



# wwPDB X-ray Structure Validation Summary Report

Nov 4, 2024 – 06:31 PM EST


PDB ID : 9D7R  
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with Fva1 antimicrobial peptide, mRNA, A-site release factor 1, and deacylated P-site and E-site tRNA<sub>phe</sub> at 2.70Å resolution  
Authors : Aleksandrova, E.V.; Huang, W.; Baliga, C.; Atkinson, G.C.; Vazquez-Laslop, N.; Mankin, A.S.; Polikanov, Y.S.  
Deposited on : 2024-08-17  
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

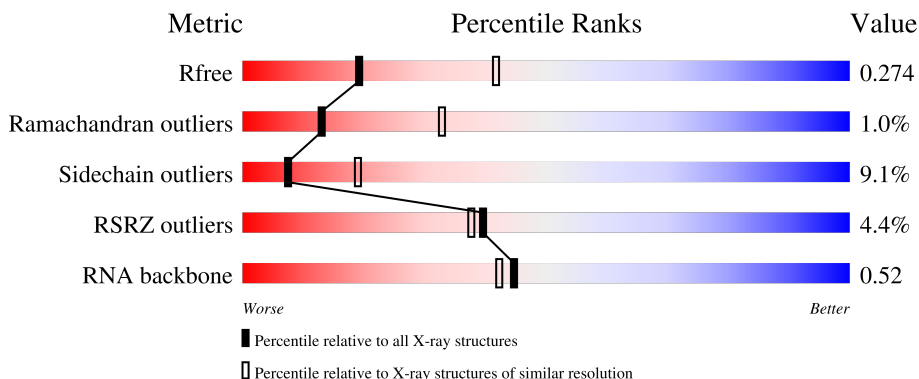
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



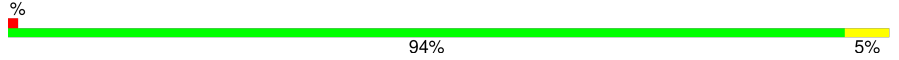
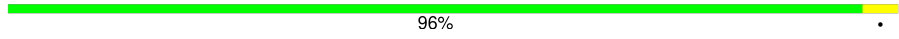
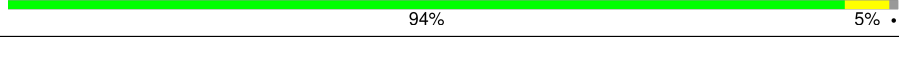
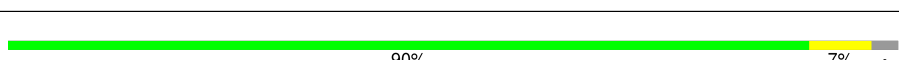
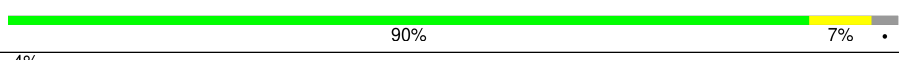
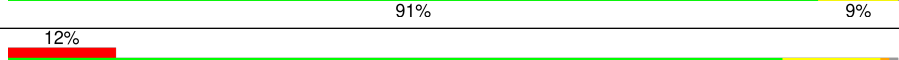
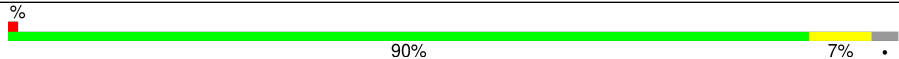

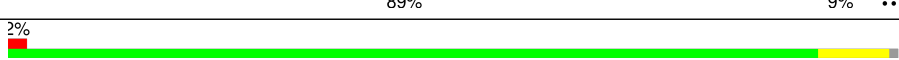
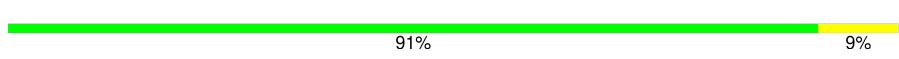
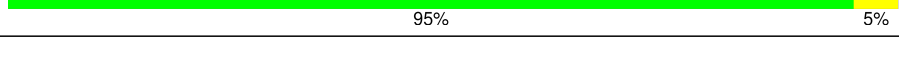
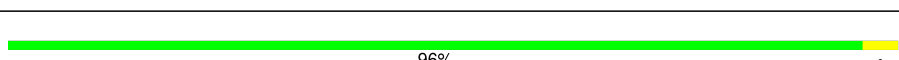
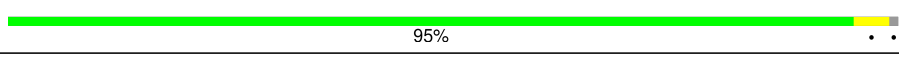
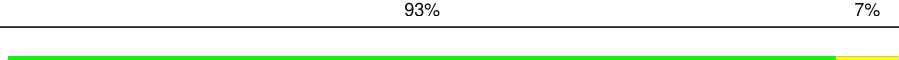
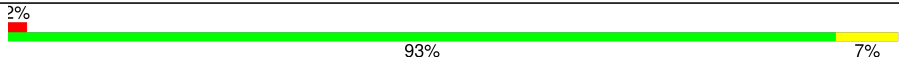
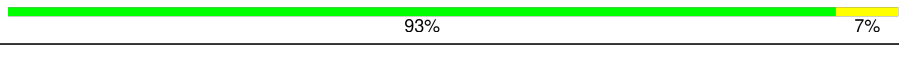
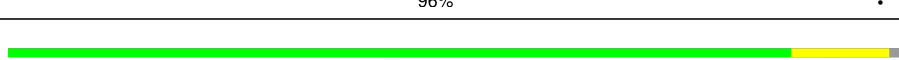




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)
RNA backbone	3690	1028 (2.94-2.46)

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	 4% 82% 16% ..
1	2A	2915	 4% 79% 17% .
2	1B	121	 89% 10% .
2	2B	121	 3% 87% 12% .

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	276	 % 94% 5%
3	2D	276	 96% .
4	1E	206	 94% 5% .
4	2E	206	 91% 8% .
5	1F	210	 90% 7% .
5	2F	210	 90% 7% .
6	1G	182	 4% 91% 9% .
6	2G	182	 12% 87% 11% ..
7	1H	180	 % 90% 7% .
7	2H	180	 6% 88% 9% .
8	1I	148	 2% 89% 9% ..
8	2I	148	 2% 91% 8% .
9	1N	140	 91% 9%
9	2N	140	 % 95% 5%
10	1O	122	 95% 5%
10	2O	122	 96% .
11	1P	150	 95% . .
11	2P	150	 93% 7% .
12	1Q	141	 93% 7%
12	2Q	141	 2% 93% 7%
13	1R	118	 93% 7%
13	2R	118	96% .
14	1S	112	88% 11% .
14	2S	112	7% 86% 12% .
15	1T	146	2% 79% 10% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	% 86% 10%
16	1U	118	95%
16	2U	118	93% 5%
17	1V	101	94% 5%
17	2V	101	% 91% 8%
18	1W	113	95%
18	2W	113	95%
19	1X	96	2% 95%
19	2X	96	2% 92% 7%
20	1Y	110	90% 7%
20	2Y	110	6% 92% 5%
21	1Z	206	82% 7% 11%
21	2Z	206	4% 83% 8% 10%
22	10	85	2% 85% 5% 11%
22	20	85	4% 87% 9%
23	11	98	% 93% 6%
23	21	98	2% 92% 7%
24	12	72	90% 7%
24	22	72	6% 90% 7%
25	13	60	90% 8%
25	23	60	95%
26	14	71	7% 80% 15%
26	24	71	21% 83% 10%
27	15	60	95%
27	25	60	2% 92% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	54	94% . .
28	26	54	2% 81% 17% .
29	17	49	6% 90% 8% .
29	27	49	8% 92% 6% .
30	18	65	92% 6% .
30	28	65	2% 88% 11% .
31	19	37	100%
31	29	37	97% .
32	1a	1521	5% 77% 21% .
32	2a	1521	5% 78% 20% . .
33	1b	256	5% 78% 11% . 10%
33	2b	256	14% 76% 14% 10%
34	1c	239	6% 75% 11% 14%
34	2c	239	6% 79% 7% 14%
35	1d	209	6% 90% 10%
35	2d	209	3% 90% 9%
36	1e	162	% 82% 9% 9%
36	2e	162	2% 83% 9% 9%
37	1f	101	4% 93% 6% .
37	2f	101	2% 90% 9% .
38	1g	156	6% 92% 7% .
38	2g	156	13% 88% 11% .
39	1h	138	91% 9% .
39	2h	138	4% 96% . .
40	1i	128	16% 90% 9% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	2i	128	23% 84% 12%
41	1j	105	22% 82% 11% 7%
41	2j	105	27% 78% 12% 9%
42	1k	129	3% 85% 12%
42	2k	129	3% 84% 12%
43	1l	132	3% 85% 8% 8%
43	2l	132	3% 84% 8% 8%
44	1m	126	11% 85% 9% 6%
44	2m	126	17% 84% 7% 9%
45	1n	61	10% 87% 11%
45	2n	61	21% 93% 5%
46	1o	89	4% 94% ..
46	2o	89	3% 88% 11%
47	1p	88	13% 84% 9% 7%
47	2p	88	91% 7%
48	1q	105	3% 86% 9% 6%
48	2q	105	3% 85% 10% 6%
49	1r	88	70% 7% 23%
49	2r	88	5% 68% 9% 23%
50	1s	93	19% 77% 12% 11%
50	2s	93	20% 77% 12% 11%
51	1t	106	6% 75% 15% 9%
51	2t	106	7% 78% 11% 9%
52	1u	27	19% 85% 15%
52	2u	27	26% 78% 7% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	76	
55	1y	76	
55	2x	76	
55	2y	76	
56	1z	20	
56	2z	20	

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
57	MG	2A	3026	-	-	-	X
57	MG	2a	1666	-	-	-	X

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 299076 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1A	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
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	Total	C	N	O	S	0	0	0
			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
			Total	C	N	O	S			
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

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



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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			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
			746	485	134	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
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	183	Total	C	N	O	S	0	0	0
			1437	919	256	260	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1451	928	256	265	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			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
			548	347	99	97	5			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	68	Total	C	N	O	S	0	0	0
			517	330	92	90	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
			511	328	99	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
			1554	977	302	274	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
			1659	1040	326	286	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
			1130	714	214	199	3			

- 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	513	143	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			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	123	Total	C	N	O	0	0	0
			940	593	185	162			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	98	Total	C	N	O	0	0	0
			721	449	140	132			
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
			Total	C	N	O	S			
42	2k	114	833	519	156	155	3	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	118	923	569	191	161	2	0	0	0
44	2m	115	889	546	183	158	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	1n	60	492	312	104	72	4	0	0	0
45	2n	60	486	309	101	72	4	0	0	0

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

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

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

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



- Molecule 48 is a protein called 30S ribosomal protein 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
			551	353	108	90				

- 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 PHE-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			
53	2v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1954	1208	361	377	8			

- Molecule 55 is a RNA chain called P-site and E-site Deacylated tRNA<sup>phe</sup>.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	1y	74	Total	C	N	O	P	S	0	0	0
			1590	712	285	517	74	2			
55	2x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	2y	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			

- Molecule 56 is a protein called Fva1 Antimicrobial Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	1z	14	Total	C	N	O	0	0	0
			121	79	25	17			
56	2z	14	Total	C	N	O	0	0	0
			121	79	25	17			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	795	Total	Mg	0	0
			795	795		
57	1B	20	Total	Mg	0	0
			20	20		
57	1D	8	Total	Mg	0	0
			8	8		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1E	9	Total Mg 9 9	0	0
57	1F	11	Total Mg 11 11	0	0
57	1G	3	Total Mg 3 3	0	0
57	1N	4	Total Mg 4 4	0	0
57	1O	1	Total Mg 1 1	0	0
57	1P	4	Total Mg 4 4	0	0
57	1Q	6	Total Mg 6 6	0	0
57	1R	3	Total Mg 3 3	0	0
57	1U	7	Total Mg 7 7	0	0
57	1V	5	Total Mg 5 5	0	0
57	1W	5	Total Mg 5 5	0	0
57	1X	2	Total Mg 2 2	0	0
57	1Z	1	Total Mg 1 1	0	0
57	10	5	Total Mg 5 5	0	0
57	11	4	Total Mg 4 4	0	0
57	12	2	Total Mg 2 2	0	0
57	13	2	Total Mg 2 2	0	0
57	14	1	Total Mg 1 1	0	0
57	15	4	Total Mg 4 4	0	0
57	16	1	Total Mg 1 1	0	0
57	17	7	Total Mg 7 7	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	18	2	Total 2	Mg 2	0	0
57	19	2	Total 2	Mg 2	0	0
57	1a	189	Total 189	Mg 189	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1v	2	Total 2	Mg 2	0	0
57	1w	3	Total 3	Mg 3	0	0
57	1x	9	Total 9	Mg 9	0	0
57	1y	1	Total 1	Mg 1	0	0
57	2A	640	Total 640	Mg 640	0	0
57	2B	11	Total 11	Mg 11	0	0
57	2D	8	Total 8	Mg 8	0	0
57	2E	5	Total 5	Mg 5	0	0
57	2F	7	Total 7	Mg 7	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	3	Total 3	Mg 3	0	0

*Continued on next page...*

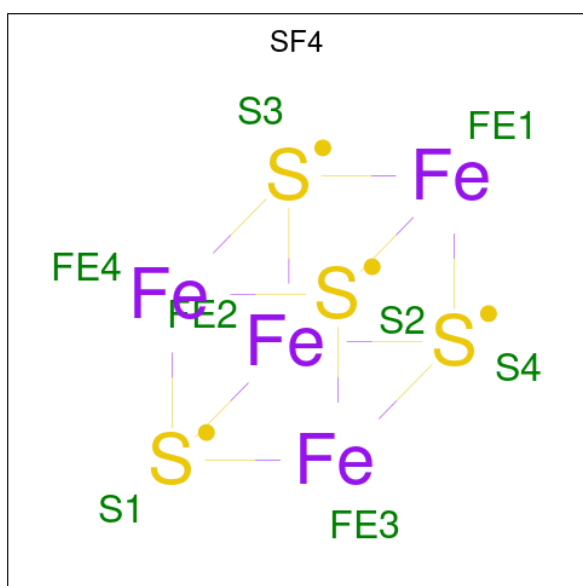
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2R	3	Total Mg 3 3	0	0
57	2U	1	Total Mg 1 1	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	1	Total Mg 1 1	0	0
57	2X	3	Total Mg 3 3	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	23	1	Total Mg 1 1	0	0
57	25	1	Total Mg 1 1	0	0
57	26	1	Total Mg 1 1	0	0
57	28	1	Total Mg 1 1	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	168	Total Mg 168 168	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	3	Total Mg 3 3	0	0
57	2f	1	Total Mg 1 1	0	0
57	2j	2	Total Mg 2 2	0	0
57	2k	2	Total Mg 2 2	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	1	Total Mg 1 1	0	0
57	2x	9	Total Mg 9 9	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1395	Total	O	0	0
			1395	1395		
60	1B	27	Total	O	0	0
			27	27		
60	1D	15	Total	O	0	0
			15	15		
60	1E	13	Total	O	0	0
			13	13		
60	1F	8	Total	O	0	0
			8	8		
60	1G	1	Total	O	0	0
			1	1		
60	1N	3	Total	O	0	0
			3	3		
60	1O	3	Total	O	0	0
			3	3		
60	1P	15	Total	O	0	0
			15	15		
60	1Q	6	Total	O	0	0
			6	6		
60	1R	3	Total	O	0	0
			3	3		
60	1T	1	Total	O	0	0
			1	1		
60	1U	4	Total	O	0	0
			4	4		
60	1V	1	Total	O	0	0
			1	1		
60	1W	3	Total	O	0	0
			3	3		
60	1X	3	Total	O	0	0
			3	3		
60	1Z	1	Total	O	0	0
			1	1		
60	10	2	Total	O	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	11	3	Total O 3 3	0	0
60	13	2	Total O 2 2	0	0
60	15	3	Total O 3 3	0	0
60	16	1	Total O 1 1	0	0
60	17	2	Total O 2 2	0	0
60	18	7	Total O 7 7	0	0
60	1a	180	Total O 180 180	0	0
60	1d	1	Total O 1 1	0	0
60	1l	1	Total O 1 1	0	0
60	1v	4	Total O 4 4	0	0
60	1w	2	Total O 2 2	0	0
60	1x	24	Total O 24 24	0	0
60	2A	946	Total O 946 946	0	0
60	2B	6	Total O 6 6	0	0
60	2D	18	Total O 18 18	0	0
60	2E	7	Total O 7 7	0	0
60	2F	5	Total O 5 5	0	0
60	2N	1	Total O 1 1	0	0
60	2O	2	Total O 2 2	0	0
60	2P	16	Total O 16 16	0	0
60	2Q	3	Total O 3 3	0	0

*Continued on next page...*



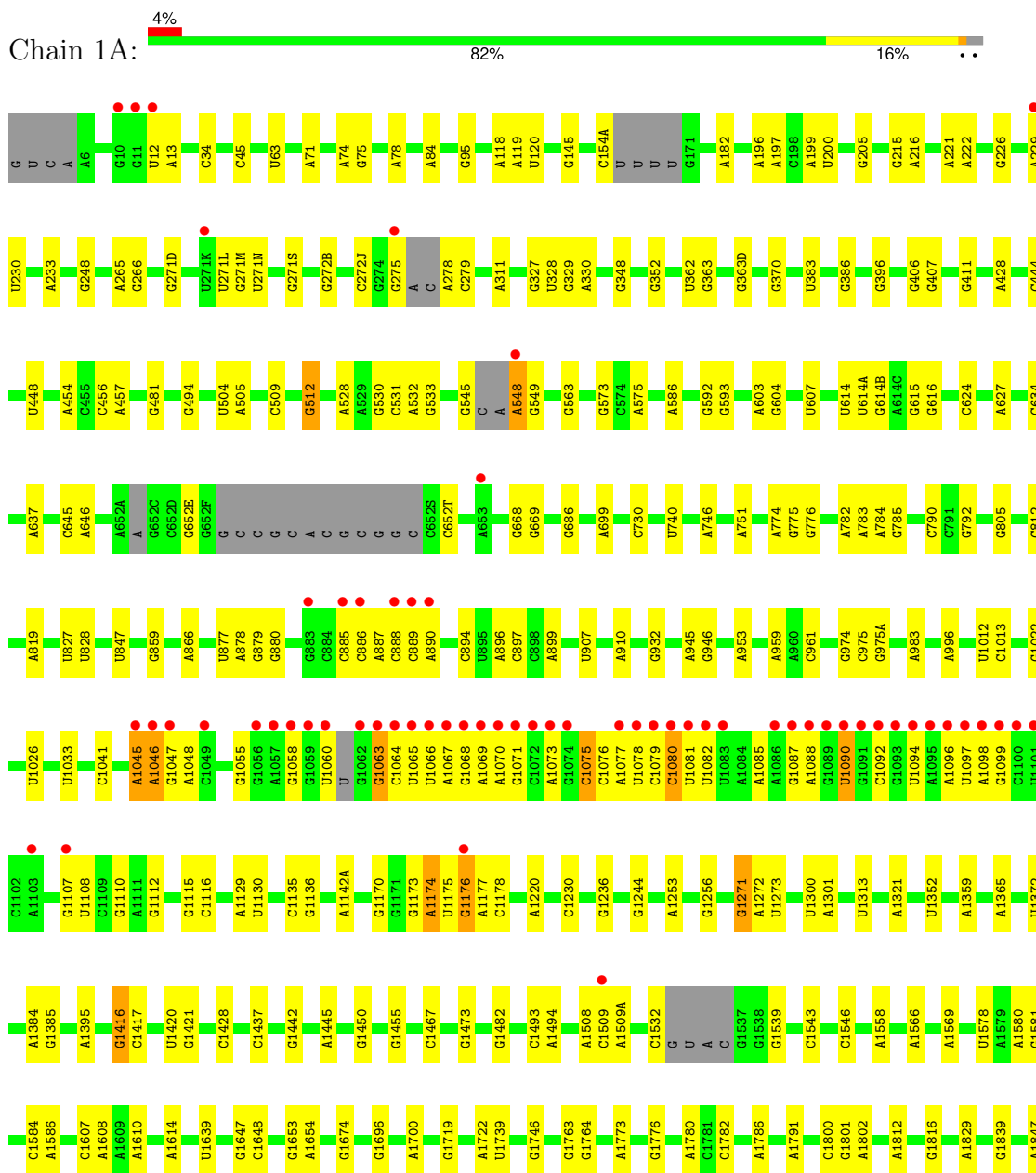
*Continued from previous page...*

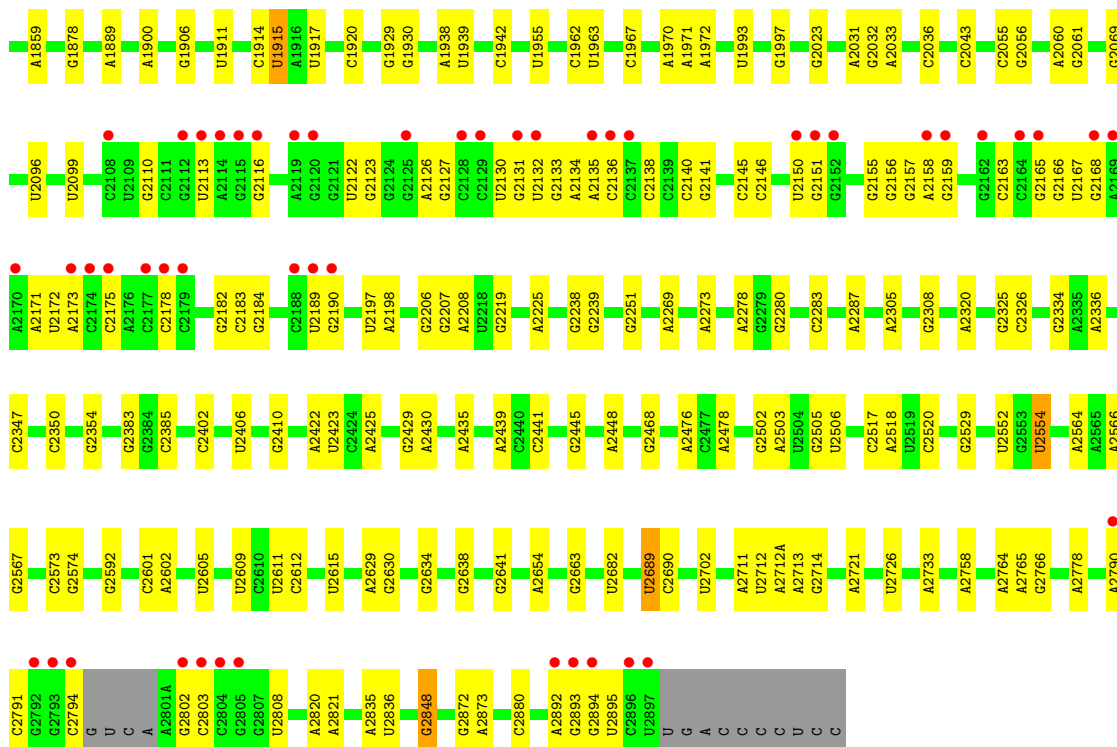
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2R	2	Total 2	O 2	0	0
60	2U	1	Total 1	O 1	0	0
60	2X	3	Total 3	O 3	0	0
60	2Y	2	Total 2	O 2	0	0
60	20	4	Total 4	O 4	0	0
60	21	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	25	2	Total 2	O 2	0	0
60	27	4	Total 4	O 4	0	0
60	28	4	Total 4	O 4	0	0
60	2a	152	Total 152	O 152	0	0
60	2d	1	Total 1	O 1	0	0
60	2j	1	Total 1	O 1	0	0
60	2q	1	Total 1	O 1	0	0
60	2t	1	Total 1	O 1	0	0
60	2w	1	Total 1	O 1	0	0
60	2x	13	Total 13	O 13	0	0
60	2z	2	Total 2	O 2	0	0

### 3 Residue-property plots i

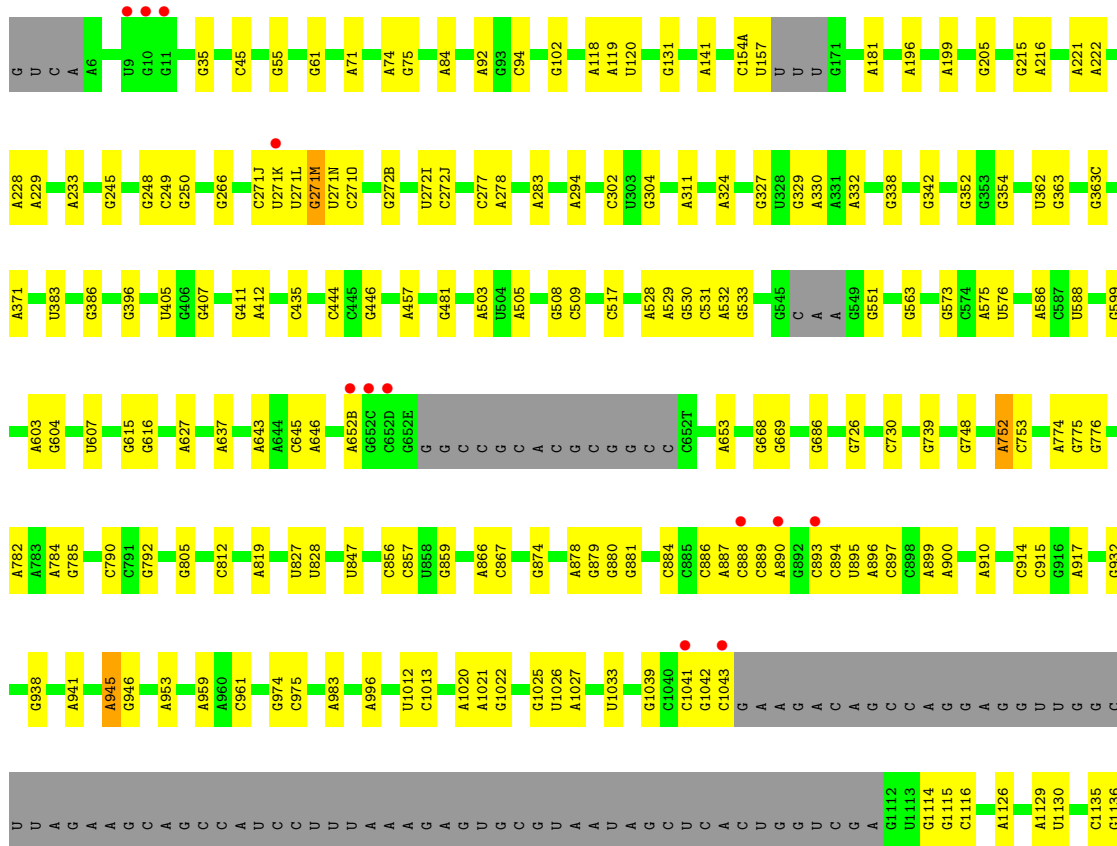
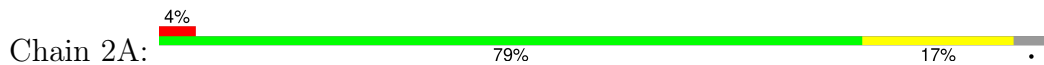
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

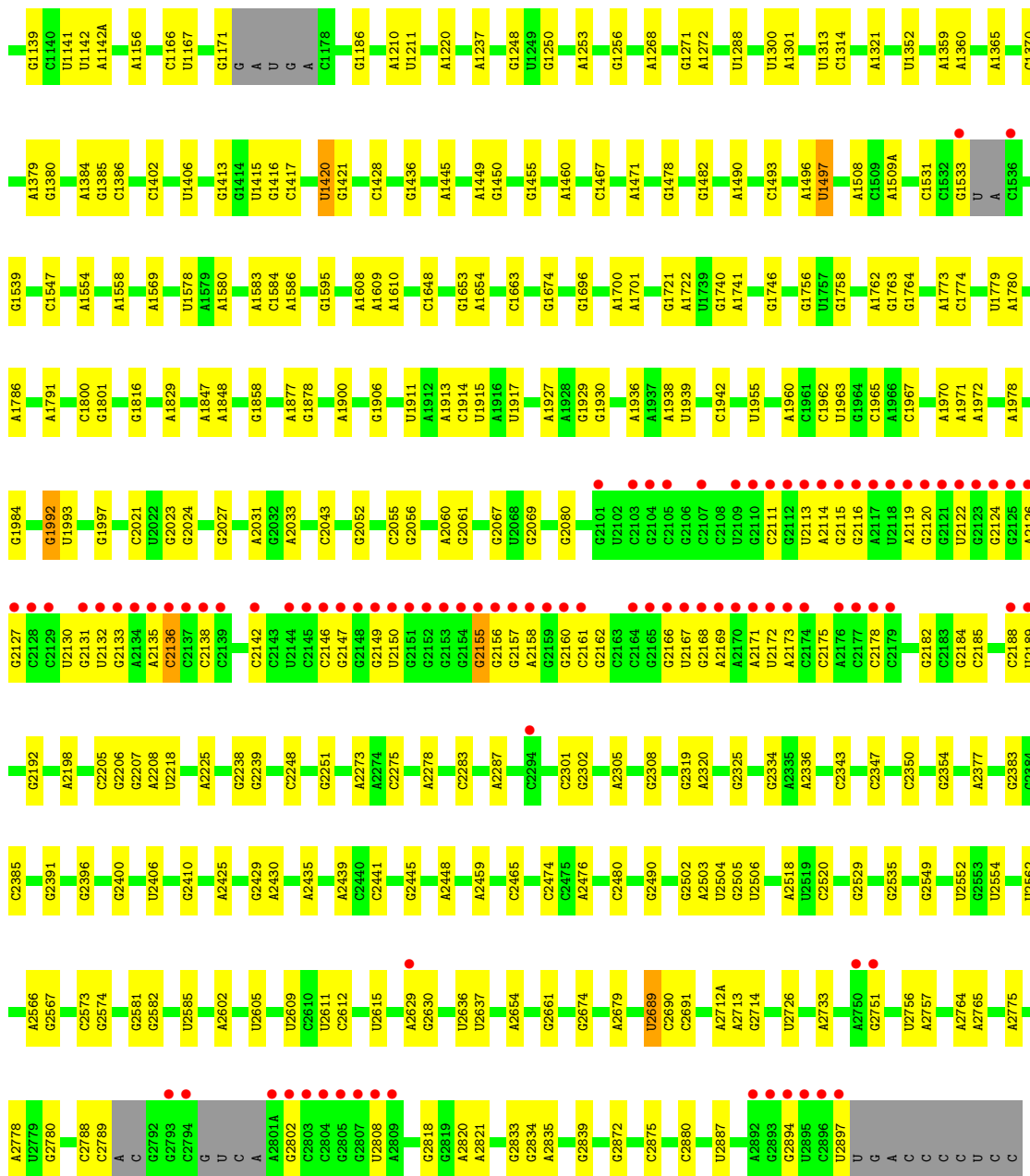
- Molecule 1: 23S Ribosomal RNA



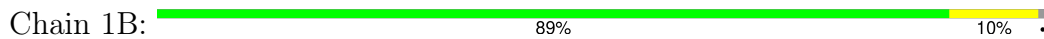


• Molecule 1: 23S Ribosomal RNA

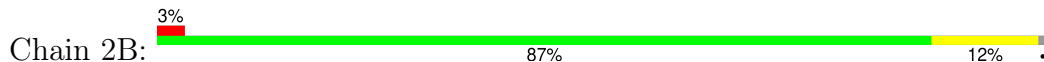




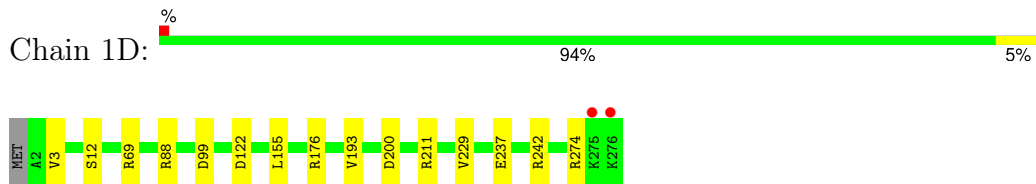
• Molecule 2: 5S Ribosomal RNA



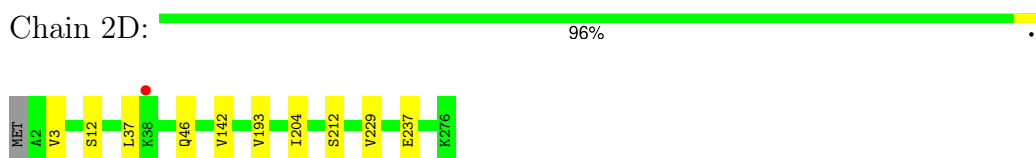
• Molecule 2: 5S Ribosomal RNA



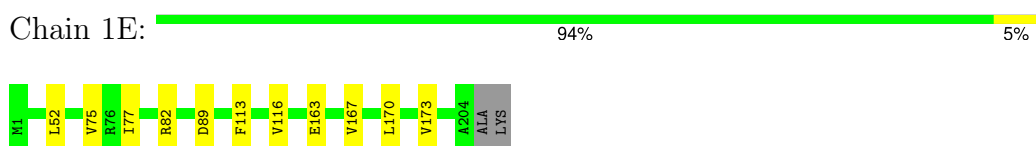
- Molecule 3: 50S ribosomal protein L2



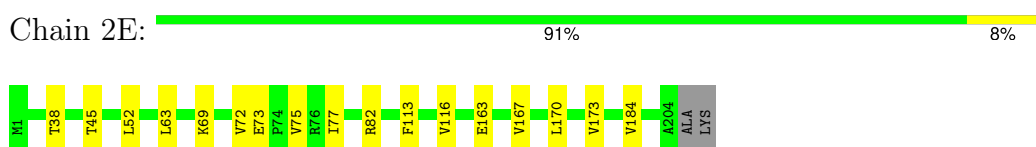
- Molecule 3: 50S ribosomal protein L2



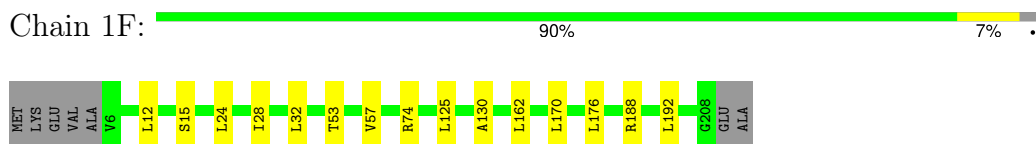
- Molecule 4: 50S ribosomal protein L3



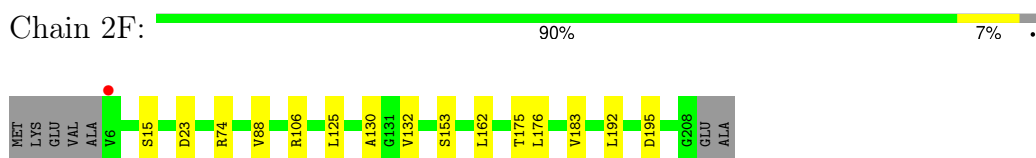
- Molecule 4: 50S ribosomal protein L3



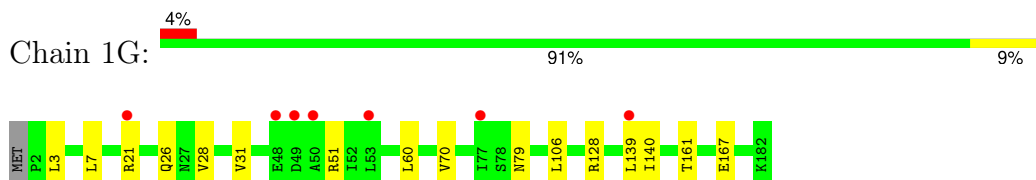
- Molecule 5: 50S ribosomal protein L4



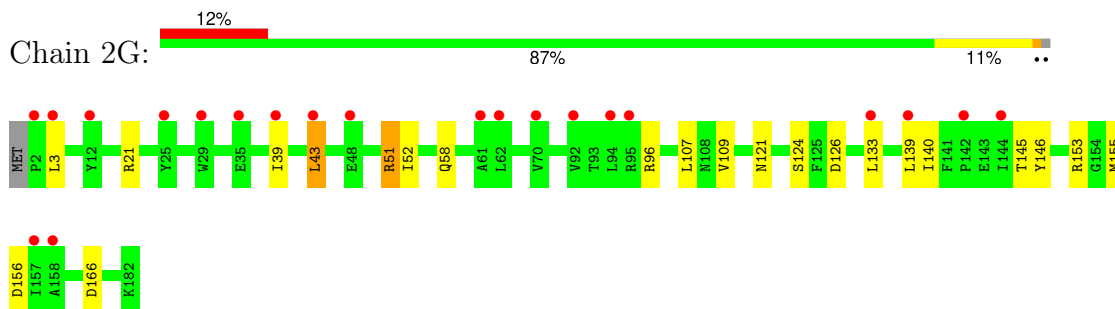
- Molecule 5: 50S ribosomal protein L4



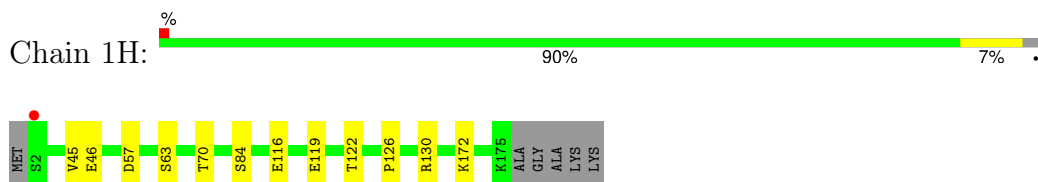
- Molecule 6: 50S ribosomal protein L5



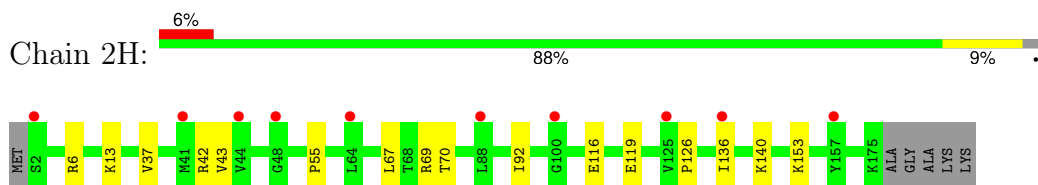
- Molecule 6: 50S ribosomal protein L5



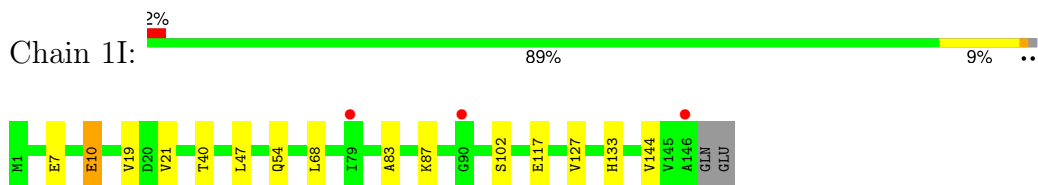
- Molecule 7: 50S ribosomal protein L6



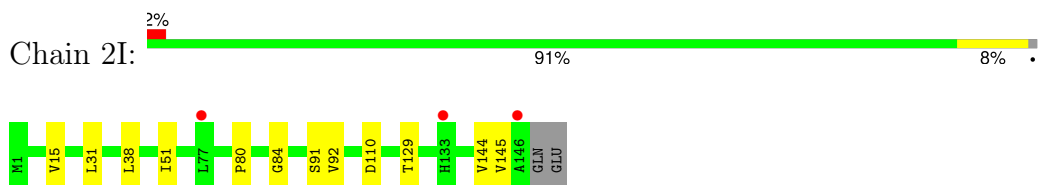
- Molecule 7: 50S ribosomal protein L6



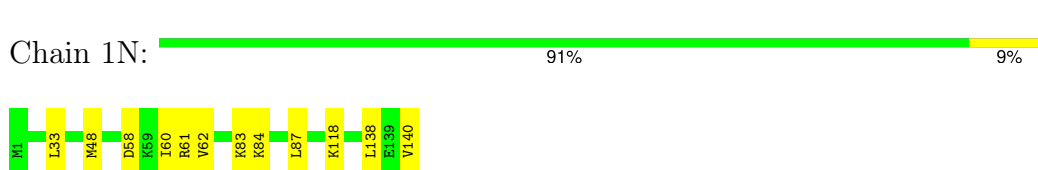
- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



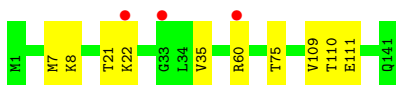
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

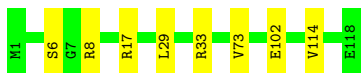


- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  93% 7%




- Molecule 13: 50S ribosomal protein L17

Chain 2R:  96%




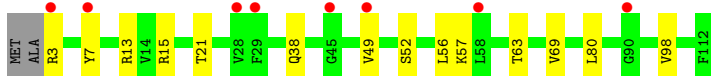
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  88% 11%




- Molecule 14: 50S ribosomal protein L18

Chain 2S:  7% 86% 12%




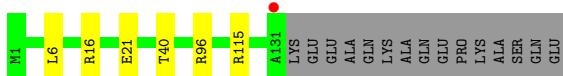
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  2% 79% 10% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T:  1% 86% 10%



- Molecule 16: 50S ribosomal protein L20

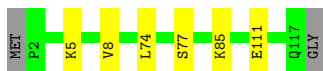
Chain 1U:  95%



- Molecule 16: 50S ribosomal protein L20



Chain 2U:  93% 5%



• Molecule 17: 50S ribosomal protein L21

Chain 1V:  94% 5%



• Molecule 17: 50S ribosomal protein L21

Chain 2V:  91% 8%



• Molecule 18: 50S ribosomal protein L22

Chain 1W:  95%



• Molecule 18: 50S ribosomal protein L22

Chain 2W:  95%



• Molecule 19: 50S ribosomal protein L23

Chain 1X:  95%



• Molecule 19: 50S ribosomal protein L23

Chain 2X:  92% 7%



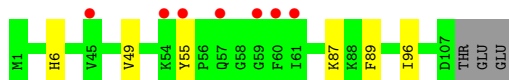
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:  90% 7%




- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  6% 92% 5%




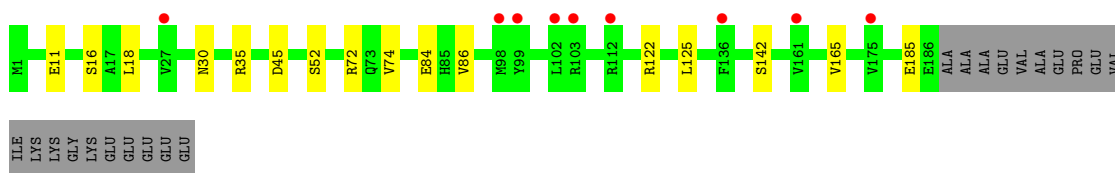
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  82% 7% 11%




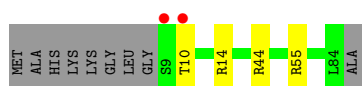
- Molecule 21: 50S ribosomal protein L25

Chain 2Z:  4% 83% 8% 10%




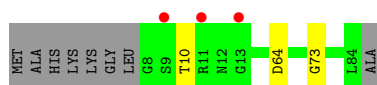
- Molecule 22: 50S ribosomal protein L27

Chain 10:  2% 85% 5% 11%



- Molecule 22: 50S ribosomal protein L27

Chain 20:  4% 87% 9%

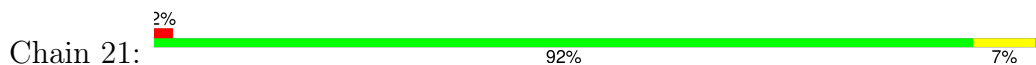


- Molecule 23: 50S ribosomal protein L28

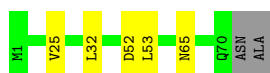
Chain 11:  % 93% 6%



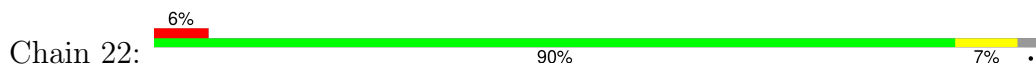
- Molecule 23: 50S ribosomal protein L28



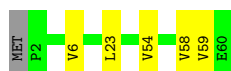
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



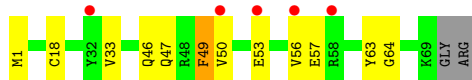
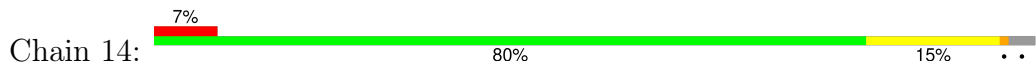
- Molecule 25: 50S ribosomal protein L30



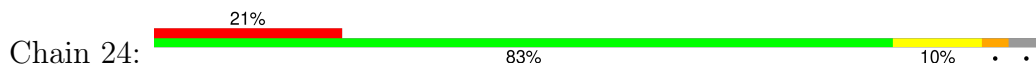
- Molecule 25: 50S ribosomal protein L30

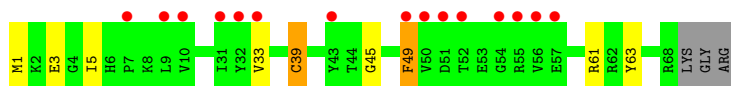


- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31





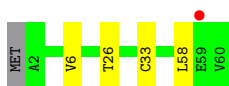
- Molecule 27: 50S ribosomal protein L32

Chain 15: 95%



- Molecule 27: 50S ribosomal protein L32

Chain 25: 92%



- Molecule 28: 50S ribosomal protein L33

Chain 16: 94%



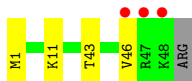
- Molecule 28: 50S ribosomal protein L33

Chain 26: 81%



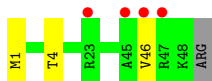
- Molecule 29: 50S ribosomal protein L34

Chain 17: 90%



- Molecule 29: 50S ribosomal protein L34

Chain 27: 92%




- Molecule 30: 50S ribosomal protein L35

Chain 18:  92% 6%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  88% 11% 2%



- Molecule 31: 50S ribosomal protein L36

Chain 19:  100%


There are no outlier residues recorded for this chain.

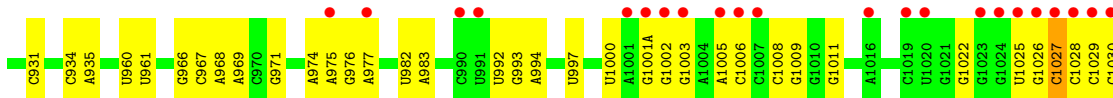
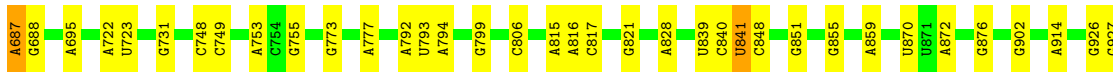
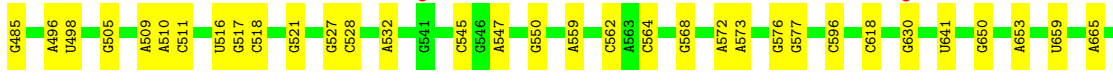
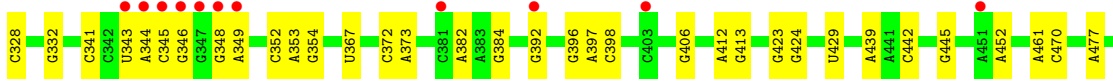
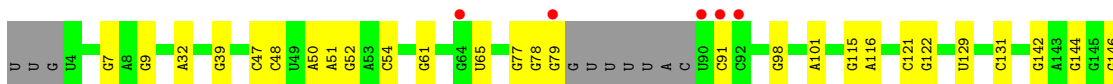
- Molecule 31: 50S ribosomal protein L36

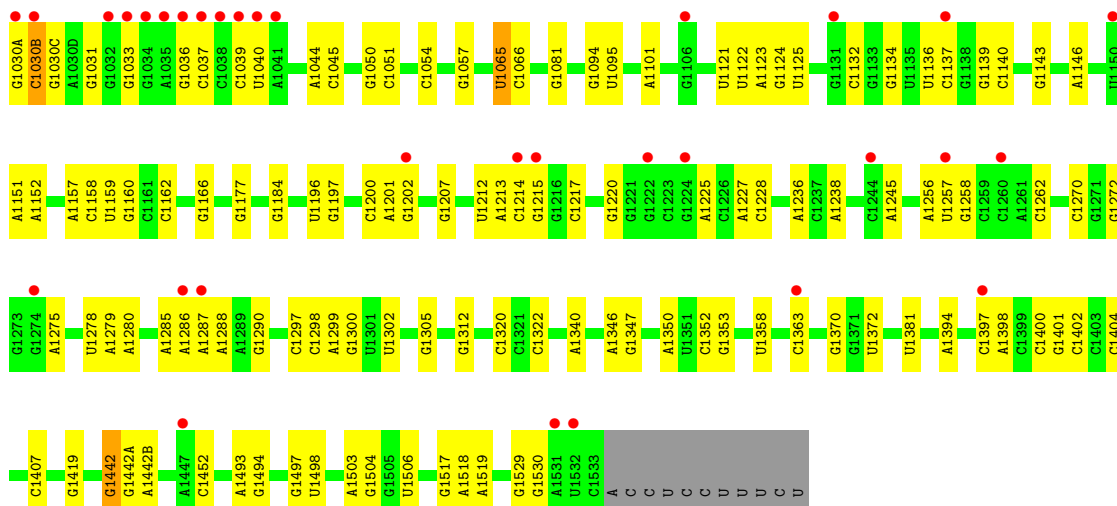
Chain 29:  97%



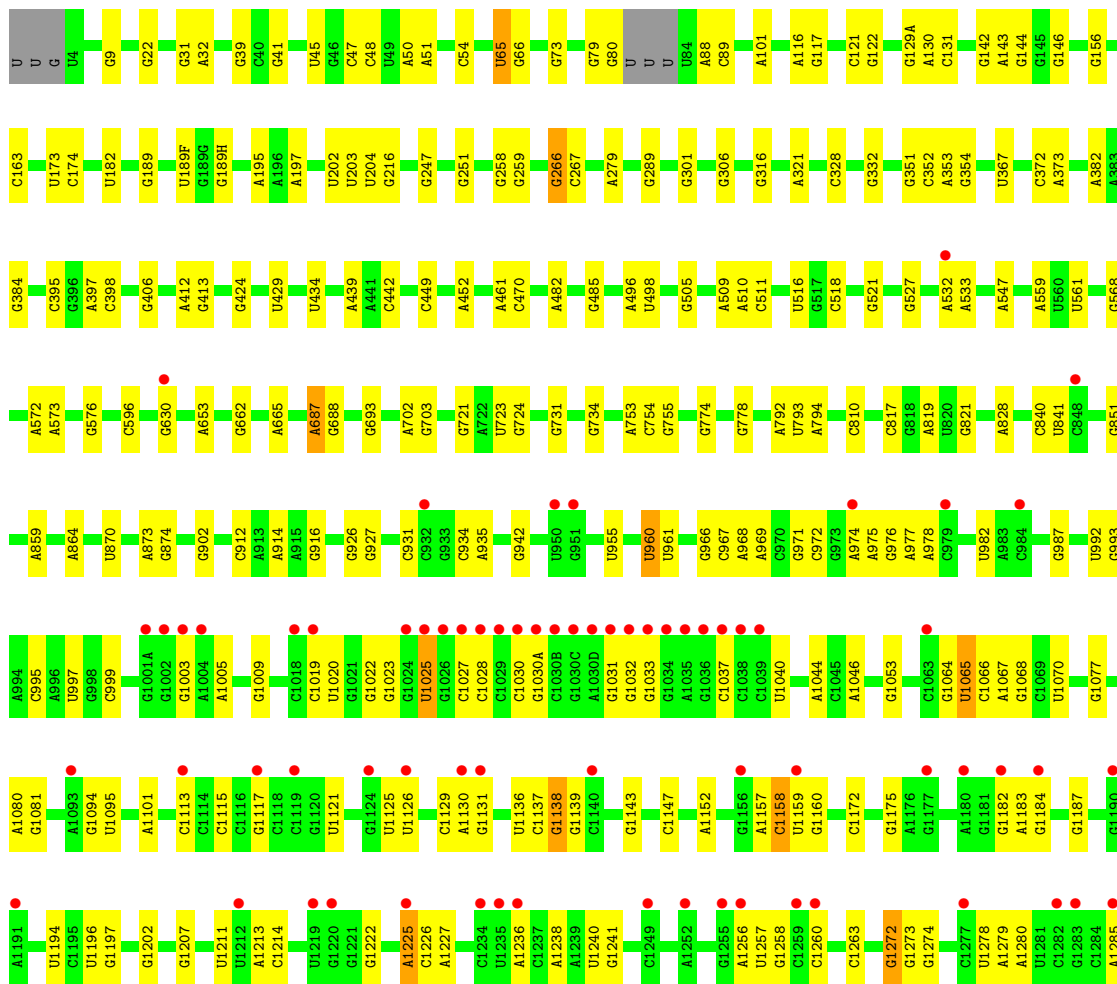
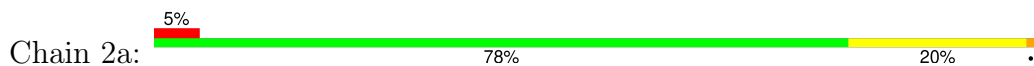
- Molecule 32: 16S Ribosomal RNA

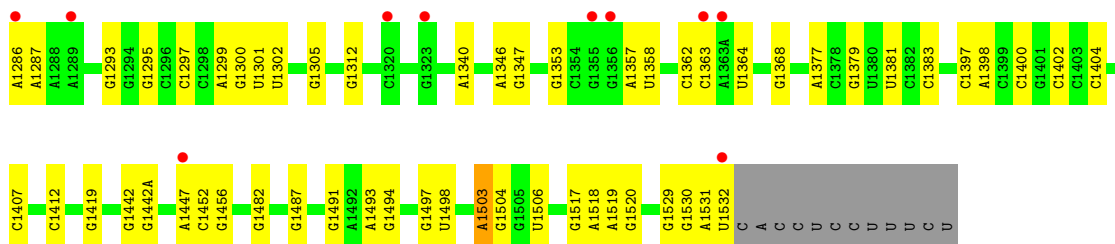
Chain 1a:  77% 21% 5%



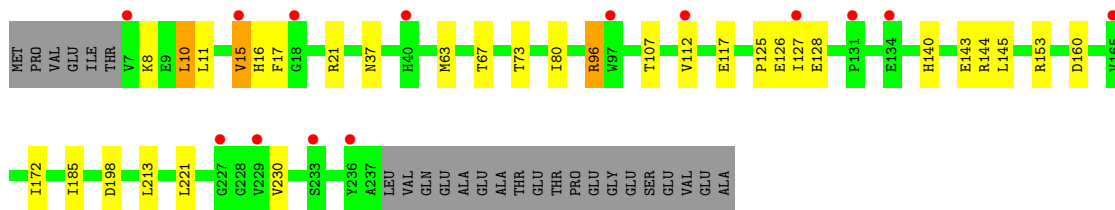
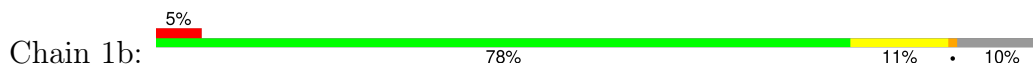


- Molecule 32: 16S Ribosomal RNA

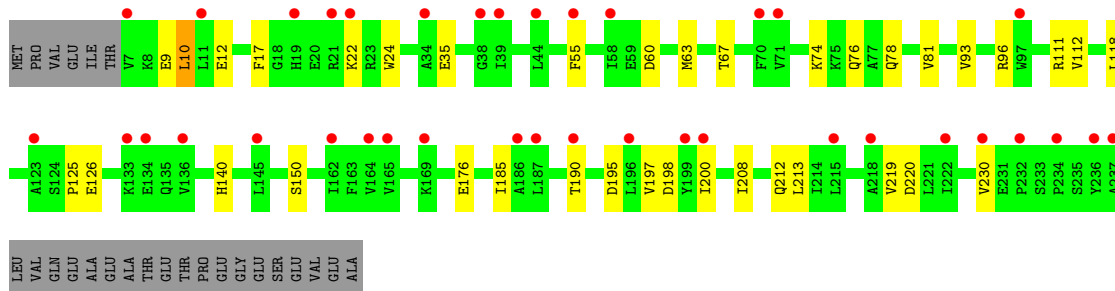
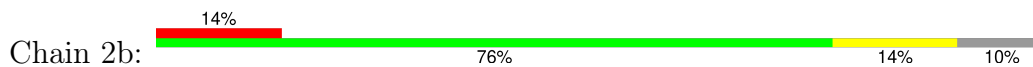




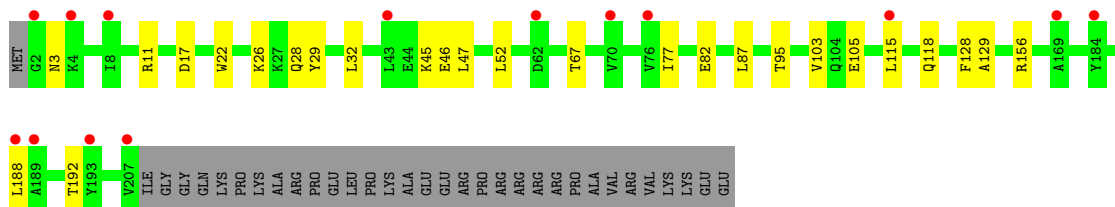
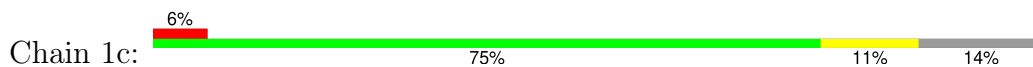
• Molecule 33: 30S ribosomal protein S2



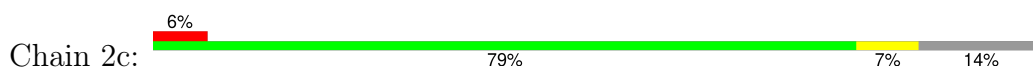
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3

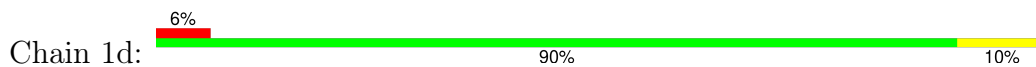


• Molecule 34: 30S ribosomal protein S3

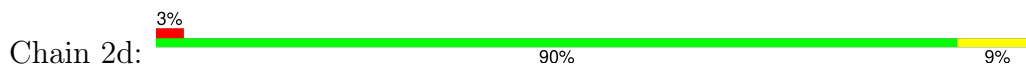


LYS  
PRO  
LYS  
ALA  
ARG  
PRO  
GLU  
LEU  
PRO  
LYS  
ALA  
GLU  
GLU  
ARG  
PRO  
ARG  
ARG  
ARG  
PRO  
ALA  
VAL  
ARG  
VAL  
LYS  
LYS  
GLU  
GLU

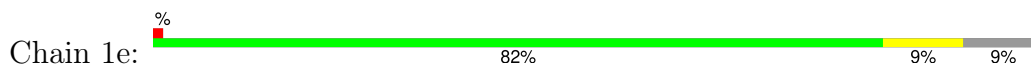
- Molecule 35: 30S ribosomal protein S4



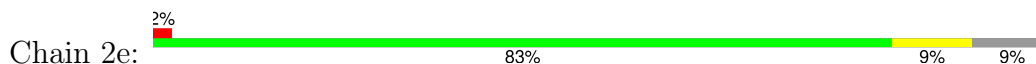
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



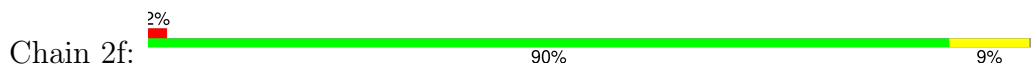
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6



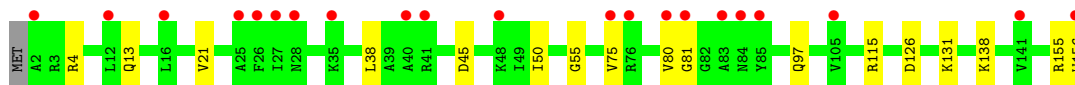
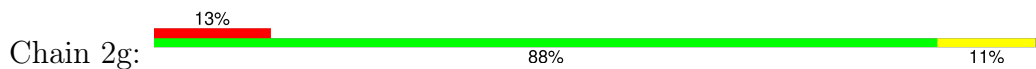
- Molecule 38: 30S ribosomal protein S7







- Molecule 38: 30S ribosomal protein S7



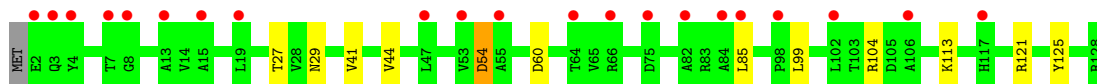
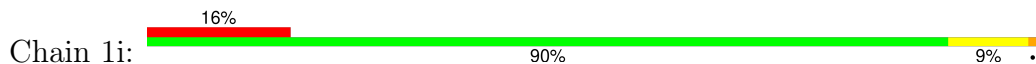
- Molecule 39: 30S ribosomal protein S8



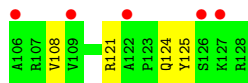
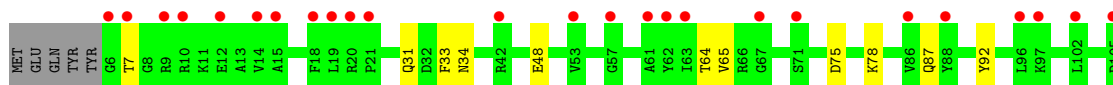
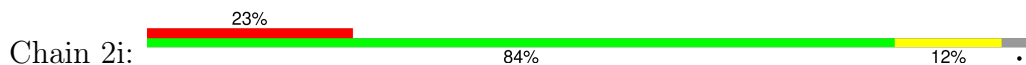
- Molecule 39: 30S ribosomal protein S8



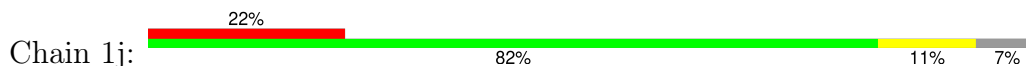
- Molecule 40: 30S ribosomal protein S9

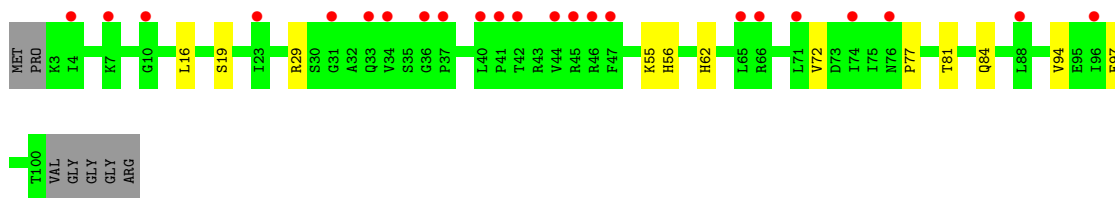


- Molecule 40: 30S ribosomal protein S9

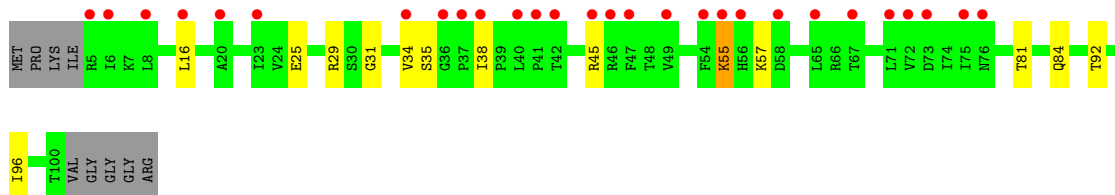
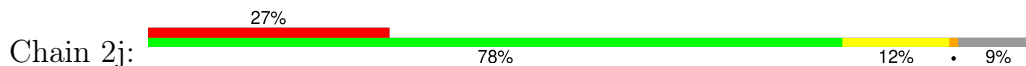


- Molecule 41: 30S ribosomal protein S10

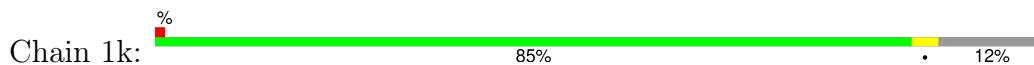




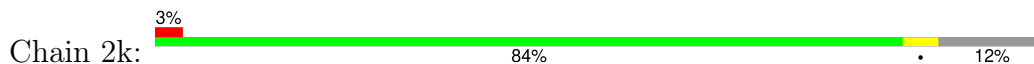
- Molecule 41: 30S ribosomal protein S10



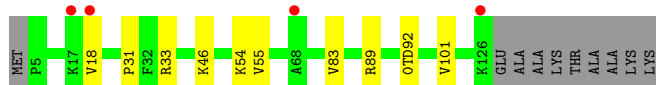
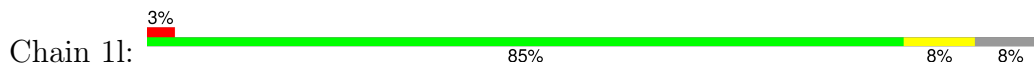
- Molecule 42: 30S ribosomal protein S11



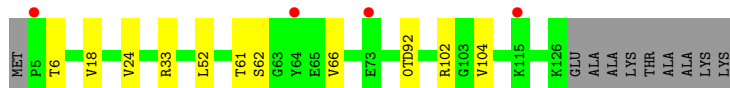
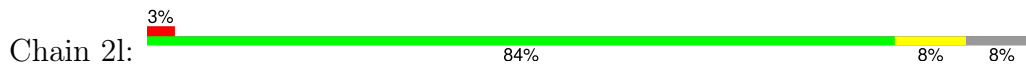
- Molecule 42: 30S ribosomal protein S11



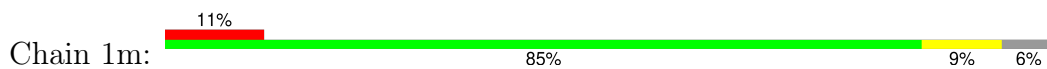
- Molecule 43: 30S ribosomal protein S12



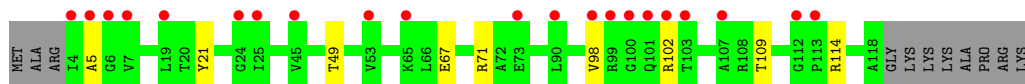
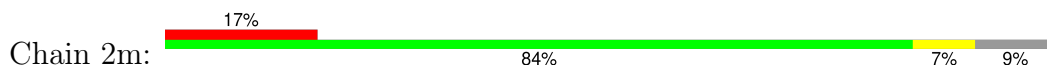
- Molecule 43: 30S ribosomal protein S12



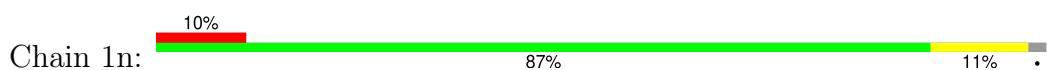
- Molecule 44: 30S ribosomal protein S13



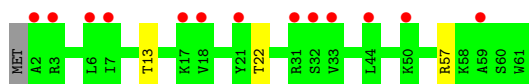
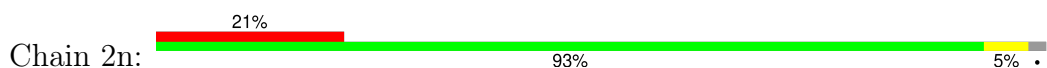
- Molecule 44: 30S ribosomal protein S13



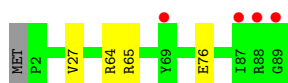
- Molecule 45: 30S ribosomal protein S14 type Z



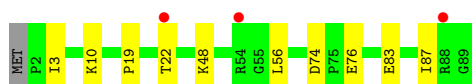
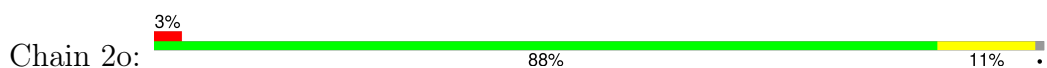
- Molecule 45: 30S ribosomal protein S14 type Z



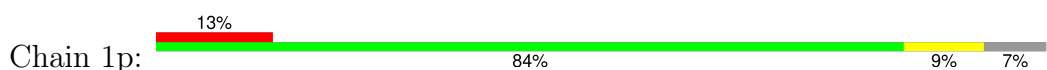
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

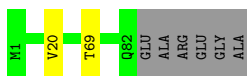


- Molecule 47: 30S ribosomal protein S16




- Molecule 47: 30S ribosomal protein S16

Chain 2p:  91% 7%




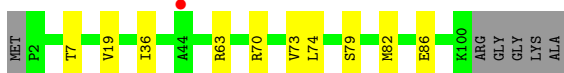
- Molecule 48: 30S ribosomal protein S17

Chain 1q:  86% 9% 6%



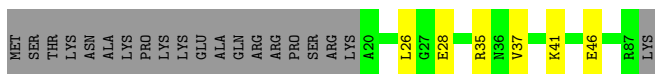
- Molecule 48: 30S ribosomal protein S17

Chain 2q:  85% 10% 6%



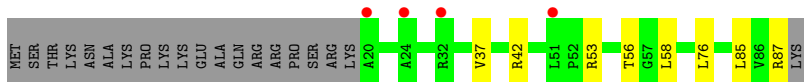
- Molecule 49: 30S ribosomal protein S18

Chain 1r:  70% 7% 23%




- Molecule 49: 30S ribosomal protein S18

Chain 2r:  68% 9% 23%




- Molecule 50: 30S ribosomal protein S19

Chain 1s:  77% 19% 12% 11%

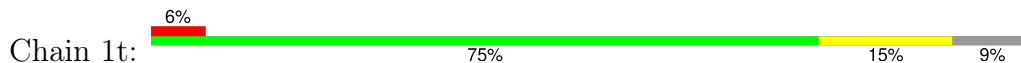


- Molecule 50: 30S ribosomal protein S19

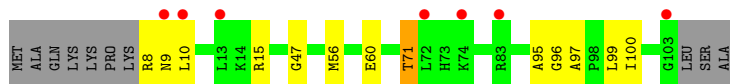
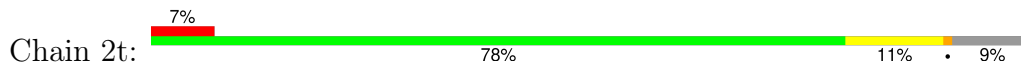
Chain 2s:  77% 20% 12% 11%



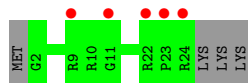
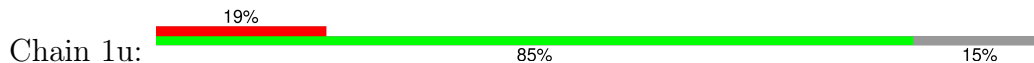
● Molecule 51: 30S ribosomal protein S20



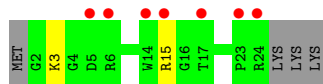
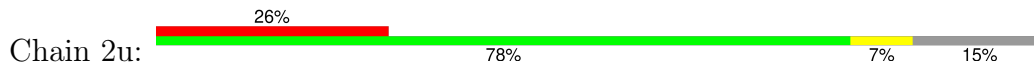
● Molecule 51: 30S ribosomal protein S20



● Molecule 52: 30S ribosomal protein Thx



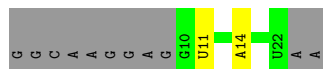
● Molecule 52: 30S ribosomal protein Thx



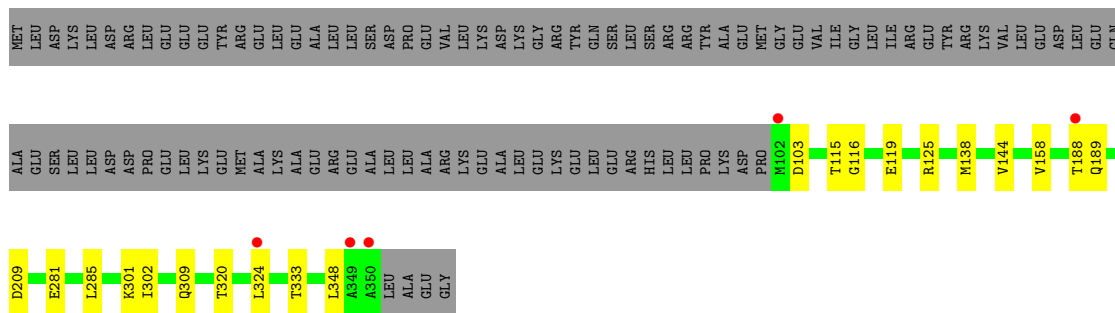
● Molecule 53: PHE-Stop mRNA



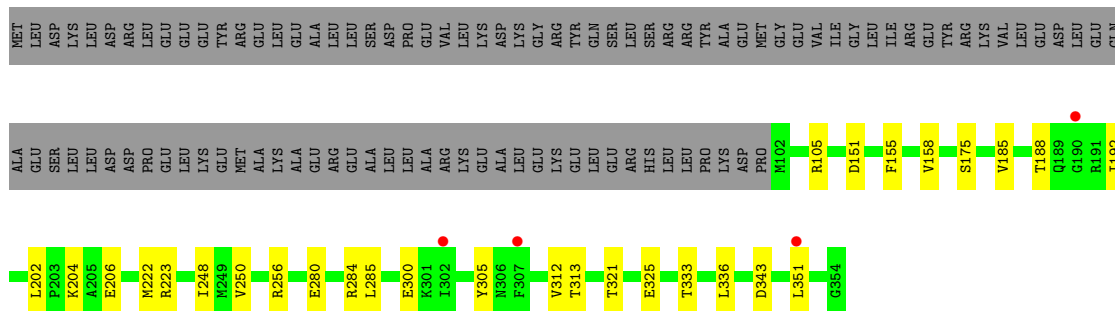
● Molecule 53: PHE-Stop mRNA



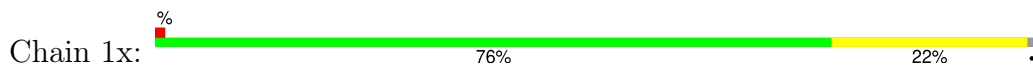
● Molecule 54: Peptide chain release factor 1



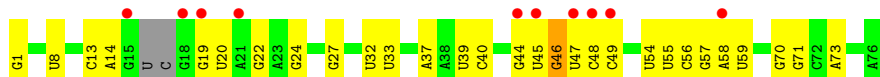
• Molecule 54: Peptide chain release factor 1



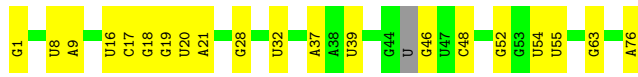
• Molecule 55: P-site and E-site Deacylated tRNAphe



• Molecule 55: P-site and E-site Deacylated tRNAphe

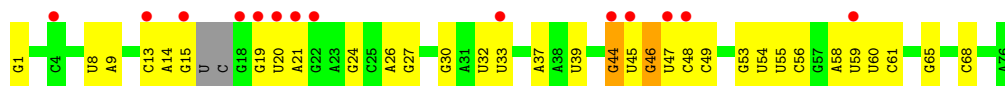


• Molecule 55: P-site and E-site Deacylated tRNAphe

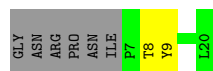


• Molecule 55: P-site and E-site Deacylated tRNAphe

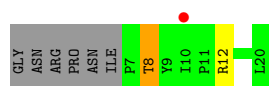




- Molecule 56: Fva1 Antimicrobial Peptide



- Molecule 56: Fva1 Antimicrobial Peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.39Å 451.41Å 623.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.02 – 2.70 37.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (37.02-2.70) 96.7 (37.02-2.70)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.226 , 0.275 0.226 , 0.274	Depositor DCC
$R_{free}$ test set	80443 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtrriage
Anisotropy	0.172	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	299076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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: OMU, ZN, 4OC, SF4, MA6, OMG, OMC, MG, 2MA, MIA, M2G, 4SU, 0TD, MEQ, UR3, 5MC, 5MU, 2MG, G7M, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.51	0/69011	0.95	46/107720 (0.0%)
1	2A	0.38	0/67295	0.85	21/105042 (0.0%)
2	1B	0.37	0/2881	0.83	0/4494
2	2B	0.32	0/2881	0.80	0/4494
3	1D	0.34	0/2186	0.55	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.36	0/1592	0.54	0/2149
4	2E	0.31	0/1592	0.49	0/2149
5	1F	0.33	0/1619	0.54	0/2193
5	2F	0.30	0/1615	0.49	0/2188
6	1G	0.30	0/1450	0.48	0/1959
6	2G	0.30	0/1449	0.49	0/1958
7	1H	0.32	0/1356	0.53	0/1834
7	2H	0.28	0/1356	0.45	0/1834
8	1I	0.29	0/1100	0.50	0/1501
8	2I	0.27	0/1076	0.47	0/1471
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.46	0/1543
10	1O	0.35	0/943	0.54	0/1269
10	2O	0.30	0/943	0.51	0/1269
11	1P	0.33	0/1152	0.57	0/1533
11	2P	0.30	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.33	0/982	0.54	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/887	0.51	0/1180
14	2S	0.28	0/880	0.48	0/1172
15	1T	0.31	0/1105	0.51	0/1477
15	2T	0.29	0/1097	0.51	0/1468
16	1U	0.39	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.30	0/977	0.43	0/1301
17	1V	0.38	0/782	0.54	0/1049
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.37	0/897	0.52	0/1205
18	2W	0.30	0/897	0.48	0/1205
19	1X	0.34	0/764	0.52	0/1025
19	2X	0.31	0/760	0.47	0/1021
20	1Y	0.33	0/819	0.53	0/1095
20	2Y	0.30	0/823	0.50	0/1100
21	1Z	0.30	0/1469	0.51	0/1998
21	2Z	0.30	0/1483	0.50	0/2018
22	10	0.33	0/612	0.55	0/816
22	20	0.28	0/616	0.50	0/821
23	11	0.31	0/762	0.54	0/1014
23	21	0.30	0/762	0.48	0/1014
24	12	0.32	0/590	0.48	0/781
24	22	0.29	0/590	0.43	0/781
25	13	0.36	0/474	0.52	0/635
25	23	0.30	0/469	0.48	0/630
26	14	0.31	0/561	0.49	0/756
26	24	0.36	0/530	0.57	0/719
27	15	0.34	0/469	0.54	0/635
27	25	0.32	0/469	0.49	0/635
28	16	0.33	0/460	0.53	0/613
28	26	0.29	0/456	0.49	0/608
29	17	0.36	0/426	0.52	0/561
29	27	0.29	0/426	0.51	0/561
30	18	0.34	0/519	0.54	0/684
30	28	0.27	0/525	0.48	0/691
31	19	0.36	0/310	0.51	0/407
31	29	0.34	0/310	0.53	0/407
32	1a	0.36	0/35795	0.86	20/55864 (0.0%)
32	2a	0.36	3/35886 (0.0%)	0.88	35/56005 (0.1%)
33	1b	0.30	0/1881	0.49	0/2542
33	2b	0.32	0/1860	0.51	1/2518 (0.0%)
34	1c	0.30	0/1578	0.48	0/2133
34	2c	0.28	0/1566	0.46	0/2119
35	1d	0.28	0/1689	0.46	0/2267
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.51	0/1543
36	2e	0.29	0/1146	0.52	0/1545
37	1f	0.29	0/823	0.48	0/1116
37	2f	0.29	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.28	0/1250	0.41	0/1679
38	2g	0.29	0/1254	0.45	0/1683
39	1h	0.29	0/1108	0.49	0/1494
39	2h	0.29	0/1108	0.48	0/1494
40	1i	0.32	0/1002	0.50	0/1346
40	2i	0.31	0/957	0.51	0/1288
41	1j	0.28	0/734	0.49	0/997
41	2j	0.30	0/727	0.50	0/988
42	1k	0.28	0/844	0.49	0/1145
42	2k	0.28	0/848	0.47	0/1149
43	1l	0.29	0/937	0.51	0/1260
43	2l	0.29	0/937	0.50	0/1260
44	1m	0.28	0/933	0.49	0/1254
44	2m	0.29	0/899	0.50	0/1212
45	1n	0.30	0/501	0.49	0/664
45	2n	0.30	0/495	0.50	0/657
46	1o	0.27	0/739	0.43	0/985
46	2o	0.28	0/739	0.42	0/985
47	1p	0.29	0/697	0.50	0/939
47	2p	0.28	0/693	0.47	0/935
48	1q	0.28	0/836	0.49	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.29	0/560	0.47	0/746
49	2r	0.27	0/556	0.50	0/741
50	1s	0.29	0/667	0.48	0/900
50	2s	0.28	0/661	0.48	0/893
51	1t	0.29	0/730	0.42	0/965
51	2t	0.27	0/729	0.45	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.25	0/203	0.51	0/266
53	1v	0.46	0/306	0.92	0/473
53	2v	0.37	0/306	0.95	0/473
54	1w	0.30	0/1956	0.48	0/2634
54	2w	0.29	0/1971	0.47	0/2654
55	1x	0.49	1/1629 (0.1%)	0.96	0/2535
55	1y	0.49	1/1602 (0.1%)	1.02	2/2488 (0.1%)
55	2x	0.45	1/1629 (0.1%)	0.88	0/2535
55	2y	0.51	1/1606 (0.1%)	0.99	1/2497 (0.0%)
56	1z	0.36	0/128	0.55	0/175
56	2z	0.26	0/128	0.43	0/175
All	All	0.39	7/317654 (0.0%)	0.80	126/474763 (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
11	1P	0	1
11	2P	0	1
14	1S	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1y	1	G	OP3-P	-10.37	1.48	1.61
55	1x	1	G	OP3-P	-10.32	1.48	1.61
55	2x	1	G	OP3-P	-10.26	1.48	1.61
55	2y	1	G	OP3-P	-10.19	1.49	1.61
32	2a	1272	G	N1-C2	-7.57	1.31	1.37

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	21.42	131.75	118.90
32	2a	1272	G	N3-C2-N2	17.71	132.30	119.90
32	2a	1272	G	C5-C6-O6	17.30	138.98	128.60
32	2a	1272	G	N1-C2-N2	-14.32	103.31	116.20
32	2a	1263	C	C2-N3-C4	13.02	126.41	119.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
14	1S	58	LEU	Peptide
11	2P	35	HIS	Peptide

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	25	49
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	25	49
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	25	49
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	25	49
6	1G	179/182 (98%)	153 (86%)	26 (14%)	0	100	100
6	2G	179/182 (98%)	150 (84%)	23 (13%)	6 (3%)	3	7
7	1H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	22	45
7	2H	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	7	20
8	1I	144/148 (97%)	125 (87%)	16 (11%)	3 (2%)	5	15
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	24
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	24
11	2P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	24
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	42
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	35
14	2S	108/112 (96%)	96 (89%)	9 (8%)	3 (3%)	4	10
15	1T	129/146 (88%)	122 (95%)	4 (3%)	3 (2%)	5	14

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	13	33
17	2V	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	3	9
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	12	30
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	92 (88%)	13 (12%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	181/206 (88%)	162 (90%)	17 (9%)	2 (1%)	12	30
21	2Z	184/206 (89%)	159 (86%)	24 (13%)	1 (0%)	25	49
22	10	74/85 (87%)	70 (95%)	3 (4%)	1 (1%)	9	24
22	20	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	10	26
23	11	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	12	30
23	21	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	12	30
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	7	18
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	11 (16%)	6 (9%)	0	0
26	24	66/71 (93%)	36 (54%)	27 (41%)	3 (4%)	2	4
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	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%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	7
33	2b	229/256 (90%)	189 (82%)	35 (15%)	5 (2%)	5	15
34	1c	204/239 (85%)	166 (81%)	37 (18%)	1 (0%)	25	49
34	2c	204/239 (85%)	177 (87%)	24 (12%)	3 (2%)	8	22
35	1d	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	13	33
35	2d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	13	33
36	1e	146/162 (90%)	126 (86%)	17 (12%)	3 (2%)	5	15
36	2e	146/162 (90%)	127 (87%)	16 (11%)	3 (2%)	5	15
37	1f	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
37	2f	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
38	1g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	6	16
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	16
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	14 (11%)	3 (2%)	5	13
40	2i	121/128 (94%)	96 (79%)	25 (21%)	0	100	100
41	1j	96/105 (91%)	78 (81%)	13 (14%)	5 (5%)	1	3
41	2j	94/105 (90%)	81 (86%)	11 (12%)	2 (2%)	5	15
42	1k	112/129 (87%)	93 (83%)	18 (16%)	1 (1%)	14	35
42	2k	112/129 (87%)	95 (85%)	16 (14%)	1 (1%)	14	35
43	1l	119/132 (90%)	104 (87%)	14 (12%)	1 (1%)	16	38
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	100 (86%)	15 (13%)	1 (1%)	14	35
44	2m	113/126 (90%)	93 (82%)	17 (15%)	3 (3%)	4	10
45	1n	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	7
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11	28
47	1p	80/88 (91%)	68 (85%)	12 (15%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	70 (88%)	10 (12%)	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%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	22
50	1s	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4	12
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	11	28
51	1t	94/106 (89%)	79 (84%)	12 (13%)	3 (3%)	3	8
51	2t	94/106 (89%)	78 (83%)	8 (8%)	8 (8%)	0	1
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	3
54	1w	246/354 (70%)	230 (94%)	15 (6%)	1 (0%)	30	55
54	2w	250/354 (71%)	231 (92%)	19 (8%)	0	100	100
56	1z	12/20 (60%)	9 (75%)	3 (25%)	0	100	100
56	2z	12/20 (60%)	10 (83%)	1 (8%)	1 (8%)	0	1
All	All	11922/12876 (93%)	10759 (90%)	1039 (9%)	124 (1%)	13	33

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	126	PRO
8	1I	10	GLU
17	1V	79	VAL
21	1Z	53	ILE
26	14	18	CYS

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	200 (93%)	15 (7%)	12	31

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2D	215/218 (99%)	205 (95%)	10 (5%)	22	49
4	1E	164/166 (99%)	154 (94%)	10 (6%)	15	36
4	2E	164/166 (99%)	148 (90%)	16 (10%)	6	16
5	1F	160/166 (96%)	146 (91%)	14 (9%)	8	20
5	2F	159/166 (96%)	145 (91%)	14 (9%)	8	20
6	1G	143/156 (92%)	127 (89%)	16 (11%)	5	12
6	2G	142/156 (91%)	124 (87%)	18 (13%)	3	9
7	1H	144/148 (97%)	133 (92%)	11 (8%)	11	27
7	2H	144/148 (97%)	131 (91%)	13 (9%)	8	19
8	1I	110/124 (89%)	97 (88%)	13 (12%)	4	10
8	2I	104/124 (84%)	94 (90%)	10 (10%)	7	17
9	1N	118/119 (99%)	106 (90%)	12 (10%)	6	15
9	2N	118/119 (99%)	111 (94%)	7 (6%)	16	38
10	1O	100/100 (100%)	94 (94%)	6 (6%)	16	38
10	2O	100/100 (100%)	95 (95%)	5 (5%)	20	46
11	1P	115/116 (99%)	112 (97%)	3 (3%)	41	70
11	2P	115/116 (99%)	108 (94%)	7 (6%)	15	36
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	9	23
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	8	19
13	1R	101/101 (100%)	93 (92%)	8 (8%)	10	25
13	2R	101/101 (100%)	96 (95%)	5 (5%)	20	46
14	1S	87/88 (99%)	77 (88%)	10 (12%)	4	11
14	2S	85/88 (97%)	74 (87%)	11 (13%)	3	8
15	1T	115/127 (91%)	103 (90%)	12 (10%)	5	14
15	2T	113/127 (89%)	107 (95%)	6 (5%)	19	43
16	1U	93/94 (99%)	89 (96%)	4 (4%)	25	52
16	2U	93/94 (99%)	87 (94%)	6 (6%)	14	34
17	1V	80/82 (98%)	74 (92%)	6 (8%)	11	28
17	2V	80/82 (98%)	73 (91%)	7 (9%)	8	20
18	1W	90/92 (98%)	85 (94%)	5 (6%)	17	41
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17	41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27	56
19	2X	76/78 (97%)	69 (91%)	7 (9%)	7	18
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	7	18
20	2Y	86/91 (94%)	80 (93%)	6 (7%)	12	31
21	1Z	155/179 (87%)	143 (92%)	12 (8%)	10	26
21	2Z	155/179 (87%)	140 (90%)	15 (10%)	6	17
22	10	61/67 (91%)	58 (95%)	3 (5%)	21	47
22	20	61/67 (91%)	59 (97%)	2 (3%)	33	62
23	11	80/83 (96%)	75 (94%)	5 (6%)	15	35
23	21	80/83 (96%)	74 (92%)	6 (8%)	11	28
24	12	65/67 (97%)	60 (92%)	5 (8%)	10	26
24	22	65/67 (97%)	60 (92%)	5 (8%)	10	26
25	13	51/52 (98%)	47 (92%)	4 (8%)	10	26
25	23	50/52 (96%)	48 (96%)	2 (4%)	27	55
26	14	58/63 (92%)	51 (88%)	7 (12%)	4	10
26	24	51/63 (81%)	43 (84%)	8 (16%)	2	6
27	15	50/52 (96%)	48 (96%)	2 (4%)	27	55
27	25	50/52 (96%)	46 (92%)	4 (8%)	10	24
28	16	51/52 (98%)	49 (96%)	2 (4%)	27	56
28	26	50/52 (96%)	41 (82%)	9 (18%)	1	4
29	17	41/42 (98%)	37 (90%)	4 (10%)	6	16
29	27	41/42 (98%)	38 (93%)	3 (7%)	11	29
30	18	53/55 (96%)	49 (92%)	4 (8%)	11	28
30	28	54/55 (98%)	47 (87%)	7 (13%)	3	8
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	67
33	1b	192/220 (87%)	165 (86%)	27 (14%)	3	7
33	2b	187/220 (85%)	155 (83%)	32 (17%)	1	4
34	1c	144/188 (77%)	119 (83%)	25 (17%)	1	4
34	2c	140/188 (74%)	127 (91%)	13 (9%)	7	18
35	1d	170/181 (94%)	152 (89%)	18 (11%)	5	13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	156 (90%)	17 (10%)	6	16
36	1e	113/123 (92%)	101 (89%)	12 (11%)	5	13
36	2e	113/123 (92%)	102 (90%)	11 (10%)	6	17
37	1f	84/90 (93%)	78 (93%)	6 (7%)	12	30
37	2f	85/90 (94%)	76 (89%)	9 (11%)	5	13
38	1g	119/127 (94%)	111 (93%)	8 (7%)	13	33
38	2g	120/127 (94%)	106 (88%)	14 (12%)	4	11
39	1h	114/119 (96%)	102 (90%)	12 (10%)	5	14
39	2h	114/119 (96%)	109 (96%)	5 (4%)	24	51
40	1i	90/99 (91%)	80 (89%)	10 (11%)	5	12
40	2i	86/99 (87%)	71 (83%)	15 (17%)	1	4
41	1j	68/92 (74%)	61 (90%)	7 (10%)	6	14
41	2j	69/92 (75%)	56 (81%)	13 (19%)	1	3
42	1k	82/99 (83%)	79 (96%)	3 (4%)	29	58
42	2k	83/99 (84%)	79 (95%)	4 (5%)	21	48
43	1l	96/108 (89%)	88 (92%)	8 (8%)	9	22
43	2l	96/108 (89%)	86 (90%)	10 (10%)	5	14
44	1m	90/101 (89%)	80 (89%)	10 (11%)	5	12
44	2m	85/101 (84%)	79 (93%)	6 (7%)	12	30
45	1n	49/50 (98%)	44 (90%)	5 (10%)	6	15
45	2n	48/50 (96%)	45 (94%)	3 (6%)	15	35
46	1o	78/80 (98%)	74 (95%)	4 (5%)	20	45
46	2o	78/80 (98%)	69 (88%)	9 (12%)	4	11
47	1p	69/74 (93%)	61 (88%)	8 (12%)	4	11
47	2p	68/74 (92%)	66 (97%)	2 (3%)	37	67
48	1q	94/97 (97%)	85 (90%)	9 (10%)	7	17
48	2q	94/97 (97%)	84 (89%)	10 (11%)	5	13
49	1r	59/77 (77%)	53 (90%)	6 (10%)	6	15
49	2r	58/77 (75%)	51 (88%)	7 (12%)	4	10
50	1s	69/80 (86%)	60 (87%)	9 (13%)	3	8
50	2s	67/80 (84%)	57 (85%)	10 (15%)	2	6

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	57 (81%)	13 (19%)	1	3
51	2t	70/82 (85%)	64 (91%)	6 (9%)	8	21
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17	41
54	1w	203/298 (68%)	184 (91%)	19 (9%)	7	18
54	2w	202/298 (68%)	173 (86%)	29 (14%)	2	7
56	1z	14/19 (74%)	12 (86%)	2 (14%)	2	7
56	2z	14/19 (74%)	12 (86%)	2 (14%)	2	7
All	All	9747/10698 (91%)	8860 (91%)	887 (9%)	7	19

5 of 887 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	2F	88	VAL
56	2z	12	ARG
17	2V	18	LEU
54	2w	312	VAL
43	2l	66	VAL

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

Mol	Chain	Res	Type
40	2i	87	GLN
42	2k	93	GLN
54	2w	315	HIS
39	1h	15	ASN
38	1g	13	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	442 (15%)	28 (0%)
1	2A	2790/2915 (95%)	481 (17%)	22 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1494/1521 (98%)	305 (20%)	0
32	2a	1498/1521 (98%)	297 (19%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	1v	11/24 (45%)	3 (27%)	0
53	2v	11/24 (45%)	2 (18%)	0
55	1x	72/76 (94%)	9 (12%)	0
55	1y	70/76 (92%)	21 (30%)	0
55	2x	72/76 (94%)	12 (16%)	0
55	2y	71/76 (93%)	26 (36%)	0
All	All	9190/9466 (97%)	1625 (17%)	50 (0%)

5 of 1625 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	63	U

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	196	A
1	2A	774	A
1	2A	2756	U
1	2A	228	A
1	2A	277	C

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

78 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
55	MIA	1y	37	55	24,31,32	2.10	5 (20%)	22,44,47	2.54	6 (27%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.48	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	PSU	1x	39	55	18,21,22	1.39	2 (11%)	21,30,33	1.90	3 (14%)
1	5MU	1A	1939	1,57	19,22,23	1.39	5 (26%)	27,32,35	2.39	6 (22%)
1	PSU	1A	1917	1	18,21,22	1.43	2 (11%)	21,30,33	1.99	3 (14%)
55	PSU	1y	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
55	G7M	2x	46	55	20,26,27	1.25	2 (10%)	16,39,42	0.71	0
1	PSU	2A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.11	6 (28%)
32	5MC	2a	967	32,57	19,22,23	1.67	3 (15%)	26,32,35	1.14	3 (11%)
55	PSU	2x	32	55	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
32	4OC	2a	1402	32,57	20,23,24	0.78	0	25,32,35	0.96	1 (4%)
1	2MA	2A	2503	1,57	17,25,26	1.05	1 (5%)	16,37,40	1.40	3 (18%)
55	PSU	2x	39	55	18,21,22	1.40	3 (16%)	21,30,33	1.82	4 (19%)
55	PSU	2y	32	55	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
1	2MA	1A	2503	1,57	17,25,26	0.99	1 (5%)	16,37,40	1.34	3 (18%)
32	2MG	1a	1207	32,57	18,26,27	0.91	1 (5%)	16,38,41	1.39	3 (18%)
32	4OC	1a	1402	32,57	20,23,24	0.79	0	25,32,35	1.05	3 (12%)
55	PSU	2y	39	55	18,21,22	1.36	2 (11%)	21,30,33	1.87	3 (14%)
1	5MU	2A	1939	1	19,22,23	1.48	6 (31%)	27,32,35	2.25	7 (25%)
55	G7M	1x	46	55	20,26,27	1.24	2 (10%)	16,39,42	0.63	0
55	PSU	1x	32	55	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
1	5MU	1A	1915	1,57	19,22,23	1.44	5 (26%)	27,32,35	2.10	5 (18%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	2.05	3 (16%)
32	MA6	2a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	1.91	3 (16%)
55	4SU	2y	8	55	18,21,22	1.74	4 (22%)	25,30,33	2.00	4 (16%)
54	MEQ	1w	230	54	8,9,10	0.98	0	5,10,12	0.69	0
55	4SU	1y	8	55	18,21,22	1.79	4 (22%)	25,30,33	2.01	5 (20%)
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.25	2 (7%)
1	OMU	2A	2552	1,57	19,22,23	1.27	3 (15%)	25,31,34	1.86	5 (20%)
55	PSU	1x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.01	4 (19%)
55	5MU	2y	54	55	19,22,23	1.47	5 (26%)	27,32,35	2.41	8 (29%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
55	4SU	1x	8	55	18,21,22	1.78	4 (22%)	25,30,33	1.91	4 (16%)
32	M2G	2a	966	32	20,27,28	1.32	3 (15%)	19,40,43	1.04	2 (10%)
55	MIA	2x	37	55	24,31,32	2.29	3 (12%)	22,44,47	2.49	7 (31%)
32	5MC	2a	1407	32	19,22,23	1.58	3 (15%)	26,32,35	1.07	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.96	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	G7M	1y	46	55	20,26,27	1.28	2 (10%)	16,39,42	0.61	0
1	5MU	2A	1915	1	19,22,23	1.45	5 (26%)	27,32,35	2.12	5 (18%)
55	PSU	1y	39	55	18,21,22	1.45	3 (16%)	21,30,33	1.73	3 (14%)
32	M2G	1a	966	32	20,27,28	1.41	3 (15%)	19,40,43	1.09	1 (5%)
1	PSU	2A	1917	1	18,21,22	1.42	3 (16%)	21,30,33	2.05	4 (19%)
1	OMG	1A	2251	1,57,55	19,26,27	1.00	1 (5%)	21,38,41	1.11	2 (9%)
32	G7M	1a	527	32	20,26,27	1.22	2 (10%)	16,39,42	0.57	0
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	1.91	6 (22%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)
43	0TD	1l	92	43	8,9,10	4.21	2 (25%)	6,11,13	9.98	3 (50%)
1	5MC	2A	1942	1	19,22,23	1.66	3 (15%)	26,32,35	1.22	3 (11%)
1	OMU	1A	2552	1,57	19,22,23	1.33	4 (21%)	25,31,34	2.01	5 (20%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
55	G7M	2y	46	55	20,26,27	1.29	1 (5%)	16,39,42	0.71	0
55	MIA	2y	37	55	24,31,32	2.26	4 (16%)	22,44,47	2.79	7 (31%)
1	5MC	2A	1962	1,57	19,22,23	1.52	3 (15%)	26,32,35	1.03	2 (7%)
1	OMG	2A	2251	1,57,55	19,26,27	0.92	1 (5%)	21,38,41	1.04	1 (4%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	2.00	3 (16%)
55	4SU	2x	8	57,55	18,21,22	1.88	4 (22%)	25,30,33	1.69	4 (16%)
1	OMC	2A	1920	1,57	19,22,23	0.80	0	25,31,34	0.88	0
55	PSU	2y	55	55	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.24	3 (11%)
54	MEQ	2w	230	54	8,9,10	0.92	0	5,10,12	0.46	0
32	MA6	1a	1518	32	19,26,27	1.03	2 (10%)	18,38,41	1.92	3 (16%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.28	2 (11%)	21,30,33	2.08	4 (19%)
1	5MC	1A	1962	1,57	19,22,23	1.62	3 (15%)	26,32,35	1.08	1 (3%)
32	5MC	1a	1407	32	19,22,23	1.44	3 (15%)	26,32,35	1.03	2 (7%)
32	5MC	1a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.17	2 (7%)
55	PSU	1y	32	55	18,21,22	1.39	2 (11%)	21,30,33	1.95	3 (14%)
32	PSU	1a	516	32,57	18,21,22	1.40	2 (11%)	21,30,33	2.03	5 (23%)
32	UR3	2a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.73	3 (11%)
1	PSU	1A	2605	1,57	18,21,22	1.41	3 (16%)	21,30,33	2.02	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.70	5 (19%)
55	5MU	1y	54	55	19,22,23	1.42	5 (26%)	27,32,35	1.77	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
43	0TD	2l	92	43	8,9,10	4.48	2 (25%)	6,11,13	4.62	3 (50%)
55	MIA	1x	37	55	24,31,32	2.41	4 (16%)	22,44,47	2.30	7 (31%)
32	G7M	2a	527	32	20,26,27	1.21	2 (10%)	16,39,42	0.73	0
32	5MC	1a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.11	3 (11%)
32	PSU	2a	516	32,57	18,21,22	1.38	2 (11%)	21,30,33	1.98	5 (23%)
55	5MU	1x	54	55	19,22,23	1.44	3 (15%)	27,32,35	1.76	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	MIA	1y	37	55	-	3/11/33/34	0/3/3/3
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	1y	55	55	-	2/7/25/26	0/2/2/2
55	G7M	2x	46	55	-	3/3/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32,57	-	0/7/25/26	0/2/2/2
55	PSU	2x	32	55	-	1/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	2/9/29/30	0/2/2/2
1	2MA	2A	2503	1,57	-	3/3/25/26	0/3/3/3
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
55	PSU	2y	32	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	2/3/25/26	0/3/3/3
32	2MG	1a	1207	32,57	-	0/5/27/28	0/3/3/3
32	4OC	1a	1402	32,57	-	2/9/29/30	0/2/2/2
55	PSU	2y	39	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
55	G7M	1x	46	55	-	3/3/25/26	0/3/3/3
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,57	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
55	4SU	2y	8	55	-	0/7/25/26	0/2/2/2
54	MEQ	1w	230	54	-	3/8/9/11	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	1y	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	5MU	2y	54	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
55	MIA	2x	37	55	-	5/11/33/34	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	G7M	1y	46	55	-	3/3/25/26	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	PSU	1y	39	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	1/5/27/28	0/3/3/3
32	G7M	1a	527	32	-	1/3/25/26	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	6/7/12/14	-
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	G7M	2y	46	55	-	3/3/25/26	0/3/3/3
55	MIA	2y	37	55	-	2/11/33/34	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,57,55	-	0/5/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
55	4SU	2x	8	57,55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1,57	-	2/9/27/28	0/2/2/2
55	PSU	2y	55	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	MEQ	2w	230	54	-	1/8/9/11	-
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	PSU	1y	32	55	-	0/7/25/26	0/2/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	5MU	1y	54	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	5/7/12/14	-
55	MIA	1x	37	55	-	7/11/33/34	0/3/3/3
32	G7M	2a	527	32	-	0/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,57	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2

The worst 5 of 195 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.03	1.70	1.82
43	1l	92	0TD	CB-SB	-11.42	1.70	1.82
55	1x	37	MIA	C2-S10	-7.91	1.69	1.75
55	2x	37	MIA	C2-S10	-7.23	1.69	1.75
55	1x	37	MIA	C13-C14	7.14	1.53	1.32

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	23.93	145.39	102.36
43	2l	92	0TD	CSB-SB-CB	10.13	120.57	102.36
55	2y	37	MIA	C12-C13-C14	-9.50	109.96	127.01
55	1y	37	MIA	C12-C13-C14	-9.26	110.38	127.01
55	2x	37	MIA	C12-C13-C14	-8.67	111.45	127.01

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
55	1x	37	MIA	C12-C13-C14-C15

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2022 ligands modelled in this entry, 2020 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
59	SF4	1d	302	35	0,12,12	-	-	-		
59	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	302	35	-	-	0/6/5/5
59	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	-0.62	112 (3%) 44 42	10, 27, 82, 98	0
1	2A	2789/2915 (95%)	-0.12	105 (3%) 44 42	25, 49, 84, 97	0
2	1B	120/121 (99%)	-0.39	0 100 100	23, 45, 58, 73	0
2	2B	120/121 (99%)	0.74	4 (3%) 49 47	55, 73, 84, 84	0
3	1D	275/276 (99%)	-0.53	2 (0%) 84 83	12, 27, 44, 70	0
3	2D	275/276 (99%)	-0.08	1 (0%) 89 88	21, 43, 56, 67	0
4	1E	204/206 (99%)	-0.54	0 100 100	11, 28, 48, 74	0
4	2E	204/206 (99%)	-0.04	0 100 100	27, 47, 60, 75	0
5	1F	203/210 (96%)	-0.38	0 100 100	12, 33, 55, 70	0
5	2F	203/210 (96%)	0.24	1 (0%) 87 86	27, 55, 70, 77	0
6	1G	181/182 (99%)	0.29	7 (3%) 44 42	36, 52, 69, 80	0
6	2G	181/182 (99%)	1.11	21 (11%) 11 10	61, 72, 78, 85	0
7	1H	174/180 (96%)	-0.16	1 (0%) 85 85	29, 43, 55, 60	0
7	2H	174/180 (96%)	0.79	10 (5%) 30 28	54, 69, 78, 85	0
8	1I	146/148 (98%)	0.35	3 (2%) 63 63	37, 60, 70, 74	0
8	2I	146/148 (98%)	0.48	3 (2%) 63 63	46, 65, 72, 76	0
9	1N	140/140 (100%)	-0.56	0 100 100	17, 27, 52, 61	0
9	2N	140/140 (100%)	0.14	1 (0%) 84 83	37, 54, 68, 71	0
10	1O	122/122 (100%)	-0.49	0 100 100	18, 30, 49, 55	0
10	2O	122/122 (100%)	-0.29	0 100 100	32, 42, 56, 61	0
11	1P	149/150 (99%)	-0.29	0 100 100	12, 36, 56, 63	0
11	2P	149/150 (99%)	0.39	0 100 100	29, 57, 71, 79	0
12	1Q	141/141 (100%)	-0.44	0 100 100	19, 32, 45, 59	0
12	2Q	141/141 (100%)	0.29	3 (2%) 63 63	39, 54, 63, 76	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%)	-0.58	0 100 100	16, 27, 40, 53	0
13	2R	118/118 (100%)	-0.03	0 100 100	31, 46, 55, 64	0
14	1S	110/112 (98%)	-0.15	0 100 100	34, 45, 55, 57	0
14	2S	110/112 (98%)	0.82	8 (7%) 22 20	58, 67, 73, 75	0
15	1T	131/146 (89%)	-0.30	3 (2%) 61 60	24, 36, 62, 75	0
15	2T	131/146 (89%)	-0.01	1 (0%) 82 82	34, 48, 65, 74	0
16	1U	116/118 (98%)	-0.63	0 100 100	12, 21, 36, 53	0
16	2U	116/118 (98%)	0.05	0 100 100	35, 50, 61, 67	0
17	1V	101/101 (100%)	-0.64	0 100 100	12, 28, 43, 49	0
17	2V	101/101 (100%)	0.30	1 (0%) 79 79	33, 60, 69, 74	0
18	1W	112/113 (99%)	-0.67	0 100 100	10, 21, 38, 69	0
18	2W	112/113 (99%)	-0.23	0 100 100	32, 42, 61, 82	0
19	1X	95/96 (98%)	-0.40	2 (2%) 63 63	20, 30, 48, 64	0
19	2X	95/96 (98%)	0.42	2 (2%) 63 63	44, 56, 67, 78	0
20	1Y	107/110 (97%)	-0.19	0 100 100	26, 39, 59, 70	0
20	2Y	107/110 (97%)	0.63	7 (6%) 26 24	48, 61, 72, 79	0
21	1Z	183/206 (88%)	0.10	0 100 100	33, 49, 61, 72	0
21	2Z	186/206 (90%)	0.72	9 (4%) 36 35	54, 67, 74, 80	0
22	10	76/85 (89%)	-0.38	2 (2%) 57 56	20, 30, 49, 61	0
22	20	77/85 (90%)	0.35	3 (3%) 44 42	46, 54, 64, 71	0
23	11	97/98 (98%)	-0.24	1 (1%) 79 79	19, 33, 58, 66	0
23	21	97/98 (98%)	0.17	2 (2%) 63 63	34, 49, 66, 73	0
24	12	70/72 (97%)	-0.11	0 100 100	27, 39, 51, 68	0
24	22	70/72 (97%)	0.51	4 (5%) 30 28	53, 62, 69, 77	0
25	13	59/60 (98%)	-0.52	0 100 100	17, 26, 48, 60	0
25	23	59/60 (98%)	0.05	0 100 100	41, 53, 64, 68	0
26	14	69/71 (97%)	0.72	5 (7%) 23 21	50, 69, 80, 83	0
26	24	68/71 (95%)	1.36	15 (22%) 3 3	67, 78, 86, 88	0
27	15	59/60 (98%)	-0.71	0 100 100	10, 26, 41, 48	0
27	25	59/60 (98%)	-0.08	1 (1%) 69 68	26, 45, 60, 69	0
28	16	53/54 (98%)	-0.40	0 100 100	27, 37, 49, 54	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%)	0.20	1 (1%) 66 65	49, 56, 64, 69	0
29	17	48/49 (97%)	-0.36	3 (6%) 27 25	13, 20, 48, 68	0
29	27	48/49 (97%)	0.14	4 (8%) 19 17	26, 36, 60, 66	0
30	18	64/65 (98%)	-0.59	0 100 100	18, 25, 33, 38	0
30	28	64/65 (98%)	0.13	1 (1%) 70 70	35, 46, 52, 63	0
31	19	37/37 (100%)	-0.44	0 100 100	22, 30, 40, 47	0
31	29	37/37 (100%)	0.52	0 100 100	46, 57, 65, 70	0
32	1a	1488/1521 (97%)	0.54	81 (5%) 32 30	23, 64, 86, 97	0
32	2a	1491/1521 (98%)	0.55	80 (5%) 32 30	35, 66, 85, 97	0
33	1b	231/256 (90%)	0.82	14 (6%) 28 26	54, 69, 78, 83	0
33	2b	231/256 (90%)	1.14	37 (16%) 6 5	61, 73, 80, 89	0
34	1c	206/239 (86%)	0.89	14 (6%) 25 23	58, 70, 76, 78	0
34	2c	206/239 (86%)	0.86	15 (7%) 22 20	62, 71, 76, 79	0
35	1d	208/209 (99%)	0.78	13 (6%) 27 25	45, 65, 74, 79	0
35	2d	208/209 (99%)	0.50	6 (2%) 54 52	46, 59, 67, 71	0
36	1e	148/162 (91%)	0.39	1 (0%) 84 83	42, 56, 67, 70	0
36	2e	148/162 (91%)	0.56	4 (2%) 56 54	48, 60, 69, 81	0
37	1f	100/101 (99%)	0.44	4 (4%) 43 41	49, 60, 67, 71	0
37	2f	100/101 (99%)	0.50	2 (2%) 64 64	55, 64, 72, 77	0
38	1g	155/156 (99%)	0.75	10 (6%) 26 24	57, 66, 74, 77	0
38	2g	155/156 (99%)	1.04	21 (13%) 8 7	61, 71, 78, 81	0
39	1h	137/138 (99%)	0.37	0 100 100	48, 57, 65, 69	0
39	2h	137/138 (99%)	0.50	6 (4%) 39 38	49, 62, 68, 72	0
40	1i	127/128 (99%)	1.25	21 (16%) 5 5	55, 70, 77, 81	0
40	2i	123/128 (96%)	1.51	30 (24%) 2 2	66, 75, 82, 87	0
41	1j	98/105 (93%)	1.47	23 (23%) 2 3	59, 72, 78, 80	0
41	2j	96/105 (91%)	1.60	28 (29%) 1 2	66, 77, 82, 84	0
42	1k	114/129 (88%)	0.39	1 (0%) 81 80	38, 57, 68, 74	0
42	2k	114/129 (88%)	0.71	4 (3%) 47 45	53, 66, 73, 82	0
43	1l	121/132 (91%)	0.31	4 (3%) 49 47	38, 51, 62, 66	0
43	2l	121/132 (91%)	0.23	4 (3%) 49 47	40, 52, 59, 69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	1.04	14 (11%) 10 9	55, 68, 76, 78	0
44	2m	115/126 (91%)	1.31	21 (18%) 4 4	63, 73, 79, 82	0
45	1n	60/61 (98%)	1.18	6 (10%) 14 13	58, 68, 75, 78	0
45	2n	60/61 (98%)	1.41	13 (21%) 3 3	63, 72, 77, 78	0
46	1o	88/89 (98%)	0.27	4 (4%) 39 37	39, 56, 67, 72	0
46	2o	88/89 (98%)	0.47	3 (3%) 48 46	50, 61, 71, 75	0
47	1p	82/88 (93%)	1.03	11 (13%) 8 7	53, 64, 72, 76	0
47	2p	82/88 (93%)	0.56	0 100 100	47, 57, 65, 73	0
48	1q	99/105 (94%)	0.38	1 (1%) 79 79	44, 56, 66, 72	0
48	2q	99/105 (94%)	0.42	1 (1%) 79 79	48, 58, 65, 76	0
49	1r	68/88 (77%)	0.45	0 100 100	44, 55, 69, 76	0
49	2r	68/88 (77%)	0.70	4 (5%) 29 27	54, 64, 72, 76	0
50	1s	83/93 (89%)	1.36	18 (21%) 3 3	63, 74, 78, 84	0
50	2s	83/93 (89%)	1.35	19 (22%) 2 3	62, 75, 82, 83	0
51	1t	96/106 (90%)	0.64	6 (6%) 27 25	50, 60, 71, 73	0
51	2t	96/106 (90%)	0.68	7 (7%) 22 20	46, 62, 70, 72	0
52	1u	23/27 (85%)	1.43	5 (21%) 3 3	60, 65, 70, 73	0
52	2u	23/27 (85%)	1.59	7 (30%) 1 2	66, 72, 75, 78	0
53	1v	13/24 (54%)	0.33	0 100 100	42, 52, 82, 86	0
53	2v	13/24 (54%)	0.84	0 100 100	56, 65, 85, 88	0
54	1w	248/354 (70%)	0.19	5 (2%) 64 64	25, 58, 72, 80	0
54	2w	252/354 (71%)	0.32	4 (1%) 70 70	40, 64, 76, 82	0
55	1x	68/76 (89%)	-0.10	1 (1%) 71 71	20, 51, 64, 84	0
55	1y	67/76 (88%)	0.99	10 (14%) 7 6	32, 79, 87, 93	0
55	2x	68/76 (89%)	0.22	0 100 100	37, 65, 74, 84	0
55	2y	67/76 (88%)	1.44	14 (20%) 3 3	50, 88, 93, 96	0
56	1z	14/20 (70%)	0.25	0 100 100	25, 35, 61, 67	0
56	2z	14/20 (70%)	0.88	1 (7%) 23 21	43, 58, 70, 73	0
All	All	21290/22342 (95%)	0.17	947 (4%) 39 38	10, 55, 79, 98	0

The worst 5 of 947 RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
1	1A	1088	A	7.9
32	1a	1026	G	6.7
1	1A	1068	G	6.6
38	1g	80	VAL	6.4
1	1A	1057	A	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
55	5MU	2y	54	21/22	0.57	0.17	82,91,101,116	0
55	G7M	2y	46	24/25	0.58	0.18	81,91,99,115	0
55	4SU	2y	8	20/21	0.68	0.13	83,87,95,108	0
55	PSU	2y	55	20/21	0.68	0.14	82,90,97,106	0
43	0TD	1l	92	10/11	0.71	0.15	40,51,63,71	0
55	G7M	1y	46	24/25	0.71	0.15	74,84,96,109	0
55	PSU	1y	55	20/21	0.75	0.14	71,81,91,98	0
55	5MU	1y	54	21/22	0.77	0.14	71,81,92,108	0
55	PSU	2y	32	20/21	0.80	0.15	70,80,83,90	0
55	PSU	2y	39	20/21	0.81	0.12	71,80,87,89	0
55	4SU	1y	8	20/21	0.81	0.12	74,80,87,90	0
55	PSU	1y	39	20/21	0.82	0.12	58,75,78,79	0
32	2MG	1a	1207	24/25	0.83	0.14	70,75,81,86	0
55	PSU	1y	32	20/21	0.83	0.11	60,70,75,76	0
32	2MG	2a	1207	24/25	0.83	0.12	60,75,81,87	0
55	MIA	2y	37	29/30	0.84	0.14	68,75,84,94	0
55	G7M	2x	46	24/25	0.85	0.13	62,68,74,93	0
43	0TD	2l	92	10/11	0.86	0.14	53,58,65,74	0
55	MIA	1y	37	29/30	0.87	0.12	58,68,71,82	0
55	PSU	2x	55	20/21	0.87	0.10	55,67,73,78	0
55	PSU	2x	32	20/21	0.87	0.12	61,68,76,77	0
32	M2G	1a	966	25/26	0.88	0.13	42,53,64,65	0
1	5MU	2A	1915	21/22	0.88	0.11	52,57,68,75	0
55	PSU	2x	39	20/21	0.91	0.11	46,64,69,74	0
32	5MC	2a	967	21/22	0.91	0.11	59,63,70,80	0
1	PSU	2A	1911	20/21	0.91	0.09	47,52,58,59	0
55	G7M	1x	46	24/25	0.91	0.09	40,47,62,79	0
32	PSU	2a	516	20/21	0.91	0.11	57,65,72,73	0
32	M2G	2a	966	25/26	0.92	0.11	54,62,72,75	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	5MU	2x	54	21/22	0.92	0.09	60,65,69,74	0
55	4SU	2x	8	20/21	0.92	0.12	58,65,70,72	0
32	PSU	1a	516	20/21	0.92	0.10	50,58,68,69	0
32	G7M	2a	527	24/25	0.92	0.11	54,62,65,68	0
32	5MC	2a	1400	21/22	0.93	0.10	55,62,66,67	0
32	G7M	1a	527	24/25	0.93	0.10	43,56,63,63	0
55	5MU	1x	54	21/22	0.93	0.11	48,55,60,64	0
1	OMC	2A	1920	21/22	0.93	0.09	44,50,54,55	0
55	PSU	1x	39	20/21	0.93	0.10	35,51,57,59	0
32	MA6	2a	1518	24/25	0.94	0.10	41,51,57,59	0
1	PSU	2A	1917	20/21	0.94	0.07	44,50,57,59	0
32	5MC	1a	967	21/22	0.94	0.10	46,53,63,67	0
32	4OC	2a	1402	22/23	0.94	0.09	46,50,54,59	0
32	5MC	2a	1404	21/22	0.94	0.11	30,44,48,50	0
1	PSU	1A	1911	20/21	0.95	0.10	35,46,53,54	0
54	MEQ	2w	230	10/11	0.95	0.12	42,44,50,51	0
1	5MU	1A	1915	21/22	0.95	0.08	42,48,54,61	0
55	PSU	1x	32	20/21	0.95	0.09	42,51,58,67	0
55	MIA	2x	37	29/30	0.95	0.11	54,62,67,68	0
32	UR3	2a	1498	21/22	0.95	0.10	42,49,55,58	0
55	PSU	1x	55	20/21	0.95	0.09	50,53,60,61	0
32	MA6	2a	1519	24/25	0.95	0.10	41,49,54,57	0
32	5MC	2a	1407	21/22	0.96	0.08	36,42,50,57	0
1	OMC	1A	1920	21/22	0.96	0.09	33,41,45,48	0
55	4SU	1x	8	20/21	0.96	0.07	32,40,47,52	0
1	PSU	1A	1917	20/21	0.96	0.07	34,42,52,54	0
55	MIA	1x	37	29/30	0.96	0.08	37,47,56,58	0
32	5MC	1a	1400	21/22	0.96	0.10	39,47,57,59	0
32	4OC	1a	1402	22/23	0.96	0.09	35,40,44,50	0
32	5MC	1a	1404	21/22	0.96	0.08	30,35,41,48	0
32	MA6	1a	1518	24/25	0.96	0.10	23,35,43,47	0
32	MA6	1a	1519	24/25	0.96	0.09	31,34,38,42	0
54	MEQ	1w	230	10/11	0.97	0.09	20,25,27,29	0
1	5MC	1A	1942	21/22	0.97	0.07	21,28,32,37	0
1	5MC	1A	1962	21/22	0.97	0.07	18,26,29,34	0
1	5MU	2A	1939	21/22	0.97	0.07	28,31,36,36	0
1	5MC	2A	1942	21/22	0.97	0.06	32,38,44,46	0
1	5MC	2A	1962	21/22	0.97	0.08	25,32,36,48	0
1	OMG	2A	2251	24/25	0.97	0.08	25,34,37,45	0
1	2MA	2A	2503	23/24	0.97	0.07	24,29,32,34	0
32	5MC	1a	1407	21/22	0.97	0.07	27,35,39,43	0
1	5MU	1A	1939	21/22	0.98	0.07	13,20,24,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	OMG	1A	2251	24/25	0.98	0.06	10,15,18,24	0
1	OMU	2A	2552	21/22	0.98	0.06	22,27,31,35	0
1	PSU	2A	2605	20/21	0.98	0.07	21,28,33,37	0
1	2MA	1A	2503	23/24	0.98	0.06	10,14,17,17	0
1	OMU	1A	2552	21/22	0.98	0.06	12,17,20,23	0
32	UR3	1a	1498	21/22	0.98	0.07	29,34,37,39	0
1	PSU	1A	2605	20/21	0.98	0.07	13,18,22,29	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2a	1766	1/1	0.47	0.20	64,64,64,64	0
57	MG	1A	3716	1/1	0.53	0.17	42,42,42,42	0
57	MG	1a	1770	1/1	0.55	0.22	73,73,73,73	0
57	MG	2a	1763	1/1	0.55	0.25	82,82,82,82	0
57	MG	1A	3631	1/1	0.55	0.23	65,65,65,65	0
57	MG	1a	1738	1/1	0.59	0.30	55,55,55,55	0
57	MG	2j	202	1/1	0.60	0.23	77,77,77,77	0
57	MG	2A	3024	1/1	0.64	0.23	64,64,64,64	0
57	MG	1A	3751	1/1	0.66	0.24	56,56,56,56	0
57	MG	2A	3585	1/1	0.69	0.18	49,49,49,49	0
57	MG	2A	3634	1/1	0.69	0.16	70,70,70,70	0
57	MG	2a	1759	1/1	0.69	0.32	69,69,69,69	0
57	MG	2A	3625	1/1	0.70	0.17	62,62,62,62	0
57	MG	2A	3478	1/1	0.70	0.24	57,57,57,57	0
57	MG	1A	3365	1/1	0.71	0.12	8,8,8,8	0
57	MG	2A	3402	1/1	0.71	0.18	65,65,65,65	0
57	MG	1A	3352	1/1	0.71	0.16	46,46,46,46	0
57	MG	2a	1666	1/1	0.71	0.43	58,58,58,58	0
57	MG	1A	3549	1/1	0.72	0.17	10,10,10,10	0
57	MG	2A	3504	1/1	0.72	0.18	60,60,60,60	0
57	MG	1a	1747	1/1	0.72	0.18	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
57	MG	2A	3046	1/1	0.72	0.22	59,59,59,59	0
57	MG	1a	1751	1/1	0.72	0.23	63,63,63,63	0
57	MG	2A	3087	1/1	0.73	0.31	65,65,65,65	0
57	MG	2A	3524	1/1	0.73	0.21	70,70,70,70	0
57	MG	2a	1669	1/1	0.73	0.30	65,65,65,65	0
57	MG	2a	1749	1/1	0.73	0.30	65,65,65,65	0
57	MG	2A	3545	1/1	0.74	0.14	63,63,63,63	0
57	MG	14	502	1/1	0.74	0.13	70,70,70,70	0
57	MG	2A	3607	1/1	0.74	0.19	61,61,61,61	0
57	MG	2A	3037	1/1	0.74	0.17	54,54,54,54	0
57	MG	2a	1753	1/1	0.75	0.17	63,63,63,63	0
57	MG	2a	1627	1/1	0.75	0.20	62,62,62,62	0
57	MG	2A	3621	1/1	0.75	0.12	66,66,66,66	0
57	MG	1A	3333	1/1	0.75	0.13	24,24,24,24	0
57	MG	2A	3068	1/1	0.75	0.24	64,64,64,64	0
57	MG	2D	308	1/1	0.76	0.14	48,48,48,48	0
57	MG	2A	3614	1/1	0.76	0.22	66,66,66,66	0
57	MG	1A	3760	1/1	0.76	0.17	54,54,54,54	0
57	MG	2A	3509	1/1	0.76	0.21	48,48,48,48	0
57	MG	1A	3793	1/1	0.76	0.15	48,48,48,48	0
57	MG	1A	3361	1/1	0.77	0.15	21,21,21,21	0
57	MG	2a	1760	1/1	0.77	0.12	52,52,52,52	0
57	MG	2a	1725	1/1	0.77	0.15	58,58,58,58	0
57	MG	2A	3531	1/1	0.77	0.16	68,68,68,68	0
57	MG	10	103	1/1	0.77	0.20	57,57,57,57	0
57	MG	2x	108	1/1	0.77	0.30	65,65,65,65	0
57	MG	2A	3393	1/1	0.78	0.17	67,67,67,67	0
57	MG	2A	3399	1/1	0.78	0.14	53,53,53,53	0
57	MG	1A	3648	1/1	0.78	0.19	46,46,46,46	0
57	MG	2A	3446	1/1	0.78	0.14	55,55,55,55	0
57	MG	1A	3487	1/1	0.78	0.34	60,60,60,60	0
57	MG	2a	1764	1/1	0.78	0.22	62,62,62,62	0
57	MG	2a	1667	1/1	0.78	0.39	69,69,69,69	0
57	MG	2A	3340	1/1	0.78	0.19	60,60,60,60	0
57	MG	2A	3392	1/1	0.78	0.28	63,63,63,63	0
57	MG	1a	1701	1/1	0.79	0.23	70,70,70,70	0
57	MG	1a	1732	1/1	0.79	0.20	58,58,58,58	0
57	MG	2A	3112	1/1	0.79	0.21	55,55,55,55	0
57	MG	2A	3140	1/1	0.79	0.23	62,62,62,62	0
57	MG	1a	1646	1/1	0.79	0.32	56,56,56,56	0
57	MG	2A	3469	1/1	0.79	0.20	74,74,74,74	0
57	MG	2A	3556	1/1	0.79	0.14	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1a	1765	1/1	0.80	0.14	52,52,52,52	0
57	MG	1a	1769	1/1	0.80	0.14	62,62,62,62	0
57	MG	2a	1689	1/1	0.80	0.20	48,48,48,48	0
57	MG	1A	3368	1/1	0.80	0.14	46,46,46,46	0
57	MG	2a	1729	1/1	0.80	0.15	68,68,68,68	0
57	MG	2a	1736	1/1	0.80	0.35	73,73,73,73	0
57	MG	2A	3599	1/1	0.80	0.24	46,46,46,46	0
57	MG	1w	403	1/1	0.80	0.19	54,54,54,54	0
57	MG	1a	1605	1/1	0.80	0.17	61,61,61,61	0
57	MG	2A	3472	1/1	0.80	0.12	39,39,39,39	0
57	MG	2A	3272	1/1	0.80	0.13	49,49,49,49	0
57	MG	2A	3326	1/1	0.80	0.12	27,27,27,27	0
57	MG	2A	3026	1/1	0.80	0.51	49,49,49,49	0
57	MG	2A	3360	1/1	0.80	0.22	68,68,68,68	0
57	MG	2k	201	1/1	0.80	0.34	67,67,67,67	0
57	MG	1a	1761	1/1	0.80	0.18	42,42,42,42	0
57	MG	2a	1697	1/1	0.81	0.18	60,60,60,60	0
57	MG	2A	3162	1/1	0.81	0.18	48,48,48,48	0
57	MG	2a	1726	1/1	0.81	0.23	69,69,69,69	0
57	MG	2A	3415	1/1	0.81	0.18	55,55,55,55	0
57	MG	2a	1735	1/1	0.81	0.18	62,62,62,62	0
57	MG	1A	3607	1/1	0.81	0.11	38,38,38,38	0
57	MG	2A	3275	1/1	0.81	0.16	30,30,30,30	0
57	MG	2A	3277	1/1	0.81	0.19	67,67,67,67	0
57	MG	2a	1756	1/1	0.81	0.25	63,63,63,63	0
57	MG	2A	3296	1/1	0.81	0.12	36,36,36,36	0
57	MG	1A	3588	1/1	0.81	0.17	14,14,14,14	0
57	MG	2A	3050	1/1	0.81	0.26	60,60,60,60	0
57	MG	1A	3764	1/1	0.81	0.15	31,31,31,31	0
57	MG	1a	1618	1/1	0.81	0.24	56,56,56,56	0
57	MG	1A	3741	1/1	0.81	0.13	36,36,36,36	0
57	MG	1a	1648	1/1	0.81	0.30	60,60,60,60	0
57	MG	2A	3562	1/1	0.81	0.15	61,61,61,61	0
57	MG	1A	3018	1/1	0.82	0.20	37,37,37,37	0
57	MG	1A	3127	1/1	0.82	0.25	71,71,71,71	0
57	MG	2A	3520	1/1	0.82	0.18	63,63,63,63	0
57	MG	2a	1698	1/1	0.82	0.16	68,68,68,68	0
57	MG	1A	3385	1/1	0.82	0.15	39,39,39,39	0
57	MG	1A	3626	1/1	0.82	0.13	36,36,36,36	0
57	MG	1A	3474	1/1	0.82	0.14	30,30,30,30	0
57	MG	2a	1734	1/1	0.82	0.27	65,65,65,65	0
57	MG	1A	3485	1/1	0.82	0.22	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
57	MG	2A	3077	1/1	0.82	0.19	56,56,56,56	0
57	MG	2A	3398	1/1	0.82	0.14	47,47,47,47	0
57	MG	1A	3664	1/1	0.82	0.13	39,39,39,39	0
57	MG	1a	1601	1/1	0.82	0.26	62,62,62,62	0
57	MG	2A	3414	1/1	0.82	0.22	33,33,33,33	0
57	MG	1A	3683	1/1	0.82	0.21	60,60,60,60	0
57	MG	2A	3436	1/1	0.82	0.14	60,60,60,60	0
57	MG	1a	1614	1/1	0.82	0.20	71,71,71,71	0
57	MG	2A	3461	1/1	0.82	0.17	33,33,33,33	0
57	MG	2A	3167	1/1	0.82	0.33	50,50,50,50	0
57	MG	1A	3331	1/1	0.82	0.13	24,24,24,24	0
57	MG	1a	1632	1/1	0.82	0.26	52,52,52,52	0
57	MG	2A	3252	1/1	0.83	0.15	53,53,53,53	0
57	MG	2A	3466	1/1	0.83	0.25	58,58,58,58	0
57	MG	2A	3258	1/1	0.83	0.17	42,42,42,42	0
57	MG	2A	3270	1/1	0.83	0.17	52,52,52,52	0
57	MG	1A	3027	1/1	0.83	0.14	44,44,44,44	0
57	MG	1a	1658	1/1	0.83	0.33	52,52,52,52	0
57	MG	1A	3723	1/1	0.83	0.25	25,25,25,25	0
57	MG	2a	1711	1/1	0.83	0.20	57,57,57,57	0
57	MG	2A	3293	1/1	0.83	0.17	56,56,56,56	0
57	MG	1A	3735	1/1	0.83	0.10	12,12,12,12	0
57	MG	1A	3589	1/1	0.83	0.12	16,16,16,16	0
57	MG	2A	3543	1/1	0.83	0.20	51,51,51,51	0
57	MG	1A	3398	1/1	0.83	0.16	48,48,48,48	0
57	MG	2A	3054	1/1	0.83	0.25	53,53,53,53	0
57	MG	1A	3759	1/1	0.83	0.15	53,53,53,53	0
57	MG	2A	3578	1/1	0.83	0.18	59,59,59,59	0
57	MG	2a	1755	1/1	0.83	0.14	64,64,64,64	0
57	MG	1A	3562	1/1	0.83	0.10	26,26,26,26	0
57	MG	2A	3597	1/1	0.83	0.11	56,56,56,56	0
57	MG	1a	1625	1/1	0.83	0.16	56,56,56,56	0
57	MG	1A	3707	1/1	0.83	0.12	47,47,47,47	0
57	MG	1A	3768	1/1	0.83	0.16	33,33,33,33	0
57	MG	1a	1784	1/1	0.83	0.16	62,62,62,62	0
57	MG	1a	1787	1/1	0.83	0.27	49,49,49,49	0
57	MG	2A	3209	1/1	0.83	0.26	47,47,47,47	0
57	MG	2x	106	1/1	0.83	0.26	72,72,72,72	0
57	MG	2A	3239	1/1	0.83	0.13	30,30,30,30	0
57	MG	1a	1704	1/1	0.84	0.14	64,64,64,64	0
57	MG	1a	1721	1/1	0.84	0.19	63,63,63,63	0
57	MG	2A	3051	1/1	0.84	0.13	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3262	1/1	0.84	0.20	40,40,40,40	0
57	MG	2a	1670	1/1	0.84	0.23	72,72,72,72	0
57	MG	2a	1680	1/1	0.84	0.25	59,59,59,59	0
57	MG	2A	3057	1/1	0.84	0.25	58,58,58,58	0
57	MG	1A	3372	1/1	0.84	0.13	32,32,32,32	0
57	MG	2A	3358	1/1	0.84	0.21	62,62,62,62	0
57	MG	1A	3374	1/1	0.84	0.12	26,26,26,26	0
57	MG	1a	1616	1/1	0.84	0.29	58,58,58,58	0
57	MG	2A	3546	1/1	0.84	0.23	60,60,60,60	0
57	MG	1A	3519	1/1	0.84	0.11	39,39,39,39	0
57	MG	1A	3109	1/1	0.84	0.20	50,50,50,50	0
57	MG	2A	3574	1/1	0.84	0.15	68,68,68,68	0
57	MG	1A	3730	1/1	0.84	0.23	65,65,65,65	0
57	MG	1a	1640	1/1	0.84	0.21	69,69,69,69	0
57	MG	2A	3183	1/1	0.84	0.39	56,56,56,56	0
57	MG	1E	305	1/1	0.84	0.24	57,57,57,57	0
57	MG	1a	1647	1/1	0.84	0.24	47,47,47,47	0
57	MG	1U	204	1/1	0.84	0.18	37,37,37,37	0
57	MG	2A	3452	1/1	0.84	0.19	55,55,55,55	0
57	MG	1A	3638	1/1	0.84	0.09	26,26,26,26	0
57	MG	2A	3633	1/1	0.84	0.14	73,73,73,73	0
57	MG	1a	1688	1/1	0.84	0.25	55,55,55,55	0
57	MG	1A	3050	1/1	0.84	0.12	40,40,40,40	0
57	MG	2N	201	1/1	0.84	0.07	61,61,61,61	0
57	MG	2a	1618	1/1	0.84	0.21	61,61,61,61	0
57	MG	2a	1626	1/1	0.84	0.26	48,48,48,48	0
57	MG	1A	3515	1/1	0.85	0.14	31,31,31,31	0
57	MG	2A	3444	1/1	0.85	0.26	59,59,59,59	0
57	MG	1E	309	1/1	0.85	0.14	30,30,30,30	0
57	MG	1a	1781	1/1	0.85	0.14	53,53,53,53	0
57	MG	2A	3596	1/1	0.85	0.17	58,58,58,58	0
57	MG	2A	3290	1/1	0.85	0.23	44,44,44,44	0
57	MG	1Q	205	1/1	0.85	0.13	48,48,48,48	0
57	MG	1a	1706	1/1	0.85	0.16	45,45,45,45	0
57	MG	2A	3612	1/1	0.85	0.18	49,49,49,49	0
57	MG	2A	3117	1/1	0.85	0.22	65,65,65,65	0
57	MG	1A	3276	1/1	0.85	0.09	52,52,52,52	0
57	MG	2A	3499	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3145	1/1	0.85	0.21	56,56,56,56	0
57	MG	1x	108	1/1	0.85	0.11	42,42,42,42	0
57	MG	2A	3638	1/1	0.85	0.16	45,45,45,45	0
57	MG	2B	204	1/1	0.85	0.28	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
57	MG	1A	3729	1/1	0.85	0.13	22,22,22,22	0
57	MG	1A	3390	1/1	0.85	0.17	50,50,50,50	0
57	MG	2X	103	1/1	0.85	0.16	71,71,71,71	0
57	MG	1A	3320	1/1	0.85	0.10	41,41,41,41	0
57	MG	1A	3785	1/1	0.85	0.30	58,58,58,58	0
57	MG	2f	201	1/1	0.85	0.14	64,64,64,64	0
57	MG	1a	1651	1/1	0.85	0.11	66,66,66,66	0
57	MG	1A	3577	1/1	0.85	0.09	30,30,30,30	0
57	MG	2A	3550	1/1	0.85	0.19	55,55,55,55	0
57	MG	1a	1768	1/1	0.85	0.34	71,71,71,71	0
57	MG	2A	3346	1/1	0.86	0.11	50,50,50,50	0
57	MG	1v	101	1/1	0.86	0.13	65,65,65,65	0
57	MG	2a	1644	1/1	0.86	0.24	66,66,66,66	0
57	MG	2a	1646	1/1	0.86	0.32	59,59,59,59	0
57	MG	2a	1664	1/1	0.86	0.26	50,50,50,50	0
57	MG	1A	3358	1/1	0.86	0.13	38,38,38,38	0
57	MG	2A	3537	1/1	0.86	0.18	53,53,53,53	0
57	MG	2A	3383	1/1	0.86	0.28	54,54,54,54	0
57	MG	2A	3390	1/1	0.86	0.16	43,43,43,43	0
57	MG	2a	1673	1/1	0.86	0.27	61,61,61,61	0
57	MG	1x	106	1/1	0.86	0.13	52,52,52,52	0
57	MG	2A	3158	1/1	0.86	0.19	60,60,60,60	0
57	MG	1B	202	1/1	0.86	0.21	43,43,43,43	0
57	MG	2A	3002	1/1	0.86	0.13	52,52,52,52	0
57	MG	2A	3401	1/1	0.86	0.10	52,52,52,52	0
57	MG	2a	1716	1/1	0.86	0.17	61,61,61,61	0
57	MG	2A	3012	1/1	0.86	0.10	52,52,52,52	0
57	MG	2A	3581	1/1	0.86	0.08	69,69,69,69	0
57	MG	1a	1742	1/1	0.86	0.17	48,48,48,48	0
57	MG	2A	3590	1/1	0.86	0.10	48,48,48,48	0
57	MG	1B	206	1/1	0.86	0.16	34,34,34,34	0
57	MG	1A	3595	1/1	0.86	0.10	38,38,38,38	0
57	MG	1a	1752	1/1	0.86	0.18	60,60,60,60	0
57	MG	1a	1680	1/1	0.86	0.24	61,61,61,61	0
57	MG	1a	1686	1/1	0.86	0.18	48,48,48,48	0
57	MG	1A	3600	1/1	0.86	0.13	29,29,29,29	0
57	MG	1A	3111	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	3680	1/1	0.86	0.10	41,41,41,41	0
57	MG	2A	3073	1/1	0.86	0.26	61,61,61,61	0
57	MG	1A	3019	1/1	0.86	0.16	47,47,47,47	0
57	MG	2A	3480	1/1	0.86	0.17	65,65,65,65	0
57	MG	2A	3490	1/1	0.86	0.13	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
57	MG	2A	3313	1/1	0.86	0.20	41,41,41,41	0
57	MG	1a	1719	1/1	0.86	0.14	54,54,54,54	0
57	MG	2A	3507	1/1	0.86	0.17	37,37,37,37	0
57	MG	1A	3737	1/1	0.86	0.14	32,32,32,32	0
57	MG	1A	3281	1/1	0.87	0.19	49,49,49,49	0
57	MG	2A	3487	1/1	0.87	0.13	66,66,66,66	0
57	MG	2A	3053	1/1	0.87	0.22	58,58,58,58	0
57	MG	2a	1602	1/1	0.87	0.14	64,64,64,64	0
57	MG	2A	3493	1/1	0.87	0.20	69,69,69,69	0
57	MG	1a	1653	1/1	0.87	0.16	63,63,63,63	0
57	MG	2A	3297	1/1	0.87	0.12	47,47,47,47	0
57	MG	2a	1630	1/1	0.87	0.11	56,56,56,56	0
57	MG	2a	1635	1/1	0.87	0.15	58,58,58,58	0
57	MG	11	103	1/1	0.87	0.29	48,48,48,48	0
57	MG	2A	3508	1/1	0.87	0.13	49,49,49,49	0
57	MG	2a	1654	1/1	0.87	0.28	63,63,63,63	0
57	MG	2a	1659	1/1	0.87	0.29	53,53,53,53	0
57	MG	1a	1679	1/1	0.87	0.37	67,67,67,67	0
57	MG	1A	3475	1/1	0.87	0.14	39,39,39,39	0
57	MG	2A	3345	1/1	0.87	0.08	67,67,67,67	0
57	MG	1a	1771	1/1	0.87	0.14	67,67,67,67	0
57	MG	18	101	1/1	0.87	0.17	38,38,38,38	0
57	MG	1a	1782	1/1	0.87	0.15	74,74,74,74	0
57	MG	1A	3359	1/1	0.87	0.10	34,34,34,34	0
57	MG	2A	3122	1/1	0.87	0.34	59,59,59,59	0
57	MG	1A	3784	1/1	0.87	0.22	50,50,50,50	0
57	MG	1n	101	1/1	0.87	0.13	63,63,63,63	0
57	MG	1A	3601	1/1	0.87	0.09	18,18,18,18	0
57	MG	2a	1713	1/1	0.87	0.24	60,60,60,60	0
57	MG	1A	3377	1/1	0.87	0.12	40,40,40,40	0
57	MG	2a	1719	1/1	0.87	0.21	53,53,53,53	0
57	MG	1A	3311	1/1	0.87	0.11	24,24,24,24	0
57	MG	2A	3169	1/1	0.87	0.24	47,47,47,47	0
57	MG	2A	3583	1/1	0.87	0.11	40,40,40,40	0
57	MG	2a	1730	1/1	0.87	0.10	54,54,54,54	0
57	MG	2A	3405	1/1	0.87	0.16	42,42,42,42	0
57	MG	1A	3336	1/1	0.87	0.11	32,32,32,32	0
57	MG	2A	3592	1/1	0.87	0.17	51,51,51,51	0
57	MG	2a	1739	1/1	0.87	0.27	61,61,61,61	0
57	MG	2A	3193	1/1	0.87	0.21	57,57,57,57	0
57	MG	2A	3416	1/1	0.87	0.11	33,33,33,33	0
57	MG	1a	1627	1/1	0.87	0.17	67,67,67,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1a	1735	1/1	0.87	0.16	54,54,54,54	0
57	MG	2A	3610	1/1	0.87	0.16	51,51,51,51	0
57	MG	1A	3392	1/1	0.87	0.11	24,24,24,24	0
57	MG	1A	3224	1/1	0.87	0.12	59,59,59,59	0
57	MG	1N	204	1/1	0.87	0.12	33,33,33,33	0
57	MG	2A	3465	1/1	0.87	0.18	49,49,49,49	0
57	MG	2A	3043	1/1	0.87	0.15	50,50,50,50	0
57	MG	1A	3408	1/1	0.87	0.09	29,29,29,29	0
57	MG	1A	3426	1/1	0.87	0.09	21,21,21,21	0
57	MG	2A	3640	1/1	0.87	0.12	49,49,49,49	0
57	MG	2A	3278	1/1	0.87	0.09	49,49,49,49	0
57	MG	2F	305	1/1	0.88	0.28	45,45,45,45	0
57	MG	1A	3620	1/1	0.88	0.15	51,51,51,51	0
57	MG	1a	1740	1/1	0.88	0.14	43,43,43,43	0
57	MG	1a	1634	1/1	0.88	0.35	60,60,60,60	0
57	MG	2a	1603	1/1	0.88	0.19	62,62,62,62	0
57	MG	2a	1617	1/1	0.88	0.29	56,56,56,56	0
57	MG	1B	209	1/1	0.88	0.22	51,51,51,51	0
57	MG	1a	1749	1/1	0.88	0.09	51,51,51,51	0
57	MG	2A	3492	1/1	0.88	0.18	58,58,58,58	0
57	MG	1A	3446	1/1	0.88	0.12	52,52,52,52	0
57	MG	2a	1632	1/1	0.88	0.25	56,56,56,56	0
57	MG	1A	3452	1/1	0.88	0.13	19,19,19,19	0
57	MG	1A	3460	1/1	0.88	0.13	29,29,29,29	0
57	MG	1A	3149	1/1	0.88	0.12	29,29,29,29	0
57	MG	1R	203	1/1	0.88	0.17	42,42,42,42	0
57	MG	2a	1655	1/1	0.88	0.16	68,68,68,68	0
57	MG	1A	3384	1/1	0.88	0.09	53,53,53,53	0
57	MG	2a	1662	1/1	0.88	0.13	50,50,50,50	0
57	MG	2A	3513	1/1	0.88	0.07	36,36,36,36	0
57	MG	1a	1678	1/1	0.88	0.34	56,56,56,56	0
57	MG	2A	3344	1/1	0.88	0.13	37,37,37,37	0
57	MG	1A	3591	1/1	0.88	0.08	29,29,29,29	0
57	MG	2A	3113	1/1	0.88	0.23	64,64,64,64	0
57	MG	1a	1774	1/1	0.88	0.20	82,82,82,82	0
57	MG	2a	1676	1/1	0.88	0.23	61,61,61,61	0
57	MG	2a	1677	1/1	0.88	0.20	50,50,50,50	0
57	MG	1A	3354	1/1	0.88	0.12	22,22,22,22	0
57	MG	2A	3361	1/1	0.88	0.08	52,52,52,52	0
57	MG	2A	3127	1/1	0.88	0.14	45,45,45,45	0
57	MG	2A	3386	1/1	0.88	0.11	60,60,60,60	0
57	MG	2A	3558	1/1	0.88	0.18	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3688	1/1	0.88	0.15	25,25,25,25	0
57	MG	1A	3415	1/1	0.88	0.09	26,26,26,26	0
57	MG	1a	1698	1/1	0.88	0.22	53,53,53,53	0
57	MG	2A	3395	1/1	0.88	0.15	48,48,48,48	0
57	MG	1A	3715	1/1	0.88	0.15	35,35,35,35	0
57	MG	2a	1728	1/1	0.88	0.18	64,64,64,64	0
57	MG	1A	3235	1/1	0.88	0.23	49,49,49,49	0
57	MG	1A	3720	1/1	0.88	0.17	21,21,21,21	0
57	MG	2A	3171	1/1	0.88	0.33	59,59,59,59	0
57	MG	2A	3178	1/1	0.88	0.16	52,52,52,52	0
57	MG	2A	3408	1/1	0.88	0.12	27,27,27,27	0
57	MG	2a	1738	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3410	1/1	0.88	0.19	53,53,53,53	0
57	MG	2A	3182	1/1	0.88	0.11	48,48,48,48	0
57	MG	1a	1712	1/1	0.88	0.17	65,65,65,65	0
57	MG	2a	1754	1/1	0.88	0.18	58,58,58,58	0
57	MG	1a	1717	1/1	0.88	0.09	69,69,69,69	0
57	MG	2A	3418	1/1	0.88	0.20	61,61,61,61	0
57	MG	2A	3206	1/1	0.88	0.07	61,61,61,61	0
57	MG	1A	3795	1/1	0.88	0.11	47,47,47,47	0
57	MG	2A	3216	1/1	0.88	0.25	57,57,57,57	0
57	MG	2A	3236	1/1	0.88	0.16	68,68,68,68	0
57	MG	2a	1765	1/1	0.88	0.18	53,53,53,53	0
57	MG	1B	201	1/1	0.88	0.10	43,43,43,43	0
57	MG	1A	3429	1/1	0.88	0.17	54,54,54,54	0
57	MG	1B	203	1/1	0.88	0.13	54,54,54,54	0
57	MG	2B	209	1/1	0.88	0.24	45,45,45,45	0
57	MG	2D	306	1/1	0.88	0.10	55,55,55,55	0
57	MG	2A	3264	1/1	0.88	0.10	28,28,28,28	0
57	MG	2x	109	1/1	0.88	0.18	51,51,51,51	0
58	ZN	14	501	1/1	0.88	0.17	124,124,124,124	0
57	MG	2A	3058	1/1	0.89	0.16	50,50,50,50	0
57	MG	2A	3368	1/1	0.89	0.16	57,57,57,57	0
57	MG	2A	3066	1/1	0.89	0.10	46,46,46,46	0
57	MG	1A	3586	1/1	0.89	0.08	16,16,16,16	0
57	MG	2A	3387	1/1	0.89	0.14	54,54,54,54	0
57	MG	2A	3623	1/1	0.89	0.11	46,46,46,46	0
57	MG	1a	1727	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3391	1/1	0.89	0.10	22,22,22,22	0
57	MG	2A	3074	1/1	0.89	0.08	54,54,54,54	0
57	MG	1a	1731	1/1	0.89	0.12	39,39,39,39	0
57	MG	2A	3394	1/1	0.89	0.13	22,22,22,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3587	1/1	0.89	0.09	27,27,27,27	0
57	MG	2B	206	1/1	0.89	0.24	55,55,55,55	0
57	MG	2B	208	1/1	0.89	0.21	54,54,54,54	0
57	MG	2A	3095	1/1	0.89	0.38	61,61,61,61	0
57	MG	1a	1734	1/1	0.89	0.20	65,65,65,65	0
57	MG	1A	3432	1/1	0.89	0.14	54,54,54,54	0
57	MG	1A	3029	1/1	0.89	0.11	56,56,56,56	0
57	MG	1A	3590	1/1	0.89	0.15	34,34,34,34	0
57	MG	2P	202	1/1	0.89	0.19	72,72,72,72	0
57	MG	1A	3448	1/1	0.89	0.13	54,54,54,54	0
57	MG	26	101	1/1	0.89	0.11	62,62,62,62	0
57	MG	1a	1744	1/1	0.89	0.12	55,55,55,55	0
57	MG	1a	1745	1/1	0.89	0.25	59,59,59,59	0
57	MG	2a	1612	1/1	0.89	0.19	58,58,58,58	0
57	MG	2A	3155	1/1	0.89	0.63	44,44,44,44	0
57	MG	1a	1746	1/1	0.89	0.11	49,49,49,49	0
57	MG	2a	1625	1/1	0.89	0.20	49,49,49,49	0
57	MG	1A	3758	1/1	0.89	0.21	28,28,28,28	0
57	MG	2A	3423	1/1	0.89	0.10	43,43,43,43	0
57	MG	1a	1621	1/1	0.89	0.20	57,57,57,57	0
57	MG	2A	3437	1/1	0.89	0.09	36,36,36,36	0
57	MG	1A	3383	1/1	0.89	0.10	23,23,23,23	0
57	MG	1A	3454	1/1	0.89	0.13	36,36,36,36	0
57	MG	1A	3263	1/1	0.89	0.10	48,48,48,48	0
57	MG	2A	3454	1/1	0.89	0.37	43,43,43,43	0
57	MG	1A	3765	1/1	0.89	0.25	50,50,50,50	0
57	MG	2A	3464	1/1	0.89	0.12	58,58,58,58	0
57	MG	2a	1660	1/1	0.89	0.17	45,45,45,45	0
57	MG	1a	1635	1/1	0.89	0.32	56,56,56,56	0
57	MG	1a	1638	1/1	0.89	0.23	54,54,54,54	0
57	MG	1A	3471	1/1	0.89	0.11	57,57,57,57	0
57	MG	1a	1641	1/1	0.89	0.27	63,63,63,63	0
57	MG	2a	1668	1/1	0.89	0.12	52,52,52,52	0
57	MG	2A	3477	1/1	0.89	0.20	46,46,46,46	0
57	MG	1a	1773	1/1	0.89	0.32	62,62,62,62	0
57	MG	2A	3222	1/1	0.89	0.40	50,50,50,50	0
57	MG	2A	3228	1/1	0.89	0.18	51,51,51,51	0
57	MG	2A	3230	1/1	0.89	0.17	48,48,48,48	0
57	MG	1A	3161	1/1	0.89	0.11	24,24,24,24	0
57	MG	1A	3191	1/1	0.89	0.06	48,48,48,48	0
57	MG	2a	1692	1/1	0.89	0.13	27,27,27,27	0
57	MG	2A	3247	1/1	0.89	0.18	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3503	1/1	0.89	0.16	61,61,61,61	0
57	MG	2a	1702	1/1	0.89	0.15	61,61,61,61	0
57	MG	1A	3786	1/1	0.89	0.09	49,49,49,49	0
57	MG	2A	3253	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3286	1/1	0.89	0.15	44,44,44,44	0
57	MG	2a	1717	1/1	0.89	0.12	40,40,40,40	0
57	MG	1A	3114	1/1	0.89	0.17	42,42,42,42	0
57	MG	2A	3269	1/1	0.89	0.11	39,39,39,39	0
57	MG	1A	3509	1/1	0.89	0.08	14,14,14,14	0
57	MG	1a	1668	1/1	0.89	0.13	55,55,55,55	0
57	MG	2A	3525	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3527	1/1	0.89	0.16	39,39,39,39	0
57	MG	1A	3659	1/1	0.89	0.15	39,39,39,39	0
57	MG	2A	3533	1/1	0.89	0.11	63,63,63,63	0
57	MG	1A	3225	1/1	0.89	0.27	47,47,47,47	0
57	MG	1A	3410	1/1	0.89	0.10	14,14,14,14	0
57	MG	2A	3286	1/1	0.89	0.13	61,61,61,61	0
57	MG	2a	1747	1/1	0.89	0.19	62,62,62,62	0
57	MG	1A	3540	1/1	0.89	0.07	12,12,12,12	0
57	MG	2a	1752	1/1	0.89	0.21	48,48,48,48	0
57	MG	2A	3547	1/1	0.89	0.10	41,41,41,41	0
57	MG	1a	1687	1/1	0.89	0.38	64,64,64,64	0
57	MG	1A	3323	1/1	0.89	0.16	39,39,39,39	0
57	MG	1a	1693	1/1	0.89	0.22	60,60,60,60	0
57	MG	2A	3300	1/1	0.89	0.07	34,34,34,34	0
57	MG	2A	3568	1/1	0.89	0.10	66,66,66,66	0
57	MG	2A	3307	1/1	0.89	0.12	47,47,47,47	0
57	MG	1A	3030	1/1	0.89	0.25	49,49,49,49	0
57	MG	2A	3319	1/1	0.89	0.10	49,49,49,49	0
57	MG	1A	3711	1/1	0.89	0.08	33,33,33,33	0
57	MG	1A	3568	1/1	0.89	0.09	30,30,30,30	0
57	MG	1A	3247	1/1	0.89	0.08	40,40,40,40	0
57	MG	1A	3582	1/1	0.89	0.10	33,33,33,33	0
57	MG	2A	3593	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3583	1/1	0.89	0.09	55,55,55,55	0
57	MG	1a	1718	1/1	0.89	0.10	59,59,59,59	0
57	MG	1A	3724	1/1	0.89	0.42	48,48,48,48	0
57	MG	1A	3477	1/1	0.90	0.12	44,44,44,44	0
57	MG	1A	3205	1/1	0.90	0.27	39,39,39,39	0
57	MG	2E	304	1/1	0.90	0.12	24,24,24,24	0
57	MG	1A	3703	1/1	0.90	0.11	22,22,22,22	0
57	MG	2A	3251	1/1	0.90	0.13	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
57	MG	1A	3219	1/1	0.90	0.20	50,50,50,50	0
57	MG	2R	203	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3292	1/1	0.90	0.10	37,37,37,37	0
57	MG	20	101	1/1	0.90	0.11	49,49,49,49	0
57	MG	1A	3714	1/1	0.90	0.13	13,13,13,13	0
57	MG	1a	1737	1/1	0.90	0.13	44,44,44,44	0
57	MG	1A	3124	1/1	0.90	0.19	51,51,51,51	0
57	MG	1A	3045	1/1	0.90	0.09	47,47,47,47	0
57	MG	1A	3534	1/1	0.90	0.12	10,10,10,10	0
57	MG	1A	3020	1/1	0.90	0.19	56,56,56,56	0
57	MG	2A	3064	1/1	0.90	0.26	50,50,50,50	0
57	MG	2A	3483	1/1	0.90	0.21	46,46,46,46	0
57	MG	1A	3618	1/1	0.90	0.11	38,38,38,38	0
57	MG	2A	3279	1/1	0.90	0.17	51,51,51,51	0
57	MG	2A	3284	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3067	1/1	0.90	0.28	58,58,58,58	0
57	MG	2a	1642	1/1	0.90	0.11	37,37,37,37	0
57	MG	2A	3496	1/1	0.90	0.12	47,47,47,47	0
57	MG	2A	3497	1/1	0.90	0.14	50,50,50,50	0
57	MG	2a	1648	1/1	0.90	0.19	49,49,49,49	0
57	MG	1A	3728	1/1	0.90	0.10	27,27,27,27	0
57	MG	1a	1650	1/1	0.90	0.18	32,32,32,32	0
57	MG	1F	309	1/1	0.90	0.32	38,38,38,38	0
57	MG	1A	3326	1/1	0.90	0.11	16,16,16,16	0
57	MG	1a	1656	1/1	0.90	0.14	55,55,55,55	0
57	MG	1a	1755	1/1	0.90	0.21	47,47,47,47	0
57	MG	2A	3312	1/1	0.90	0.13	30,30,30,30	0
57	MG	2A	3515	1/1	0.90	0.20	52,52,52,52	0
57	MG	2A	3103	1/1	0.90	0.20	59,59,59,59	0
57	MG	1P	204	1/1	0.90	0.09	32,32,32,32	0
57	MG	1a	1660	1/1	0.90	0.26	64,64,64,64	0
57	MG	2A	3329	1/1	0.90	0.07	29,29,29,29	0
57	MG	2A	3116	1/1	0.90	0.18	51,51,51,51	0
57	MG	1A	3329	1/1	0.90	0.14	6,6,6,6	0
57	MG	1Q	206	1/1	0.90	0.13	32,32,32,32	0
57	MG	2a	1685	1/1	0.90	0.22	52,52,52,52	0
57	MG	2a	1686	1/1	0.90	0.23	49,49,49,49	0
57	MG	2A	3539	1/1	0.90	0.21	56,56,56,56	0
57	MG	2A	3123	1/1	0.90	0.23	44,44,44,44	0
57	MG	1A	3630	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3132	1/1	0.90	0.12	45,45,45,45	0
57	MG	2a	1701	1/1	0.90	0.15	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
57	MG	2A	3138	1/1	0.90	0.06	50,50,50,50	0
57	MG	2a	1708	1/1	0.90	0.18	57,57,57,57	0
57	MG	1A	3246	1/1	0.90	0.06	28,28,28,28	0
57	MG	2A	3373	1/1	0.90	0.13	56,56,56,56	0
57	MG	2A	3382	1/1	0.90	0.13	65,65,65,65	0
57	MG	1a	1685	1/1	0.90	0.12	35,35,35,35	0
57	MG	2A	3384	1/1	0.90	0.12	49,49,49,49	0
57	MG	2A	3573	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3101	1/1	0.90	0.18	28,28,28,28	0
57	MG	2A	3577	1/1	0.90	0.09	61,61,61,61	0
57	MG	1A	3643	1/1	0.90	0.07	22,22,22,22	0
57	MG	12	101	1/1	0.90	0.10	32,32,32,32	0
57	MG	2a	1733	1/1	0.90	0.22	46,46,46,46	0
57	MG	1A	3755	1/1	0.90	0.20	25,25,25,25	0
57	MG	15	104	1/1	0.90	0.27	35,35,35,35	0
57	MG	1a	1789	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3172	1/1	0.90	0.09	38,38,38,38	0
57	MG	2A	3173	1/1	0.90	0.24	49,49,49,49	0
57	MG	1k	201	1/1	0.90	0.13	52,52,52,52	0
57	MG	2A	3180	1/1	0.90	0.25	51,51,51,51	0
57	MG	1A	3177	1/1	0.90	0.17	35,35,35,35	0
57	MG	1A	3117	1/1	0.90	0.08	24,24,24,24	0
57	MG	1w	401	1/1	0.90	0.21	51,51,51,51	0
57	MG	2A	3200	1/1	0.90	0.28	62,62,62,62	0
57	MG	2A	3613	1/1	0.90	0.16	41,41,41,41	0
57	MG	2A	3409	1/1	0.90	0.07	34,34,34,34	0
57	MG	2A	3204	1/1	0.90	0.11	46,46,46,46	0
57	MG	2a	1761	1/1	0.90	0.18	57,57,57,57	0
57	MG	2A	3413	1/1	0.90	0.14	58,58,58,58	0
57	MG	1a	1603	1/1	0.90	0.18	46,46,46,46	0
57	MG	2A	3626	1/1	0.90	0.13	67,67,67,67	0
57	MG	2A	3207	1/1	0.90	0.20	66,66,66,66	0
57	MG	2d	301	1/1	0.90	0.32	56,56,56,56	0
57	MG	1x	103	1/1	0.90	0.19	60,60,60,60	0
57	MG	1A	3196	1/1	0.90	0.13	29,29,29,29	0
57	MG	1A	3674	1/1	0.90	0.13	41,41,41,41	0
57	MG	2x	101	1/1	0.90	0.15	54,54,54,54	0
57	MG	2A	3426	1/1	0.90	0.13	58,58,58,58	0
57	MG	2A	3430	1/1	0.90	0.11	25,25,25,25	0
57	MG	1A	3678	1/1	0.90	0.15	50,50,50,50	0
57	MG	1A	3357	1/1	0.90	0.10	43,43,43,43	0
57	MG	1A	3767	1/1	0.91	0.12	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3151	1/1	0.91	0.07	45,45,45,45	0
57	MG	1a	1756	1/1	0.91	0.21	65,65,65,65	0
57	MG	1A	3520	1/1	0.91	0.19	48,48,48,48	0
57	MG	1a	1763	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3163	1/1	0.91	0.14	36,36,36,36	0
57	MG	1a	1764	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3769	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3782	1/1	0.91	0.12	39,39,39,39	0
57	MG	2A	3403	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3636	1/1	0.91	0.12	46,46,46,46	0
57	MG	1A	3783	1/1	0.91	0.10	27,27,27,27	0
57	MG	2A	3407	1/1	0.91	0.12	38,38,38,38	0
57	MG	2B	202	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3234	1/1	0.91	0.11	40,40,40,40	0
57	MG	2B	205	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3174	1/1	0.91	0.22	63,63,63,63	0
57	MG	2B	207	1/1	0.91	0.38	57,57,57,57	0
57	MG	1A	3539	1/1	0.91	0.09	16,16,16,16	0
57	MG	2A	3411	1/1	0.91	0.11	40,40,40,40	0
57	MG	2A	3412	1/1	0.91	0.22	35,35,35,35	0
57	MG	1A	3431	1/1	0.91	0.12	17,17,17,17	0
57	MG	1A	3666	1/1	0.91	0.26	38,38,38,38	0
57	MG	1A	3543	1/1	0.91	0.10	36,36,36,36	0
57	MG	2A	3186	1/1	0.91	0.09	57,57,57,57	0
57	MG	2A	3417	1/1	0.91	0.10	40,40,40,40	0
57	MG	2R	202	1/1	0.91	0.30	44,44,44,44	0
57	MG	2A	3191	1/1	0.91	0.24	54,54,54,54	0
57	MG	1a	1655	1/1	0.91	0.20	40,40,40,40	0
57	MG	2A	3199	1/1	0.91	0.32	59,59,59,59	0
57	MG	1A	3201	1/1	0.91	0.33	33,33,33,33	0
57	MG	2A	3432	1/1	0.91	0.19	60,60,60,60	0
57	MG	2A	3434	1/1	0.91	0.08	31,31,31,31	0
57	MG	2A	3203	1/1	0.91	0.15	48,48,48,48	0
57	MG	2a	1615	1/1	0.91	0.18	52,52,52,52	0
57	MG	1a	1657	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3443	1/1	0.91	0.09	37,37,37,37	0
57	MG	2a	1623	1/1	0.91	0.33	54,54,54,54	0
57	MG	2A	3205	1/1	0.91	0.17	51,51,51,51	0
57	MG	1A	3561	1/1	0.91	0.07	12,12,12,12	0
57	MG	2A	3451	1/1	0.91	0.21	47,47,47,47	0
57	MG	1d	301	1/1	0.91	0.21	34,34,34,34	0
57	MG	1A	3168	1/1	0.91	0.09	19,19,19,19	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3387	1/1	0.91	0.13	36,36,36,36	0
57	MG	2a	1636	1/1	0.91	0.26	48,48,48,48	0
57	MG	2a	1637	1/1	0.91	0.18	43,43,43,43	0
57	MG	1a	1671	1/1	0.91	0.20	50,50,50,50	0
57	MG	1A	3693	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3699	1/1	0.91	0.07	42,42,42,42	0
57	MG	1A	3116	1/1	0.91	0.28	42,42,42,42	0
57	MG	2a	1651	1/1	0.91	0.10	46,46,46,46	0
57	MG	1a	1684	1/1	0.91	0.20	59,59,59,59	0
57	MG	1A	3298	1/1	0.91	0.09	45,45,45,45	0
57	MG	1N	203	1/1	0.91	0.10	26,26,26,26	0
57	MG	1A	3367	1/1	0.91	0.19	54,54,54,54	0
57	MG	2a	1661	1/1	0.91	0.17	39,39,39,39	0
57	MG	1A	3462	1/1	0.91	0.12	44,44,44,44	0
57	MG	2A	3254	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3464	1/1	0.91	0.10	16,16,16,16	0
57	MG	2A	3032	1/1	0.91	0.17	47,47,47,47	0
57	MG	2A	3265	1/1	0.91	0.07	25,25,25,25	0
57	MG	2A	3494	1/1	0.91	0.11	47,47,47,47	0
57	MG	2A	3495	1/1	0.91	0.08	35,35,35,35	0
57	MG	1a	1694	1/1	0.91	0.17	61,61,61,61	0
57	MG	2a	1674	1/1	0.91	0.35	63,63,63,63	0
57	MG	1A	3469	1/1	0.91	0.08	35,35,35,35	0
57	MG	1A	3399	1/1	0.91	0.09	14,14,14,14	0
57	MG	1a	1703	1/1	0.91	0.21	55,55,55,55	0
57	MG	1A	3403	1/1	0.91	0.06	15,15,15,15	0
57	MG	1W	201	1/1	0.91	0.23	47,47,47,47	0
57	MG	1A	3404	1/1	0.91	0.09	17,17,17,17	0
57	MG	2A	3281	1/1	0.91	0.13	36,36,36,36	0
57	MG	1A	3067	1/1	0.91	0.15	30,30,30,30	0
57	MG	1A	3599	1/1	0.91	0.10	52,52,52,52	0
57	MG	13	102	1/1	0.91	0.07	13,13,13,13	0
57	MG	1a	1720	1/1	0.91	0.13	59,59,59,59	0
57	MG	1A	3482	1/1	0.91	0.14	37,37,37,37	0
57	MG	15	101	1/1	0.91	0.27	26,26,26,26	0
57	MG	2A	3529	1/1	0.91	0.12	52,52,52,52	0
57	MG	2a	1714	1/1	0.91	0.14	34,34,34,34	0
57	MG	2A	3069	1/1	0.91	0.16	44,44,44,44	0
57	MG	2A	3532	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	3338	1/1	0.91	0.09	33,33,33,33	0
57	MG	2a	1723	1/1	0.91	0.24	62,62,62,62	0
57	MG	2A	3534	1/1	0.91	0.13	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
57	MG	1A	3316	1/1	0.91	0.12	40,40,40,40	0
57	MG	1A	3738	1/1	0.91	0.24	27,27,27,27	0
57	MG	2A	3079	1/1	0.91	0.11	50,50,50,50	0
57	MG	2A	3325	1/1	0.91	0.09	39,39,39,39	0
57	MG	1A	3613	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3327	1/1	0.91	0.14	53,53,53,53	0
57	MG	1a	1736	1/1	0.91	0.10	61,61,61,61	0
57	MG	2A	3551	1/1	0.91	0.13	25,25,25,25	0
57	MG	2A	3102	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3742	1/1	0.91	0.08	43,43,43,43	0
57	MG	2a	1743	1/1	0.91	0.16	64,64,64,64	0
57	MG	2A	3559	1/1	0.91	0.12	57,57,57,57	0
57	MG	2A	3104	1/1	0.91	0.24	49,49,49,49	0
57	MG	2A	3563	1/1	0.91	0.18	54,54,54,54	0
57	MG	1a	1612	1/1	0.91	0.17	50,50,50,50	0
57	MG	2A	3570	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3493	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3114	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3752	1/1	0.91	0.08	33,33,33,33	0
57	MG	2A	3366	1/1	0.91	0.16	51,51,51,51	0
57	MG	1A	3500	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	3420	1/1	0.91	0.06	11,11,11,11	0
57	MG	2A	3374	1/1	0.91	0.07	26,26,26,26	0
57	MG	2A	3589	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3628	1/1	0.91	0.12	38,38,38,38	0
57	MG	1a	1626	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	3513	1/1	0.91	0.21	48,48,48,48	0
57	MG	2A	3137	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	3091	1/1	0.91	0.09	42,42,42,42	0
57	MG	2A	3388	1/1	0.91	0.19	59,59,59,59	0
57	MG	2x	104	1/1	0.91	0.18	48,48,48,48	0
57	MG	2x	105	1/1	0.91	0.15	36,36,36,36	0
57	MG	2A	3600	1/1	0.91	0.14	56,56,56,56	0
57	MG	2A	3601	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3606	1/1	0.91	0.13	50,50,50,50	0
57	MG	1A	3428	1/1	0.91	0.10	15,15,15,15	0
57	MG	1A	3113	1/1	0.92	0.28	57,57,57,57	0
57	MG	2D	304	1/1	0.92	0.69	41,41,41,41	0
57	MG	1A	3212	1/1	0.92	0.23	28,28,28,28	0
57	MG	1A	3542	1/1	0.92	0.08	21,21,21,21	0
57	MG	2A	3083	1/1	0.92	0.27	48,48,48,48	0
57	MG	2A	3455	1/1	0.92	0.25	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
57	MG	2A	3086	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3463	1/1	0.92	0.16	37,37,37,37	0
57	MG	1A	3632	1/1	0.92	0.14	49,49,49,49	0
57	MG	1a	1662	1/1	0.92	0.23	34,34,34,34	0
57	MG	2A	3101	1/1	0.92	0.41	45,45,45,45	0
57	MG	1A	3270	1/1	0.92	0.15	26,26,26,26	0
57	MG	11	102	1/1	0.92	0.17	32,32,32,32	0
57	MG	2A	3475	1/1	0.92	0.16	46,46,46,46	0
57	MG	1A	3639	1/1	0.92	0.08	10,10,10,10	0
57	MG	1a	1767	1/1	0.92	0.06	71,71,71,71	0
57	MG	1A	3011	1/1	0.92	0.09	31,31,31,31	0
57	MG	2A	3285	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	3220	1/1	0.92	0.20	37,37,37,37	0
57	MG	1a	1681	1/1	0.92	0.08	44,44,44,44	0
57	MG	2a	1624	1/1	0.92	0.11	41,41,41,41	0
57	MG	2A	3491	1/1	0.92	0.16	55,55,55,55	0
57	MG	1a	1682	1/1	0.92	0.14	44,44,44,44	0
57	MG	2A	3295	1/1	0.92	0.09	37,37,37,37	0
57	MG	2A	3121	1/1	0.92	0.17	39,39,39,39	0
57	MG	1A	3343	1/1	0.92	0.09	30,30,30,30	0
57	MG	2a	1634	1/1	0.92	0.15	50,50,50,50	0
57	MG	1A	3350	1/1	0.92	0.08	25,25,25,25	0
57	MG	2A	3301	1/1	0.92	0.11	25,25,25,25	0
57	MG	2A	3305	1/1	0.92	0.10	44,44,44,44	0
57	MG	1a	1775	1/1	0.92	0.20	58,58,58,58	0
57	MG	2A	3310	1/1	0.92	0.09	39,39,39,39	0
57	MG	2A	3130	1/1	0.92	0.19	54,54,54,54	0
57	MG	1a	1776	1/1	0.92	0.20	49,49,49,49	0
57	MG	2a	1649	1/1	0.92	0.20	60,60,60,60	0
57	MG	2A	3314	1/1	0.92	0.09	28,28,28,28	0
57	MG	2A	3511	1/1	0.92	0.13	58,58,58,58	0
57	MG	1A	3665	1/1	0.92	0.06	31,31,31,31	0
57	MG	2A	3514	1/1	0.92	0.08	57,57,57,57	0
57	MG	2A	3320	1/1	0.92	0.09	29,29,29,29	0
57	MG	17	106	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	3396	1/1	0.92	0.12	35,35,35,35	0
57	MG	2A	3143	1/1	0.92	0.30	54,54,54,54	0
57	MG	1A	3673	1/1	0.92	0.08	46,46,46,46	0
57	MG	2A	3330	1/1	0.92	0.12	51,51,51,51	0
57	MG	2A	3331	1/1	0.92	0.12	30,30,30,30	0
57	MG	2A	3146	1/1	0.92	0.15	40,40,40,40	0
57	MG	2A	3147	1/1	0.92	0.13	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
57	MG	1a	1788	1/1	0.92	0.11	66,66,66,66	0
57	MG	2A	3535	1/1	0.92	0.10	47,47,47,47	0
57	MG	1a	1602	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3348	1/1	0.92	0.09	60,60,60,60	0
57	MG	2A	3357	1/1	0.92	0.15	60,60,60,60	0
57	MG	2a	1682	1/1	0.92	0.13	52,52,52,52	0
57	MG	2a	1684	1/1	0.92	0.09	55,55,55,55	0
57	MG	2A	3156	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3031	1/1	0.92	0.09	20,20,20,20	0
57	MG	2A	3159	1/1	0.92	0.32	58,58,58,58	0
57	MG	2a	1691	1/1	0.92	0.16	44,44,44,44	0
57	MG	1A	3287	1/1	0.92	0.10	31,31,31,31	0
57	MG	1a	1611	1/1	0.92	0.15	46,46,46,46	0
57	MG	1A	3355	1/1	0.92	0.13	33,33,33,33	0
57	MG	1v	102	1/1	0.92	0.13	44,44,44,44	0
57	MG	1A	3288	1/1	0.92	0.26	30,30,30,30	0
57	MG	2a	1703	1/1	0.92	0.18	39,39,39,39	0
57	MG	2a	1705	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3001	1/1	0.92	0.10	20,20,20,20	0
57	MG	1x	102	1/1	0.92	0.11	33,33,33,33	0
57	MG	2A	3566	1/1	0.92	0.10	60,60,60,60	0
57	MG	1A	3185	1/1	0.92	0.13	25,25,25,25	0
57	MG	1A	3122	1/1	0.92	0.15	33,33,33,33	0
57	MG	1a	1624	1/1	0.92	0.23	56,56,56,56	0
57	MG	1y	101	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3315	1/1	0.92	0.11	17,17,17,17	0
57	MG	2A	3008	1/1	0.92	0.16	46,46,46,46	0
57	MG	2A	3187	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3593	1/1	0.92	0.13	61,61,61,61	0
57	MG	1a	1725	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3194	1/1	0.92	0.12	29,29,29,29	0
57	MG	2A	3197	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3499	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1728	1/1	0.92	0.15	46,46,46,46	0
57	MG	2A	3034	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3404	1/1	0.92	0.18	34,34,34,34	0
57	MG	1a	1730	1/1	0.92	0.17	59,59,59,59	0
57	MG	1a	1629	1/1	0.92	0.12	51,51,51,51	0
57	MG	2a	1745	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3421	1/1	0.92	0.10	16,16,16,16	0
57	MG	1A	3366	1/1	0.92	0.13	7,7,7,7	0
57	MG	2a	1750	1/1	0.92	0.19	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3208	1/1	0.92	0.25	48,48,48,48	0
57	MG	1A	3511	1/1	0.92	0.11	30,30,30,30	0
57	MG	2A	3212	1/1	0.92	0.21	45,45,45,45	0
57	MG	1A	3603	1/1	0.92	0.07	36,36,36,36	0
57	MG	2A	3221	1/1	0.92	0.18	34,34,34,34	0
57	MG	2A	3619	1/1	0.92	0.08	45,45,45,45	0
57	MG	1E	304	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3227	1/1	0.92	0.26	45,45,45,45	0
57	MG	1A	3721	1/1	0.92	0.14	24,24,24,24	0
57	MG	1A	3240	1/1	0.92	0.08	31,31,31,31	0
57	MG	2A	3631	1/1	0.92	0.28	58,58,58,58	0
57	MG	2A	3231	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3235	1/1	0.92	0.13	51,51,51,51	0
57	MG	2e	201	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3429	1/1	0.92	0.20	45,45,45,45	0
57	MG	1A	3006	1/1	0.92	0.09	41,41,41,41	0
57	MG	2A	3238	1/1	0.92	0.11	56,56,56,56	0
57	MG	2v	101	1/1	0.92	0.11	59,59,59,59	0
57	MG	2B	201	1/1	0.92	0.14	59,59,59,59	0
57	MG	2x	102	1/1	0.92	0.24	55,55,55,55	0
57	MG	2x	103	1/1	0.92	0.16	46,46,46,46	0
57	MG	1A	3059	1/1	0.92	0.11	30,30,30,30	0
57	MG	1A	3255	1/1	0.92	0.10	67,67,67,67	0
57	MG	1A	3439	1/1	0.92	0.07	39,39,39,39	0
57	MG	2A	3438	1/1	0.92	0.10	48,48,48,48	0
57	MG	1Q	204	1/1	0.92	0.08	31,31,31,31	0
57	MG	1A	3627	1/1	0.92	0.09	39,39,39,39	0
57	MG	2A	3609	1/1	0.93	0.09	31,31,31,31	0
57	MG	1A	3481	1/1	0.93	0.10	18,18,18,18	0
57	MG	2A	3611	1/1	0.93	0.10	46,46,46,46	0
57	MG	1A	3391	1/1	0.93	0.11	38,38,38,38	0
57	MG	1a	1633	1/1	0.93	0.15	50,50,50,50	0
57	MG	1A	3761	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3763	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3161	1/1	0.93	0.18	58,58,58,58	0
57	MG	1A	3230	1/1	0.93	0.11	35,35,35,35	0
57	MG	2A	3624	1/1	0.93	0.22	37,37,37,37	0
57	MG	1A	3159	1/1	0.93	0.09	55,55,55,55	0
57	MG	1a	1772	1/1	0.93	0.13	62,62,62,62	0
57	MG	2A	3630	1/1	0.93	0.07	57,57,57,57	0
57	MG	2A	3396	1/1	0.93	0.15	29,29,29,29	0
57	MG	1A	3489	1/1	0.93	0.16	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
57	MG	1A	3491	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3400	1/1	0.93	0.16	28,28,28,28	0
57	MG	1A	3007	1/1	0.93	0.09	31,31,31,31	0
57	MG	2A	3639	1/1	0.93	0.10	24,24,24,24	0
57	MG	1A	3071	1/1	0.93	0.07	39,39,39,39	0
57	MG	1A	3173	1/1	0.93	0.10	29,29,29,29	0
57	MG	1A	3506	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3174	1/1	0.93	0.20	41,41,41,41	0
57	MG	2A	3406	1/1	0.93	0.12	51,51,51,51	0
57	MG	1a	1654	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3250	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3791	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3115	1/1	0.93	0.09	28,28,28,28	0
57	MG	2B	211	1/1	0.93	0.08	56,56,56,56	0
57	MG	1A	3646	1/1	0.93	0.27	42,42,42,42	0
57	MG	1m	3001	1/1	0.93	0.10	58,58,58,58	0
57	MG	1a	1659	1/1	0.93	0.26	35,35,35,35	0
57	MG	2E	301	1/1	0.93	0.19	35,35,35,35	0
57	MG	2A	3195	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3351	1/1	0.93	0.04	10,10,10,10	0
57	MG	2A	3198	1/1	0.93	0.34	53,53,53,53	0
57	MG	1A	3653	1/1	0.93	0.16	34,34,34,34	0
57	MG	1A	3073	1/1	0.93	0.28	53,53,53,53	0
57	MG	2A	3420	1/1	0.93	0.06	35,35,35,35	0
57	MG	1A	3661	1/1	0.93	0.07	34,34,34,34	0
57	MG	1a	1674	1/1	0.93	0.15	48,48,48,48	0
57	MG	1a	1676	1/1	0.93	0.37	54,54,54,54	0
57	MG	1x	104	1/1	0.93	0.12	34,34,34,34	0
57	MG	1a	1677	1/1	0.93	0.20	41,41,41,41	0
57	MG	2a	1608	1/1	0.93	0.17	55,55,55,55	0
57	MG	1A	3186	1/1	0.93	0.11	33,33,33,33	0
57	MG	2a	1614	1/1	0.93	0.14	53,53,53,53	0
57	MG	1B	210	1/1	0.93	0.15	48,48,48,48	0
57	MG	2a	1616	1/1	0.93	0.18	41,41,41,41	0
57	MG	1B	213	1/1	0.93	0.11	47,47,47,47	0
57	MG	1A	3521	1/1	0.93	0.06	34,34,34,34	0
57	MG	2A	3440	1/1	0.93	0.13	53,53,53,53	0
57	MG	2A	3442	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3528	1/1	0.93	0.13	33,33,33,33	0
57	MG	2A	3018	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3020	1/1	0.93	0.12	49,49,49,49	0
57	MG	2a	1629	1/1	0.93	0.19	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3672	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3529	1/1	0.93	0.09	17,17,17,17	0
57	MG	2a	1633	1/1	0.93	0.17	51,51,51,51	0
57	MG	1F	310	1/1	0.93	0.07	39,39,39,39	0
57	MG	2A	3232	1/1	0.93	0.10	44,44,44,44	0
57	MG	1G	201	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3035	1/1	0.93	0.12	31,31,31,31	0
57	MG	1G	203	1/1	0.93	0.09	51,51,51,51	0
57	MG	1N	202	1/1	0.93	0.05	31,31,31,31	0
57	MG	2a	1645	1/1	0.93	0.11	45,45,45,45	0
57	MG	1A	3086	1/1	0.93	0.08	23,23,23,23	0
57	MG	2A	3468	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3249	1/1	0.93	0.22	52,52,52,52	0
57	MG	2A	3470	1/1	0.93	0.11	59,59,59,59	0
57	MG	2a	1653	1/1	0.93	0.35	47,47,47,47	0
57	MG	2A	3471	1/1	0.93	0.18	43,43,43,43	0
57	MG	2A	3047	1/1	0.93	0.16	57,57,57,57	0
57	MG	2a	1656	1/1	0.93	0.20	55,55,55,55	0
57	MG	2A	3049	1/1	0.93	0.18	58,58,58,58	0
57	MG	2A	3476	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3195	1/1	0.93	0.15	33,33,33,33	0
57	MG	1a	1699	1/1	0.93	0.24	70,70,70,70	0
57	MG	2a	1663	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3479	1/1	0.93	0.11	35,35,35,35	0
57	MG	2A	3052	1/1	0.93	0.29	65,65,65,65	0
57	MG	1A	3046	1/1	0.93	0.07	18,18,18,18	0
57	MG	1Q	201	1/1	0.93	0.30	38,38,38,38	0
57	MG	2A	3268	1/1	0.93	0.13	67,67,67,67	0
57	MG	1A	3682	1/1	0.93	0.10	38,38,38,38	0
57	MG	1A	3197	1/1	0.93	0.24	41,41,41,41	0
57	MG	2A	3271	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3059	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3198	1/1	0.93	0.14	39,39,39,39	0
57	MG	1a	1716	1/1	0.93	0.20	48,48,48,48	0
57	MG	1A	3546	1/1	0.93	0.10	23,23,23,23	0
57	MG	1A	3438	1/1	0.93	0.10	20,20,20,20	0
57	MG	1A	3550	1/1	0.93	0.10	18,18,18,18	0
57	MG	2A	3072	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3706	1/1	0.93	0.08	25,25,25,25	0
57	MG	1A	3559	1/1	0.93	0.08	25,25,25,25	0
57	MG	1A	3710	1/1	0.93	0.08	17,17,17,17	0
57	MG	2a	1695	1/1	0.93	0.15	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
57	MG	2A	3510	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3292	1/1	0.93	0.10	19,19,19,19	0
57	MG	1A	3021	1/1	0.93	0.07	24,24,24,24	0
57	MG	2A	3081	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3051	1/1	0.93	0.09	29,29,29,29	0
57	MG	2A	3517	1/1	0.93	0.09	35,35,35,35	0
57	MG	2A	3084	1/1	0.93	0.18	45,45,45,45	0
57	MG	2a	1710	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3521	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3206	1/1	0.93	0.18	44,44,44,44	0
57	MG	1A	3450	1/1	0.93	0.09	39,39,39,39	0
57	MG	2a	1715	1/1	0.93	0.10	63,63,63,63	0
57	MG	2A	3091	1/1	0.93	0.07	40,40,40,40	0
57	MG	2A	3528	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3093	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3094	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3311	1/1	0.93	0.07	26,26,26,26	0
57	MG	1A	3580	1/1	0.93	0.10	18,18,18,18	0
57	MG	2a	1727	1/1	0.93	0.25	40,40,40,40	0
57	MG	1A	3300	1/1	0.93	0.23	31,31,31,31	0
57	MG	17	107	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3315	1/1	0.93	0.10	27,27,27,27	0
57	MG	2a	1732	1/1	0.93	0.12	48,48,48,48	0
57	MG	2A	3538	1/1	0.93	0.12	28,28,28,28	0
57	MG	1A	3309	1/1	0.93	0.10	30,30,30,30	0
57	MG	1A	3457	1/1	0.93	0.07	16,16,16,16	0
57	MG	1A	3310	1/1	0.93	0.08	13,13,13,13	0
57	MG	1a	1739	1/1	0.93	0.20	45,45,45,45	0
57	MG	1A	3128	1/1	0.93	0.06	26,26,26,26	0
57	MG	2a	1740	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3378	1/1	0.93	0.06	38,38,38,38	0
57	MG	1A	3466	1/1	0.93	0.11	25,25,25,25	0
57	MG	2a	1746	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3118	1/1	0.93	0.18	56,56,56,56	0
57	MG	2A	3333	1/1	0.93	0.17	55,55,55,55	0
57	MG	2A	3338	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3339	1/1	0.93	0.09	26,26,26,26	0
57	MG	1A	3130	1/1	0.93	0.05	15,15,15,15	0
57	MG	1A	3132	1/1	0.93	0.11	15,15,15,15	0
57	MG	1A	3133	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3569	1/1	0.93	0.11	38,38,38,38	0
57	MG	2A	3126	1/1	0.93	0.19	45,45,45,45	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	2A	3572	1/1	0.93	0.12	42,42,42,42	0
57	MG	1A	3597	1/1	0.93	0.11	22,22,22,22	0
57	MG	2A	3352	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3356	1/1	0.93	0.14	45,45,45,45	0
57	MG	1a	1620	1/1	0.93	0.06	55,55,55,55	0
57	MG	1A	3322	1/1	0.93	0.20	48,48,48,48	0
57	MG	2A	3582	1/1	0.93	0.06	42,42,42,42	0
57	MG	1a	1754	1/1	0.93	0.17	64,64,64,64	0
57	MG	1A	3476	1/1	0.93	0.10	19,19,19,19	0
57	MG	1A	3032	1/1	0.93	0.07	23,23,23,23	0
57	MG	1a	1758	1/1	0.93	0.22	49,49,49,49	0
57	MG	2t	201	1/1	0.93	0.14	48,48,48,48	0
57	MG	2A	3591	1/1	0.93	0.13	46,46,46,46	0
57	MG	2A	3370	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3371	1/1	0.93	0.08	58,58,58,58	0
57	MG	2A	3372	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3144	1/1	0.93	0.06	67,67,67,67	0
57	MG	1A	3756	1/1	0.93	0.09	14,14,14,14	0
57	MG	2A	3381	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	1762	1/1	0.93	0.17	62,62,62,62	0
57	MG	1A	3480	1/1	0.93	0.11	37,37,37,37	0
57	MG	2A	3150	1/1	0.93	0.27	51,51,51,51	0
57	MG	1A	3486	1/1	0.94	0.08	26,26,26,26	0
57	MG	2A	3202	1/1	0.94	0.16	45,45,45,45	0
57	MG	2A	3023	1/1	0.94	0.27	47,47,47,47	0
57	MG	1a	1696	1/1	0.94	0.22	41,41,41,41	0
57	MG	1A	3364	1/1	0.94	0.07	33,33,33,33	0
57	MG	1A	3062	1/1	0.94	0.11	36,36,36,36	0
57	MG	2A	3033	1/1	0.94	0.09	63,63,63,63	0
57	MG	1a	1700	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3312	1/1	0.94	0.12	32,32,32,32	0
57	MG	2A	3210	1/1	0.94	0.12	33,33,33,33	0
57	MG	2B	203	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3036	1/1	0.94	0.15	47,47,47,47	0
57	MG	2A	3214	1/1	0.94	0.07	39,39,39,39	0
57	MG	2A	3419	1/1	0.94	0.07	44,44,44,44	0
57	MG	1a	1702	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3219	1/1	0.94	0.21	48,48,48,48	0
57	MG	1A	3239	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3044	1/1	0.94	0.13	56,56,56,56	0
57	MG	2A	3225	1/1	0.94	0.15	42,42,42,42	0
57	MG	1W	202	1/1	0.94	0.07	22,22,22,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3192	1/1	0.94	0.10	20,20,20,20	0
57	MG	2A	3048	1/1	0.94	0.21	54,54,54,54	0
57	MG	2E	303	1/1	0.94	0.08	51,51,51,51	0
57	MG	1a	1707	1/1	0.94	0.13	36,36,36,36	0
57	MG	2F	303	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3141	1/1	0.94	0.06	23,23,23,23	0
57	MG	2F	307	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3598	1/1	0.94	0.05	40,40,40,40	0
57	MG	1A	3096	1/1	0.94	0.35	29,29,29,29	0
57	MG	2Q	201	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3508	1/1	0.94	0.10	20,20,20,20	0
57	MG	1A	3375	1/1	0.94	0.05	12,12,12,12	0
57	MG	2A	3445	1/1	0.94	0.13	35,35,35,35	0
57	MG	2A	3244	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3448	1/1	0.94	0.16	46,46,46,46	0
57	MG	1A	3445	1/1	0.94	0.09	13,13,13,13	0
57	MG	1A	3156	1/1	0.94	0.18	50,50,50,50	0
57	MG	2a	1605	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3250	1/1	0.94	0.08	38,38,38,38	0
57	MG	2a	1610	1/1	0.94	0.24	53,53,53,53	0
57	MG	2a	1611	1/1	0.94	0.14	55,55,55,55	0
57	MG	1a	1723	1/1	0.94	0.17	24,24,24,24	0
57	MG	2a	1613	1/1	0.94	0.20	51,51,51,51	0
57	MG	2A	3458	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3459	1/1	0.94	0.07	66,66,66,66	0
57	MG	2A	3460	1/1	0.94	0.17	60,60,60,60	0
57	MG	2A	3061	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3610	1/1	0.94	0.43	21,21,21,21	0
57	MG	2a	1620	1/1	0.94	0.19	52,52,52,52	0
57	MG	2a	1621	1/1	0.94	0.07	43,43,43,43	0
57	MG	2a	1622	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3254	1/1	0.94	0.09	21,21,21,21	0
57	MG	2A	3256	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3614	1/1	0.94	0.09	21,21,21,21	0
57	MG	2A	3259	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3739	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3615	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3070	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3382	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3473	1/1	0.94	0.09	31,31,31,31	0
57	MG	1a	1604	1/1	0.94	0.16	43,43,43,43	0
57	MG	1A	3744	1/1	0.94	0.11	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3076	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3745	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3078	1/1	0.94	0.15	51,51,51,51	0
57	MG	2a	1643	1/1	0.94	0.20	40,40,40,40	0
57	MG	1A	3748	1/1	0.94	0.06	12,12,12,12	0
57	MG	2A	3482	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3080	1/1	0.94	0.12	33,33,33,33	0
57	MG	2a	1647	1/1	0.94	0.28	44,44,44,44	0
57	MG	1A	3750	1/1	0.94	0.08	15,15,15,15	0
57	MG	2A	3282	1/1	0.94	0.10	42,42,42,42	0
57	MG	2a	1650	1/1	0.94	0.14	53,53,53,53	0
57	MG	2A	3082	1/1	0.94	0.13	37,37,37,37	0
57	MG	1A	3327	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3064	1/1	0.94	0.06	19,19,19,19	0
57	MG	2A	3289	1/1	0.94	0.08	32,32,32,32	0
57	MG	1A	3522	1/1	0.94	0.07	29,29,29,29	0
57	MG	1A	3526	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3088	1/1	0.94	0.14	38,38,38,38	0
57	MG	1A	3456	1/1	0.94	0.12	40,40,40,40	0
57	MG	1A	3104	1/1	0.94	0.08	32,32,32,32	0
57	MG	1A	3204	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3505	1/1	0.94	0.08	36,36,36,36	0
57	MG	2A	3506	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3299	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3635	1/1	0.94	0.44	19,19,19,19	0
57	MG	1A	3762	1/1	0.94	0.13	33,33,33,33	0
57	MG	1A	3538	1/1	0.94	0.09	25,25,25,25	0
57	MG	1a	1753	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3308	1/1	0.94	0.13	22,22,22,22	0
57	MG	1A	3461	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3110	1/1	0.94	0.13	72,72,72,72	0
57	MG	2a	1679	1/1	0.94	0.38	52,52,52,52	0
57	MG	2A	3111	1/1	0.94	0.16	34,34,34,34	0
57	MG	2a	1681	1/1	0.94	0.21	49,49,49,49	0
57	MG	1A	3640	1/1	0.94	0.07	25,25,25,25	0
57	MG	2a	1683	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3641	1/1	0.94	0.14	26,26,26,26	0
57	MG	1A	3269	1/1	0.94	0.34	50,50,50,50	0
57	MG	1a	1759	1/1	0.94	0.22	40,40,40,40	0
57	MG	2A	3526	1/1	0.94	0.11	68,68,68,68	0
57	MG	1a	1639	1/1	0.94	0.16	34,34,34,34	0
57	MG	2A	3321	1/1	0.94	0.17	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
57	MG	1A	3644	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3777	1/1	0.94	0.09	16,16,16,16	0
57	MG	1A	3780	1/1	0.94	0.09	14,14,14,14	0
57	MG	2a	1699	1/1	0.94	0.18	41,41,41,41	0
57	MG	2a	1700	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3645	1/1	0.94	0.12	35,35,35,35	0
57	MG	2A	3124	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	3541	1/1	0.94	0.09	29,29,29,29	0
57	MG	1A	3463	1/1	0.94	0.07	13,13,13,13	0
57	MG	2A	3334	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3335	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3540	1/1	0.94	0.16	75,75,75,75	0
57	MG	2A	3129	1/1	0.94	0.41	53,53,53,53	0
57	MG	2A	3544	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3162	1/1	0.94	0.09	51,51,51,51	0
57	MG	1a	1652	1/1	0.94	0.24	51,51,51,51	0
57	MG	1A	3655	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3658	1/1	0.94	0.13	34,34,34,34	0
57	MG	2a	1721	1/1	0.94	0.15	45,45,45,45	0
57	MG	1A	3107	1/1	0.94	0.21	51,51,51,51	0
57	MG	2A	3553	1/1	0.94	0.08	25,25,25,25	0
57	MG	2A	3555	1/1	0.94	0.15	54,54,54,54	0
57	MG	1A	3467	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3350	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3351	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3169	1/1	0.94	0.15	33,33,33,33	0
57	MG	2A	3353	1/1	0.94	0.13	38,38,38,38	0
57	MG	1A	3558	1/1	0.94	0.08	51,51,51,51	0
57	MG	1a	1778	1/1	0.94	0.19	45,45,45,45	0
57	MG	1A	3126	1/1	0.94	0.10	30,30,30,30	0
57	MG	1A	3670	1/1	0.94	0.06	67,67,67,67	0
57	MG	2a	1737	1/1	0.94	0.16	43,43,43,43	0
57	MG	1A	3472	1/1	0.94	0.16	43,43,43,43	0
57	MG	2A	3362	1/1	0.94	0.22	50,50,50,50	0
57	MG	1a	1786	1/1	0.94	0.08	47,47,47,47	0
57	MG	2a	1741	1/1	0.94	0.20	58,58,58,58	0
57	MG	2A	3575	1/1	0.94	0.12	47,47,47,47	0
57	MG	1a	1663	1/1	0.94	0.31	47,47,47,47	0
57	MG	1a	1664	1/1	0.94	0.24	46,46,46,46	0
57	MG	2A	3580	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3017	1/1	0.94	0.06	20,20,20,20	0
57	MG	1A	3563	1/1	0.94	0.08	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
57	MG	1f	201	1/1	0.94	0.06	34,34,34,34	0
57	MG	1E	303	1/1	0.94	0.08	9,9,9,9	0
57	MG	2A	3586	1/1	0.94	0.06	59,59,59,59	0
57	MG	2A	3164	1/1	0.94	0.16	29,29,29,29	0
57	MG	1A	3677	1/1	0.94	0.12	22,22,22,22	0
57	MG	2a	1758	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3223	1/1	0.94	0.25	44,44,44,44	0
57	MG	1A	3015	1/1	0.94	0.25	36,36,36,36	0
57	MG	1A	3579	1/1	0.94	0.14	43,43,43,43	0
57	MG	1A	3052	1/1	0.94	0.13	20,20,20,20	0
57	MG	1A	3684	1/1	0.94	0.11	37,37,37,37	0
57	MG	2A	3389	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3175	1/1	0.94	0.15	29,29,29,29	0
57	MG	2a	1767	1/1	0.94	0.12	62,62,62,62	0
57	MG	2a	1768	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3177	1/1	0.94	0.18	40,40,40,40	0
57	MG	1x	101	1/1	0.94	0.10	36,36,36,36	0
57	MG	2e	202	1/1	0.94	0.07	54,54,54,54	0
57	MG	2e	203	1/1	0.94	0.15	43,43,43,43	0
57	MG	1A	3581	1/1	0.94	0.10	46,46,46,46	0
57	MG	2j	201	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3608	1/1	0.94	0.08	43,43,43,43	0
57	MG	1a	1683	1/1	0.94	0.20	45,45,45,45	0
57	MG	2k	202	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3226	1/1	0.94	0.08	24,24,24,24	0
57	MG	1A	3697	1/1	0.94	0.11	24,24,24,24	0
57	MG	1A	3411	1/1	0.94	0.06	12,12,12,12	0
57	MG	2A	3190	1/1	0.94	0.21	34,34,34,34	0
57	MG	1A	3047	1/1	0.94	0.09	18,18,18,18	0
57	MG	1A	3704	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3004	1/1	0.94	0.22	58,58,58,58	0
57	MG	1a	1690	1/1	0.94	0.17	45,45,45,45	0
57	MG	1a	1692	1/1	0.94	0.25	46,46,46,46	0
57	MG	2A	3014	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3190	1/1	0.94	0.22	22,22,22,22	0
58	ZN	24	501	1/1	0.94	0.18	137,137,137,137	0
57	MG	1A	3308	1/1	0.95	0.08	36,36,36,36	0
57	MG	1B	215	1/1	0.95	0.09	29,29,29,29	0
57	MG	1D	306	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3642	1/1	0.95	0.10	30,30,30,30	0
57	MG	1a	1722	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3502	1/1	0.95	0.08	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
57	MG	2A	3616	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3618	1/1	0.95	0.05	45,45,45,45	0
57	MG	1A	3148	1/1	0.95	0.42	34,34,34,34	0
57	MG	2A	3367	1/1	0.95	0.15	30,30,30,30	0
57	MG	1a	1726	1/1	0.95	0.23	55,55,55,55	0
57	MG	1E	307	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3079	1/1	0.95	0.07	38,38,38,38	0
57	MG	1F	301	1/1	0.95	0.09	34,34,34,34	0
57	MG	1F	302	1/1	0.95	0.11	21,21,21,21	0
57	MG	1A	3393	1/1	0.95	0.15	42,42,42,42	0
57	MG	2A	3376	1/1	0.95	0.17	45,45,45,45	0
57	MG	2A	3380	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3394	1/1	0.95	0.11	29,29,29,29	0
57	MG	2A	3134	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3651	1/1	0.95	0.08	32,32,32,32	0
57	MG	1A	3213	1/1	0.95	0.10	28,28,28,28	0
57	MG	2A	3139	1/1	0.95	0.15	43,43,43,43	0
57	MG	1N	201	1/1	0.95	0.17	25,25,25,25	0
57	MG	2A	3142	1/1	0.95	0.32	42,42,42,42	0
57	MG	1A	3654	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3514	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3217	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3313	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3400	1/1	0.95	0.08	13,13,13,13	0
57	MG	1A	3663	1/1	0.95	0.09	36,36,36,36	0
57	MG	2B	210	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3401	1/1	0.95	0.09	24,24,24,24	0
57	MG	1A	3314	1/1	0.95	0.15	42,42,42,42	0
57	MG	1R	201	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3523	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3668	1/1	0.95	0.06	23,23,23,23	0
57	MG	2A	3160	1/1	0.95	0.24	44,44,44,44	0
57	MG	1U	205	1/1	0.95	0.16	39,39,39,39	0
57	MG	1V	205	1/1	0.95	0.05	37,37,37,37	0
57	MG	1A	3669	1/1	0.95	0.14	41,41,41,41	0
57	MG	1A	3218	1/1	0.95	0.13	26,26,26,26	0
57	MG	1a	1757	1/1	0.95	0.15	42,42,42,42	0
57	MG	1W	205	1/1	0.95	0.09	26,26,26,26	0
57	MG	1Z	301	1/1	0.95	0.08	34,34,34,34	0
57	MG	2Q	203	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3405	1/1	0.95	0.08	33,33,33,33	0
57	MG	1A	3406	1/1	0.95	0.07	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2V	202	1/1	0.95	0.23	45,45,45,45	0
57	MG	2X	101	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3533	1/1	0.95	0.14	30,30,30,30	0
57	MG	11	104	1/1	0.95	0.09	32,32,32,32	0
57	MG	20	102	1/1	0.95	0.13	57,57,57,57	0
57	MG	1A	3150	1/1	0.95	0.06	31,31,31,31	0
57	MG	29	101	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3318	1/1	0.95	0.06	8,8,8,8	0
57	MG	1A	3319	1/1	0.95	0.11	29,29,29,29	0
57	MG	2a	1604	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3681	1/1	0.95	0.20	40,40,40,40	0
57	MG	2a	1607	1/1	0.95	0.28	42,42,42,42	0
57	MG	1A	3152	1/1	0.95	0.22	27,27,27,27	0
57	MG	2a	1609	1/1	0.95	0.14	54,54,54,54	0
57	MG	2A	3185	1/1	0.95	0.23	43,43,43,43	0
57	MG	16	101	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3154	1/1	0.95	0.08	26,26,26,26	0
57	MG	1A	3004	1/1	0.95	0.09	14,14,14,14	0
57	MG	2A	3424	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3425	1/1	0.95	0.09	28,28,28,28	0
57	MG	1A	3425	1/1	0.95	0.13	22,22,22,22	0
57	MG	2A	3428	1/1	0.95	0.16	51,51,51,51	0
57	MG	19	102	1/1	0.95	0.09	44,44,44,44	0
57	MG	2a	1619	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3689	1/1	0.95	0.12	20,20,20,20	0
57	MG	1A	3692	1/1	0.95	0.08	35,35,35,35	0
57	MG	1a	1780	1/1	0.95	0.08	55,55,55,55	0
57	MG	2A	3435	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3325	1/1	0.95	0.09	28,28,28,28	0
57	MG	1A	3063	1/1	0.95	0.15	31,31,31,31	0
57	MG	1A	3698	1/1	0.95	0.10	33,33,33,33	0
57	MG	1a	1785	1/1	0.95	0.08	58,58,58,58	0
57	MG	2a	1628	1/1	0.95	0.06	34,34,34,34	0
57	MG	1a	1609	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3160	1/1	0.95	0.10	32,32,32,32	0
57	MG	1A	3551	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3557	1/1	0.95	0.05	24,24,24,24	0
57	MG	1A	3229	1/1	0.95	0.09	38,38,38,38	0
57	MG	1a	1617	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3093	1/1	0.95	0.14	34,34,34,34	0
57	MG	1A	3560	1/1	0.95	0.07	17,17,17,17	0
57	MG	2a	1638	1/1	0.95	0.18	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3436	1/1	0.95	0.12	42,42,42,42	0
57	MG	1A	3332	1/1	0.95	0.11	37,37,37,37	0
57	MG	2A	3456	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3215	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3028	1/1	0.95	0.23	31,31,31,31	0
57	MG	2A	3217	1/1	0.95	0.05	35,35,35,35	0
57	MG	2A	3218	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3566	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3220	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3718	1/1	0.95	0.07	43,43,43,43	0
57	MG	2a	1652	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3121	1/1	0.95	0.07	15,15,15,15	0
57	MG	2A	3223	1/1	0.95	0.19	35,35,35,35	0
57	MG	1a	1630	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3572	1/1	0.95	0.14	37,37,37,37	0
57	MG	2a	1658	1/1	0.95	0.34	53,53,53,53	0
57	MG	1A	3576	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3033	1/1	0.95	0.14	16,16,16,16	0
57	MG	1A	3727	1/1	0.95	0.12	43,43,43,43	0
57	MG	1A	3341	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3234	1/1	0.95	0.11	45,45,45,45	0
57	MG	2A	3001	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3449	1/1	0.95	0.11	24,24,24,24	0
57	MG	2A	3237	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3170	1/1	0.95	0.07	39,39,39,39	0
57	MG	2A	3481	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3005	1/1	0.95	0.20	40,40,40,40	0
57	MG	2a	1671	1/1	0.95	0.29	49,49,49,49	0
57	MG	2a	1672	1/1	0.95	0.12	43,43,43,43	0
57	MG	2A	3240	1/1	0.95	0.17	40,40,40,40	0
57	MG	2A	3486	1/1	0.95	0.29	34,34,34,34	0
57	MG	2A	3241	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3489	1/1	0.95	0.10	45,45,45,45	0
57	MG	2a	1678	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3242	1/1	0.95	0.08	34,34,34,34	0
57	MG	1A	3733	1/1	0.95	0.07	33,33,33,33	0
57	MG	2A	3246	1/1	0.95	0.18	50,50,50,50	0
57	MG	2A	3009	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3248	1/1	0.95	0.14	40,40,40,40	0
57	MG	1a	1642	1/1	0.95	0.22	55,55,55,55	0
57	MG	1A	3451	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3344	1/1	0.95	0.06	36,36,36,36	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2a	1687	1/1	0.95	0.27	44,44,44,44	0
57	MG	1A	3345	1/1	0.95	0.05	13,13,13,13	0
57	MG	2A	3500	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3501	1/1	0.95	0.09	53,53,53,53	0
57	MG	2a	1693	1/1	0.95	0.08	38,38,38,38	0
57	MG	1a	1649	1/1	0.95	0.22	41,41,41,41	0
57	MG	1A	3347	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3349	1/1	0.95	0.08	10,10,10,10	0
57	MG	2A	3257	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3028	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3243	1/1	0.95	0.07	27,27,27,27	0
57	MG	2A	3262	1/1	0.95	0.06	36,36,36,36	0
57	MG	1A	3123	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3102	1/1	0.95	0.17	28,28,28,28	0
57	MG	2A	3512	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3267	1/1	0.95	0.09	30,30,30,30	0
57	MG	1A	3746	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	1712	1/1	0.95	0.18	54,54,54,54	0
57	MG	1A	3249	1/1	0.95	0.05	30,30,30,30	0
57	MG	1A	3176	1/1	0.95	0.15	33,33,33,33	0
57	MG	2A	3518	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3519	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3039	1/1	0.95	0.18	22,22,22,22	0
57	MG	1A	3596	1/1	0.95	0.07	24,24,24,24	0
57	MG	2A	3522	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3273	1/1	0.95	0.13	43,43,43,43	0
57	MG	2a	1724	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3253	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3754	1/1	0.95	0.09	29,29,29,29	0
57	MG	1a	1661	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3125	1/1	0.95	0.14	27,27,27,27	0
57	MG	1A	3468	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	3182	1/1	0.95	0.31	35,35,35,35	0
57	MG	1a	1665	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3103	1/1	0.95	0.07	34,34,34,34	0
57	MG	1a	1669	1/1	0.95	0.20	50,50,50,50	0
57	MG	2A	3288	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3602	1/1	0.95	0.08	19,19,19,19	0
57	MG	2A	3056	1/1	0.95	0.13	26,26,26,26	0
57	MG	1a	1673	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3068	1/1	0.95	0.22	41,41,41,41	0
57	MG	2A	3541	1/1	0.95	0.13	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
57	MG	1A	3265	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3608	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3268	1/1	0.95	0.13	29,29,29,29	0
57	MG	2A	3298	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3105	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3129	1/1	0.95	0.14	28,28,28,28	0
57	MG	1A	3478	1/1	0.95	0.09	32,32,32,32	0
57	MG	2a	1751	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3479	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3771	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3774	1/1	0.95	0.07	24,24,24,24	0
57	MG	1A	3775	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3619	1/1	0.95	0.14	33,33,33,33	0
57	MG	2a	1757	1/1	0.95	0.17	49,49,49,49	0
57	MG	1A	3778	1/1	0.95	0.07	57,57,57,57	0
57	MG	1A	3002	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3621	1/1	0.95	0.13	33,33,33,33	0
57	MG	1A	3623	1/1	0.95	0.14	23,23,23,23	0
57	MG	2A	3317	1/1	0.95	0.11	35,35,35,35	0
57	MG	1A	3280	1/1	0.95	0.15	25,25,25,25	0
57	MG	1A	3072	1/1	0.95	0.19	40,40,40,40	0
57	MG	1a	1695	1/1	0.95	0.35	49,49,49,49	0
57	MG	2A	3323	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3285	1/1	0.95	0.06	26,26,26,26	0
57	MG	1A	3026	1/1	0.95	0.16	27,27,27,27	0
57	MG	2d	302	1/1	0.95	0.17	48,48,48,48	0
57	MG	1A	3792	1/1	0.95	0.09	11,11,11,11	0
57	MG	1A	3134	1/1	0.95	0.32	28,28,28,28	0
57	MG	1A	3488	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3089	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3332	1/1	0.95	0.12	30,30,30,30	0
57	MG	1A	3633	1/1	0.95	0.26	25,25,25,25	0
57	MG	1A	3634	1/1	0.95	0.08	49,49,49,49	0
57	MG	1A	3136	1/1	0.95	0.13	27,27,27,27	0
57	MG	1B	205	1/1	0.95	0.11	47,47,47,47	0
57	MG	1A	3139	1/1	0.95	0.17	22,22,22,22	0
57	MG	1a	1708	1/1	0.95	0.09	33,33,33,33	0
57	MG	2A	3342	1/1	0.95	0.07	27,27,27,27	0
57	MG	1a	1710	1/1	0.95	0.20	48,48,48,48	0
57	MG	1a	1711	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3105	1/1	0.95	0.29	60,60,60,60	0
57	MG	2A	3108	1/1	0.95	0.27	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
57	MG	2A	3109	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3112	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3143	1/1	0.95	0.16	32,32,32,32	0
57	MG	1B	211	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3594	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3085	1/1	0.96	0.07	7,7,7,7	0
57	MG	1A	3483	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3598	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3283	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3789	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3085	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3790	1/1	0.96	0.11	43,43,43,43	0
57	MG	2A	3337	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3376	1/1	0.96	0.06	13,13,13,13	0
57	MG	1A	3284	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3010	1/1	0.96	0.07	26,26,26,26	0
57	MG	1a	1691	1/1	0.96	0.20	49,49,49,49	0
57	MG	1A	3380	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3381	1/1	0.96	0.07	19,19,19,19	0
57	MG	1A	3151	1/1	0.96	0.18	16,16,16,16	0
57	MG	2A	3615	1/1	0.96	0.09	54,54,54,54	0
57	MG	2A	3347	1/1	0.96	0.11	21,21,21,21	0
57	MG	2A	3617	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3495	1/1	0.96	0.04	23,23,23,23	0
57	MG	1B	204	1/1	0.96	0.10	28,28,28,28	0
57	MG	1a	1697	1/1	0.96	0.06	36,36,36,36	0
57	MG	2A	3622	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3088	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3208	1/1	0.96	0.10	25,25,25,25	0
57	MG	1B	207	1/1	0.96	0.07	22,22,22,22	0
57	MG	1A	3290	1/1	0.96	0.07	11,11,11,11	0
57	MG	2A	3627	1/1	0.96	0.15	51,51,51,51	0
57	MG	2A	3628	1/1	0.96	0.09	41,41,41,41	0
57	MG	1A	3505	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3386	1/1	0.96	0.10	22,22,22,22	0
57	MG	2A	3632	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3090	1/1	0.96	0.07	15,15,15,15	0
57	MG	1B	214	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3647	1/1	0.96	0.05	31,31,31,31	0
57	MG	2A	3637	1/1	0.96	0.16	61,61,61,61	0
57	MG	1B	216	1/1	0.96	0.10	35,35,35,35	0
57	MG	1B	219	1/1	0.96	0.10	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3369	1/1	0.96	0.08	50,50,50,50	0
57	MG	1D	304	1/1	0.96	0.24	25,25,25,25	0
57	MG	1A	3118	1/1	0.96	0.15	33,33,33,33	0
57	MG	1a	1713	1/1	0.96	0.07	52,52,52,52	0
57	MG	1a	1714	1/1	0.96	0.10	37,37,37,37	0
57	MG	1D	307	1/1	0.96	0.16	31,31,31,31	0
57	MG	2A	3375	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3650	1/1	0.96	0.07	44,44,44,44	0
57	MG	2A	3378	1/1	0.96	0.09	31,31,31,31	0
57	MG	1A	3215	1/1	0.96	0.18	22,22,22,22	0
57	MG	2A	3128	1/1	0.96	0.49	58,58,58,58	0
57	MG	1A	3302	1/1	0.96	0.52	21,21,21,21	0
57	MG	2D	301	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3306	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3131	1/1	0.96	0.26	49,49,49,49	0
57	MG	2D	307	1/1	0.96	0.08	54,54,54,54	0
57	MG	1E	308	1/1	0.96	0.08	23,23,23,23	0
57	MG	1A	3157	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3136	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3158	1/1	0.96	0.12	20,20,20,20	0
57	MG	2E	305	1/1	0.96	0.09	33,33,33,33	0
57	MG	2F	302	1/1	0.96	0.04	26,26,26,26	0
57	MG	1A	3397	1/1	0.96	0.08	15,15,15,15	0
57	MG	2F	304	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3014	1/1	0.96	0.09	17,17,17,17	0
57	MG	1A	3662	1/1	0.96	0.08	49,49,49,49	0
57	MG	2A	3141	1/1	0.96	0.10	25,25,25,25	0
57	MG	2P	201	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3048	1/1	0.96	0.30	36,36,36,36	0
57	MG	1A	3222	1/1	0.96	0.11	44,44,44,44	0
57	MG	2Q	202	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3094	1/1	0.96	0.10	18,18,18,18	0
57	MG	1A	3039	1/1	0.96	0.22	24,24,24,24	0
57	MG	1A	3166	1/1	0.96	0.05	25,25,25,25	0
57	MG	2U	201	1/1	0.96	0.25	48,48,48,48	0
57	MG	1A	3530	1/1	0.96	0.10	12,12,12,12	0
57	MG	2A	3149	1/1	0.96	0.06	36,36,36,36	0
57	MG	1P	202	1/1	0.96	0.23	16,16,16,16	0
57	MG	2Y	201	1/1	0.96	0.07	58,58,58,58	0
57	MG	1P	203	1/1	0.96	0.13	27,27,27,27	0
57	MG	2A	3152	1/1	0.96	0.24	43,43,43,43	0
57	MG	1A	3167	1/1	0.96	0.09	20,20,20,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1A	3671	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3317	1/1	0.96	0.08	41,41,41,41	0
57	MG	1a	1741	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3537	1/1	0.96	0.07	13,13,13,13	0
57	MG	1A	3407	1/1	0.96	0.15	51,51,51,51	0
57	MG	2a	1606	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3675	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3227	1/1	0.96	0.07	21,21,21,21	0
57	MG	1U	202	1/1	0.96	0.23	32,32,32,32	0
57	MG	1A	3100	1/1	0.96	0.16	19,19,19,19	0
57	MG	2A	3168	1/1	0.96	0.12	40,40,40,40	0
57	MG	1a	1750	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3679	1/1	0.96	0.08	8,8,8,8	0
57	MG	1V	202	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3042	1/1	0.96	0.08	16,16,16,16	0
57	MG	1A	3413	1/1	0.96	0.05	15,15,15,15	0
57	MG	2A	3421	1/1	0.96	0.09	27,27,27,27	0
57	MG	1A	3414	1/1	0.96	0.07	14,14,14,14	0
57	MG	2A	3176	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3321	1/1	0.96	0.07	19,19,19,19	0
57	MG	1X	101	1/1	0.96	0.07	39,39,39,39	0
57	MG	2A	3427	1/1	0.96	0.11	30,30,30,30	0
57	MG	1X	102	1/1	0.96	0.06	18,18,18,18	0
57	MG	1A	3548	1/1	0.96	0.12	17,17,17,17	0
57	MG	10	101	1/1	0.96	0.08	36,36,36,36	0
57	MG	2A	3184	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3433	1/1	0.96	0.10	37,37,37,37	0
57	MG	10	102	1/1	0.96	0.11	38,38,38,38	0
57	MG	1A	3686	1/1	0.96	0.14	11,11,11,11	0
57	MG	11	101	1/1	0.96	0.18	32,32,32,32	0
57	MG	2A	3188	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3418	1/1	0.96	0.07	13,13,13,13	0
57	MG	2A	3439	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3069	1/1	0.96	0.24	48,48,48,48	0
57	MG	2A	3441	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3192	1/1	0.96	0.09	24,24,24,24	0
57	MG	1A	3690	1/1	0.96	0.14	46,46,46,46	0
57	MG	2a	1639	1/1	0.96	0.23	49,49,49,49	0
57	MG	2a	1641	1/1	0.96	0.13	60,60,60,60	0
57	MG	1A	3044	1/1	0.96	0.14	17,17,17,17	0
57	MG	12	102	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3552	1/1	0.96	0.08	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3694	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3449	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3696	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3556	1/1	0.96	0.05	14,14,14,14	0
57	MG	1A	3324	1/1	0.96	0.06	42,42,42,42	0
57	MG	17	103	1/1	0.96	0.21	24,24,24,24	0
57	MG	1A	3237	1/1	0.96	0.20	24,24,24,24	0
57	MG	1a	1779	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3700	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3238	1/1	0.96	0.31	25,25,25,25	0
57	MG	1A	3054	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3462	1/1	0.96	0.18	51,51,51,51	0
57	MG	1A	3430	1/1	0.96	0.13	37,37,37,37	0
57	MG	1A	3328	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3708	1/1	0.96	0.27	52,52,52,52	0
57	MG	2A	3213	1/1	0.96	0.12	25,25,25,25	0
57	MG	2A	3467	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	3709	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3025	1/1	0.96	0.20	30,30,30,30	0
57	MG	2a	1665	1/1	0.96	0.23	53,53,53,53	0
57	MG	1a	1607	1/1	0.96	0.12	15,15,15,15	0
57	MG	1A	3565	1/1	0.96	0.09	12,12,12,12	0
57	MG	1A	3713	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3241	1/1	0.96	0.04	26,26,26,26	0
57	MG	2A	3474	1/1	0.96	0.11	51,51,51,51	0
57	MG	1a	1613	1/1	0.96	0.12	32,32,32,32	0
57	MG	1A	3567	1/1	0.96	0.08	32,32,32,32	0
57	MG	1a	1615	1/1	0.96	0.05	44,44,44,44	0
57	MG	1A	3106	1/1	0.96	0.20	31,31,31,31	0
57	MG	1A	3244	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3719	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3440	1/1	0.96	0.05	23,23,23,23	0
57	MG	2A	3229	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3442	1/1	0.96	0.05	7,7,7,7	0
57	MG	1a	1622	1/1	0.96	0.05	42,42,42,42	0
57	MG	1a	1623	1/1	0.96	0.25	41,41,41,41	0
57	MG	1x	105	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3444	1/1	0.96	0.13	12,12,12,12	0
57	MG	1x	107	1/1	0.96	0.05	49,49,49,49	0
57	MG	1A	3245	1/1	0.96	0.06	21,21,21,21	0
57	MG	1A	3179	1/1	0.96	0.13	37,37,37,37	0
57	MG	2a	1688	1/1	0.96	0.18	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
57	MG	1A	3447	1/1	0.96	0.07	22,22,22,22	0
57	MG	2a	1690	1/1	0.96	0.18	57,57,57,57	0
57	MG	1a	1628	1/1	0.96	0.30	49,49,49,49	0
57	MG	1A	3074	1/1	0.96	0.19	34,34,34,34	0
57	MG	1A	3584	1/1	0.96	0.06	10,10,10,10	0
57	MG	2A	3006	1/1	0.96	0.12	48,48,48,48	0
57	MG	2a	1696	1/1	0.96	0.22	42,42,42,42	0
57	MG	1A	3342	1/1	0.96	0.06	12,12,12,12	0
57	MG	1A	3248	1/1	0.96	0.08	24,24,24,24	0
57	MG	2A	3010	1/1	0.96	0.14	31,31,31,31	0
57	MG	2A	3011	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3183	1/1	0.96	0.31	23,23,23,23	0
57	MG	2A	3013	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3184	1/1	0.96	0.08	27,27,27,27	0
57	MG	2a	1704	1/1	0.96	0.17	48,48,48,48	0
57	MG	2A	3016	1/1	0.96	0.12	45,45,45,45	0
57	MG	2a	1706	1/1	0.96	0.20	59,59,59,59	0
57	MG	2a	1707	1/1	0.96	0.14	47,47,47,47	0
57	MG	1a	1636	1/1	0.96	0.14	25,25,25,25	0
57	MG	2a	1709	1/1	0.96	0.06	36,36,36,36	0
57	MG	2A	3019	1/1	0.96	0.07	32,32,32,32	0
57	MG	1a	1637	1/1	0.96	0.08	34,34,34,34	0
57	MG	2A	3021	1/1	0.96	0.06	17,17,17,17	0
57	MG	1A	3453	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	3740	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3263	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3252	1/1	0.96	0.05	28,28,28,28	0
57	MG	2A	3027	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3266	1/1	0.96	0.15	30,30,30,30	0
57	MG	2a	1720	1/1	0.96	0.13	40,40,40,40	0
57	MG	1A	3455	1/1	0.96	0.08	16,16,16,16	0
57	MG	2a	1722	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3031	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3594	1/1	0.96	0.12	14,14,14,14	0
57	MG	2A	3523	1/1	0.96	0.11	35,35,35,35	0
57	MG	1a	1643	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3348	1/1	0.96	0.04	30,30,30,30	0
57	MG	1A	3108	1/1	0.96	0.14	16,16,16,16	0
57	MG	1A	3747	1/1	0.96	0.08	17,17,17,17	0
57	MG	1A	3077	1/1	0.96	0.09	41,41,41,41	0
57	MG	2a	1731	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3188	1/1	0.96	0.07	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
57	MG	2A	3530	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3040	1/1	0.96	0.25	40,40,40,40	0
57	MG	1A	3256	1/1	0.96	0.08	21,21,21,21	0
57	MG	1A	3259	1/1	0.96	0.13	36,36,36,36	0
57	MG	2A	3045	1/1	0.96	0.24	48,48,48,48	0
57	MG	2A	3283	1/1	0.96	0.07	43,43,43,43	0
57	MG	1A	3189	1/1	0.96	0.18	14,14,14,14	0
57	MG	1A	3465	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3356	1/1	0.96	0.06	27,27,27,27	0
57	MG	2a	1742	1/1	0.96	0.12	48,48,48,48	0
57	MG	1A	3604	1/1	0.96	0.10	15,15,15,15	0
57	MG	1A	3605	1/1	0.96	0.06	33,33,33,33	0
57	MG	2A	3542	1/1	0.96	0.22	51,51,51,51	0
57	MG	1A	3110	1/1	0.96	0.11	33,33,33,33	0
57	MG	2A	3291	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3140	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3266	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3612	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3549	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3055	1/1	0.96	0.19	51,51,51,51	0
57	MG	1A	3267	1/1	0.96	0.16	14,14,14,14	0
57	MG	1A	3362	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	3363	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3617	1/1	0.96	0.07	16,16,16,16	0
57	MG	1a	1666	1/1	0.96	0.08	49,49,49,49	0
57	MG	2A	3303	1/1	0.96	0.11	20,20,20,20	0
57	MG	2A	3560	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3304	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3062	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3564	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3565	1/1	0.96	0.12	59,59,59,59	0
57	MG	2A	3063	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3567	1/1	0.96	0.08	29,29,29,29	0
57	MG	1a	1667	1/1	0.96	0.14	50,50,50,50	0
57	MG	2A	3065	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3060	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3770	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3142	1/1	0.96	0.11	36,36,36,36	0
57	MG	1a	1672	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3081	1/1	0.96	0.13	22,22,22,22	0
57	MG	2A	3316	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3272	1/1	0.96	0.06	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
57	MG	2A	3579	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3318	1/1	0.96	0.07	39,39,39,39	0
57	MG	1a	1675	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	3776	1/1	0.96	0.06	7,7,7,7	0
57	MG	2A	3075	1/1	0.96	0.09	35,35,35,35	0
57	MG	2A	3584	1/1	0.96	0.09	67,67,67,67	0
57	MG	1A	3622	1/1	0.96	0.12	26,26,26,26	0
57	MG	2A	3324	1/1	0.96	0.13	56,56,56,56	0
57	MG	1A	3146	1/1	0.96	0.11	31,31,31,31	0
57	MG	2x	107	1/1	0.96	0.06	68,68,68,68	0
57	MG	1A	3625	1/1	0.96	0.08	32,32,32,32	0
57	MG	1A	3369	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3328	1/1	0.96	0.18	42,42,42,42	0
58	ZN	2Y	202	1/1	0.96	0.07	99,99,99,99	0
57	MG	1A	3083	1/1	0.96	0.30	33,33,33,33	0
58	ZN	2n	501	1/1	0.96	0.06	94,94,94,94	0
57	MG	1A	3277	1/1	0.97	0.17	21,21,21,21	0
57	MG	1A	3279	1/1	0.97	0.23	31,31,31,31	0
57	MG	2V	201	1/1	0.97	0.12	55,55,55,55	0
57	MG	1A	3334	1/1	0.97	0.06	32,32,32,32	0
57	MG	2W	201	1/1	0.97	0.13	54,54,54,54	0
57	MG	1A	3656	1/1	0.97	0.08	20,20,20,20	0
57	MG	1a	1619	1/1	0.97	0.14	37,37,37,37	0
57	MG	1a	1760	1/1	0.97	0.08	22,22,22,22	0
57	MG	2A	3294	1/1	0.97	0.04	39,39,39,39	0
57	MG	1A	3657	1/1	0.97	0.05	21,21,21,21	0
57	MG	23	101	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3145	1/1	0.97	0.23	27,27,27,27	0
57	MG	28	101	1/1	0.97	0.14	55,55,55,55	0
57	MG	2A	3484	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3485	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	3395	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3087	1/1	0.97	0.26	39,39,39,39	0
57	MG	1A	3339	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3340	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3564	1/1	0.97	0.07	33,33,33,33	0
57	MG	2A	3302	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3282	1/1	0.97	0.17	29,29,29,29	0
57	MG	2A	3125	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3236	1/1	0.97	0.13	16,16,16,16	0
57	MG	1A	3022	1/1	0.97	0.06	14,14,14,14	0
57	MG	1A	3089	1/1	0.97	0.11	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	2A	3309	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3787	1/1	0.97	0.15	29,29,29,29	0
57	MG	1A	3788	1/1	0.97	0.07	16,16,16,16	0
57	MG	2A	3502	1/1	0.97	0.04	50,50,50,50	0
57	MG	1A	3570	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3571	1/1	0.97	0.07	32,32,32,32	0
57	MG	2A	3133	1/1	0.97	0.10	17,17,17,17	0
57	MG	1A	3199	1/1	0.97	0.12	17,17,17,17	0
57	MG	2A	3135	1/1	0.97	0.16	42,42,42,42	0
57	MG	1A	3573	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3346	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3171	1/1	0.97	0.12	19,19,19,19	0
57	MG	1A	3676	1/1	0.97	0.09	45,45,45,45	0
57	MG	1a	1783	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3578	1/1	0.97	0.06	14,14,14,14	0
57	MG	1A	3202	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3242	1/1	0.97	0.17	22,22,22,22	0
57	MG	2a	1631	1/1	0.97	0.21	42,42,42,42	0
57	MG	1a	1644	1/1	0.97	0.30	59,59,59,59	0
57	MG	1a	1645	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	3203	1/1	0.97	0.17	40,40,40,40	0
57	MG	1A	3293	1/1	0.97	0.15	34,34,34,34	0
57	MG	1A	3035	1/1	0.97	0.14	19,19,19,19	0
57	MG	1A	3076	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3301	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3175	1/1	0.97	0.09	28,28,28,28	0
57	MG	2a	1640	1/1	0.97	0.15	37,37,37,37	0
57	MG	2A	3154	1/1	0.97	0.05	36,36,36,36	0
57	MG	1B	212	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3687	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3419	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3492	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3303	1/1	0.97	0.05	14,14,14,14	0
57	MG	1B	218	1/1	0.97	0.04	42,42,42,42	0
57	MG	2A	3343	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3691	1/1	0.97	0.12	22,22,22,22	0
57	MG	1B	220	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3494	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3592	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3305	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3349	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3695	1/1	0.97	0.06	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
57	MG	2A	3170	1/1	0.97	0.12	52,52,52,52	0
57	MG	2a	1657	1/1	0.97	0.15	45,45,45,45	0
57	MG	1x	109	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3496	1/1	0.97	0.06	20,20,20,20	0
57	MG	1A	3497	1/1	0.97	0.03	10,10,10,10	0
57	MG	1E	306	1/1	0.97	0.08	15,15,15,15	0
57	MG	1A	3422	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3423	1/1	0.97	0.08	15,15,15,15	0
57	MG	1A	3501	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3701	1/1	0.97	0.10	30,30,30,30	0
57	MG	2A	3363	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3552	1/1	0.97	0.18	23,23,23,23	0
57	MG	1A	3702	1/1	0.97	0.13	37,37,37,37	0
57	MG	2A	3554	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3181	1/1	0.97	0.18	41,41,41,41	0
57	MG	1F	303	1/1	0.97	0.27	33,33,33,33	0
57	MG	1F	305	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3207	1/1	0.97	0.04	30,30,30,30	0
57	MG	1A	3504	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3561	1/1	0.97	0.13	31,31,31,31	0
57	MG	1A	3360	1/1	0.97	0.04	7,7,7,7	0
57	MG	2A	3015	1/1	0.97	0.11	45,45,45,45	0
57	MG	1G	202	1/1	0.97	0.07	31,31,31,31	0
57	MG	2A	3017	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3307	1/1	0.97	0.07	33,33,33,33	0
57	MG	2A	3377	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	3507	1/1	0.97	0.06	49,49,49,49	0
57	MG	2A	3379	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3119	1/1	0.97	0.13	15,15,15,15	0
57	MG	2A	3571	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3209	1/1	0.97	0.19	24,24,24,24	0
57	MG	1A	3606	1/1	0.97	0.04	18,18,18,18	0
57	MG	1O	201	1/1	0.97	0.10	31,31,31,31	0
57	MG	2A	3025	1/1	0.97	0.14	49,49,49,49	0
57	MG	2A	3576	1/1	0.97	0.10	32,32,32,32	0
57	MG	1P	201	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3510	1/1	0.97	0.21	29,29,29,29	0
57	MG	2A	3201	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3211	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3030	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3512	1/1	0.97	0.05	11,11,11,11	0
57	MG	1a	1689	1/1	0.97	0.05	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3611	1/1	0.97	0.20	48,48,48,48	0
57	MG	1A	3717	1/1	0.97	0.14	22,22,22,22	0
57	MG	1A	3120	1/1	0.97	0.06	9,9,9,9	0
57	MG	2A	3588	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3178	1/1	0.97	0.24	24,24,24,24	0
57	MG	2A	3397	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3155	1/1	0.97	0.28	28,28,28,28	0
57	MG	1R	202	1/1	0.97	0.22	33,33,33,33	0
57	MG	1A	3516	1/1	0.97	0.14	26,26,26,26	0
57	MG	2A	3041	1/1	0.97	0.07	34,34,34,34	0
57	MG	2A	3042	1/1	0.97	0.15	32,32,32,32	0
57	MG	1U	201	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3722	1/1	0.97	0.19	21,21,21,21	0
57	MG	1A	3616	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3066	1/1	0.97	0.14	18,18,18,18	0
57	MG	1U	206	1/1	0.97	0.12	24,24,24,24	0
57	MG	2A	3602	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3604	1/1	0.97	0.25	34,34,34,34	0
57	MG	2a	1718	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3605	1/1	0.97	0.06	46,46,46,46	0
57	MG	1U	207	1/1	0.97	0.12	22,22,22,22	0
57	MG	1A	3725	1/1	0.97	0.25	18,18,18,18	0
57	MG	1V	203	1/1	0.97	0.10	22,22,22,22	0
57	MG	2A	3224	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3726	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3137	1/1	0.97	0.18	22,22,22,22	0
57	MG	1A	3441	1/1	0.97	0.06	24,24,24,24	0
57	MG	1a	1709	1/1	0.97	0.06	29,29,29,29	0
57	MG	1W	204	1/1	0.97	0.06	17,17,17,17	0
57	MG	1A	3370	1/1	0.97	0.11	17,17,17,17	0
57	MG	1A	3371	1/1	0.97	0.05	33,33,33,33	0
57	MG	2A	3233	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3731	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3732	1/1	0.97	0.14	37,37,37,37	0
57	MG	2A	3620	1/1	0.97	0.24	42,42,42,42	0
57	MG	1a	1715	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3257	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3527	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3373	1/1	0.97	0.06	18,18,18,18	0
57	MG	10	104	1/1	0.97	0.07	42,42,42,42	0
57	MG	10	105	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3138	1/1	0.97	0.04	15,15,15,15	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3260	1/1	0.97	0.13	23,23,23,23	0
57	MG	2A	3629	1/1	0.97	0.05	43,43,43,43	0
57	MG	2a	1744	1/1	0.97	0.10	65,65,65,65	0
57	MG	2A	3431	1/1	0.97	0.06	43,43,43,43	0
57	MG	2A	3245	1/1	0.97	0.12	20,20,20,20	0
57	MG	1A	3532	1/1	0.97	0.07	31,31,31,31	0
57	MG	2a	1748	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3261	1/1	0.97	0.05	39,39,39,39	0
57	MG	2A	3071	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3037	1/1	0.97	0.15	20,20,20,20	0
57	MG	1A	3743	1/1	0.97	0.14	13,13,13,13	0
57	MG	1A	3535	1/1	0.97	0.12	29,29,29,29	0
57	MG	1A	3536	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3055	1/1	0.97	0.07	14,14,14,14	0
57	MG	1A	3264	1/1	0.97	0.31	31,31,31,31	0
57	MG	2A	3255	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3636	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3749	1/1	0.97	0.14	58,58,58,58	0
57	MG	17	105	1/1	0.97	0.16	31,31,31,31	0
57	MG	1A	3187	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3009	1/1	0.97	0.05	7,7,7,7	0
57	MG	1A	3040	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3163	1/1	0.97	0.10	32,32,32,32	0
57	MG	1A	3165	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3453	1/1	0.97	0.12	25,25,25,25	0
57	MG	1A	3545	1/1	0.97	0.11	14,14,14,14	0
57	MG	2D	303	1/1	0.97	0.11	38,38,38,38	0
57	MG	1a	1743	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	3458	1/1	0.97	0.07	17,17,17,17	0
57	MG	2A	3457	1/1	0.97	0.14	31,31,31,31	0
57	MG	1A	3459	1/1	0.97	0.07	5,5,5,5	0
57	MG	1A	3008	1/1	0.97	0.14	17,17,17,17	0
57	MG	1A	3193	1/1	0.97	0.05	21,21,21,21	0
57	MG	1a	1748	1/1	0.97	0.05	57,57,57,57	0
57	MG	1A	3388	1/1	0.97	0.10	42,42,42,42	0
57	MG	2F	301	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3096	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3276	1/1	0.97	0.05	25,25,25,25	0
57	MG	2A	3099	1/1	0.97	0.09	53,53,53,53	0
57	MG	2A	3100	1/1	0.97	0.12	25,25,25,25	0
57	MG	2F	306	1/1	0.97	0.15	38,38,38,38	0
57	MG	1a	1610	1/1	0.97	0.14	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1A	3649	1/1	0.97	0.12	35,35,35,35	0
57	MG	2O	201	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3233	1/1	0.97	0.24	30,30,30,30	0
57	MG	1A	3553	1/1	0.97	0.10	12,12,12,12	0
57	MG	1A	3652	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3106	1/1	0.97	0.09	40,40,40,40	0
58	ZN	1n	102	1/1	0.97	0.04	85,85,85,85	0
57	MG	2A	3107	1/1	0.97	0.16	38,38,38,38	0
57	MG	2R	201	1/1	0.97	0.13	26,26,26,26	0
57	MG	2A	3287	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3531	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3766	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3189	1/1	0.98	0.15	60,60,60,60	0
57	MG	1a	1766	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3295	1/1	0.98	0.17	31,31,31,31	0
57	MG	1A	3685	1/1	0.98	0.04	37,37,37,37	0
57	MG	1V	201	1/1	0.98	0.14	17,17,17,17	0
57	MG	1A	3296	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3297	1/1	0.98	0.07	26,26,26,26	0
57	MG	2A	3196	1/1	0.98	0.11	34,34,34,34	0
57	MG	1A	3402	1/1	0.98	0.10	22,22,22,22	0
57	MG	1A	3773	1/1	0.98	0.08	11,11,11,11	0
57	MG	1A	3147	1/1	0.98	0.11	19,19,19,19	0
57	MG	1W	203	1/1	0.98	0.22	27,27,27,27	0
57	MG	1a	1670	1/1	0.98	0.20	35,35,35,35	0
57	MG	1A	3299	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3210	1/1	0.98	0.13	14,14,14,14	0
57	MG	1A	3097	1/1	0.98	0.16	29,29,29,29	0
57	MG	1A	3470	1/1	0.98	0.10	25,25,25,25	0
57	MG	1A	3779	1/1	0.98	0.06	29,29,29,29	0
57	MG	2A	3336	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3098	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3781	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3180	1/1	0.98	0.12	15,15,15,15	0
57	MG	1A	3473	1/1	0.98	0.04	11,11,11,11	0
57	MG	2A	3341	1/1	0.98	0.13	24,24,24,24	0
57	MG	2A	3211	1/1	0.98	0.22	29,29,29,29	0
57	MG	1A	3544	1/1	0.98	0.08	14,14,14,14	0
57	MG	2a	1675	1/1	0.98	0.12	32,32,32,32	0
57	MG	2A	3090	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3409	1/1	0.98	0.08	20,20,20,20	0
57	MG	2A	3092	1/1	0.98	0.09	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3214	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3547	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3181	1/1	0.98	0.04	19,19,19,19	0
57	MG	2A	3488	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3216	1/1	0.98	0.04	26,26,26,26	0
57	MG	2A	3097	1/1	0.98	0.06	44,44,44,44	0
57	MG	2A	3098	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3635	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3013	1/1	0.98	0.09	17,17,17,17	0
57	MG	2A	3354	1/1	0.98	0.12	35,35,35,35	0
57	MG	1A	3258	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3705	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3416	1/1	0.98	0.07	19,19,19,19	0
57	MG	2A	3359	1/1	0.98	0.12	50,50,50,50	0
57	MG	2A	3498	1/1	0.98	0.04	32,32,32,32	0
57	MG	2a	1694	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3226	1/1	0.98	0.09	44,44,44,44	0
57	MG	15	102	1/1	0.98	0.14	33,33,33,33	0
57	MG	1w	402	1/1	0.98	0.21	34,34,34,34	0
57	MG	1A	3629	1/1	0.98	0.06	61,61,61,61	0
57	MG	1A	3417	1/1	0.98	0.07	12,12,12,12	0
57	MG	17	102	1/1	0.98	0.22	24,24,24,24	0
57	MG	1A	3554	1/1	0.98	0.08	11,11,11,11	0
57	MG	1A	3003	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3078	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3712	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3153	1/1	0.98	0.15	21,21,21,21	0
57	MG	18	102	1/1	0.98	0.12	22,22,22,22	0
57	MG	2D	305	1/1	0.98	0.08	32,32,32,32	0
57	MG	19	101	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3221	1/1	0.98	0.09	27,27,27,27	0
57	MG	1B	208	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3005	1/1	0.98	0.09	34,34,34,34	0
57	MG	2E	302	1/1	0.98	0.15	37,37,37,37	0
57	MG	2A	3119	1/1	0.98	0.14	19,19,19,19	0
57	MG	2A	3516	1/1	0.98	0.04	55,55,55,55	0
57	MG	2A	3243	1/1	0.98	0.06	23,23,23,23	0
57	MG	2A	3120	1/1	0.98	0.08	46,46,46,46	0
57	MG	1A	3080	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3016	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3490	1/1	0.98	0.06	33,33,33,33	0
57	MG	1a	1606	1/1	0.98	0.21	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1A	3082	1/1	0.98	0.12	9,9,9,9	0
57	MG	1a	1608	1/1	0.98	0.12	49,49,49,49	0
57	MG	1A	3427	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3038	1/1	0.98	0.20	19,19,19,19	0
57	MG	1A	3131	1/1	0.98	0.08	19,19,19,19	0
57	MG	1A	3084	1/1	0.98	0.14	17,17,17,17	0
57	MG	1A	3569	1/1	0.98	0.08	52,52,52,52	0
57	MG	1A	3065	1/1	0.98	0.12	27,27,27,27	0
57	MG	1D	302	1/1	0.98	0.19	33,33,33,33	0
57	MG	1D	303	1/1	0.98	0.05	15,15,15,15	0
57	MG	1A	3271	1/1	0.98	0.10	17,17,17,17	0
57	MG	2A	3260	1/1	0.98	0.04	20,20,20,20	0
57	MG	2A	3261	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3434	1/1	0.98	0.04	8,8,8,8	0
57	MG	1A	3435	1/1	0.98	0.04	21,21,21,21	0
57	MG	1D	308	1/1	0.98	0.07	24,24,24,24	0
57	MG	1E	301	1/1	0.98	0.27	25,25,25,25	0
57	MG	2X	102	1/1	0.98	0.04	36,36,36,36	0
57	MG	1a	1724	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3574	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3575	1/1	0.98	0.03	35,35,35,35	0
57	MG	1A	3231	1/1	0.98	0.08	25,25,25,25	0
57	MG	1A	3273	1/1	0.98	0.24	24,24,24,24	0
57	MG	25	101	1/1	0.98	0.05	49,49,49,49	0
57	MG	1a	1729	1/1	0.98	0.15	53,53,53,53	0
57	MG	1A	3503	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3734	1/1	0.98	0.05	28,28,28,28	0
57	MG	2a	1601	1/1	0.98	0.16	35,35,35,35	0
57	MG	2A	3274	1/1	0.98	0.09	26,26,26,26	0
57	MG	2A	3148	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3274	1/1	0.98	0.19	25,25,25,25	0
57	MG	1A	3194	1/1	0.98	0.10	25,25,25,25	0
57	MG	1A	3379	1/1	0.98	0.10	45,45,45,45	0
57	MG	1a	1631	1/1	0.98	0.10	41,41,41,41	0
57	MG	2A	3153	1/1	0.98	0.11	29,29,29,29	0
57	MG	2A	3038	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3012	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3660	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3157	1/1	0.98	0.09	22,22,22,22	0
57	MG	2A	3422	1/1	0.98	0.10	49,49,49,49	0
57	MG	1A	3443	1/1	0.98	0.09	14,14,14,14	0
57	MG	1A	3135	1/1	0.98	0.18	18,18,18,18	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	1A	3023	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3041	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	3053	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3200	1/1	0.98	0.08	17,17,17,17	0
57	MG	1A	3667	1/1	0.98	0.04	27,27,27,27	0
57	MG	2A	3166	1/1	0.98	0.17	39,39,39,39	0
57	MG	1A	3024	1/1	0.98	0.04	14,14,14,14	0
57	MG	1A	3335	1/1	0.98	0.07	17,17,17,17	0
57	MG	1A	3043	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	3517	1/1	0.98	0.05	21,21,21,21	0
57	MG	1A	3518	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3753	1/1	0.98	0.10	48,48,48,48	0
57	MG	1A	3389	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3092	1/1	0.98	0.14	35,35,35,35	0
57	MG	1Q	202	1/1	0.98	0.12	22,22,22,22	0
57	MG	1Q	203	1/1	0.98	0.09	18,18,18,18	0
57	MG	1A	3056	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3057	1/1	0.98	0.07	9,9,9,9	0
57	MG	2A	3306	1/1	0.98	0.15	33,33,33,33	0
57	MG	2A	3179	1/1	0.98	0.04	28,28,28,28	0
57	MG	2A	3060	1/1	0.98	0.08	48,48,48,48	0
57	MG	1A	3289	1/1	0.98	0.16	7,7,7,7	0
57	MG	2A	3587	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3447	1/1	0.98	0.14	59,59,59,59	0
57	MG	1A	3144	1/1	0.98	0.21	17,17,17,17	0
57	MG	1A	3291	1/1	0.98	0.10	22,22,22,22	0
57	MG	2A	3450	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3095	1/1	0.98	0.17	23,23,23,23	0
57	MG	1A	3075	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3294	1/1	0.98	0.10	37,37,37,37	0
57	MG	2A	3595	1/1	0.98	0.12	65,65,65,65	0
59	SF4	1d	302	8/8	0.98	0.04	52,61,71,77	0
59	SF4	2d	303	8/8	0.98	0.04	49,56,67,71	0
57	MG	2A	3029	1/1	0.99	0.05	29,29,29,29	0
57	MG	1a	1733	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3058	1/1	0.99	0.07	16,16,16,16	0
57	MG	1A	3099	1/1	0.99	0.09	21,21,21,21	0
57	MG	17	101	1/1	0.99	0.03	23,23,23,23	0
57	MG	1D	301	1/1	0.99	0.04	26,26,26,26	0
57	MG	1A	3049	1/1	0.99	0.08	20,20,20,20	0
57	MG	17	104	1/1	0.99	0.07	20,20,20,20	0
57	MG	1A	3555	1/1	0.99	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
57	MG	1A	3330	1/1	0.99	0.03	21,21,21,21	0
57	MG	2A	3322	1/1	0.99	0.07	19,19,19,19	0
57	MG	2A	3385	1/1	0.99	0.03	47,47,47,47	0
57	MG	1D	305	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3172	1/1	0.99	0.06	9,9,9,9	0
57	MG	1A	3637	1/1	0.99	0.10	23,23,23,23	0
57	MG	1A	3609	1/1	0.99	0.04	13,13,13,13	0
57	MG	1A	3164	1/1	0.99	0.04	24,24,24,24	0
57	MG	1U	203	1/1	0.99	0.04	21,21,21,21	0
57	MG	1E	302	1/1	0.99	0.10	22,22,22,22	0
57	MG	1A	3757	1/1	0.99	0.14	29,29,29,29	0
57	MG	1A	3228	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3585	1/1	0.99	0.05	8,8,8,8	0
57	MG	1A	3424	1/1	0.99	0.04	14,14,14,14	0
57	MG	1A	3275	1/1	0.99	0.14	26,26,26,26	0
57	MG	1A	3794	1/1	0.99	0.05	15,15,15,15	0
57	MG	2D	302	1/1	0.99	0.09	20,20,20,20	0
57	MG	1a	1705	1/1	0.99	0.12	42,42,42,42	0
57	MG	1V	204	1/1	0.99	0.08	17,17,17,17	0
57	MG	2A	3165	1/1	0.99	0.16	28,28,28,28	0
57	MG	2A	3280	1/1	0.99	0.15	31,31,31,31	0
57	MG	1A	3304	1/1	0.99	0.12	29,29,29,29	0
57	MG	1A	3353	1/1	0.99	0.08	19,19,19,19	0
57	MG	2a	1762	1/1	0.99	0.10	36,36,36,36	0
57	MG	1A	3251	1/1	0.99	0.05	25,25,25,25	0
57	MG	1A	3337	1/1	0.99	0.04	27,27,27,27	0
57	MG	2A	3003	1/1	0.99	0.11	17,17,17,17	0
57	MG	1F	304	1/1	0.99	0.22	18,18,18,18	0
57	MG	2A	3115	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3070	1/1	0.99	0.03	28,28,28,28	0
57	MG	1F	306	1/1	0.99	0.08	19,19,19,19	0
57	MG	2A	3536	1/1	0.99	0.04	52,52,52,52	0
57	MG	2A	3007	1/1	0.99	0.03	33,33,33,33	0
57	MG	2A	3603	1/1	0.99	0.05	29,29,29,29	0
57	MG	1F	307	1/1	0.99	0.09	17,17,17,17	0
57	MG	1F	308	1/1	0.99	0.10	17,17,17,17	0
57	MG	1A	3736	1/1	0.99	0.05	14,14,14,14	0
57	MG	1A	3278	1/1	0.99	0.11	22,22,22,22	0
57	MG	1F	311	1/1	0.99	0.03	21,21,21,21	0
57	MG	2A	3355	1/1	0.99	0.10	26,26,26,26	0
57	MG	1A	3412	1/1	0.99	0.07	8,8,8,8	0
57	MG	1A	3498	1/1	0.99	0.06	8,8,8,8	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	1A	3034	1/1	0.99	0.14	8,8,8,8	0
57	MG	1A	3772	1/1	0.99	0.03	15,15,15,15	0
57	MG	1A	3624	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3061	1/1	0.99	0.10	32,32,32,32	0
57	MG	1A	3232	1/1	0.99	0.13	22,22,22,22	0
57	MG	1A	3524	1/1	0.99	0.02	28,28,28,28	0
57	MG	2A	3364	1/1	0.99	0.07	34,34,34,34	0
57	MG	1a	1777	1/1	0.99	0.06	50,50,50,50	0
57	MG	2A	3022	1/1	0.99	0.04	34,34,34,34	0
58	ZN	1Y	501	1/1	0.99	0.03	51,51,51,51	0
57	MG	13	101	1/1	0.99	0.12	20,20,20,20	0
58	ZN	16	102	1/1	0.99	0.02	38,38,38,38	0
58	ZN	19	103	1/1	0.99	0.04	38,38,38,38	0
57	MG	2A	3557	1/1	0.99	0.03	45,45,45,45	0
57	MG	1A	3525	1/1	0.99	0.05	12,12,12,12	0
57	MG	1A	3437	1/1	0.99	0.07	16,16,16,16	0
58	ZN	26	102	1/1	0.99	0.03	56,56,56,56	0
58	ZN	29	102	1/1	0.99	0.03	58,58,58,58	0
57	MG	1B	217	1/1	0.99	0.04	41,41,41,41	0
57	MG	1A	3036	1/1	0.99	0.15	21,21,21,21	0
57	MG	15	103	1/1	0.99	0.15	19,19,19,19	0
58	ZN	25	102	1/1	1.00	0.04	51,51,51,51	0
57	MG	2A	3548	1/1	1.00	0.03	16,16,16,16	0
57	MG	2A	3365	1/1	1.00	0.05	37,37,37,37	0
57	MG	1A	3484	1/1	1.00	0.03	10,10,10,10	0
57	MG	1A	3433	1/1	1.00	0.05	27,27,27,27	0
58	ZN	15	105	1/1	1.00	0.03	24,24,24,24	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.