97	0.04	36,36,36,36	0
56	MG	13	102	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	3707	1/1	0.97	0.11	24,24,24,24	0
56	MG	2A	3671	1/1	0.97	0.07	64,64,64,64	0
56	MG	1A	3588	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3028	1/1	0.97	0.27	33,33,33,33	0
56	MG	2A	3674	1/1	0.97	0.07	68,68,68,68	0
56	MG	2a	1780	1/1	0.97	0.06	59,59,59,59	0
56	MG	2A	3079	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3080	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3174	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3082	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3713	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3084	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3591	1/1	0.97	0.13	48,48,48,48	0
56	MG	1a	1746	1/1	0.97	0.09	54,54,54,54	0
56	MG	1a	1747	1/1	0.97	0.08	62,62,62,62	0
56	MG	1A	3397	1/1	0.97	0.40	47,47,47,47	0
56	MG	1A	3593	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3454	1/1	0.97	0.25	60,60,60,60	0
56	MG	1A	3981	1/1	0.97	0.07	72,72,72,72	0
56	MG	1A	3840	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3518	1/1	0.97	0.21	29,29,29,29	0
56	MG	2A	3690	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3296	1/1	0.97	0.18	33,33,33,33	0
56	MG	1a	1756	1/1	0.97	0.10	63,63,63,63	0
56	MG	1A	3251	1/1	0.97	0.31	60,60,60,60	0
56	MG	17	105	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3141	1/1	0.97	0.11	35,35,35,35	0
56	MG	2W	202	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3214	1/1	0.97	0.15	35,35,35,35	0
56	MG	1A	3523	1/1	0.97	0.16	33,33,33,33	0
56	MG	1a	1762	1/1	0.97	0.06	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3725	1/1	0.97	0.12	31,31,31,31	0
56	MG	18	107	1/1	0.97	0.09	43,43,43,43	0
56	MG	1B	227	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3177	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3706	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3727	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3473	1/1	0.97	0.11	79,79,79,79	0
56	MG	1A	3728	1/1	0.97	0.06	49,49,49,49	0
56	MG	1a	1770	1/1	0.97	0.07	69,69,69,69	0
56	MG	25	104	1/1	0.97	0.12	62,62,62,62	0
56	MG	1A	3052	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3302	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3180	1/1	0.97	0.10	41,41,41,41	0
56	MG	1a	1775	1/1	0.97	0.07	66,66,66,66	0
56	MG	1A	3857	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3143	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3355	1/1	0.97	0.08	40,40,40,40	0
56	MG	1D	302	1/1	0.97	0.15	48,48,48,48	0
56	MG	1A	3012	1/1	0.97	0.04	30,30,30,30	0
56	MG	2A	3722	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3306	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3104	1/1	0.97	0.04	30,30,30,30	0
56	MG	1a	1787	1/1	0.97	0.10	75,75,75,75	0
56	MG	1D	308	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3068	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3471	1/1	0.97	0.13	34,34,34,34	0
56	MG	1A	3613	1/1	0.97	0.07	37,37,37,37	0
56	MG	2a	1833	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	3310	1/1	0.97	0.16	54,54,54,54	0
56	MG	1A	3745	1/1	0.97	0.05	52,52,52,52	0
56	MG	1A	4015	1/1	0.97	0.07	33,33,33,33	0
56	MG	1a	1798	1/1	0.97	0.05	72,72,72,72	0
56	MG	1A	3473	1/1	0.97	0.23	44,44,44,44	0
56	MG	1A	4017	1/1	0.97	0.04	33,33,33,33	0
56	MG	2A	3131	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3617	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3502	1/1	0.97	0.06	60,60,60,60	0
56	MG	1E	307	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3311	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3749	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3224	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3009	1/1	0.97	0.08	25,25,25,25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3752	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3264	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3622	1/1	0.97	0.08	46,46,46,46	0
56	MG	2A	3322	1/1	0.97	0.09	59,59,59,59	0
56	MG	2q	201	1/1	0.97	0.32	65,65,65,65	0
56	MG	1A	3624	1/1	0.97	0.10	27,27,27,27	0
56	MG	1F	301	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3072	1/1	0.97	0.10	34,34,34,34	0
56	MG	1a	1635	1/1	0.97	0.15	41,41,41,41	0
56	MG	2A	3519	1/1	0.97	0.08	49,49,49,49	0
56	MG	1a	1636	1/1	0.97	0.24	66,66,66,66	0
56	MG	1F	303	1/1	0.97	0.27	33,33,33,33	0
56	MG	1F	304	1/1	0.97	0.18	35,35,35,35	0
56	MG	1F	305	1/1	0.97	0.10	40,40,40,40	0
56	MG	1F	306	1/1	0.97	0.07	49,49,49,49	0
56	MG	1F	307	1/1	0.97	0.18	28,28,28,28	0
56	MG	2A	3527	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3152	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3762	1/1	0.97	0.13	60,60,60,60	0
56	MG	1m	3001	1/1	0.97	0.12	68,68,68,68	0
56	MG	2A	3764	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3228	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3109	1/1	0.97	0.21	42,42,42,42	0
56	MG	1A	3129	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3631	1/1	0.97	0.06	39,39,39,39	0
56	MG	2x	107	1/1	0.97	0.10	57,57,57,57	0
56	MG	1G	201	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3889	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3044	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3032	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3540	1/1	0.97	0.06	51,51,51,51	0
56	MG	2A	3774	1/1	0.97	0.04	64,64,64,64	0
56	MG	1A	3195	1/1	0.97	0.23	40,40,40,40	0
56	MG	1A	3893	1/1	0.97	0.07	27,27,27,27	0
56	MG	1a	1653	1/1	0.97	0.09	53,53,53,53	0
58	A1A1F	2A	3875	34/34	0.97	0.08	38,45,52,56	0
56	MG	2A	3545	1/1	0.97	0.07	44,44,44,44	0
59	ZN	2Y	501	1/1	0.97	0.05	108,108,108,108	0
56	MG	1a	1654	1/1	0.97	0.06	61,61,61,61	0
56	MG	1A	3373	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3111	1/1	0.98	0.28	34,34,34,34	0
56	MG	1a	1771	1/1	0.98	0.05	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3908	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3607	1/1	0.98	0.14	30,30,30,30	0
56	MG	1A	3160	1/1	0.98	0.18	32,32,32,32	0
56	MG	1V	201	1/1	0.98	0.16	33,33,33,33	0
56	MG	1V	202	1/1	0.98	0.20	35,35,35,35	0
56	MG	1A	3279	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3912	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	3668	1/1	0.98	0.03	23,23,23,23	0
56	MG	1a	1780	1/1	0.98	0.04	81,81,81,81	0
56	MG	2X	102	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3161	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3670	1/1	0.98	0.06	26,26,26,26	0
56	MG	1A	3162	1/1	0.98	0.21	38,38,38,38	0
56	MG	2A	3778	1/1	0.98	0.04	57,57,57,57	0
56	MG	2A	3468	1/1	0.98	0.12	26,26,26,26	0
56	MG	1A	4022	1/1	0.98	0.04	42,42,42,42	0
56	MG	2A	3627	1/1	0.98	0.05	42,42,42,42	0
56	MG	1W	204	1/1	0.98	0.11	42,42,42,42	0
56	MG	1a	1789	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	4023	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3008	1/1	0.98	0.13	32,32,32,32	0
56	MG	1a	1792	1/1	0.98	0.04	52,52,52,52	0
56	MG	1A	3919	1/1	0.98	0.08	46,46,46,46	0
56	MG	1a	1794	1/1	0.98	0.04	60,60,60,60	0
56	MG	1A	3920	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3218	1/1	0.98	0.18	38,38,38,38	0
56	MG	1A	3833	1/1	0.98	0.05	41,41,41,41	0
56	MG	2A	3345	1/1	0.98	0.05	70,70,70,70	0
56	MG	2A	3793	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3675	1/1	0.98	0.05	30,30,30,30	0
56	MG	1A	3676	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3677	1/1	0.98	0.06	29,29,29,29	0
56	MG	1A	3678	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3188	1/1	0.98	0.11	34,34,34,34	0
56	MG	2A	3799	1/1	0.98	0.07	57,57,57,57	0
56	MG	1A	3930	1/1	0.98	0.10	50,50,50,50	0
56	MG	1A	4035	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3445	1/1	0.98	0.08	55,55,55,55	0
56	MG	1A	3686	1/1	0.98	0.03	30,30,30,30	0
56	MG	1A	3286	1/1	0.98	0.24	39,39,39,39	0
56	MG	1A	3113	1/1	0.98	0.16	42,42,42,42	0
56	MG	1D	301	1/1	0.98	0.12	38,38,38,38	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3689	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3844	1/1	0.98	0.04	31,31,31,31	0
56	MG	1D	304	1/1	0.98	0.08	18,18,18,18	0
56	MG	1A	3325	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3221	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3812	1/1	0.98	0.04	46,46,46,46	0
56	MG	2A	3499	1/1	0.98	0.08	74,74,74,74	0
56	MG	2A	3815	1/1	0.98	0.08	42,42,42,42	0
56	MG	1D	307	1/1	0.98	0.19	45,45,45,45	0
56	MG	1A	3043	1/1	0.98	0.22	37,37,37,37	0
56	MG	1A	3623	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3082	1/1	0.98	0.09	43,43,43,43	0
56	MG	1A	3944	1/1	0.98	0.06	34,34,34,34	0
56	MG	2A	3821	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	3699	1/1	0.98	0.06	20,20,20,20	0
56	MG	1A	3192	1/1	0.98	0.21	39,39,39,39	0
56	MG	1A	3853	1/1	0.98	0.04	61,61,61,61	0
56	MG	1A	3702	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3949	1/1	0.98	0.04	46,46,46,46	0
56	MG	2A	3510	1/1	0.98	0.19	50,50,50,50	0
56	MG	1A	3578	1/1	0.98	0.11	28,28,28,28	0
56	MG	1E	306	1/1	0.98	0.08	32,32,32,32	0
56	MG	2A	3513	1/1	0.98	0.17	55,55,55,55	0
56	MG	1A	4056	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3256	1/1	0.98	0.11	47,47,47,47	0
56	MG	1A	3048	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3581	1/1	0.98	0.09	38,38,38,38	0
56	MG	2A	3838	1/1	0.98	0.07	65,65,65,65	0
56	MG	1A	3582	1/1	0.98	0.24	40,40,40,40	0
56	MG	1A	3709	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3781	1/1	0.98	0.04	15,15,15,15	0
56	MG	17	101	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3117	1/1	0.98	0.13	52,52,52,52	0
56	MG	1A	3194	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3864	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3711	1/1	0.98	0.04	14,14,14,14	0
56	MG	1A	3295	1/1	0.98	0.05	49,49,49,49	0
56	MG	1A	3077	1/1	0.98	0.05	32,32,32,32	0
56	MG	18	102	1/1	0.98	0.16	46,46,46,46	0
56	MG	1A	3196	1/1	0.98	0.26	36,36,36,36	0
56	MG	1A	3715	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	4071	1/1	0.98	0.05	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	18	106	1/1	0.98	0.10	49,49,49,49	0
56	MG	1A	3870	1/1	0.98	0.11	47,47,47,47	0
56	MG	2A	3692	1/1	0.98	0.05	71,71,71,71	0
56	MG	2A	3693	1/1	0.98	0.13	58,58,58,58	0
56	MG	1F	308	1/1	0.98	0.11	30,30,30,30	0
56	MG	1A	3146	1/1	0.98	0.18	34,34,34,34	0
56	MG	1A	3147	1/1	0.98	0.15	36,36,36,36	0
56	MG	2A	3541	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3148	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	4076	1/1	0.98	0.07	17,17,17,17	0
56	MG	2A	3700	1/1	0.98	0.09	73,73,73,73	0
56	MG	1A	3232	1/1	0.98	0.22	32,32,32,32	0
56	MG	2A	3865	1/1	0.98	0.11	48,48,48,48	0
56	MG	1A	4078	1/1	0.98	0.08	34,34,34,34	0
56	MG	2A	3546	1/1	0.98	0.13	49,49,49,49	0
56	MG	1A	3795	1/1	0.98	0.08	46,46,46,46	0
56	MG	1A	3070	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3086	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3552	1/1	0.98	0.07	57,57,57,57	0
56	MG	2A	3139	1/1	0.98	0.17	48,48,48,48	0
56	MG	1A	3878	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	3120	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3556	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3009	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3974	1/1	0.98	0.07	26,26,26,26	0
56	MG	1a	1612	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3723	1/1	0.98	0.03	14,14,14,14	0
56	MG	1A	3087	1/1	0.98	0.19	30,30,30,30	0
56	MG	2A	3562	1/1	0.98	0.05	43,43,43,43	0
56	MG	1a	1732	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3649	1/1	0.98	0.06	24,24,24,24	0
56	MG	1A	4089	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3978	1/1	0.98	0.10	58,58,58,58	0
56	MG	1A	3883	1/1	0.98	0.21	34,34,34,34	0
56	MG	1A	3650	1/1	0.98	0.04	15,15,15,15	0
56	MG	1A	3805	1/1	0.98	0.08	28,28,28,28	0
56	MG	1A	3176	1/1	0.98	0.13	27,27,27,27	0
56	MG	1a	1740	1/1	0.98	0.03	42,42,42,42	0
56	MG	1a	1741	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	3307	1/1	0.98	0.04	34,34,34,34	0
56	MG	1A	3270	1/1	0.98	0.20	38,38,38,38	0
56	MG	2A	3027	1/1	0.98	0.05	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3654	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3108	1/1	0.98	0.07	32,32,32,32	0
56	MG	1P	205	1/1	0.98	0.28	31,31,31,31	0
56	MG	1A	3154	1/1	0.98	0.08	31,31,31,31	0
56	MG	1A	3065	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	3157	1/1	0.98	0.24	41,41,41,41	0
56	MG	2A	3584	1/1	0.98	0.07	51,51,51,51	0
56	MG	1a	1750	1/1	0.98	0.06	53,53,53,53	0
56	MG	2A	3586	1/1	0.98	0.09	64,64,64,64	0
56	MG	1A	3814	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3815	1/1	0.98	0.03	27,27,27,27	0
56	MG	2A	3037	1/1	0.98	0.07	50,50,50,50	0
56	MG	1A	3993	1/1	0.98	0.07	22,22,22,22	0
56	MG	1A	3351	1/1	0.98	0.23	31,31,31,31	0
56	MG	1a	1755	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	4106	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3897	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3898	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3737	1/1	0.98	0.05	35,35,35,35	0
56	MG	2F	305	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	3660	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3901	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	3740	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3903	1/1	0.98	0.08	24,24,24,24	0
56	MG	1A	3098	1/1	0.98	0.05	39,39,39,39	0
56	MG	2A	3604	1/1	0.98	0.06	66,66,66,66	0
58	A1A1F	1A	4110	34/34	0.98	0.06	21,27,30,33	0
56	MG	1a	1765	1/1	0.98	0.06	58,58,58,58	0
56	MG	1A	3212	1/1	0.98	0.05	34,34,34,34	0
59	ZN	1n	103	1/1	0.98	0.04	80,80,80,80	0
56	MG	1A	3354	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	4010	1/1	0.98	0.04	33,33,33,33	0
59	ZN	29	102	1/1	0.98	0.05	85,85,85,85	0
56	MG	1U	206	1/1	0.98	0.20	41,41,41,41	0
60	SF4	1d	302	8/8	0.98	0.05	72,79,86,88	0
60	SF4	2d	302	8/8	0.98	0.05	67,77,85,88	0
56	MG	2A	3021	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3762	1/1	0.99	0.04	28,28,28,28	0
56	MG	1A	3683	1/1	0.99	0.09	25,25,25,25	0
56	MG	1A	3685	1/1	0.99	0.04	27,27,27,27	0
56	MG	1A	3860	1/1	0.99	0.07	19,19,19,19	0
56	MG	1a	1800	1/1	0.99	0.04	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	1801	1/1	0.99	0.03	69,69,69,69	0
56	MG	1A	3067	1/1	0.99	0.12	37,37,37,37	0
56	MG	1A	3058	1/1	0.99	0.06	27,27,27,27	0
56	MG	2A	3497	1/1	0.99	0.05	70,70,70,70	0
56	MG	1A	3178	1/1	0.99	0.11	34,34,34,34	0
56	MG	1A	3627	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	3769	1/1	0.99	0.07	48,48,48,48	0
56	MG	1a	1731	1/1	0.99	0.03	35,35,35,35	0
56	MG	1A	3010	1/1	0.99	0.04	35,35,35,35	0
56	MG	2A	3870	1/1	0.99	0.04	51,51,51,51	0
56	MG	2A	3590	1/1	0.99	0.06	43,43,43,43	0
56	MG	2A	3591	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	3691	1/1	0.99	0.07	25,25,25,25	0
56	MG	1A	3013	1/1	0.99	0.23	27,27,27,27	0
56	MG	1U	201	1/1	0.99	0.13	26,26,26,26	0
56	MG	1A	3773	1/1	0.99	0.03	31,31,31,31	0
56	MG	1E	302	1/1	0.99	0.23	36,36,36,36	0
56	MG	1A	3693	1/1	0.99	0.06	31,31,31,31	0
56	MG	2A	3195	1/1	0.99	0.04	57,57,57,57	0
56	MG	1A	3566	1/1	0.99	0.13	35,35,35,35	0
56	MG	1A	3922	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	3923	1/1	0.99	0.03	30,30,30,30	0
56	MG	1A	3695	1/1	0.99	0.03	31,31,31,31	0
56	MG	1A	3696	1/1	0.99	0.07	30,30,30,30	0
56	MG	1U	210	1/1	0.99	0.30	37,37,37,37	0
56	MG	1A	4039	1/1	0.99	0.02	25,25,25,25	0
56	MG	1A	3014	1/1	0.99	0.08	25,25,25,25	0
56	MG	1A	3632	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3155	1/1	0.99	0.11	41,41,41,41	0
56	MG	1E	313	1/1	0.99	0.08	24,24,24,24	0
56	MG	1A	3739	1/1	0.99	0.08	31,31,31,31	0
56	MG	2A	3523	1/1	0.99	0.08	35,35,35,35	0
56	MG	1A	3700	1/1	0.99	0.05	26,26,26,26	0
56	MG	1A	3783	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3037	1/1	0.99	0.08	25,25,25,25	0
56	MG	1A	3074	1/1	0.99	0.02	13,13,13,13	0
56	MG	1A	3987	1/1	0.99	0.08	62,62,62,62	0
56	MG	1A	3786	1/1	0.99	0.06	31,31,31,31	0
56	MG	2A	3708	1/1	0.99	0.03	39,39,39,39	0
56	MG	1A	3787	1/1	0.99	0.04	25,25,25,25	0
56	MG	1A	3636	1/1	0.99	0.08	27,27,27,27	0
56	MG	2A	3620	1/1	0.99	0.04	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	3704	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3612	1/1	0.99	0.06	30,30,30,30	0
56	MG	1A	3939	1/1	0.99	0.02	13,13,13,13	0
56	MG	1A	3638	1/1	0.99	0.04	29,29,29,29	0
56	MG	2A	3716	1/1	0.99	0.04	59,59,59,59	0
56	MG	2A	3536	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	3995	1/1	0.99	0.08	42,42,42,42	0
56	MG	2A	3538	1/1	0.99	0.07	62,62,62,62	0
56	MG	1A	3996	1/1	0.99	0.07	26,26,26,26	0
56	MG	2A	3814	1/1	0.99	0.13	44,44,44,44	0
56	MG	1A	3997	1/1	0.99	0.08	31,31,31,31	0
56	MG	2A	3630	1/1	0.99	0.07	41,41,41,41	0
56	MG	1A	3038	1/1	0.99	0.10	36,36,36,36	0
56	MG	1A	3942	1/1	0.99	0.09	38,38,38,38	0
56	MG	2A	3725	1/1	0.99	0.06	46,46,46,46	0
56	MG	1A	3031	1/1	0.99	0.08	30,30,30,30	0
56	MG	2a	1755	1/1	0.99	0.03	78,78,78,78	0
56	MG	1A	3615	1/1	0.99	0.08	36,36,36,36	0
56	MG	2A	3822	1/1	0.99	0.03	43,43,43,43	0
56	MG	1A	3642	1/1	0.99	0.07	24,24,24,24	0
56	MG	2A	3824	1/1	0.99	0.03	57,57,57,57	0
56	MG	1A	3099	1/1	0.99	0.10	21,21,21,21	0
56	MG	2a	1761	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	4004	1/1	0.99	0.04	37,37,37,37	0
56	MG	2A	3548	1/1	0.99	0.07	39,39,39,39	0
56	MG	2A	3549	1/1	0.99	0.07	37,37,37,37	0
56	MG	1A	3282	1/1	0.99	0.07	27,27,27,27	0
56	MG	1A	3645	1/1	0.99	0.06	26,26,26,26	0
56	MG	1A	4069	1/1	0.99	0.03	39,39,39,39	0
56	MG	1A	3202	1/1	0.99	0.09	20,20,20,20	0
56	MG	1A	3404	1/1	0.99	0.05	35,35,35,35	0
56	MG	2a	1770	1/1	0.99	0.03	64,64,64,64	0
56	MG	2A	3834	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	4009	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3386	1/1	0.99	0.20	26,26,26,26	0
56	MG	1A	3203	1/1	0.99	0.07	38,38,38,38	0
56	MG	1A	3803	1/1	0.99	0.05	22,22,22,22	0
56	MG	1A	3851	1/1	0.99	0.09	37,37,37,37	0
56	MG	1a	1783	1/1	0.99	0.05	51,51,51,51	0
56	MG	1A	3804	1/1	0.99	0.05	24,24,24,24	0
56	MG	1a	1785	1/1	0.99	0.03	63,63,63,63	0
56	MG	2A	3563	1/1	0.99	0.05	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1786	1/1	0.99	0.04	59,59,59,59	0
56	MG	1P	202	1/1	0.99	0.31	33,33,33,33	0
56	MG	1A	3679	1/1	0.99	0.03	41,41,41,41	0
59	ZN	1Y	204	1/1	0.99	0.03	73,73,73,73	0
56	MG	1A	3680	1/1	0.99	0.06	27,27,27,27	0
59	ZN	15	107	1/1	0.99	0.07	50,50,50,50	0
59	ZN	16	102	1/1	0.99	0.03	42,42,42,42	0
56	MG	1A	3003	1/1	0.99	0.05	26,26,26,26	0
56	MG	1A	3033	1/1	0.99	0.30	32,32,32,32	0
56	MG	1A	4019	1/1	0.99	0.04	29,29,29,29	0
59	ZN	25	106	1/1	0.99	0.03	58,58,58,58	0
59	ZN	26	102	1/1	0.99	0.03	64,64,64,64	0
56	MG	1Q	202	1/1	0.99	0.12	29,29,29,29	0
56	MG	1Q	203	1/1	0.99	0.04	39,39,39,39	0
56	MG	2A	3573	1/1	0.99	0.07	48,48,48,48	0
56	MG	1A	4083	1/1	0.99	0.08	41,41,41,41	0
56	MG	1A	3071	1/1	1.00	0.04	13,13,13,13	0
56	MG	1A	3673	1/1	1.00	0.07	40,40,40,40	0
56	MG	1A	3917	1/1	1.00	0.04	32,32,32,32	0
56	MG	1A	3684	1/1	1.00	0.09	31,31,31,31	0
56	MG	1A	3730	1/1	1.00	0.07	26,26,26,26	0
56	MG	1A	4040	1/1	1.00	0.07	51,51,51,51	0
59	ZN	19	102	1/1	1.00	0.03	43,43,43,43	0
56	MG	2A	3514	1/1	1.00	0.08	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.