



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2024 – 07:14 PM EST

PDB ID : 9DFD
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with lasso peptide lariocidin B, mRNA, aminoacylated A-site Phe-tRNA_{Phe}, aminoacylated P-site fMet-tRNA_{Met}, and deacylated E-site tRNA_{Phe} at 2.60Å resolution
Authors : Aleksandrova, E.V.; Travin, D.Y.; Jangra, M.; Kaur, M.; Darwish, L.; Koteva, K.; Klepacki, D.; Wang, W.; Tiffany, M.; Sokaribo, A.; Coombes, B.K.; Vazquez-Laslop, N.; Wright, G.D.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2024-08-29
Resolution : 2.60 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

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)

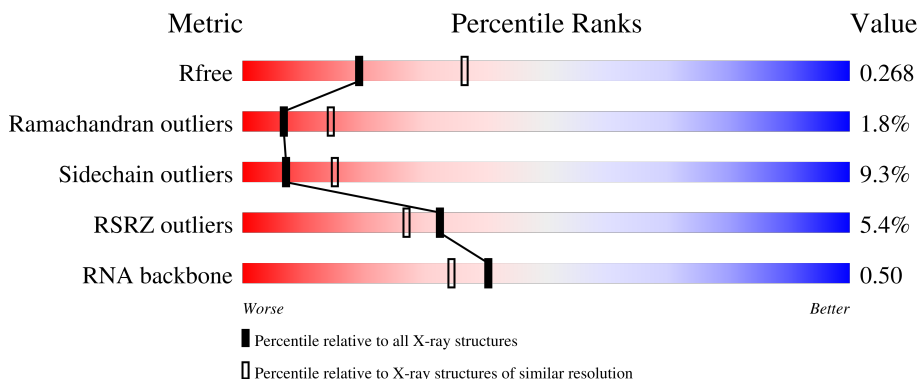
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


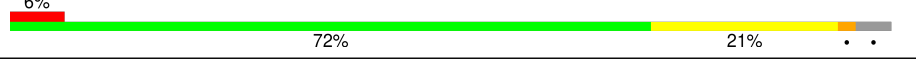

The reported resolution of this entry is 2.60 Å.

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	3775 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)
RNA backbone	3690	1025 (2.88-2.32)

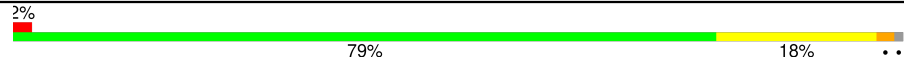
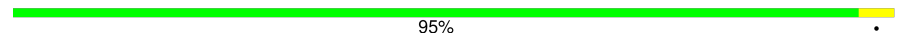
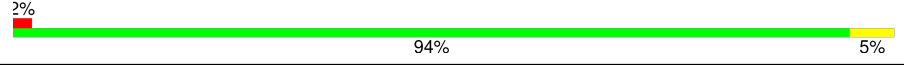
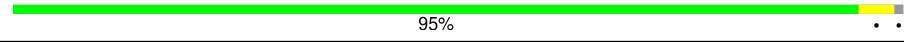
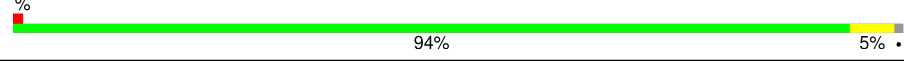

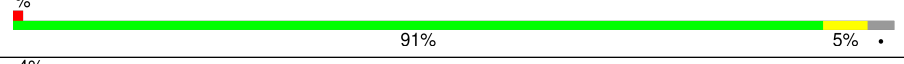
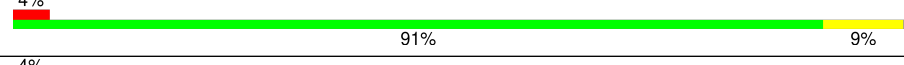
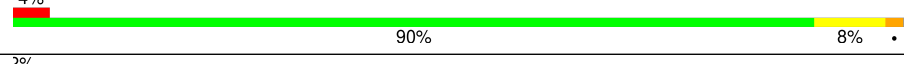
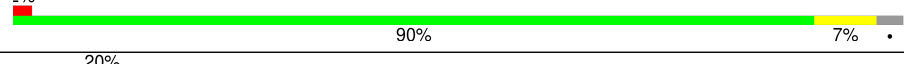
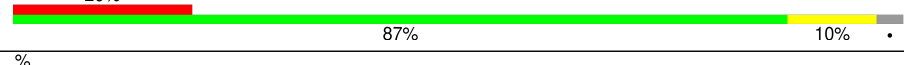
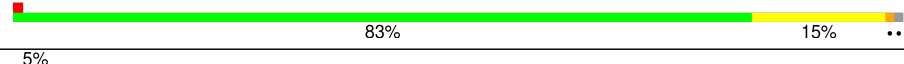
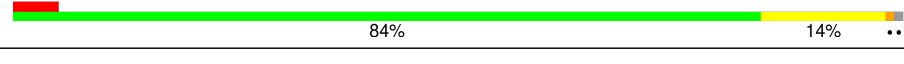
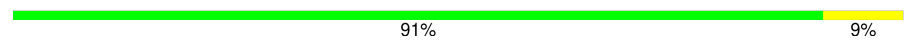
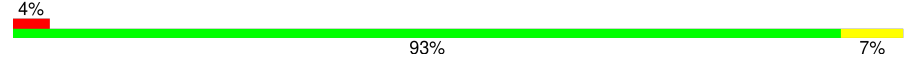
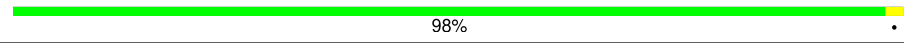
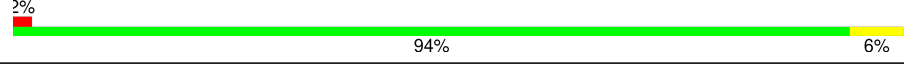
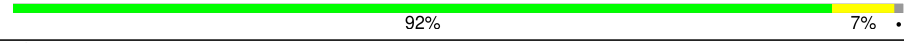
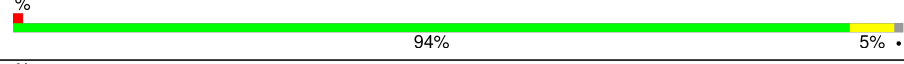
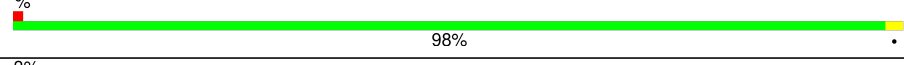
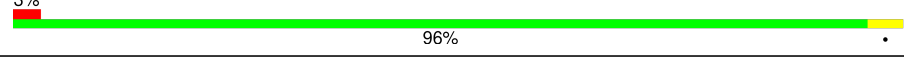
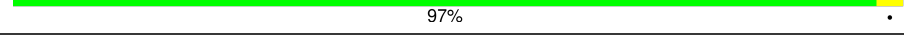
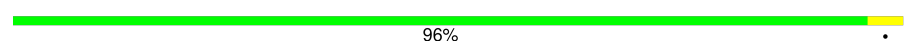
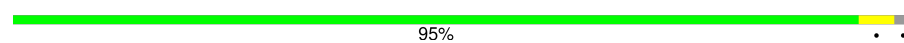
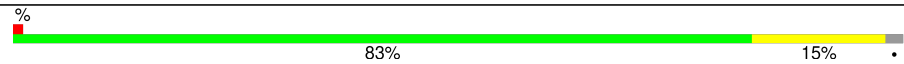
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	2A	2915	
2	1B	121	

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	 2% 79% 18%
3	1D	276	 95%
3	2D	276	 2% 94% 5%
4	1E	206	 95%
4	2E	206	 % 94% 5%
5	1F	210	 88% 8%
5	2F	210	 % 91% 5%
6	1G	182	 4% 91% 9%
6	2G	182	 4% 90% 8%
7	1H	180	 2% 90% 7%
7	2H	180	 20% 87% 10%
8	1I	148	 % 83% 15%
8	2I	148	 5% 84% 14%
9	1N	140	 91% 9%
9	2N	140	 4% 93% 7%
10	1O	122	 98%
10	2O	122	 2% 94% 6%
11	1P	150	 92% 7%
11	2P	150	 % 94% 5%
12	1Q	141	 % 98%
12	2Q	141	 3% 96%
13	1R	118	 97%
13	2R	118	 96%
14	1S	112	 95%
14	2S	112	 % 83% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	84% 5% 10% 3%
15	2T	146	86% 10% 10% 3%
16	1U	118	92% 6% 10%
16	2U	118	94% 10% 10% 3%
17	1V	101	89% 10% 10%
17	2V	101	92% 7% 10%
18	1W	113	94% 5% 10% 3%
18	2W	113	92% 7% 10% 3%
19	1X	96	95% 10% 10% 2%
19	2X	96	93% 6% 10% 2%
20	1Y	110	91% 6% 10%
20	2Y	110	85% 12% 10% 9%
21	1Z	206	68% 5% 25% 2%
21	2Z	206	65% 13% 22% 13%
22	10	85	93% 5% 10% 3%
22	20	85	94% 10% 10% 3%
23	11	98	94% 5% 10% 2%
23	21	98	95% 10% 10% 4%
24	12	72	88% 10% 10% 3%
24	22	72	90% 7% 10% 3%
25	13	60	92% 7% 10%
25	23	60	93% 5% 10% 3%
26	14	71	80% 14% 10% 10%
26	24	71	70% 24% 10% 13%
27	15	60	90% 8% 10%

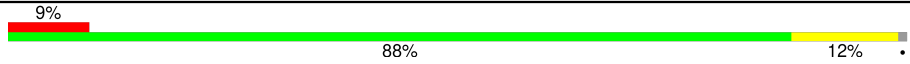
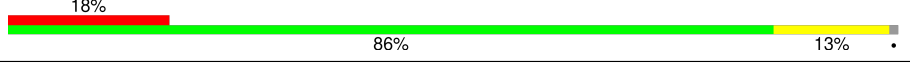
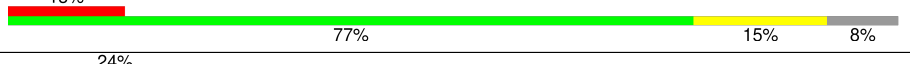


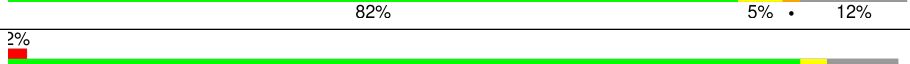
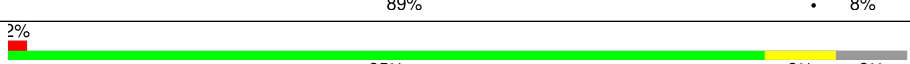
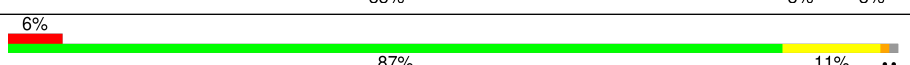
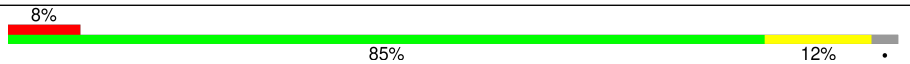


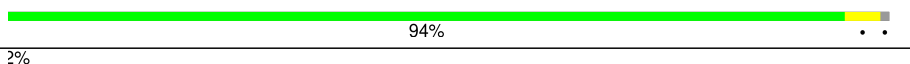
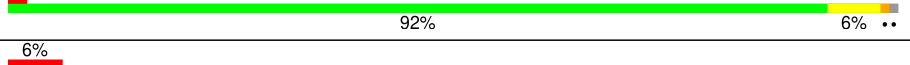

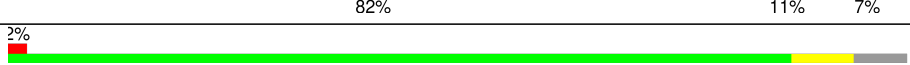










Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	95%
28	16	54	93%
28	26	54	2%
29	17	49	2%
29	27	49	8%
30	18	65	92%
30	28	65	2%
31	19	37	92%
31	29	37	3%
32	1a	1521	5%
32	2a	1521	5%
33	1b	256	10%
33	2b	256	9%
34	1c	239	2%
34	2c	239	8%
35	1d	209	12%
35	2d	209	5%
36	1e	162	%
36	2e	162	3%
37	1f	101	92%
37	2f	101	%
38	1g	156	6%
38	2g	156	10%
39	1h	138	2%
39	2h	138	%

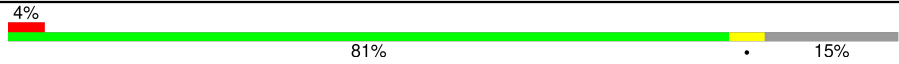
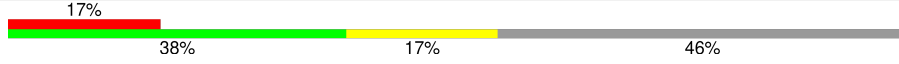
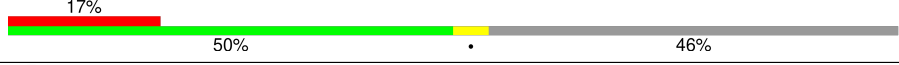

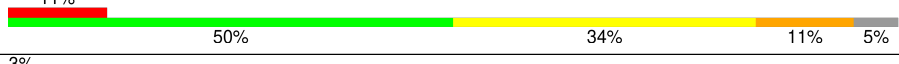
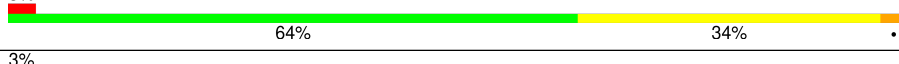
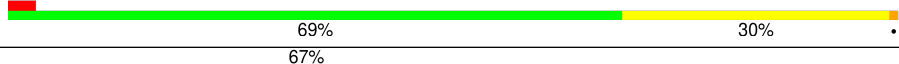



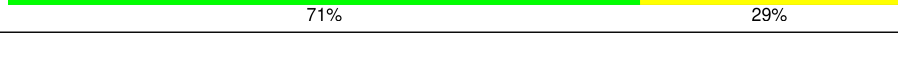
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	
57	1z	17	
57	2z	17	

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
58	MG	29	101	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 300583 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			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	125	979	604	204	169	2	0	0	0
44	2m	122	950	586	197	165	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-PHE-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
54	1w	75	Total 1623	C 731	N 289	O 526	P 75	S 2	0	0	0
54	2w	72	Total 1555	C 699	N 280	O 502	P 72	S 2	0	0	0

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNA_{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	77	Total 1656	C 740	N 299	O 538	P 77	S 2	0	0	0
55	2x	77	Total 1656	C 740	N 299	O 538	P 77	S 2	0	0	0

- Molecule 56 is a RNA chain called E-site Deacylated tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
56	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
56	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

- Molecule 57 is a protein called Lasso peptide lariocidin B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	1z	17	Total 127	C 79	N 28	O 20	0	0	0
57	2z	17	Total 127	C 79	N 28	O 20	0	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1105	Total 1105	Mg 1105	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	12	Total 12	Mg 12	0	0
58	1E	14	Total 14	Mg 14	0	0
58	1F	13	Total 13	Mg 13	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	7	Total 7	Mg 7	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	4	Total 4	Mg 4	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	4	Total 4	Mg 4	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	3	Total 3	Mg 3	0	0
58	1U	11	Total 11	Mg 11	0	0
58	1V	7	Total 7	Mg 7	0	0
58	1W	8	Total 8	Mg 8	0	0
58	1X	6	Total 6	Mg 6	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	3	Total 3	Mg 3	0	0
58	10	9	Total 9	Mg 9	0	0
58	11	6	Total 6	Mg 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	12	2	Total Mg 2 2	0	0
58	13	3	Total Mg 3 3	0	0
58	15	9	Total Mg 9 9	0	0
58	16	2	Total Mg 2 2	0	0
58	17	3	Total Mg 3 3	0	0
58	18	5	Total Mg 5 5	0	0
58	19	1	Total Mg 1 1	0	0
58	1a	218	Total Mg 218 218	0	0
58	1b	1	Total Mg 1 1	0	0
58	1d	1	Total Mg 1 1	0	0
58	1e	2	Total Mg 2 2	0	0
58	1f	2	Total Mg 2 2	0	0
58	1h	1	Total Mg 1 1	0	0
58	1l	2	Total Mg 2 2	0	0
58	1m	1	Total Mg 1 1	0	0
58	1n	1	Total Mg 1 1	0	0
58	1p	1	Total Mg 1 1	0	0
58	1s	1	Total Mg 1 1	0	0
58	1t	1	Total Mg 1 1	0	0
58	1v	2	Total Mg 2 2	0	0
58	1w	8	Total Mg 8 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1x	13	Total Mg 13 13	0	0
58	1y	1	Total Mg 1 1	0	0
58	2A	883	Total Mg 883 883	0	0
58	2B	19	Total Mg 19 19	0	0
58	2D	7	Total Mg 7 7	0	0
58	2E	11	Total Mg 11 11	0	0
58	2F	9	Total Mg 9 9	0	0
58	2G	1	Total Mg 1 1	0	0
58	2N	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2Q	3	Total Mg 3 3	0	0
58	2R	3	Total Mg 3 3	0	0
58	2S	1	Total Mg 1 1	0	0
58	2T	3	Total Mg 3 3	0	0
58	2U	2	Total Mg 2 2	0	0
58	2V	2	Total Mg 2 2	0	0
58	2W	2	Total Mg 2 2	0	0
58	2X	1	Total Mg 1 1	0	0
58	2Z	1	Total Mg 1 1	0	0
58	21	1	Total Mg 1 1	0	0
58	23	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	25	4	Total Mg 4 4	0	0
58	26	1	Total Mg 1 1	0	0
58	27	3	Total Mg 3 3	0	0
58	28	4	Total Mg 4 4	0	0
58	29	1	Total Mg 1 1	0	0
58	2a	242	Total Mg 242 242	0	0
58	2d	1	Total Mg 1 1	0	0
58	2e	1	Total Mg 1 1	0	0
58	2f	2	Total Mg 2 2	0	0
58	2g	1	Total Mg 1 1	0	0
58	2i	1	Total Mg 1 1	0	0
58	2j	1	Total Mg 1 1	0	0
58	2l	5	Total Mg 5 5	0	0
58	2p	1	Total Mg 1 1	0	0
58	2q	2	Total Mg 2 2	0	0
58	2r	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	3	Total Mg 3 3	0	0
58	2w	12	Total Mg 12 12	0	0
58	2x	5	Total Mg 5 5	0	0
58	2y	6	Total Mg 6 6	0	0

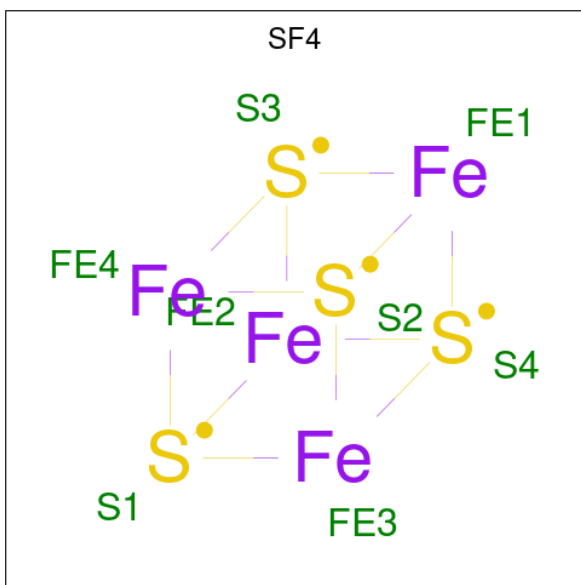
- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0
59	2x	1	Total K 1 1	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	2019	Total O 2019 2019	0	0
62	1B	63	Total O 63 63	0	0
62	1D	24	Total O 24 24	0	0
62	1E	24	Total O 24 24	0	0
62	1F	15	Total O 15 15	0	0
62	1G	2	Total O 2 2	0	0
62	1H	2	Total O 2 2	0	0
62	1I	1	Total O 1 1	0	0
62	1N	5	Total O 5 5	0	0
62	1O	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	19	Total 19	O 19	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	12	Total 12	O 12	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	9	Total 9	O 9	0	0
62	1U	15	Total 15	O 15	0	0
62	1V	8	Total 8	O 8	0	0
62	1W	9	Total 9	O 9	0	0
62	1X	4	Total 4	O 4	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	13	Total 13	O 13	0	0
62	11	11	Total 11	O 11	0	0
62	12	4	Total 4	O 4	0	0
62	13	5	Total 5	O 5	0	0
62	14	1	Total 1	O 1	0	0
62	15	5	Total 5	O 5	0	0
62	16	4	Total 4	O 4	0	0
62	17	7	Total 7	O 7	0	0
62	18	9	Total 9	O 9	0	0
62	1a	388	Total 388	O 388	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1b	1	Total O 1 1	0	0
62	1f	1	Total O 1 1	0	0
62	1l	8	Total O 8 8	0	0
62	1m	2	Total O 2 2	0	0
62	1n	1	Total O 1 1	0	0
62	1o	1	Total O 1 1	0	0
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1u	1	Total O 1 1	0	0
62	1v	6	Total O 6 6	0	0
62	1w	20	Total O 20 20	0	0
62	1x	15	Total O 15 15	0	0
62	1y	2	Total O 2 2	0	0
62	1z	1	Total O 1 1	0	0
62	2A	1153	Total O 1153 1153	0	0
62	2B	23	Total O 23 23	0	0
62	2D	24	Total O 24 24	0	0
62	2E	14	Total O 14 14	0	0
62	2F	13	Total O 13 13	0	0
62	2I	2	Total O 2 2	0	0
62	2N	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2O	3	Total 3	O 3	0	0
62	2P	14	Total 14	O 14	0	0
62	2Q	3	Total 3	O 3	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	4	Total 4	O 4	0	0
62	2U	2	Total 2	O 2	0	0
62	2W	2	Total 2	O 2	0	0
62	2X	2	Total 2	O 2	0	0
62	2Y	1	Total 1	O 1	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	3	Total 3	O 3	0	0
62	21	13	Total 13	O 13	0	0
62	23	1	Total 1	O 1	0	0
62	25	1	Total 1	O 1	0	0
62	27	5	Total 5	O 5	0	0
62	28	4	Total 4	O 4	0	0
62	29	1	Total 1	O 1	0	0
62	2a	283	Total 283	O 283	0	0
62	2c	2	Total 2	O 2	0	0
62	2d	2	Total 2	O 2	0	0
62	2e	1	Total 1	O 1	0	0

Continued on next page...

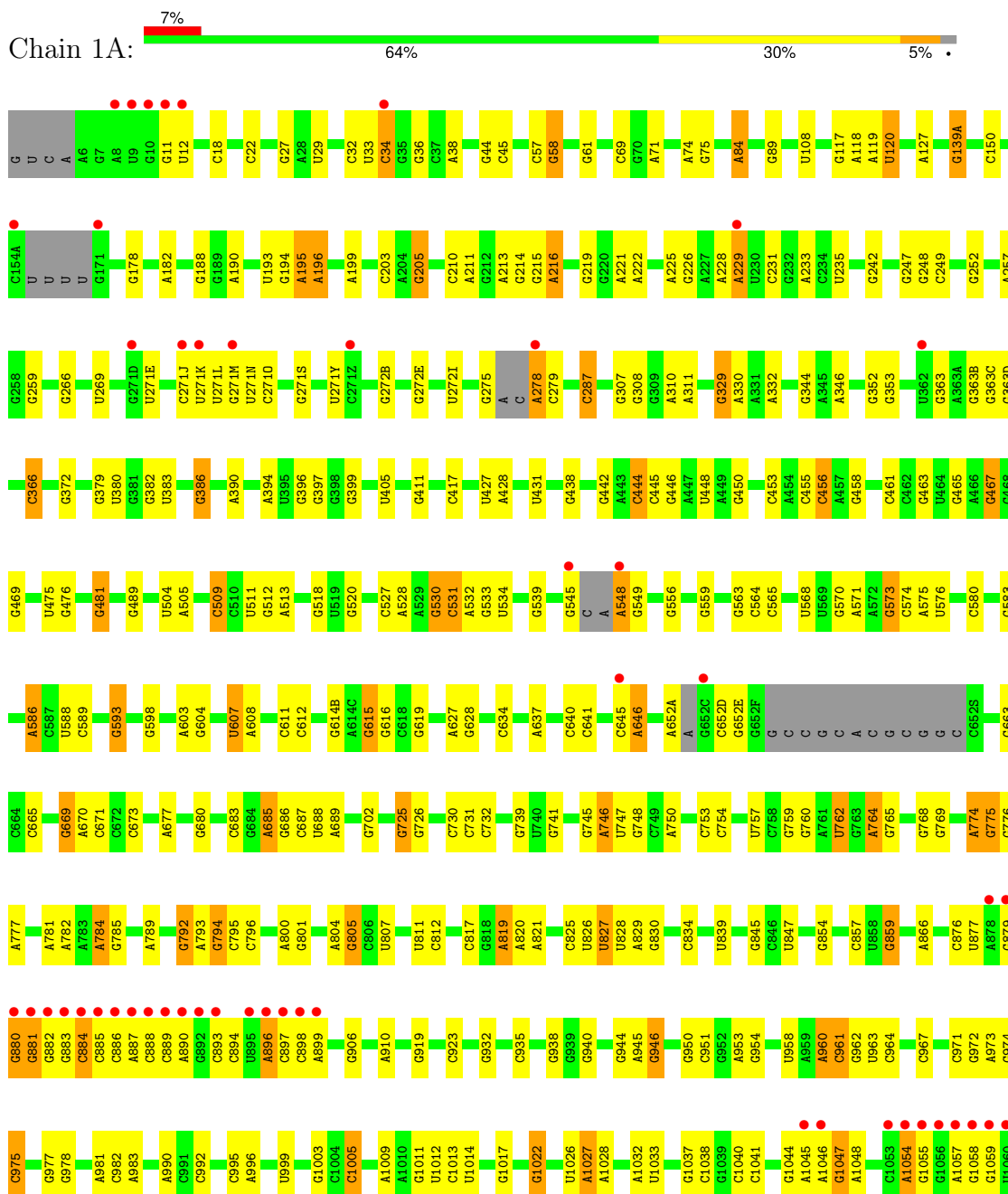
Continued from previous page...

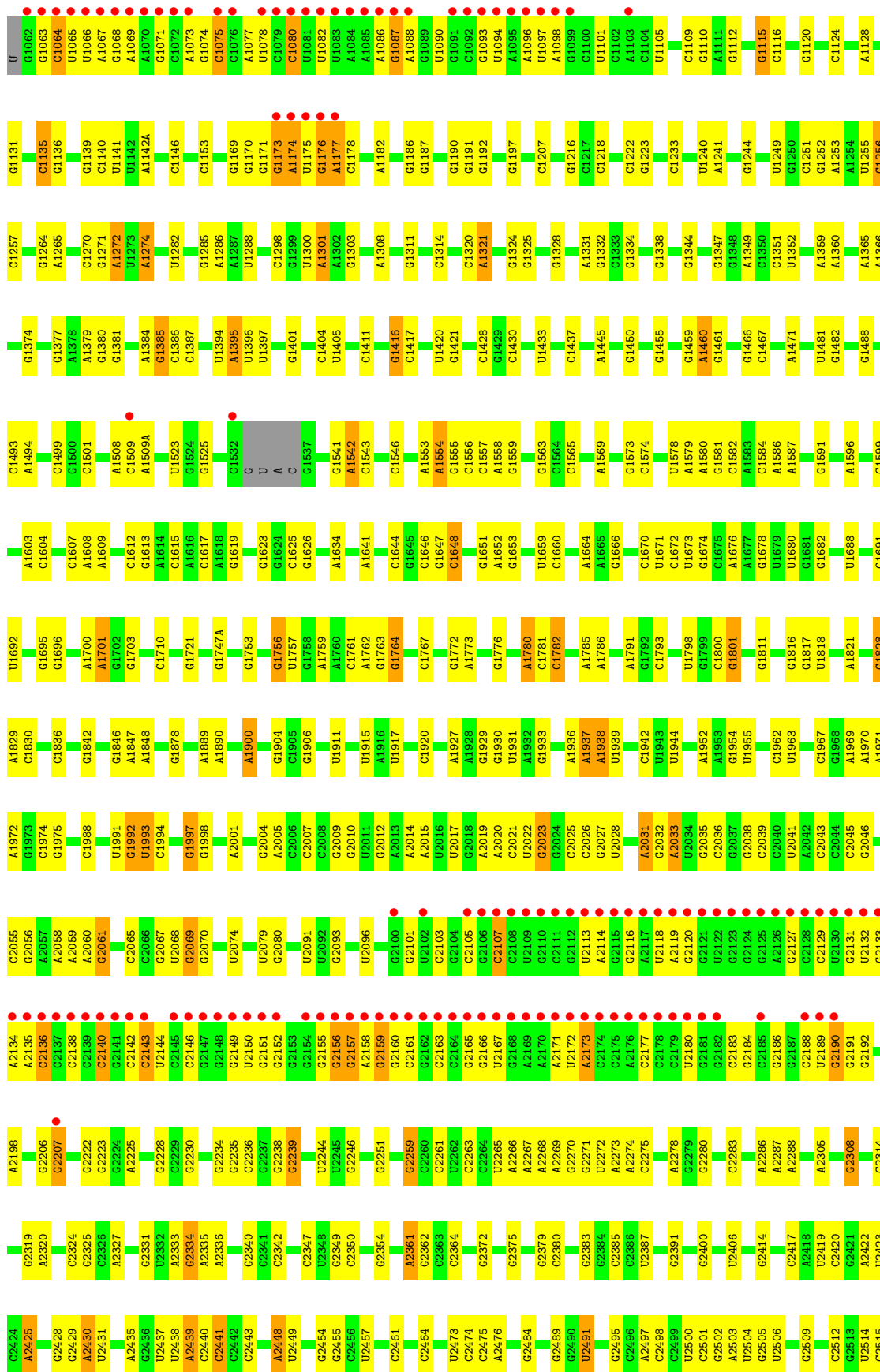
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2j	3	Total 3	O 3	0	0
62	2l	6	Total 6	O 6	0	0
62	2p	1	Total 1	O 1	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	1	Total 1	O 1	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	10	Total 10	O 10	0	0
62	2x	6	Total 6	O 6	0	0
62	2y	9	Total 9	O 9	0	0

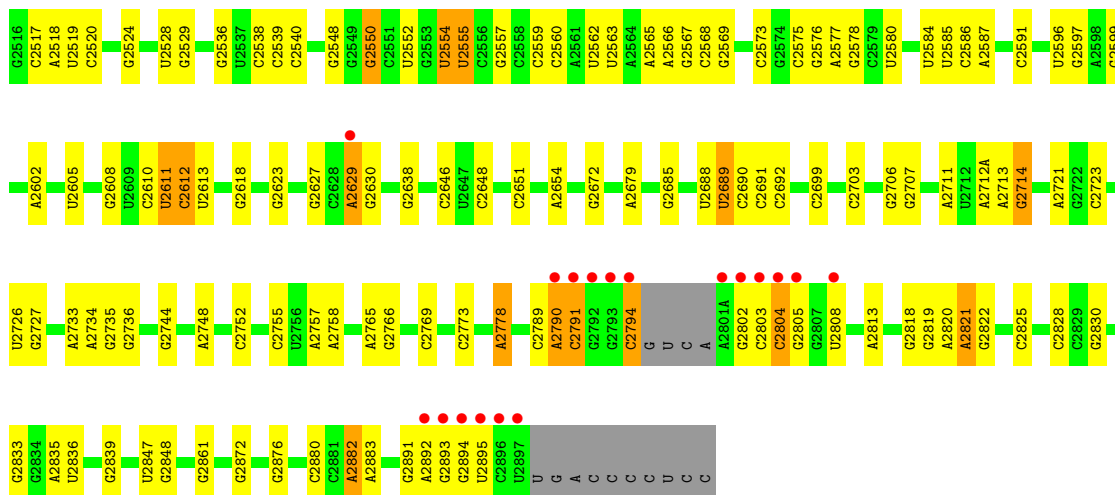
3 Residue-property plots i

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.

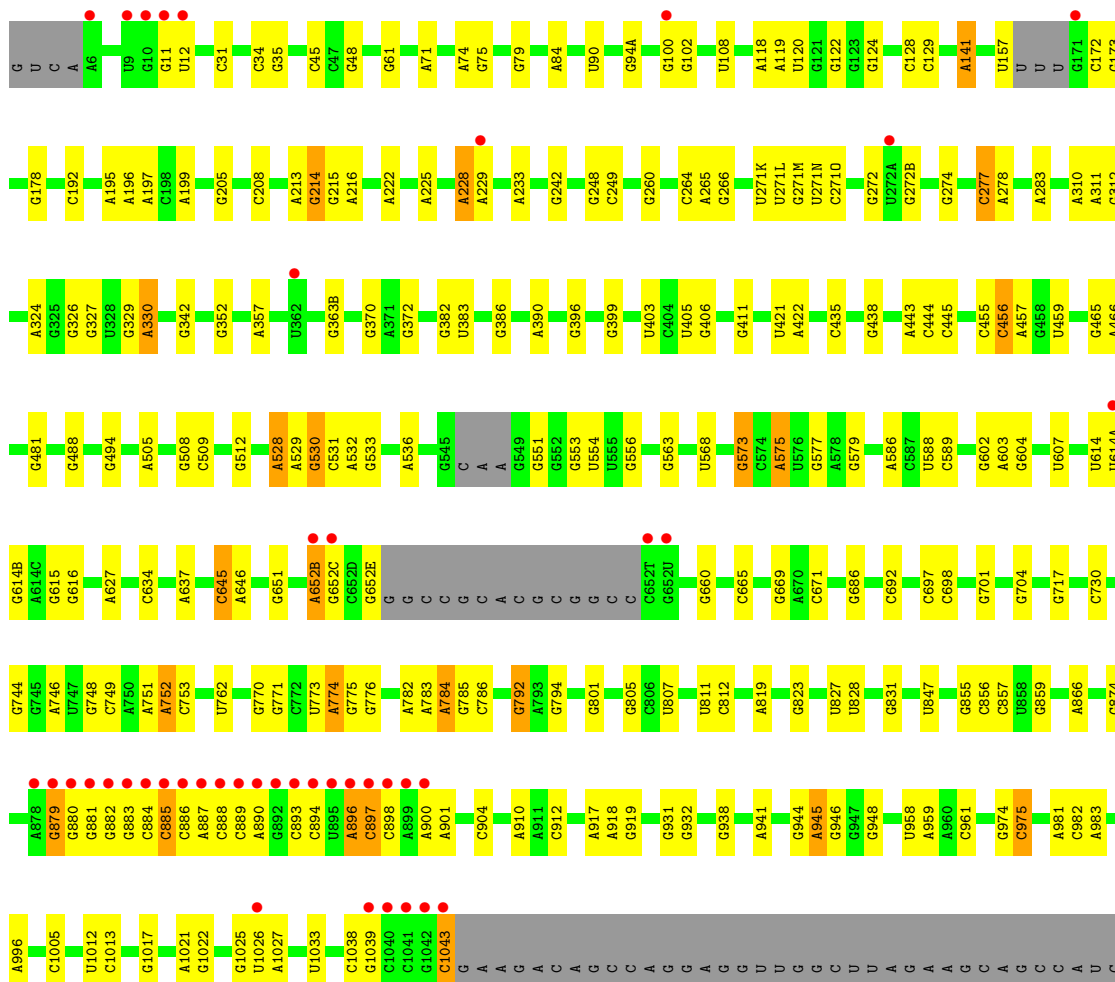
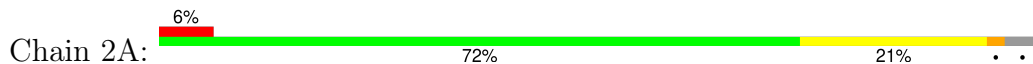
- Molecule 1: 23S Ribosomal RNA

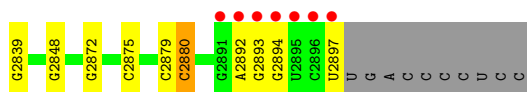






● Molecule 1: 23S Ribosomal RNA





- Molecule 2: 5S Ribosomal RNA

Chain 1B: 77% 20%



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 79% 18% 2%



- Molecule 3: 50S ribosomal protein L2

Chain 1D: 95%



- Molecule 3: 50S ribosomal protein L2

Chain 2D: 94% 5% 2%



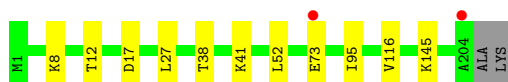
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 95%



- Molecule 4: 50S ribosomal protein L3

Chain 2E: 94% 5% 1%



- Molecule 5: 50S ribosomal protein L4

Chain 1F: 88% 8%



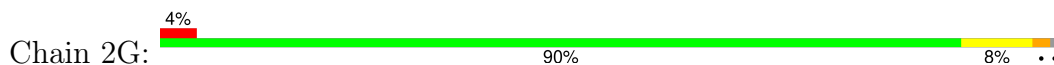
• Molecule 5: 50S ribosomal protein L4



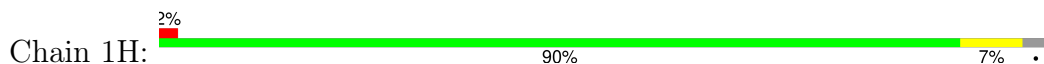
• Molecule 6: 50S ribosomal protein L5



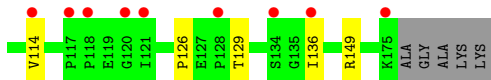
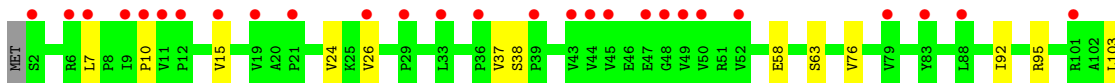
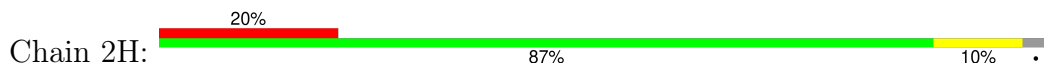
• Molecule 6: 50S ribosomal protein L5



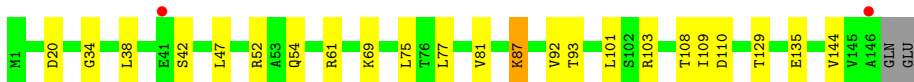
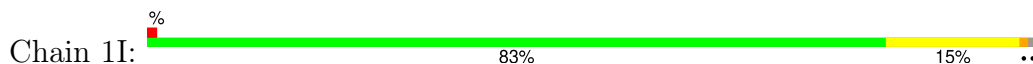
• Molecule 7: 50S ribosomal protein L6



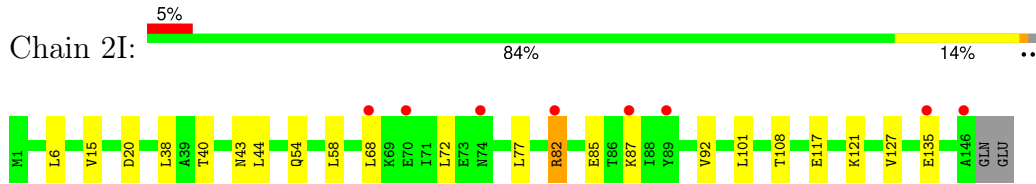
• Molecule 7: 50S ribosomal protein L6



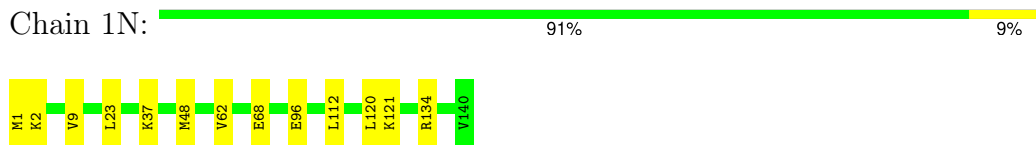
• Molecule 8: 50S ribosomal protein L9



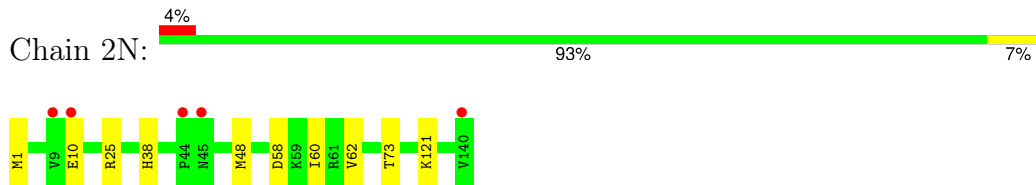
- Molecule 8: 50S ribosomal protein L9



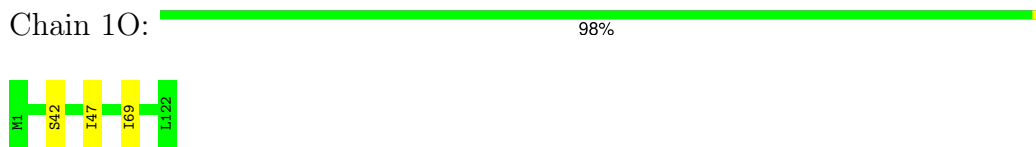
- Molecule 9: 50S ribosomal protein L13



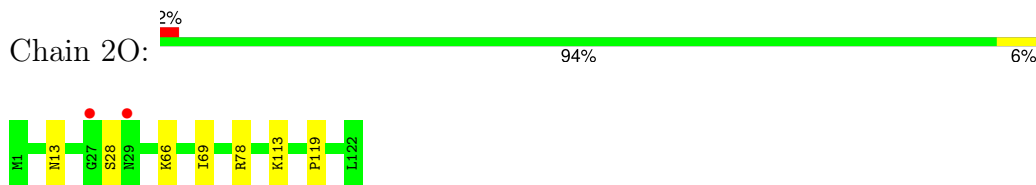
- Molecule 9: 50S ribosomal protein L13



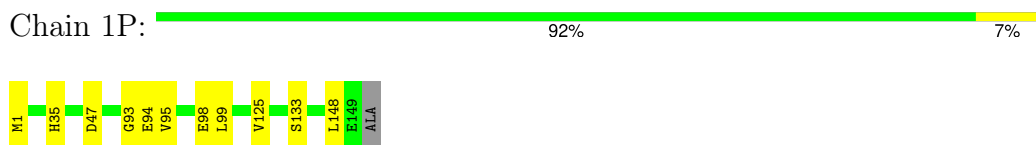
- Molecule 10: 50S ribosomal protein L14



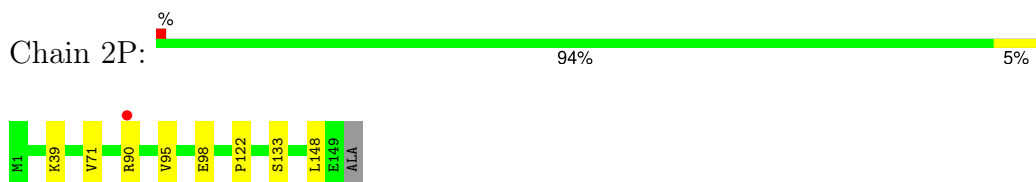
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15



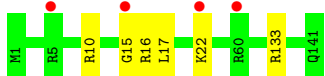
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



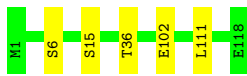
- Molecule 12: 50S ribosomal protein L16



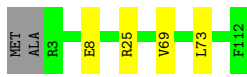
- Molecule 13: 50S ribosomal protein L17



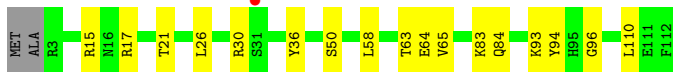
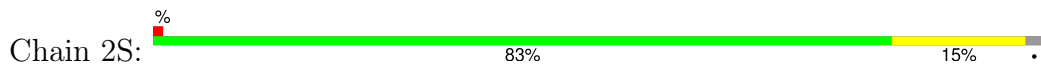
- Molecule 13: 50S ribosomal protein L17



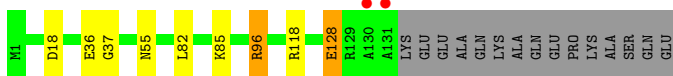
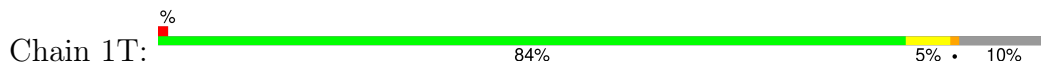
- Molecule 14: 50S ribosomal protein L18



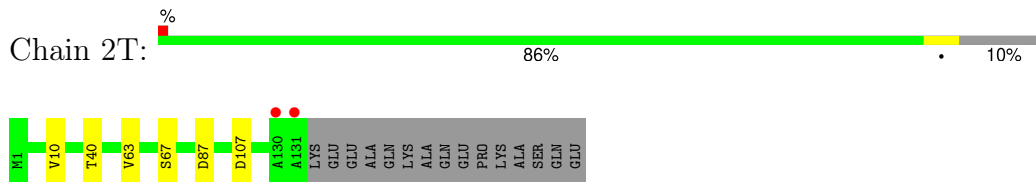
- Molecule 14: 50S ribosomal protein L18



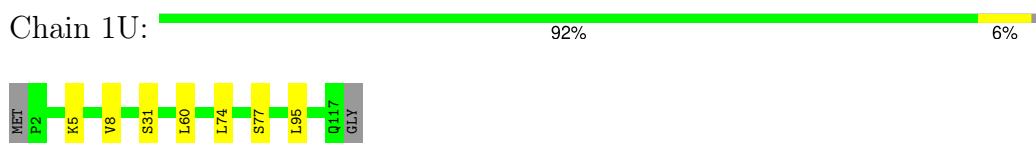
- Molecule 15: 50S ribosomal protein L19



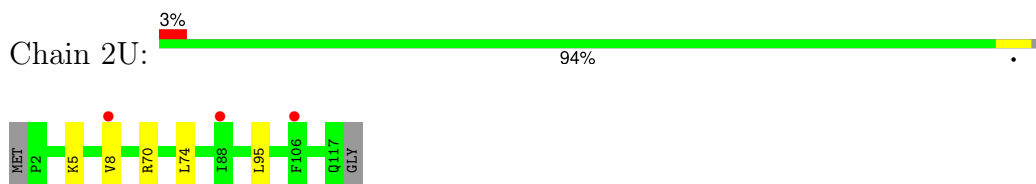
- Molecule 15: 50S ribosomal protein L19



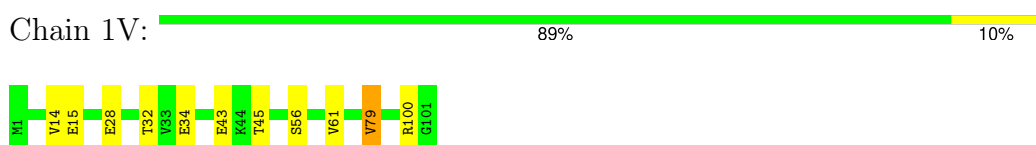
- Molecule 16: 50S ribosomal protein L20



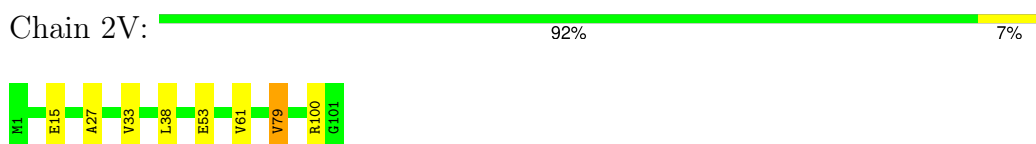
- Molecule 16: 50S ribosomal protein L20



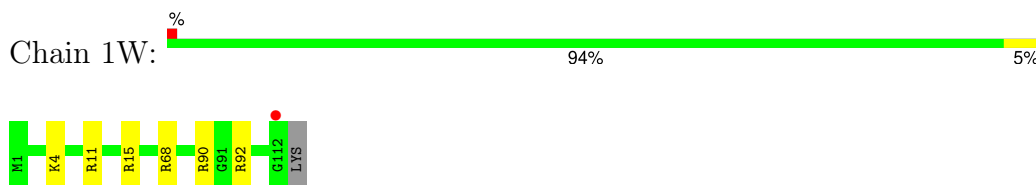
- Molecule 17: 50S ribosomal protein L21



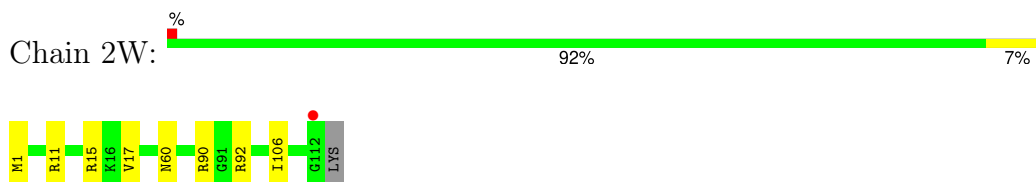
- Molecule 17: 50S ribosomal protein L21



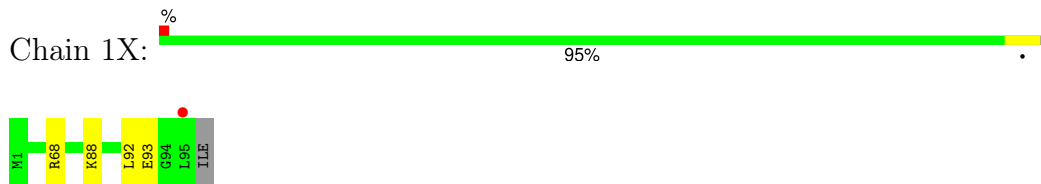
- Molecule 18: 50S ribosomal protein L22



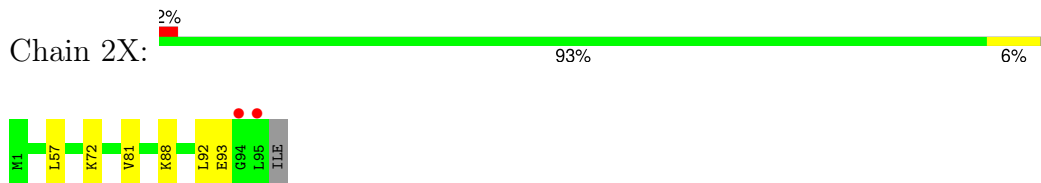
- Molecule 18: 50S ribosomal protein L22



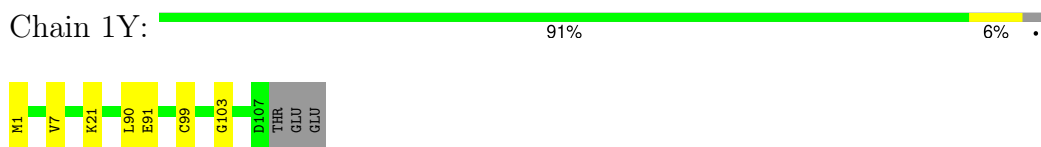
- Molecule 19: 50S ribosomal protein L23



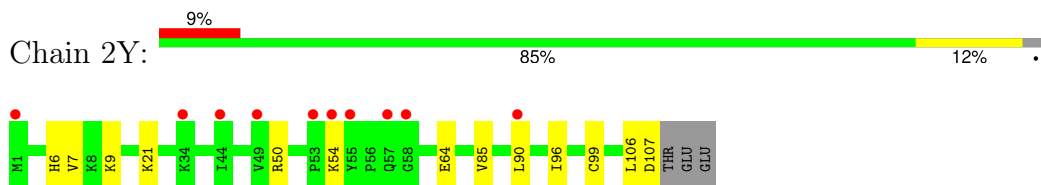
- Molecule 19: 50S ribosomal protein L23



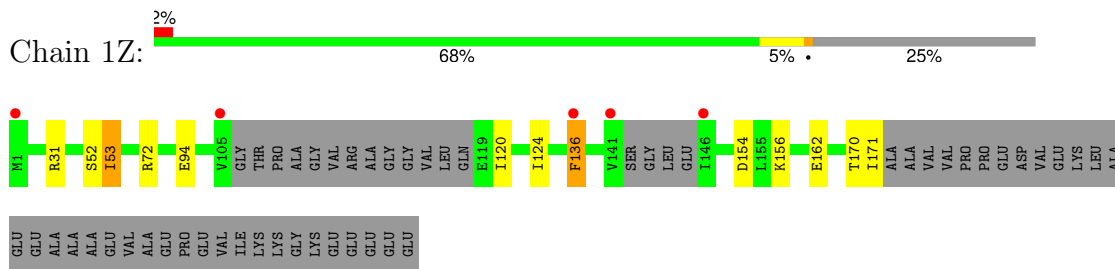
- Molecule 20: 50S ribosomal protein L24



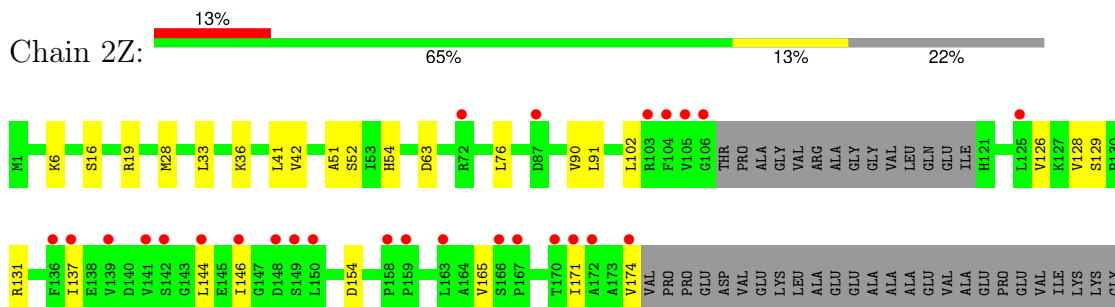
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



LYS
GLU
GLU
GLU
GLU

- Molecule 22: 50S ribosomal protein L27



MET A2 H3 E27 K49 G73 V81 L84 ALA

- Molecule 22: 50S ribosomal protein L27



MET A2 S9 T10 R11 G73 L84 ALA

- Molecule 23: 50S ribosomal protein L28



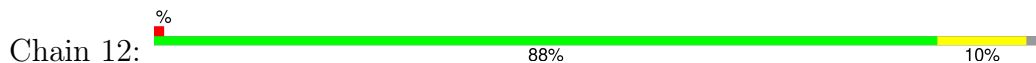
MET S2 K3 I13 R26 R40 E57 E83 L98

- Molecule 23: 50S ribosomal protein L28



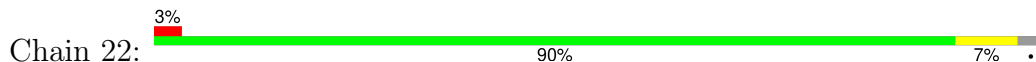
MET S2 R26 E27 Q28 R40 E63 G64 L65 L98

- Molecule 24: 50S ribosomal protein L29



M1 S4 V19 R30 S40 L53 R69 Q70 ASN ALA

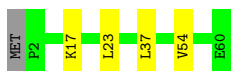
- Molecule 24: 50S ribosomal protein L29



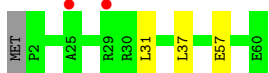
M1 R30 Q38 L53 R64 R65 Q70 ASN ALA

- Molecule 25: 50S ribosomal protein L30

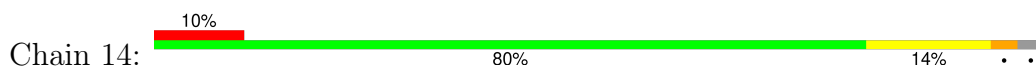




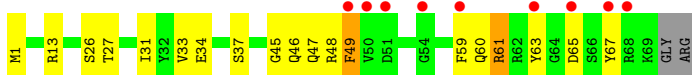
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



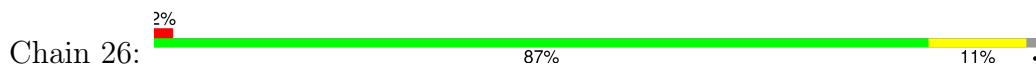
- Molecule 27: 50S ribosomal protein L32

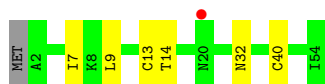


- Molecule 28: 50S ribosomal protein L33

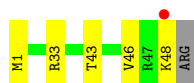
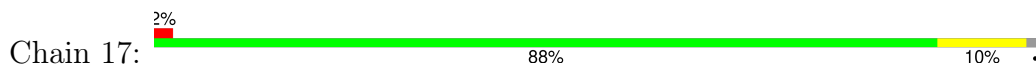


- Molecule 28: 50S ribosomal protein L33

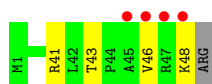
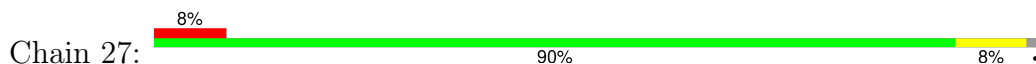




- Molecule 29: 50S ribosomal protein L34



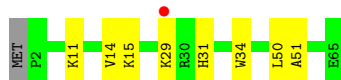
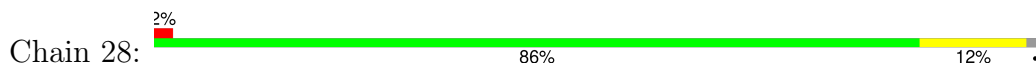
- Molecule 29: 50S ribosomal protein L34



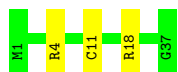
- Molecule 30: 50S ribosomal protein L35



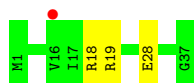
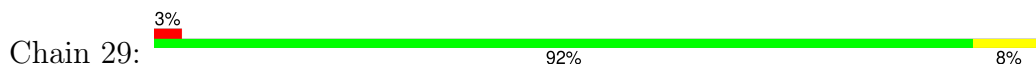
- Molecule 30: 50S ribosomal protein L35



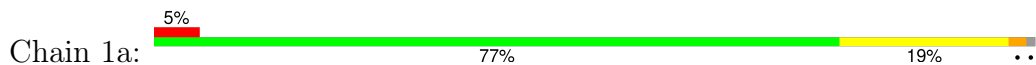
- Molecule 31: 50S ribosomal protein L36

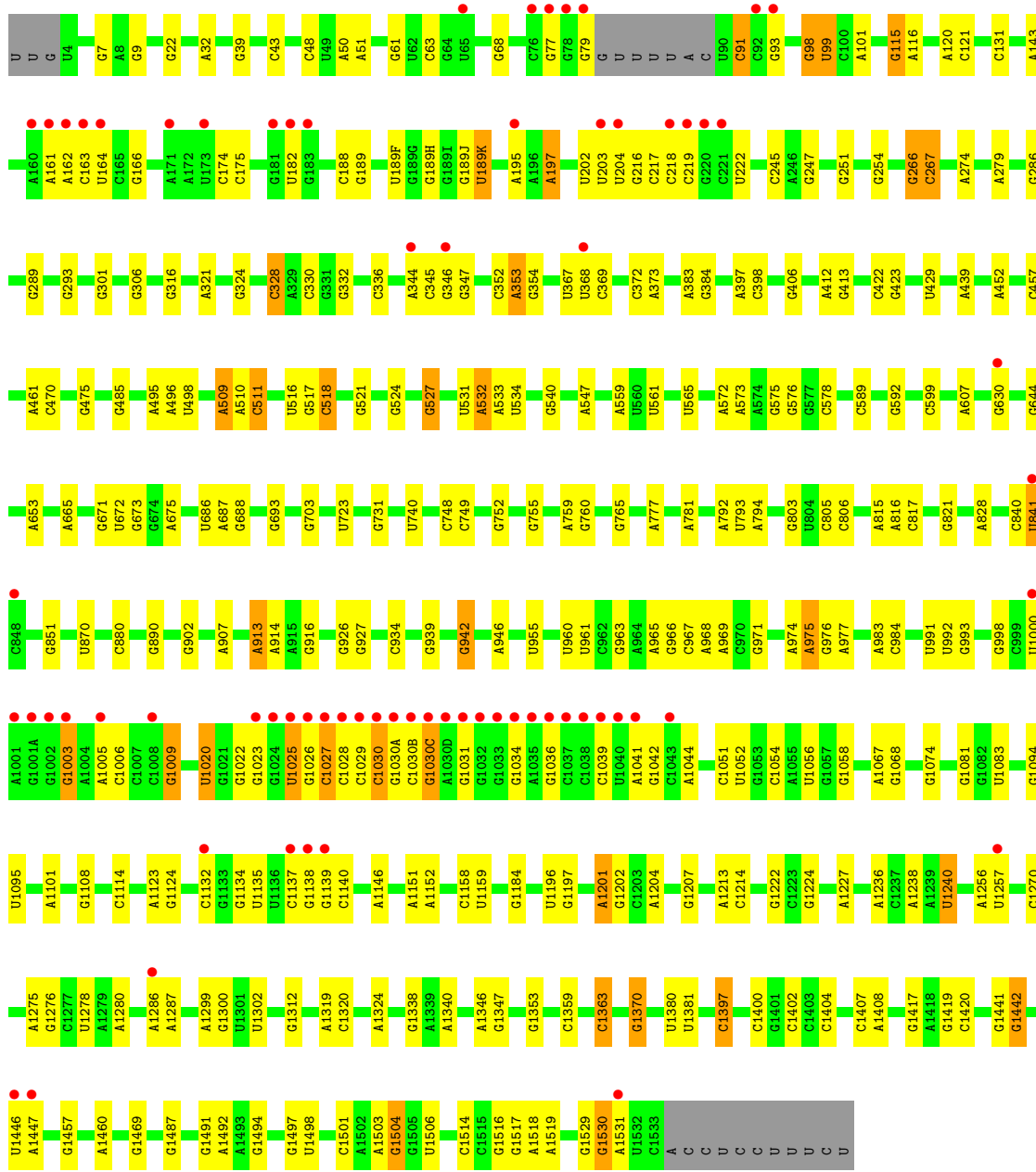


- Molecule 31: 50S ribosomal protein L36

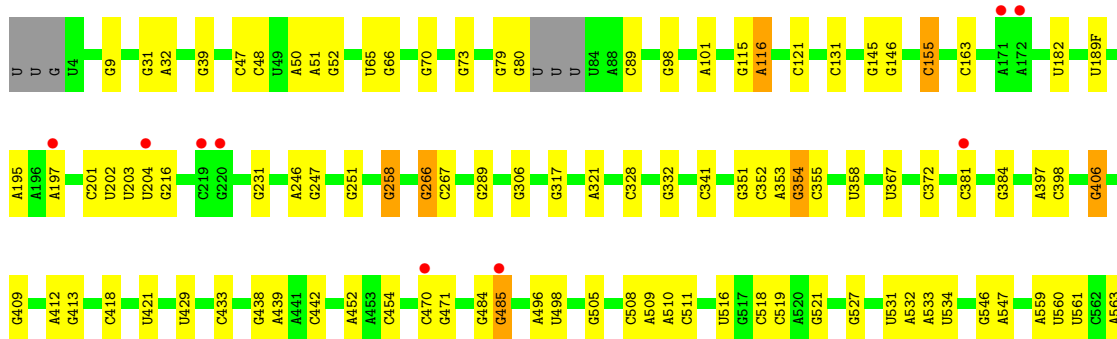
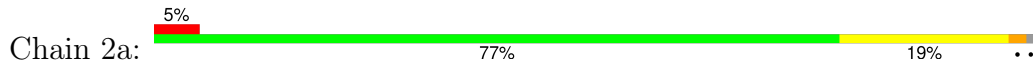


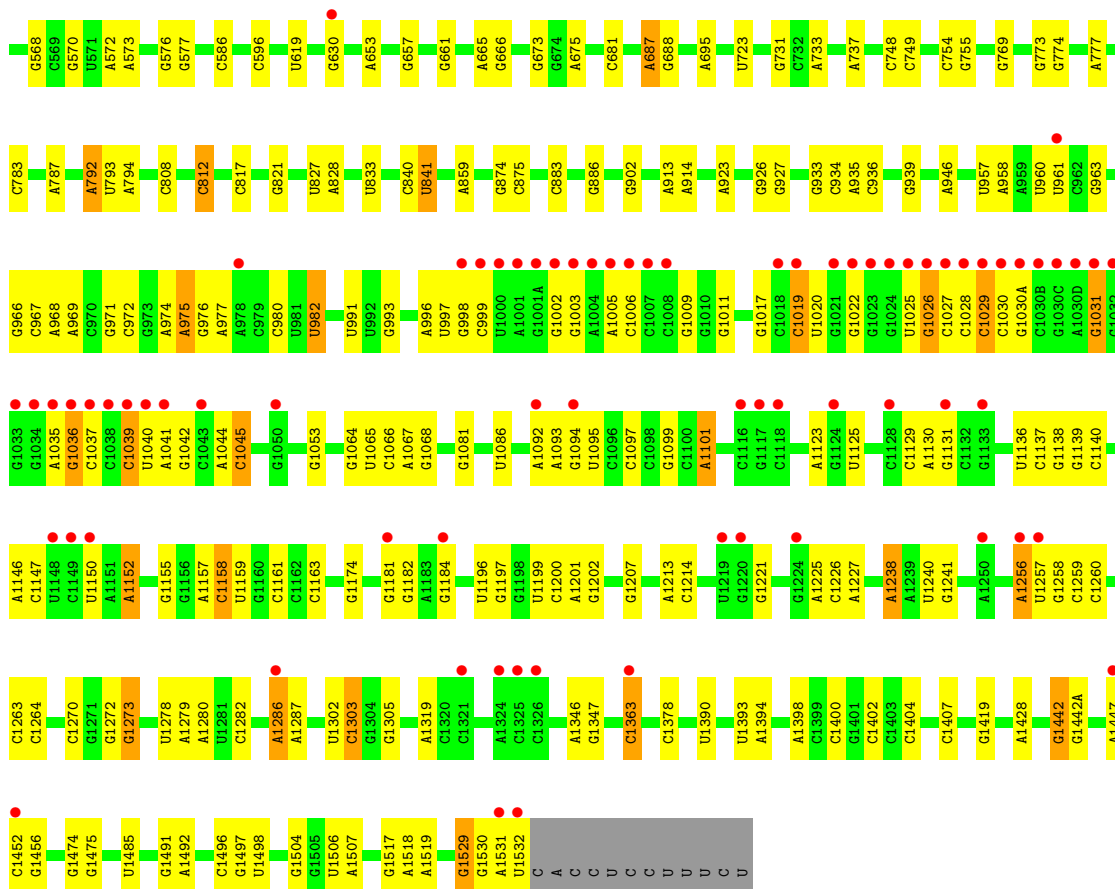
- Molecule 32: 16S Ribosomal RNA



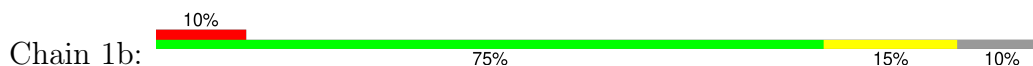


• Molecule 32: 16S Ribosomal RNA

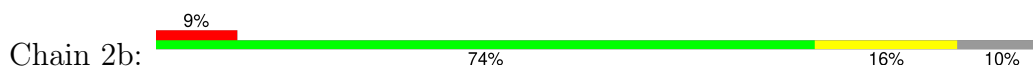




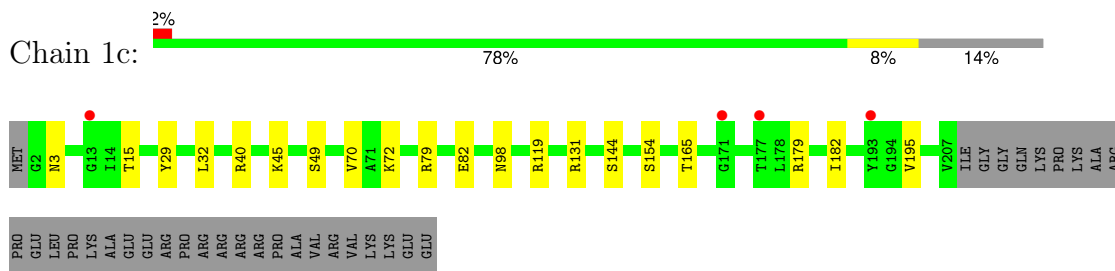
• Molecule 33: 30S ribosomal protein S2



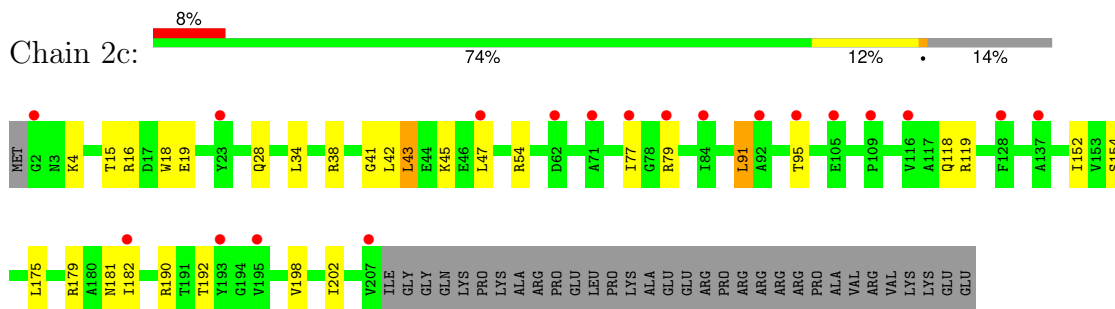
• Molecule 33: 30S ribosomal protein S2



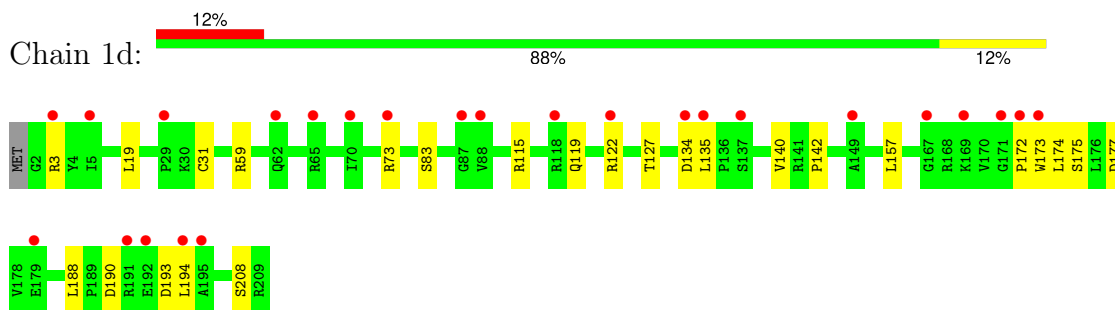
- Molecule 34: 30S ribosomal protein S3



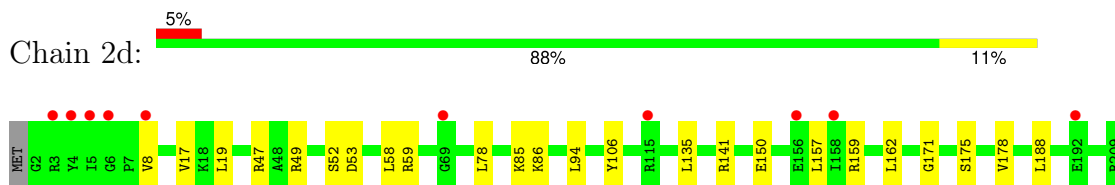
- Molecule 34: 30S ribosomal protein S3



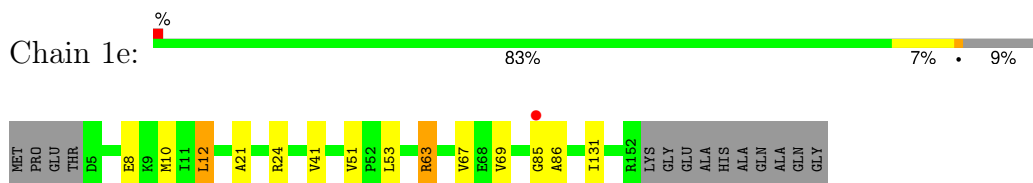
- Molecule 35: 30S ribosomal protein S4



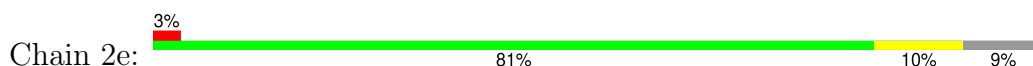
- Molecule 35: 30S ribosomal protein S4

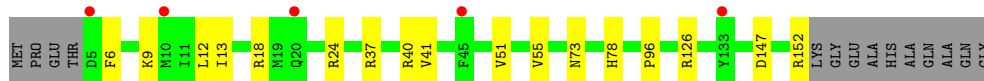


- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5





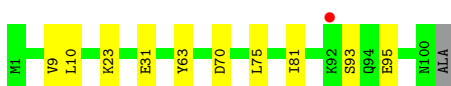
- Molecule 37: 30S ribosomal protein S6

Chain 1f: 92% 7%



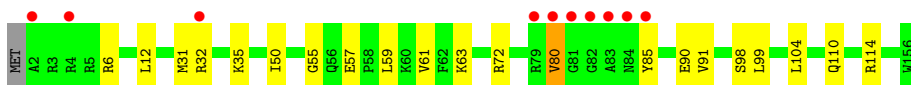
- Molecule 37: 30S ribosomal protein S6

Chain 2f: 89% 10%



- Molecule 38: 30S ribosomal protein S7

Chain 1g: 6% 86% 13%



- Molecule 38: 30S ribosomal protein S7

Chain 2g: 10% 86% 13%



- Molecule 39: 30S ribosomal protein S8

Chain 1h: 2% 95%

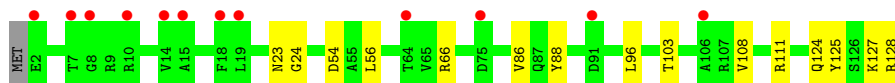
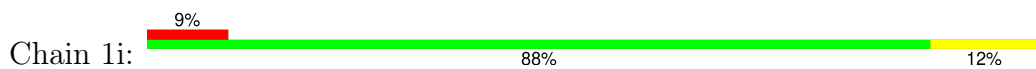


- Molecule 39: 30S ribosomal protein S8

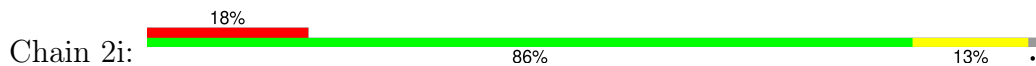
Chain 2h: 2% 88% 12%



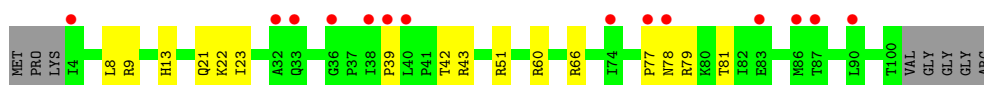
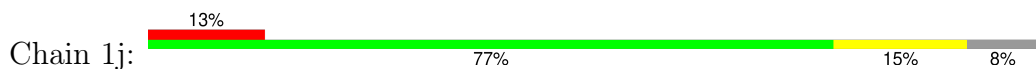
- Molecule 40: 30S ribosomal protein S9



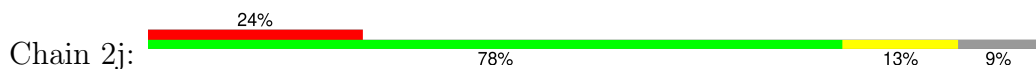
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

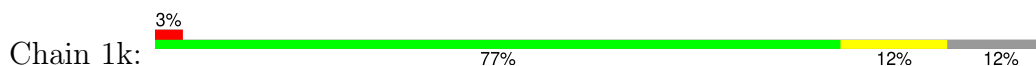


- Molecule 41: 30S ribosomal protein S10

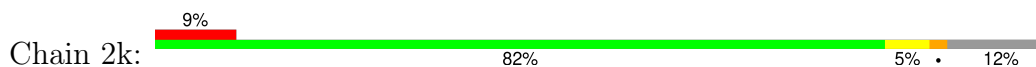


ARG

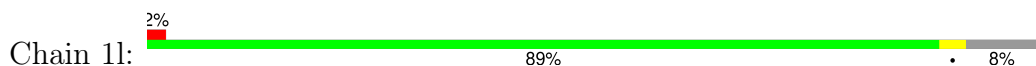
- Molecule 42: 30S ribosomal protein S11

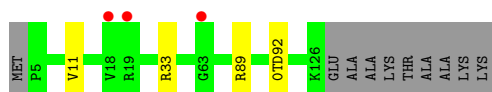


- Molecule 42: 30S ribosomal protein S11

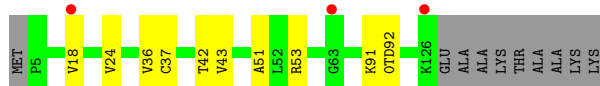
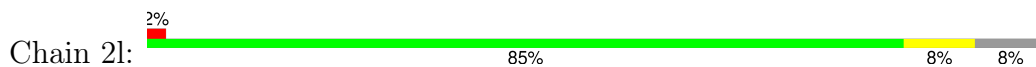


- Molecule 43: 30S ribosomal protein S12

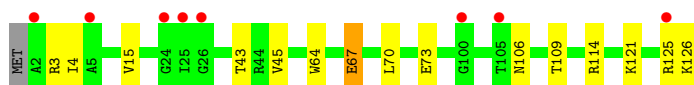
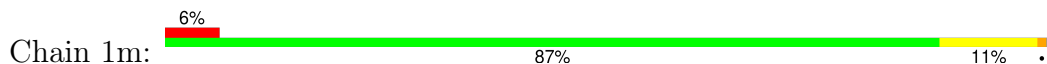




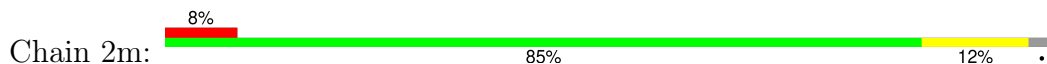
- Molecule 43: 30S ribosomal protein S12



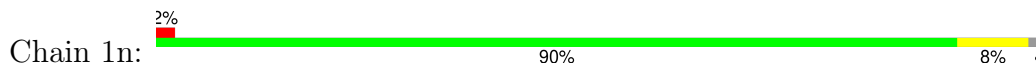
- Molecule 44: 30S ribosomal protein S13



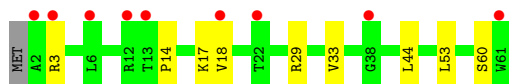
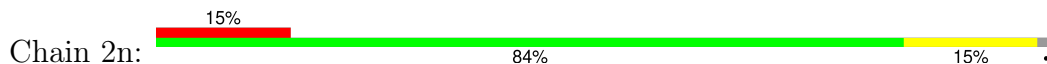
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



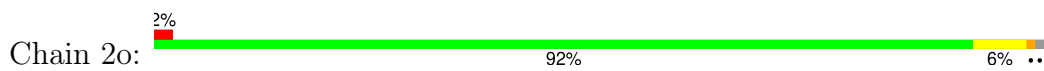
- Molecule 45: 30S ribosomal protein S14 type Z



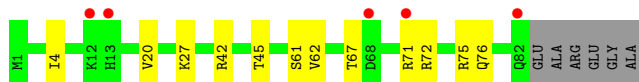
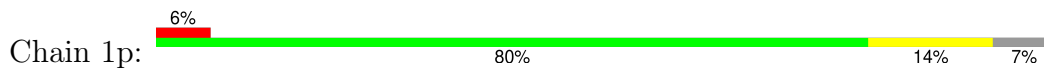
- Molecule 46: 30S ribosomal protein S15



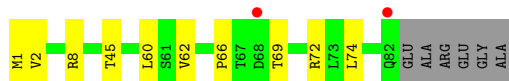
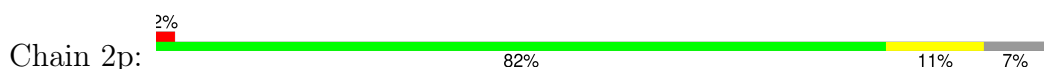
- Molecule 46: 30S ribosomal protein S15



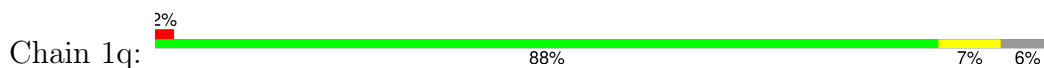
• Molecule 47: 30S ribosomal protein S16



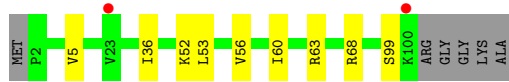
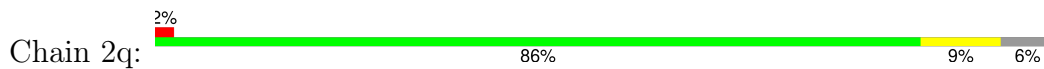
• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17



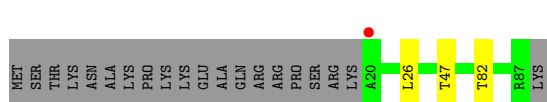
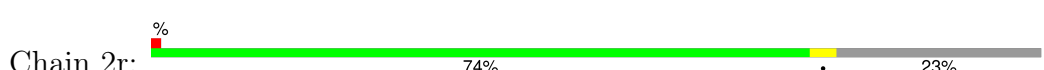
• Molecule 48: 30S ribosomal protein S17



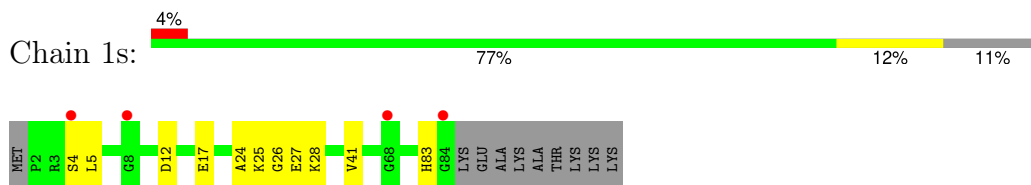
• Molecule 49: 30S ribosomal protein S18



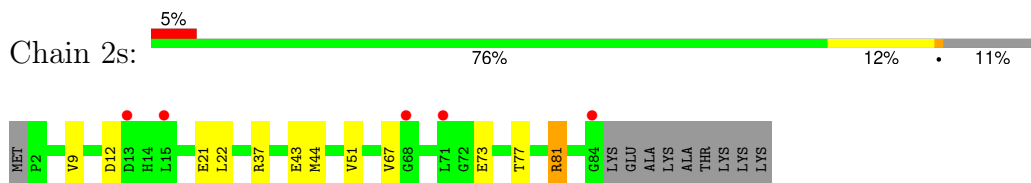
• Molecule 49: 30S ribosomal protein S18



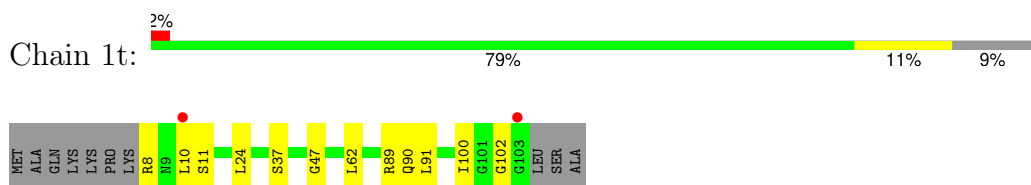
- Molecule 50: 30S ribosomal protein S19



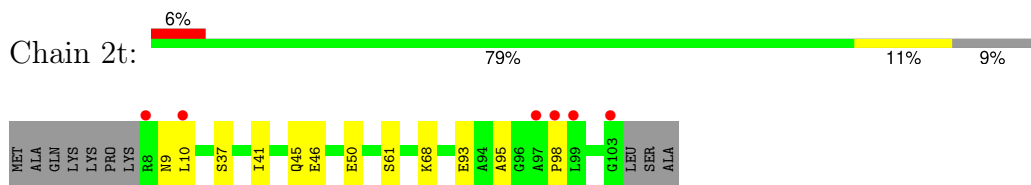
- Molecule 50: 30S ribosomal protein S19



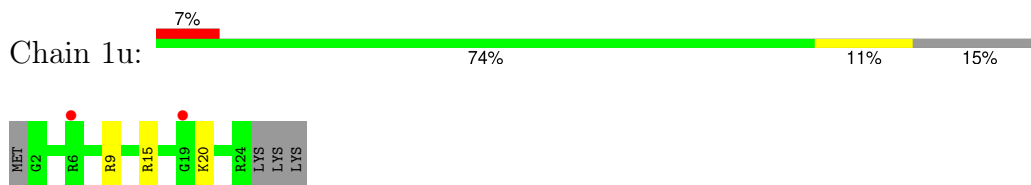
- Molecule 51: 30S ribosomal protein S20



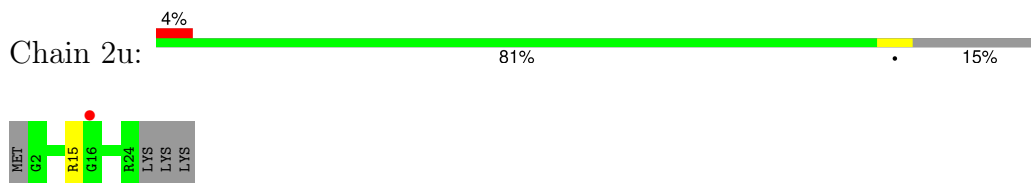
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx

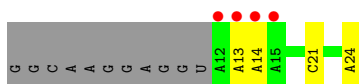


- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: MET-PHE-mRNA

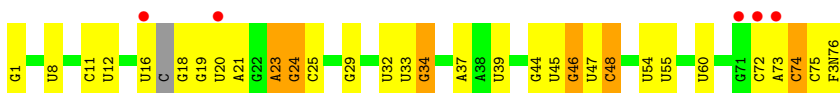




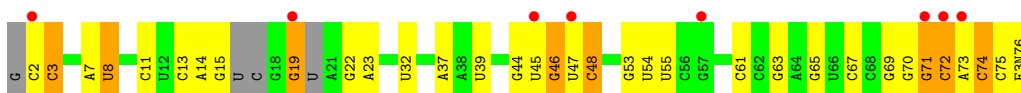
- Molecule 53: MET-PHE-mRNA



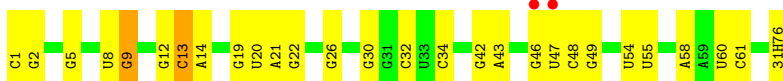
- Molecule 54: A-site Aminoacylated Phe-tRNAphe



- Molecule 54: A-site Aminoacylated Phe-tRNAphe



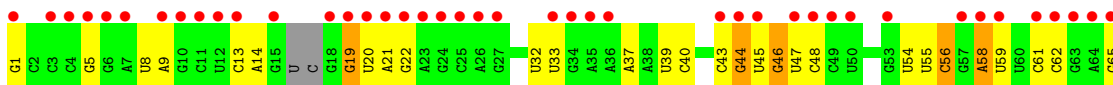
- Molecule 55: P-site Aminoacylated fMet-tRNAmet

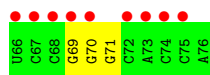


- Molecule 55: P-site Aminoacylated fMet-tRNAmet

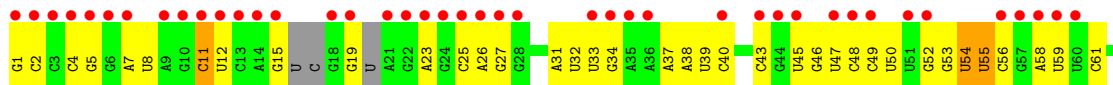
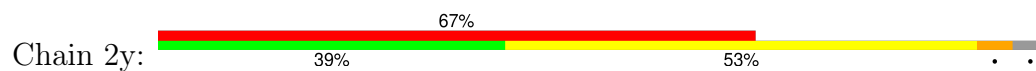


- Molecule 56: E-site Deacylated tRNAphe

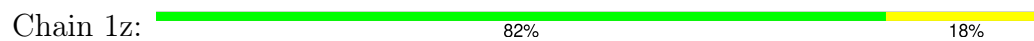




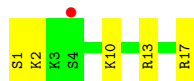
- Molecule 56: E-site Deacylated tRNA^{phe}



- Molecule 57: Lasso peptide lariocidin B



- Molecule 57: Lasso peptide lariocidin B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.29Å 450.05Å 626.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	365.48 – 2.60 365.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (365.48-2.60) 99.8 (365.48-2.60)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.62Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.215 , 0.266 0.221 , 0.268	Depositor DCC
R_{free} test set	90129 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	300583	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, ZN, 0TD, 5MC, UR3, OMU, MG, MA6, 4OC, K, OMC, 4SU, OMG, SF4, 2MA, MIA, 31H, G7M, PSU, 5MU, F3N, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	1.00	37/69011 (0.1%)	1.52	984/107720 (0.9%)
1	2A	0.79	7/67295 (0.0%)	1.31	402/105042 (0.4%)
2	1B	0.83	1/2882 (0.0%)	1.40	22/4494 (0.5%)
2	2B	0.71	1/2879 (0.0%)	1.27	10/4487 (0.2%)
3	1D	0.57	0/2186	0.74	0/2944
3	2D	0.51	0/2186	0.66	0/2944
4	1E	0.53	0/1592	0.69	0/2149
4	2E	0.43	0/1592	0.63	0/2149
5	1F	0.57	0/1619	0.75	2/2193 (0.1%)
5	2F	0.49	0/1615	0.63	0/2188
6	1G	0.50	0/1448	0.65	0/1957
6	2G	0.42	0/1453	0.59	0/1963
7	1H	0.54	0/1356	0.66	0/1834
7	2H	0.41	0/1356	0.54	0/1834
8	1I	0.45	0/1112	0.60	0/1514
8	2I	0.40	0/1079	0.64	1/1475 (0.1%)
9	1N	0.55	0/1144	0.68	0/1543
9	2N	0.46	0/1144	0.59	0/1543
10	1O	0.58	0/943	0.70	0/1269
10	2O	0.47	0/943	0.62	0/1269
11	1P	0.54	0/1152	0.75	1/1533 (0.1%)
11	2P	0.48	0/1152	0.70	0/1533
12	1Q	0.55	0/1143	0.70	0/1527
12	2Q	0.46	0/1143	0.61	0/1527
13	1R	0.57	0/982	0.74	0/1312
13	2R	0.43	0/982	0.67	0/1312
14	1S	0.50	0/883	0.71	0/1176
14	2S	0.44	0/880	0.64	0/1172
15	1T	0.52	0/1105	0.71	2/1477 (0.1%)
15	2T	0.45	0/1097	0.59	0/1468
16	1U	0.61	0/977	0.73	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.46	0/977	0.61	0/1301
17	1V	0.63	1/782 (0.1%)	0.73	0/1049
17	2V	0.47	0/782	0.66	0/1049
18	1W	0.61	0/897	0.74	1/1205 (0.1%)
18	2W	0.49	0/897	0.62	0/1205
19	1X	0.60	0/764	0.72	0/1025
19	2X	0.49	0/764	0.64	0/1025
20	1Y	0.51	0/819	0.65	0/1095
20	2Y	0.48	0/819	0.61	0/1095
21	1Z	0.49	0/1267	0.65	0/1717
21	2Z	0.44	0/1299	0.61	0/1763
22	10	0.54	0/662	0.74	0/881
22	20	0.43	0/662	0.67	0/881
23	11	0.58	0/762	0.66	0/1014
23	21	0.47	0/762	0.63	0/1014
24	12	0.56	0/590	0.69	0/781
24	22	0.44	0/590	0.56	0/781
25	13	0.53	0/474	0.70	0/635
25	23	0.43	0/469	0.60	0/630
26	14	0.55	0/565	0.64	0/761
26	24	0.46	0/545	0.68	0/737
27	15	0.57	0/469	0.76	1/635 (0.2%)
27	25	0.45	0/469	0.66	0/635
28	16	0.56	0/460	0.66	0/613
28	26	0.50	0/456	0.63	0/608
29	17	0.61	0/426	0.78	1/561 (0.2%)
29	27	0.54	0/426	0.73	0/561
30	18	0.52	0/525	0.74	0/691
30	28	0.47	0/525	0.66	0/691
31	19	0.56	0/310	0.70	0/407
31	29	0.41	0/310	0.70	0/407
32	1a	0.73	0/35795	1.27	174/55864 (0.3%)
32	2a	0.68	3/35886 (0.0%)	1.24	141/56005 (0.3%)
33	1b	0.42	0/1881	0.64	1/2542 (0.0%)
33	2b	0.50	1/1860 (0.1%)	0.59	1/2518 (0.0%)
34	1c	0.45	0/1572	0.60	0/2126
34	2c	0.44	0/1566	0.58	0/2119
35	1d	0.44	0/1685	0.61	0/2262
35	2d	0.44	0/1704	0.59	0/2284
36	1e	0.45	0/1145	0.66	1/1543 (0.1%)
36	2e	0.45	0/1149	0.63	0/1548
37	1f	0.44	0/823	0.63	0/1115
37	2f	0.45	0/829	0.63	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.40	0/1250	0.56	0/1679
38	2g	0.43	0/1254	0.55	0/1683
39	1h	0.41	0/1108	0.61	0/1494
39	2h	0.38	0/1108	0.56	0/1494
40	1i	0.40	0/1002	0.60	1/1346 (0.1%)
40	2i	0.43	0/997	0.61	0/1343
41	1j	0.42	0/722	0.59	0/982
41	2j	0.42	0/727	0.64	1/988 (0.1%)
42	1k	0.43	0/844	0.60	0/1145
42	2k	0.44	0/848	0.64	0/1149
43	1l	0.48	0/937	0.63	0/1260
43	2l	0.47	1/937 (0.1%)	0.62	1/1260 (0.1%)
44	1m	0.46	0/990	0.64	0/1327
44	2m	0.41	0/961	0.60	0/1291
45	1n	0.49	0/501	0.61	0/664
45	2n	0.48	0/501	0.62	0/664
46	1o	0.44	0/739	0.55	0/985
46	2o	0.41	0/739	0.56	0/985
47	1p	0.43	0/697	0.61	0/939
47	2p	0.41	0/693	0.62	0/935
48	1q	0.45	0/836	0.58	0/1117
48	2q	0.45	0/836	0.61	0/1117
49	1r	0.45	0/560	0.59	0/746
49	2r	0.44	0/560	0.59	0/746
50	1s	0.44	0/667	0.64	0/900
50	2s	0.44	0/661	0.65	0/893
51	1t	0.43	0/730	0.62	0/965
51	2t	0.44	0/729	0.59	0/965
52	1u	0.40	0/203	0.60	0/266
52	2u	0.41	0/203	0.58	0/266
53	1v	0.94	0/310	1.38	1/480 (0.2%)
53	2v	0.82	0/310	1.16	0/480
54	1w	0.84	1/1603 (0.1%)	1.46	24/2492 (1.0%)
54	2w	0.77	0/1531	1.42	16/2379 (0.7%)
55	1x	0.95	7/1723 (0.4%)	1.57	32/2684 (1.2%)
55	2x	0.82	7/1723 (0.4%)	1.44	31/2684 (1.2%)
56	1y	1.11	1/1606 (0.1%)	1.32	8/2497 (0.3%)
56	2y	1.09	1/1583 (0.1%)	1.48	14/2459 (0.6%)
57	1z	0.40	0/128	0.75	0/163
57	2z	0.42	0/128	0.73	0/163
All	All	0.75	69/316935 (0.0%)	1.22	1874/474426 (0.4%)

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
15	1T	0	1
21	1Z	0	1
26	14	0	1
26	24	0	1
33	1b	0	1
40	2i	0	1
44	2m	0	1
47	1p	0	1
All	All	0	8

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1272	G	C6-N1	-10.68	1.32	1.39
55	1x	1	C	OP3-P	-10.59	1.48	1.61
54	1w	1	G	OP3-P	-9.86	1.49	1.61
2	2B	1	U	OP3-P	-9.82	1.49	1.61
55	2x	1	C	OP3-P	-9.64	1.49	1.61

The worst 5 of 1874 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	28.14	135.78	118.90
32	2a	1272	G	N1-C2-N2	-23.34	95.19	116.20
32	2a	1272	G	N3-C2-N2	22.38	135.57	119.90
32	2a	1272	G	C5-C6-O6	19.69	140.41	128.60
32	2a	1263	C	N3-C2-O2	-17.15	109.90	121.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
15	1T	128	GLU	Peptide
21	1Z	136	PHE	Peptide
33	1b	122	PHE	Peptide
47	1p	4	ILE	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%)	257 (94%)	14 (5%)	2 (1%)	19	38
3	2D	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30	52
4	1E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	13	29
4	2E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	13	29
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	25	47
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	6	12
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	12	26
6	2G	179/182 (98%)	151 (84%)	24 (13%)	4 (2%)	5	10
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	22	43
7	2H	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	10
8	1I	144/148 (97%)	120 (83%)	20 (14%)	4 (3%)	4	7
8	2I	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9	19
9	1N	138/140 (99%)	133 (96%)	3 (2%)	2 (1%)	9	19
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	34
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	19
11	2P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	12
12	1Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
12	2Q	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	9	19
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
14	1S	108/112 (96%)	97 (90%)	11 (10%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	8 (7%)	3 (3%)	4	7
15	1T	129/146 (88%)	119 (92%)	7 (5%)	3 (2%)	5	10
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%)	94 (95%)	3 (3%)	2 (2%)	6	12
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	12
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	12	26
19	2X	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	12	26
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	13	29
20	2Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	13	29
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	6	12
21	2Z	156/206 (76%)	130 (83%)	22 (14%)	4 (3%)	4	7
22	10	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	11	24
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	11	24
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	12	26
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	8	18
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	51 (76%)	10 (15%)	6 (9%)	0	0
26	24	67/71 (94%)	48 (72%)	12 (18%)	7 (10%)	0	0
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	58 (94%)	3 (5%)	1 (2%)	8	17
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	183 (80%)	32 (14%)	14 (6%)	1	1
33	2b	229/256 (90%)	185 (81%)	29 (13%)	15 (7%)	1	1
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	13	29
34	2c	204/239 (85%)	162 (79%)	32 (16%)	10 (5%)	2	2
35	1d	206/209 (99%)	184 (89%)	19 (9%)	3 (2%)	8	18
35	2d	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	13	29
36	1e	146/162 (90%)	133 (91%)	8 (6%)	5 (3%)	3	5
36	2e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	5	11
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	13	29
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	12
38	2g	153/156 (98%)	130 (85%)	15 (10%)	8 (5%)	1	2
39	1h	135/138 (98%)	121 (90%)	11 (8%)	3 (2%)	5	10
39	2h	135/138 (98%)	124 (92%)	9 (7%)	2 (2%)	8	18
40	1i	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	5	9
40	2i	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	16	34
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	1
41	2j	94/105 (90%)	74 (79%)	15 (16%)	5 (5%)	1	1
42	1k	112/129 (87%)	100 (89%)	8 (7%)	4 (4%)	3	4
42	2k	112/129 (87%)	99 (88%)	9 (8%)	4 (4%)	3	4
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	9 (8%)	2 (2%)	7	16
44	1m	123/126 (98%)	110 (89%)	11 (9%)	2 (2%)	8	17
44	2m	120/126 (95%)	100 (83%)	16 (13%)	4 (3%)	3	5
45	1n	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	5
46	1o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	11	24
46	2o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	11	24
47	1p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	10	21
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	10	21
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	13	29
49	1r	66/88 (75%)	57 (86%)	8 (12%)	1 (2%)	8	18
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	6 (7%)	5 (6%)	1	1
50	2s	81/93 (87%)	67 (83%)	11 (14%)	3 (4%)	2	4
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	3
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
57	1z	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
57	2z	15/17 (88%)	10 (67%)	5 (33%)	0	100	100
All	All	11402/12162 (94%)	10291 (90%)	906 (8%)	205 (2%)	7	14

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	50	ALA
15	1T	55	ASN
23	11	3	LYS
33	1b	8	LYS

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%)	203 (94%)	12 (6%)	17	38
3	2D	215/218 (99%)	201 (94%)	14 (6%)	14	31
4	1E	164/166 (99%)	157 (96%)	7 (4%)	25	49
4	2E	164/166 (99%)	155 (94%)	9 (6%)	18	38
5	1F	160/166 (96%)	144 (90%)	16 (10%)	6	13
5	2F	159/166 (96%)	151 (95%)	8 (5%)	20	43
6	1G	143/156 (92%)	129 (90%)	14 (10%)	6	13
6	2G	143/156 (92%)	126 (88%)	17 (12%)	4	8
7	1H	144/148 (97%)	133 (92%)	11 (8%)	11	23
7	2H	144/148 (97%)	130 (90%)	14 (10%)	6	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	1	3
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	2
9	1N	118/119 (99%)	107 (91%)	11 (9%)	7	15
9	2N	118/119 (99%)	108 (92%)	10 (8%)	8	18
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	63
10	2O	100/100 (100%)	94 (94%)	6 (6%)	16	35
11	1P	115/116 (99%)	107 (93%)	8 (7%)	12	27
11	2P	115/116 (99%)	110 (96%)	5 (4%)	25	49
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	40	66
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	30	56
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	63
13	2R	101/101 (100%)	96 (95%)	5 (5%)	20	43
14	1S	86/88 (98%)	82 (95%)	4 (5%)	22	45
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	3
15	1T	115/127 (91%)	110 (96%)	5 (4%)	25	49
15	2T	113/127 (89%)	107 (95%)	6 (5%)	19	40
16	1U	93/94 (99%)	86 (92%)	7 (8%)	11	24
16	2U	93/94 (99%)	88 (95%)	5 (5%)	18	39
17	1V	80/82 (98%)	71 (89%)	9 (11%)	4	9
17	2V	80/82 (98%)	73 (91%)	7 (9%)	8	17
18	1W	90/92 (98%)	85 (94%)	5 (6%)	17	38
18	2W	90/92 (98%)	82 (91%)	8 (9%)	8	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27	53
19	2X	77/78 (99%)	72 (94%)	5 (6%)	14	31
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	12	26
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	5
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	9	20
21	2Z	137/179 (76%)	114 (83%)	23 (17%)	1	3
22	10	65/67 (97%)	62 (95%)	3 (5%)	23	46
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	62
23	11	80/83 (96%)	76 (95%)	4 (5%)	20	43
23	21	80/83 (96%)	76 (95%)	4 (5%)	20	43
24	12	65/67 (97%)	59 (91%)	6 (9%)	7	15
24	22	65/67 (97%)	60 (92%)	5 (8%)	10	22
25	13	51/52 (98%)	47 (92%)	4 (8%)	10	22
25	23	50/52 (96%)	47 (94%)	3 (6%)	16	35
26	14	59/63 (94%)	52 (88%)	7 (12%)	4	8
26	24	53/63 (84%)	40 (76%)	13 (24%)	0	1
27	15	50/52 (96%)	46 (92%)	4 (8%)	10	21
27	25	50/52 (96%)	48 (96%)	2 (4%)	27	52
28	16	51/52 (98%)	48 (94%)	3 (6%)	16	35
28	26	50/52 (96%)	44 (88%)	6 (12%)	4	8
29	17	41/42 (98%)	37 (90%)	4 (10%)	6	13
29	27	41/42 (98%)	37 (90%)	4 (10%)	6	13
30	18	54/55 (98%)	50 (93%)	4 (7%)	11	24
30	28	54/55 (98%)	47 (87%)	7 (13%)	3	6
31	19	34/34 (100%)	31 (91%)	3 (9%)	8	17
31	29	34/34 (100%)	31 (91%)	3 (9%)	8	17
33	1b	192/220 (87%)	168 (88%)	24 (12%)	3	7
33	2b	187/220 (85%)	160 (86%)	27 (14%)	2	5
34	1c	142/188 (76%)	124 (87%)	18 (13%)	3	7
34	2c	140/188 (74%)	118 (84%)	22 (16%)	2	3
35	1d	169/181 (93%)	147 (87%)	22 (13%)	3	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	151 (87%)	22 (13%)	3	7
36	1e	113/123 (92%)	103 (91%)	10 (9%)	8	17
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	8
37	1f	84/90 (93%)	78 (93%)	6 (7%)	12	26
37	2f	85/90 (94%)	75 (88%)	10 (12%)	4	8
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	3
38	2g	120/127 (94%)	107 (89%)	13 (11%)	5	10
39	1h	114/119 (96%)	110 (96%)	4 (4%)	31	57
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	8
40	1i	90/99 (91%)	79 (88%)	11 (12%)	4	8
40	2i	89/99 (90%)	74 (83%)	15 (17%)	1	3
41	1j	66/92 (72%)	56 (85%)	10 (15%)	2	4
41	2j	69/92 (75%)	61 (88%)	8 (12%)	4	9
42	1k	82/99 (83%)	71 (87%)	11 (13%)	3	6
42	2k	83/99 (84%)	77 (93%)	6 (7%)	12	26
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	62
43	2l	96/108 (89%)	91 (95%)	5 (5%)	19	41
44	1m	95/101 (94%)	81 (85%)	14 (15%)	2	4
44	2m	92/101 (91%)	82 (89%)	10 (11%)	5	10
45	1n	49/50 (98%)	45 (92%)	4 (8%)	9	20
45	2n	49/50 (98%)	42 (86%)	7 (14%)	2	5
46	1o	78/80 (98%)	75 (96%)	3 (4%)	28	54
46	2o	78/80 (98%)	72 (92%)	6 (8%)	10	22
47	1p	69/74 (93%)	59 (86%)	10 (14%)	2	4
47	2p	68/74 (92%)	59 (87%)	9 (13%)	3	6
48	1q	94/97 (97%)	87 (93%)	7 (7%)	11	24
48	2q	94/97 (97%)	86 (92%)	8 (8%)	8	18
49	1r	59/77 (77%)	54 (92%)	5 (8%)	8	18
49	2r	59/77 (77%)	56 (95%)	3 (5%)	20	42
50	1s	69/80 (86%)	63 (91%)	6 (9%)	8	17
50	2s	67/80 (84%)	57 (85%)	10 (15%)	2	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	62 (89%)	8 (11%)	4	9
51	2t	70/82 (85%)	62 (89%)	8 (11%)	4	9
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	3
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17	38
57	1z	13/13 (100%)	10 (77%)	3 (23%)	0	1
57	2z	13/13 (100%)	8 (62%)	5 (38%)	0	0
All	All	9331/10090 (92%)	8467 (91%)	864 (9%)	7	15

5 of 864 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	2I	15	VAL
21	2Z	33	LEU
44	2m	19	LEU
8	2I	92	VAL
8	2I	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
51	1t	90	GLN
44	2m	40	ASN
16	2U	94	ASN
43	2l	99	HIS
50	2s	47	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	474 (16%)	35 (1%)
1	2A	2790/2915 (95%)	481 (17%)	30 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	19 (16%)	0
32	1a	1494/1521 (98%)	234 (15%)	0
32	2a	1498/1521 (98%)	261 (17%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	71/76 (93%)	16 (22%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	2w	67/76 (88%)	22 (32%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	11 (14%)	0
56	1y	71/76 (93%)	24 (33%)	0
56	2y	69/76 (90%)	28 (40%)	0
All	All	9334/9620 (97%)	1597 (17%)	65 (0%)

5 of 1597 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	69	C

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1653	G
1	2A	1992	G
1	1A	1508	A
1	1A	1420	U
1	2A	2119	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMU	2A	2552	1,58	19,22,23	1.10	2 (10%)	25,31,34	1.81	5 (20%)
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.51	2 (9%)
56	PSU	2y	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.92	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MG	2a	1207	58,32	18,26,27	0.98	1 (5%)	16,38,41	1.58	3 (18%)
1	PSU	1A	2605	1,58	18,21,22	1.54	5 (27%)	21,30,33	1.96	5 (23%)
56	5MU	1y	54	56	19,22,23	1.58	4 (21%)	27,32,35	1.87	7 (25%)
54	F3N	2w	76	1	29,36,37	1.48	5 (17%)	28,51,54	1.44	1 (3%)
32	5MC	1a	1407	32	19,22,23	1.43	2 (10%)	26,32,35	1.07	4 (15%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.82	4 (19%)
1	5MU	1A	1915	1	19,22,23	1.39	4 (21%)	27,32,35	2.67	10 (37%)
1	5MU	1A	1939	1,58	19,22,23	1.70	6 (31%)	27,32,35	2.33	6 (22%)
32	MA6	1a	1518	32	19,26,27	1.10	2 (10%)	18,38,41	1.71	3 (16%)
55	5MU	1x	54	55	19,22,23	1.49	5 (26%)	27,32,35	2.04	6 (22%)
1	OMC	2A	1920	1	19,22,23	0.86	1 (5%)	25,31,34	1.11	2 (8%)
32	G7M	2a	527	58,32	20,26,27	1.16	1 (5%)	16,39,42	0.70	0
56	PSU	1y	39	56	18,21,22	1.55	2 (11%)	21,30,33	1.74	3 (14%)
56	MIA	2y	37	56	17,24,32	1.13	1 (5%)	16,35,47	1.31	2 (12%)
1	5MU	2A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.43	6 (22%)
56	G7M	2y	46	56	20,26,27	1.52	2 (10%)	16,39,42	0.76	0
1	OMG	1A	2251	1,58,55	19,26,27	1.16	1 (5%)	21,38,41	1.17	3 (14%)
1	5MU	2A	1939	1,58	19,22,23	1.52	4 (21%)	27,32,35	2.31	7 (25%)
54	MIA	1w	37	54	24,31,32	2.27	2 (8%)	22,44,47	2.57	7 (31%)
43	0TD	2l	92	43	8,9,10	5.12	2 (25%)	6,11,13	2.48	1 (16%)
32	MA6	1a	1519	32	19,26,27	1.08	2 (10%)	18,38,41	1.82	3 (16%)
55	5MC	2x	32	55	19,22,23	1.57	3 (15%)	26,32,35	1.56	6 (23%)
56	MIA	1y	37	56	17,24,32	1.16	1 (5%)	16,35,47	1.48	1 (6%)
32	M2G	1a	966	32	20,27,28	1.56	3 (15%)	19,40,43	1.25	2 (10%)
32	5MC	1a	1400	32	19,22,23	1.38	3 (15%)	26,32,35	1.34	4 (15%)
54	PSU	1w	32	54	18,21,22	1.35	3 (16%)	21,30,33	1.81	4 (19%)
32	MA6	2a	1518	32	19,26,27	0.98	2 (10%)	18,38,41	2.05	4 (22%)
55	PSU	1x	55	55	18,21,22	1.47	3 (16%)	21,30,33	1.78	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.16	3 (15%)	26,32,35	1.25	3 (11%)
54	4SU	1w	8	54	18,21,22	1.89	4 (22%)	25,30,33	1.87	6 (24%)
32	MA6	2a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	2.07	4 (22%)
55	4SU	2x	8	55	18,21,22	1.92	5 (27%)	25,30,33	1.18	3 (12%)
1	PSU	1A	1911	1	18,21,22	1.43	3 (16%)	21,30,33	2.04	3 (14%)
43	0TD	1l	92	43	8,9,10	3.92	2 (25%)	6,11,13	5.45	2 (33%)
54	G7M	1w	46	54	20,26,27	1.33	2 (10%)	16,39,42	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1942	1	19,22,23	1.20	3 (15%)	26,32,35	1.10	2 (7%)
1	5MC	1A	1962	1,58	19,22,23	1.90	4 (21%)	26,32,35	1.39	5 (19%)
1	2MA	2A	2503	1,58	17,25,26	1.05	1 (5%)	16,37,40	1.40	4 (25%)
54	PSU	1w	39	54	18,21,22	1.42	3 (16%)	21,30,33	2.03	4 (19%)
54	5MU	1w	54	54	19,22,23	1.48	4 (21%)	27,32,35	2.14	5 (18%)
55	31H	1x	76	58,55	27,34,35	1.20	3 (11%)	22,47,50	2.69	6 (27%)
1	PSU	2A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.05	3 (14%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	21,30,33	2.06	5 (23%)
56	5MU	2y	54	56	19,22,23	1.56	3 (15%)	27,32,35	2.14	8 (29%)
55	5MC	1x	32	55	19,22,23	1.78	3 (15%)	26,32,35	1.44	3 (11%)
54	4SU	2w	8	54	18,21,22	1.84	4 (22%)	25,30,33	2.43	5 (20%)
32	4OC	2a	1402	32	20,23,24	0.82	0	25,32,35	0.93	1 (4%)
55	31H	2x	76	59,58,55	27,34,35	1.10	3 (11%)	22,47,50	3.58	6 (27%)
32	2MG	1a	1207	58,32	18,26,27	1.00	1 (5%)	16,38,41	1.47	3 (18%)
32	PSU	1a	516	32	18,21,22	1.46	3 (16%)	21,30,33	1.79	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	1.08	2 (8%)
54	G7M	2w	46	54	20,26,27	1.16	1 (5%)	16,39,42	0.95	1 (6%)
32	5MC	1a	967	32	19,22,23	1.77	2 (10%)	26,32,35	1.29	2 (7%)
32	5MC	2a	967	32	19,22,23	1.59	2 (10%)	26,32,35	1.30	4 (15%)
56	4SU	2y	8	56,58	18,21,22	1.71	5 (27%)	25,30,33	2.10	5 (20%)
1	5MC	1A	1942	1,58	19,22,23	1.26	2 (10%)	26,32,35	1.50	5 (19%)
32	UR3	2a	1498	32	19,22,23	1.29	2 (10%)	26,32,35	1.84	5 (19%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.28	4 (19%)
56	PSU	2y	39	56	18,21,22	1.41	2 (11%)	21,30,33	1.58	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.87	3 (15%)	26,32,35	1.21	4 (15%)
56	PSU	2y	55	56	18,21,22	1.43	2 (11%)	21,30,33	2.17	4 (19%)
1	2MA	1A	2503	1,58	17,25,26	1.11	2 (11%)	16,37,40	1.51	3 (18%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	1.20	4 (16%)
54	5MU	2w	54	54	19,22,23	1.22	3 (15%)	27,32,35	2.37	8 (29%)
55	5MU	2x	54	55	19,22,23	1.37	2 (10%)	27,32,35	2.26	6 (22%)
32	G7M	1a	527	32	20,26,27	1.19	2 (10%)	16,39,42	0.64	0
56	G7M	1y	46	56	20,26,27	1.37	1 (5%)	16,39,42	0.69	0
32	5MC	2a	1400	32	19,22,23	1.74	3 (15%)	26,32,35	1.38	2 (7%)
54	MIA	2w	37	54	19,27,32	1.88	3 (15%)	18,39,47	1.59	4 (22%)
55	4SU	1x	8	55	18,21,22	2.24	5 (27%)	25,30,33	1.80	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	1y	32	56	18,21,22	1.43	2 (11%)	21,30,33	1.80	4 (19%)
56	4SU	1y	8	56	18,21,22	1.56	5 (27%)	25,30,33	1.51	4 (16%)
1	OMG	2A	2251	1,58,55	19,26,27	1.09	1 (5%)	21,38,41	1.02	2 (9%)
54	F3N	1w	76	1	29,36,37	1.40	5 (17%)	28,51,54	1.55	3 (10%)
56	PSU	1y	55	56	18,21,22	1.51	3 (16%)	21,30,33	2.02	4 (19%)
32	5MC	2a	1407	58,32	19,22,23	1.59	3 (15%)	26,32,35	1.45	4 (15%)
54	PSU	2w	55	54	18,21,22	1.47	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	1A	1917	1	18,21,22	1.33	3 (16%)	21,30,33	2.06	5 (23%)
32	M2G	2a	966	32	20,27,28	1.27	3 (15%)	19,40,43	1.16	1 (5%)
32	UR3	1a	1498	32	19,22,23	0.95	1 (5%)	26,32,35	1.73	5 (19%)
1	OMU	1A	2552	1,58	19,22,23	1.30	3 (15%)	25,31,34	2.05	5 (20%)
54	PSU	2w	32	54	18,21,22	1.41	2 (11%)	21,30,33	2.06	5 (23%)
1	5MC	2A	1962	1,58	19,22,23	1.49	3 (15%)	26,32,35	1.11	2 (7%)
55	PSU	2x	55	55	18,21,22	1.36	3 (16%)	21,30,33	1.99	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	1.81	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	58,32	-	1/5/27/28	0/3/3/3
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	1	-	4/15/37/38	0/4/4/4
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	G7M	2a	527	58,32	-	2/3/25/26	0/3/3/3
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MIA	2y	37	56	-	2/3/25/34	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	0/3/25/26	0/3/3/3
1	OMG	1A	2251	1,58,55	-	1/5/27/28	0/3/3/3
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/11/33/34	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	3/3/25/34	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,58	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	58,55	-	4/18/40/41	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
55	31H	2x	76	59,58,55	-	4/18/40/41	0/3/3/3
32	2MG	1a	1207	58,32	-	0/5/27/28	0/3/3/3
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
54	G7M	2w	46	54	-	3/3/25/26	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56,58	-	1/7/25/26	0/2/2/2
1	5MC	1A	1942	1,58	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	1,58	-	1/3/25/26	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/3/25/26	0/3/3/3
56	G7M	1y	46	56	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,58,55	-	0/5/27/28	0/3/3/3
54	F3N	1w	76	1	-	2/15/37/38	0/4/4/4
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	58,32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-13.70	1.68	1.82
43	1l	92	0TD	CB-SB	-10.44	1.71	1.82
54	1w	37	MIA	C2-S10	-7.76	1.69	1.75
1	1A	1962	5MC	C5-C4	6.84	1.49	1.44
54	1w	37	MIA	C13-C14	6.80	1.52	1.32

The worst 5 of 332 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.53	79.84	102.36
55	2x	76	31H	O4'-C1'-N9	-10.23	95.18	108.75
55	2x	76	31H	C4'-O4'-C1'	-9.67	101.06	109.92
54	1w	37	MIA	C12-C13-C14	-9.06	110.74	127.01
55	1x	76	31H	C4'-O4'-C1'	-8.93	101.75	109.92

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	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 2820 ligands modelled in this entry, 2818 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	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	302	35	0,12,12	-	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	2w	1
54	1w	1
17	1V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2w	75:C	O3'	76:F3N	P	2.56
1	1w	75:C	O3'	76:F3N	P	2.32
1	1V	34:GLU	C	35:LEU	N	1.14

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, 95th 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 ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.60	193 (6%) 25 20	11, 27, 82, 92	0
1	2A	2789/2915 (95%)	-0.11	163 (5%) 30 24	23, 44, 80, 96	0
2	1B	120/121 (99%)	-0.43	0 100 100	21, 39, 54, 74	0
2	2B	120/121 (99%)	0.27	2 (1%) 69 64	43, 57, 66, 80	0
3	1D	275/276 (99%)	-0.50	1 (0%) 89 86	13, 28, 42, 71	0
3	2D	275/276 (99%)	-0.22	5 (1%) 67 62	21, 38, 50, 68	0
4	1E	204/206 (99%)	-0.49	0 100 100	12, 30, 49, 65	0
4	2E	204/206 (99%)	0.07	2 (0%) 79 75	26, 48, 60, 69	0
5	1F	203/210 (96%)	-0.46	0 100 100	12, 31, 54, 69	0
5	2F	203/210 (96%)	0.20	3 (1%) 71 67	24, 52, 65, 71	0
6	1G	181/182 (99%)	0.15	8 (4%) 39 33	28, 44, 59, 72	0
6	2G	181/182 (99%)	0.55	8 (4%) 39 33	48, 58, 68, 76	0
7	1H	174/180 (96%)	0.02	3 (1%) 69 64	29, 43, 55, 64	0
7	2H	174/180 (96%)	1.37	36 (20%) 3 2	59, 71, 78, 88	0
8	1I	146/148 (98%)	0.46	2 (1%) 73 68	34, 59, 67, 70	0
8	2I	146/148 (98%)	0.64	8 (5%) 32 26	42, 59, 69, 73	0
9	1N	140/140 (100%)	-0.44	0 100 100	18, 28, 46, 61	0
9	2N	140/140 (100%)	0.38	5 (3%) 46 40	36, 50, 67, 73	0
10	1O	122/122 (100%)	-0.41	0 100 100	19, 31, 48, 53	0
10	2O	122/122 (100%)	0.13	2 (1%) 70 65	35, 48, 58, 62	0
11	1P	149/150 (99%)	-0.28	0 100 100	14, 37, 55, 62	0
11	2P	149/150 (99%)	0.25	1 (0%) 84 81	28, 52, 66, 73	0
12	1Q	141/141 (100%)	-0.30	1 (0%) 84 81	17, 30, 48, 62	0
12	2Q	141/141 (100%)	0.32	4 (2%) 55 49	34, 50, 62, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.67	0 100 100	17, 25, 38, 44	0
13	2R	118/118 (100%)	-0.09	0 100 100	31, 42, 54, 61	0
14	1S	110/112 (98%)	-0.17	0 100 100	26, 39, 51, 53	0
14	2S	110/112 (98%)	0.39	1 (0%) 81 77	45, 54, 62, 68	0
15	1T	131/146 (89%)	-0.28	2 (1%) 71 67	23, 35, 56, 69	0
15	2T	131/146 (89%)	0.34	2 (1%) 71 67	40, 50, 62, 68	0
16	1U	116/118 (98%)	-0.74	0 100 100	15, 21, 34, 47	0
16	2U	116/118 (98%)	0.21	3 (2%) 57 51	30, 47, 59, 64	0
17	1V	101/101 (100%)	-0.55	0 100 100	14, 27, 47, 56	0
17	2V	101/101 (100%)	0.40	0 100 100	29, 56, 62, 66	0
18	1W	112/113 (99%)	-0.65	1 (0%) 81 77	13, 22, 39, 66	0
18	2W	112/113 (99%)	-0.15	1 (0%) 81 77	30, 38, 56, 75	0
19	1X	95/96 (98%)	-0.42	1 (1%) 77 74	16, 29, 50, 65	0
19	2X	95/96 (98%)	0.08	2 (2%) 63 58	34, 44, 61, 71	0
20	1Y	107/110 (97%)	-0.12	0 100 100	24, 39, 55, 65	0
20	2Y	107/110 (97%)	0.71	10 (9%) 16 13	45, 57, 69, 75	0
21	1Z	154/206 (74%)	0.52	5 (3%) 50 45	26, 52, 70, 76	0
21	2Z	160/206 (77%)	1.14	26 (16%) 5 4	53, 66, 76, 79	0
22	10	83/85 (97%)	-0.37	1 (1%) 76 72	15, 26, 40, 51	0
22	20	83/85 (97%)	0.29	1 (1%) 76 72	35, 45, 54, 62	0
23	11	97/98 (98%)	-0.04	2 (2%) 63 58	19, 37, 58, 65	0
23	21	97/98 (98%)	0.24	4 (4%) 42 36	29, 45, 61, 67	0
24	12	70/72 (97%)	-0.17	1 (1%) 73 68	23, 37, 47, 63	0
24	22	70/72 (97%)	0.54	2 (2%) 54 48	42, 54, 64, 70	0
25	13	59/60 (98%)	-0.32	0 100 100	15, 26, 49, 62	0
25	23	59/60 (98%)	0.31	2 (3%) 48 42	40, 50, 61, 68	0
26	14	69/71 (97%)	0.60	7 (10%) 14 12	38, 59, 74, 78	0
26	24	69/71 (97%)	1.05	9 (13%) 9 6	56, 68, 76, 79	0
27	15	59/60 (98%)	-0.63	0 100 100	12, 22, 39, 46	0
27	25	59/60 (98%)	-0.05	0 100 100	28, 39, 54, 70	0
28	16	53/54 (98%)	-0.33	0 100 100	24, 32, 47, 53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.26	1 (1%) 66 61	37, 46, 54, 60	0
29	17	48/49 (97%)	-0.63	1 (2%) 63 58	14, 19, 43, 50	0
29	27	48/49 (97%)	-0.12	4 (8%) 19 15	24, 31, 51, 59	0
30	18	64/65 (98%)	-0.67	0 100 100	20, 25, 32, 46	0
30	28	64/65 (98%)	-0.06	1 (1%) 70 65	33, 40, 46, 54	0
31	19	37/37 (100%)	-0.45	0 100 100	19, 29, 45, 51	0
31	29	37/37 (100%)	0.69	1 (2%) 56 50	44, 54, 66, 68	0
32	1a	1488/1521 (97%)	0.20	70 (4%) 37 32	25, 52, 79, 94	0
32	2a	1491/1521 (98%)	0.41	83 (5%) 31 25	34, 58, 79, 96	0
33	1b	231/256 (90%)	0.91	26 (11%) 11 9	50, 64, 74, 78	0
33	2b	231/256 (90%)	1.03	23 (9%) 14 12	51, 68, 75, 79	0
34	1c	206/239 (86%)	0.56	4 (1%) 66 61	43, 56, 69, 75	0
34	2c	206/239 (86%)	1.02	19 (9%) 16 13	56, 64, 73, 77	0
35	1d	208/209 (99%)	0.98	25 (12%) 10 8	44, 56, 66, 75	0
35	2d	208/209 (99%)	0.57	10 (4%) 36 31	45, 54, 63, 71	0
36	1e	148/162 (91%)	0.29	1 (0%) 84 81	35, 51, 61, 68	0
36	2e	148/162 (91%)	0.49	5 (3%) 48 42	45, 57, 65, 75	0
37	1f	100/101 (99%)	0.46	0 100 100	43, 55, 63, 68	0
37	2f	100/101 (99%)	0.37	1 (1%) 79 75	41, 52, 60, 70	0
38	1g	155/156 (99%)	0.55	10 (6%) 26 21	47, 57, 72, 77	0
38	2g	155/156 (99%)	0.80	15 (9%) 15 12	54, 63, 72, 76	0
39	1h	137/138 (99%)	0.30	3 (2%) 62 57	42, 53, 59, 65	0
39	2h	137/138 (99%)	0.36	2 (1%) 71 67	49, 58, 64, 69	0
40	1i	127/128 (99%)	0.84	12 (9%) 15 13	41, 61, 70, 74	0
40	2i	127/128 (99%)	1.27	23 (18%) 4 3	52, 68, 73, 75	0
41	1j	97/105 (92%)	1.11	14 (14%) 7 5	43, 63, 71, 76	0
41	2j	96/105 (91%)	1.51	25 (26%) 2 2	55, 68, 76, 78	0
42	1k	114/129 (88%)	0.33	4 (3%) 47 41	33, 52, 63, 67	0
42	2k	114/129 (88%)	0.75	11 (9%) 15 12	38, 56, 67, 74	0
43	1l	121/132 (91%)	-0.03	3 (2%) 58 53	33, 40, 53, 64	0
43	2l	121/132 (91%)	0.41	3 (2%) 58 53	42, 50, 61, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	125/126 (99%)	0.45	8 (6%) 27 21	38, 52, 61, 66	0
44	2m	122/126 (96%)	0.77	10 (8%) 19 16	47, 61, 67, 69	0
45	1n	60/61 (98%)	0.60	1 (1%) 69 64	45, 52, 58, 64	0
45	2n	60/61 (98%)	1.28	9 (15%) 6 5	59, 63, 69, 75	0
46	1o	88/89 (98%)	0.17	0 100 100	36, 51, 63, 66	0
46	2o	88/89 (98%)	0.39	2 (2%) 61 55	45, 54, 67, 69	0
47	1p	82/88 (93%)	0.83	5 (6%) 28 23	41, 56, 64, 70	0
47	2p	82/88 (93%)	0.56	2 (2%) 59 54	47, 56, 64, 66	0
48	1q	99/105 (94%)	0.43	2 (2%) 64 59	41, 54, 63, 64	0
48	2q	99/105 (94%)	0.50	2 (2%) 64 59	48, 57, 66, 68	0
49	1r	68/88 (77%)	0.47	1 (1%) 71 67	44, 52, 64, 67	0
49	2r	68/88 (77%)	0.18	1 (1%) 71 67	46, 52, 61, 67	0
50	1s	83/93 (89%)	0.55	4 (4%) 36 31	46, 54, 64, 68	0
50	2s	83/93 (89%)	1.04	5 (6%) 29 23	53, 64, 73, 76	0
51	1t	96/106 (90%)	0.59	2 (2%) 63 58	46, 57, 68, 71	0
51	2t	96/106 (90%)	0.55	6 (6%) 27 22	47, 56, 67, 72	0
52	1u	23/27 (85%)	0.80	2 (8%) 17 14	46, 52, 57, 58	0
52	2u	23/27 (85%)	1.02	1 (4%) 40 34	54, 62, 65, 72	0
53	1v	13/24 (54%)	0.60	4 (30%) 1 1	32, 39, 82, 89	0
53	2v	13/24 (54%)	0.93	4 (30%) 1 1	47, 53, 81, 93	0
54	1w	67/76 (88%)	0.53	5 (7%) 22 17	18, 63, 78, 85	0
54	2w	64/76 (84%)	0.94	8 (12%) 9 7	36, 71, 80, 87	0
55	1x	72/77 (93%)	-0.02	2 (2%) 55 49	16, 48, 66, 79	0
55	2x	72/77 (93%)	0.27	2 (2%) 55 49	31, 56, 70, 87	0
56	1y	67/76 (88%)	2.51	51 (76%) 0 0	50, 85, 89, 90	0
56	2y	66/76 (86%)	2.61	51 (77%) 0 0	56, 86, 91, 93	0
57	1z	17/17 (100%)	0.03	0 100 100	40, 45, 51, 52	0
57	2z	17/17 (100%)	0.64	1 (5%) 29 24	56, 59, 65, 68	0
All	All	20910/21782 (95%)	0.13	1121 (5%) 32 27	11, 49, 74, 96	0

The worst 5 of 1121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2174	C	9.2
45	1n	2	ALA	8.5
1	1A	2174	C	8.4
1	1A	2129	C	8.2
1	2A	2802	G	7.9

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, 95th 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 ²)	Q<0.9
56	4SU	2y	8	20/21	0.46	0.20	84,89,100,114	0
56	G7M	2y	46	24/25	0.47	0.18	75,85,92,101	0
56	5MU	2y	54	21/22	0.48	0.17	78,86,96,113	0
56	5MU	1y	54	21/22	0.51	0.18	77,85,93,112	0
56	G7M	1y	46	24/25	0.52	0.19	81,86,94,100	0
56	4SU	1y	8	20/21	0.57	0.18	83,88,92,103	0
56	PSU	1y	55	20/21	0.66	0.18	83,87,96,107	0
56	MIA	1y	37	22/30	0.67	0.18	74,79,86,90	0
56	MIA	2y	37	22/30	0.68	0.17	65,84,90,108	0
56	PSU	2y	39	20/21	0.68	0.16	76,80,88,100	0
56	PSU	2y	32	20/21	0.71	0.16	79,83,88,104	0
56	PSU	2y	55	20/21	0.74	0.14	79,86,95,97	0
54	G7M	1w	46	24/25	0.77	0.14	58,66,85,96	0
56	PSU	1y	39	20/21	0.80	0.13	68,76,80,85	0
54	G7M	2w	46	24/25	0.82	0.12	69,73,87,98	0
56	PSU	1y	32	20/21	0.82	0.14	72,76,84,94	0
54	PSU	2w	55	20/21	0.86	0.13	63,68,77,78	0
54	4SU	2w	8	20/21	0.88	0.11	68,73,76,88	0
55	PSU	2x	55	20/21	0.91	0.11	54,58,63,65	0
54	5MU	2w	54	21/22	0.91	0.12	55,61,67,72	0
54	PSU	1w	55	20/21	0.91	0.11	42,57,69,69	0
55	4SU	2x	8	20/21	0.91	0.12	55,64,69,81	0
54	PSU	2w	32	20/21	0.92	0.12	47,58,63,66	0
55	5MU	2x	54	21/22	0.92	0.15	55,61,63,65	0
32	2MG	2a	1207	24/25	0.92	0.10	53,61,65,68	0
43	0TD	2l	92	10/11	0.92	0.16	45,53,56,61	0
55	5MU	1x	54	21/22	0.92	0.13	48,54,59,60	0
43	0TD	1l	92	10/11	0.93	0.11	35,41,45,48	0
32	5MC	2a	1400	21/22	0.93	0.11	43,50,55,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	PSU	2a	516	20/21	0.93	0.09	46,56,61,62	0
54	PSU	1w	32	20/21	0.94	0.09	38,41,47,49	0
55	PSU	1x	55	20/21	0.94	0.09	38,46,56,61	0
32	G7M	2a	527	24/25	0.94	0.10	47,52,59,60	0
32	M2G	2a	966	25/26	0.94	0.10	43,48,60,65	0
55	5MC	2x	32	21/22	0.94	0.11	45,52,57,59	0
32	5MC	2a	967	21/22	0.94	0.10	45,52,60,61	0
54	MIA	2w	37	25/30	0.94	0.09	29,50,59,65	0
55	5MC	1x	32	21/22	0.95	0.10	37,43,47,57	0
54	4SU	1w	8	20/21	0.95	0.09	55,63,67,67	0
32	5MC	1a	967	21/22	0.95	0.09	35,40,49,53	0
1	5MU	2A	1915	21/22	0.95	0.09	40,47,52,53	0
1	PSU	2A	1917	20/21	0.95	0.08	46,50,57,66	0
1	5MC	2A	1942	21/22	0.95	0.11	39,46,50,59	0
32	2MG	1a	1207	24/25	0.95	0.08	41,53,57,57	0
54	5MU	1w	54	21/22	0.95	0.10	38,46,51,52	0
1	PSU	1A	1917	20/21	0.95	0.10	34,38,46,47	0
55	4SU	1x	8	20/21	0.95	0.10	45,49,55,58	0
1	5MU	1A	1915	21/22	0.96	0.09	29,38,41,43	0
32	4OC	2a	1402	22/23	0.96	0.08	37,44,47,49	0
32	5MC	2a	1407	21/22	0.96	0.07	33,39,42,45	0
32	UR3	2a	1498	21/22	0.96	0.09	37,41,46,49	0
55	31H	2x	76	32/33	0.96	0.09	27,32,37,40	0
1	5MC	2A	1962	21/22	0.96	0.09	35,41,48,56	0
1	OMU	2A	2552	21/22	0.96	0.08	29,34,39,41	0
1	PSU	2A	1911	20/21	0.96	0.08	36,44,48,53	0
32	G7M	1a	527	24/25	0.96	0.07	32,37,41,44	0
32	M2G	1a	966	25/26	0.96	0.08	34,39,46,48	0
1	OMC	2A	1920	21/22	0.96	0.09	40,45,49,52	0
1	5MU	2A	1939	21/22	0.96	0.08	29,32,37,38	0
32	PSU	1a	516	20/21	0.97	0.07	32,41,45,46	0
32	MA6	2a	1518	24/25	0.97	0.08	35,43,48,49	0
32	MA6	2a	1519	24/25	0.97	0.09	31,43,47,49	0
32	5MC	1a	1400	21/22	0.97	0.10	32,36,40,42	0
54	MIA	1w	37	29/30	0.97	0.08	25,37,48,53	0
32	4OC	1a	1402	22/23	0.97	0.07	26,31,35,40	0
55	31H	1x	76	32/33	0.97	0.07	10,14,18,23	10
54	PSU	2w	39	20/21	0.97	0.08	37,49,59,61	0
32	5MC	1a	1407	21/22	0.97	0.09	26,32,35,40	0
32	5MC	2a	1404	21/22	0.97	0.07	34,37,40,42	0
1	5MC	1A	1942	21/22	0.97	0.08	23,28,31,35	0
54	F3N	2w	76	33/34	0.97	0.09	22,31,36,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	2MA	2A	2503	23/24	0.98	0.07	19,28,33,33	0
1	PSU	1A	1911	20/21	0.98	0.07	26,35,39,42	0
1	PSU	2A	2605	20/21	0.98	0.06	24,26,30,30	0
1	5MC	1A	1962	21/22	0.98	0.06	20,26,30,34	0
32	5MC	1a	1404	21/22	0.98	0.06	23,27,30,35	0
54	PSU	1w	39	20/21	0.98	0.07	28,39,42,45	0
1	2MA	1A	2503	23/24	0.98	0.05	10,15,18,20	0
32	UR3	1a	1498	21/22	0.98	0.06	22,32,34,40	0
32	MA6	1a	1519	24/25	0.98	0.07	24,28,30,31	0
54	F3N	1w	76	33/34	0.98	0.07	10,14,18,25	0
1	OMC	1A	1920	21/22	0.98	0.07	27,33,37,39	0
1	OMG	2A	2251	24/25	0.98	0.06	24,27,32,39	0
1	PSU	1A	2605	20/21	0.99	0.05	13,16,21,23	0
1	OMG	1A	2251	24/25	0.99	0.05	11,15,18,18	0
1	5MU	1A	1939	21/22	0.99	0.05	14,19,23,27	0
32	MA6	1a	1518	24/25	0.99	0.06	19,27,30,31	0
1	OMU	1A	2552	21/22	0.99	0.05	15,18,21,24	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, 95th 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(\AA^2)	Q<0.9
58	MG	2A	3272	1/1	0.41	0.35	78,78,78,78	0
58	MG	2A	3686	1/1	0.44	0.26	77,77,77,77	0
58	MG	2B	219	1/1	0.45	0.28	78,78,78,78	0
58	MG	2A	3253	1/1	0.47	0.16	76,76,76,76	0
58	MG	18	105	1/1	0.47	0.23	70,70,70,70	0
58	MG	1y	101	1/1	0.59	0.17	78,78,78,78	0
58	MG	2a	1626	1/1	0.61	0.28	65,65,65,65	0
58	MG	2a	1631	1/1	0.62	0.19	78,78,78,78	0
58	MG	2a	1810	1/1	0.62	0.18	76,76,76,76	0
58	MG	2w	102	1/1	0.62	0.16	73,73,73,73	0
58	MG	1A	3988	1/1	0.63	0.18	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2a	1745	1/1	0.64	0.17	71,71,71,71	0
58	MG	2a	1780	1/1	0.64	0.21	66,66,66,66	0
58	MG	2A	3850	1/1	0.64	0.37	65,65,65,65	0
58	MG	2A	3810	1/1	0.64	0.27	62,62,62,62	0
58	MG	2A	3701	1/1	0.65	0.19	69,69,69,69	0
58	MG	1A	4094	1/1	0.66	0.19	71,71,71,71	0
58	MG	1a	1741	1/1	0.66	0.21	67,67,67,67	0
58	MG	1A	4038	1/1	0.67	0.19	49,49,49,49	0
58	MG	2y	104	1/1	0.67	0.28	80,80,80,80	0
58	MG	2A	3608	1/1	0.68	0.24	73,73,73,73	0
58	MG	2a	1749	1/1	0.69	0.17	66,66,66,66	0
58	MG	1A	3478	1/1	0.69	0.16	52,52,52,52	0
58	MG	1B	222	1/1	0.69	0.20	57,57,57,57	0
58	MG	1D	311	1/1	0.69	0.24	59,59,59,59	0
58	MG	2A	3681	1/1	0.69	0.20	58,58,58,58	0
58	MG	1a	1779	1/1	0.70	0.15	48,48,48,48	0
58	MG	1a	1714	1/1	0.70	0.32	57,57,57,57	0
58	MG	1A	3793	1/1	0.70	0.21	72,72,72,72	0
58	MG	2A	3266	1/1	0.70	0.16	70,70,70,70	0
58	MG	1O	205	1/1	0.71	0.26	62,62,62,62	0
58	MG	29	101	1/1	0.71	0.56	63,63,63,63	0
58	MG	2a	1796	1/1	0.72	0.20	69,69,69,69	0
58	MG	2A	3176	1/1	0.72	0.34	60,60,60,60	0
58	MG	2e	201	1/1	0.72	0.12	59,59,59,59	0
58	MG	2A	3390	1/1	0.72	0.18	62,62,62,62	0
58	MG	2A	3778	1/1	0.72	0.27	51,51,51,51	0
58	MG	2A	3361	1/1	0.73	0.27	70,70,70,70	0
58	MG	1A	3426	1/1	0.73	0.34	58,58,58,58	0
58	MG	2a	1817	1/1	0.73	0.29	66,66,66,66	0
58	MG	1A	3750	1/1	0.73	0.19	60,60,60,60	0
58	MG	2A	3768	1/1	0.73	0.20	48,48,48,48	0
58	MG	2A	3769	1/1	0.73	0.24	58,58,58,58	0
58	MG	2A	3724	1/1	0.74	0.18	69,69,69,69	0
58	MG	1A	4023	1/1	0.74	0.20	55,55,55,55	0
58	MG	2A	3291	1/1	0.74	0.25	64,64,64,64	0
58	MG	2A	3344	1/1	0.74	0.17	72,72,72,72	0
58	MG	2A	3800	1/1	0.74	0.15	52,52,52,52	0
58	MG	1a	1769	1/1	0.75	0.15	70,70,70,70	0
58	MG	10	107	1/1	0.75	0.31	59,59,59,59	0
58	MG	1A	3684	1/1	0.75	0.26	67,67,67,67	0
58	MG	2A	3074	1/1	0.75	0.27	66,66,66,66	0
58	MG	2r	101	1/1	0.75	0.14	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3803	1/1	0.75	0.20	54,54,54,54	0
58	MG	1A	4100	1/1	0.75	0.14	60,60,60,60	0
58	MG	2A	3404	1/1	0.76	0.18	64,64,64,64	0
58	MG	2A	3582	1/1	0.76	0.25	70,70,70,70	0
58	MG	2A	3838	1/1	0.76	0.17	33,33,33,33	0
58	MG	2A	3340	1/1	0.76	0.19	58,58,58,58	0
58	MG	2A	3373	1/1	0.76	0.24	76,76,76,76	0
58	MG	2w	103	1/1	0.76	0.20	73,73,73,73	0
58	MG	2A	3281	1/1	0.76	0.19	66,66,66,66	0
58	MG	2j	201	1/1	0.77	0.14	64,64,64,64	0
58	MG	2l	201	1/1	0.77	0.28	63,63,63,63	0
58	MG	2A	3755	1/1	0.77	0.14	33,33,33,33	0
58	MG	2A	3710	1/1	0.77	0.17	50,50,50,50	0
58	MG	2A	3257	1/1	0.77	0.17	55,55,55,55	0
58	MG	2A	3775	1/1	0.77	0.18	71,71,71,71	0
58	MG	2a	1779	1/1	0.78	0.17	68,68,68,68	0
58	MG	1A	3212	1/1	0.78	0.26	66,66,66,66	0
58	MG	2w	105	1/1	0.78	0.12	61,61,61,61	0
58	MG	2B	202	1/1	0.78	0.20	69,69,69,69	0
58	MG	2a	1757	1/1	0.79	0.17	68,68,68,68	0
58	MG	2A	3682	1/1	0.79	0.24	60,60,60,60	0
58	MG	2A	3238	1/1	0.79	0.15	70,70,70,70	0
58	MG	1B	230	1/1	0.79	0.18	69,69,69,69	0
58	MG	1A	3773	1/1	0.79	0.13	16,16,16,16	0
58	MG	1A	3421	1/1	0.79	0.17	54,54,54,54	0
58	MG	2a	1818	1/1	0.79	0.18	63,63,63,63	0
58	MG	1B	212	1/1	0.79	0.28	46,46,46,46	0
58	MG	2A	3761	1/1	0.79	0.14	42,42,42,42	0
58	MG	2a	1610	1/1	0.79	0.14	54,54,54,54	0
58	MG	2A	3576	1/1	0.79	0.14	43,43,43,43	0
58	MG	1A	4093	1/1	0.79	0.21	55,55,55,55	0
58	MG	2a	1708	1/1	0.79	0.21	59,59,59,59	0
58	MG	1a	1705	1/1	0.79	0.19	51,51,51,51	0
58	MG	2y	101	1/1	0.79	0.19	79,79,79,79	0
58	MG	1a	1713	1/1	0.79	0.23	39,39,39,39	0
58	MG	2a	1795	1/1	0.80	0.17	64,64,64,64	0
58	MG	2A	3871	1/1	0.80	0.12	62,62,62,62	0
58	MG	1A	3951	1/1	0.80	0.14	57,57,57,57	0
58	MG	2A	3088	1/1	0.80	0.28	62,62,62,62	0
58	MG	2A	3658	1/1	0.80	0.18	41,41,41,41	0
58	MG	2a	1835	1/1	0.80	0.23	51,51,51,51	0
58	MG	1A	3585	1/1	0.80	0.19	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3773	1/1	0.80	0.17	38,38,38,38	0
58	MG	2A	3204	1/1	0.80	0.34	66,66,66,66	0
58	MG	2A	3221	1/1	0.80	0.17	49,49,49,49	0
58	MG	2A	3690	1/1	0.80	0.15	46,46,46,46	0
58	MG	1A	3774	1/1	0.80	0.13	54,54,54,54	0
58	MG	2A	3556	1/1	0.80	0.18	59,59,59,59	0
58	MG	2A	3846	1/1	0.80	0.13	60,60,60,60	0
58	MG	2A	3307	1/1	0.80	0.26	61,61,61,61	0
58	MG	2A	3709	1/1	0.81	0.24	62,62,62,62	0
58	MG	2a	1649	1/1	0.81	0.21	70,70,70,70	0
58	MG	1A	3062	1/1	0.81	0.14	56,56,56,56	0
58	MG	1A	3688	1/1	0.81	0.14	49,49,49,49	0
58	MG	2A	3097	1/1	0.81	0.15	61,61,61,61	0
58	MG	2A	3101	1/1	0.81	0.24	64,64,64,64	0
58	MG	2A	3118	1/1	0.81	0.18	47,47,47,47	0
58	MG	1a	1625	1/1	0.81	0.29	61,61,61,61	0
58	MG	1A	3740	1/1	0.81	0.11	51,51,51,51	0
58	MG	2A	3405	1/1	0.81	0.18	56,56,56,56	0
58	MG	2a	1804	1/1	0.81	0.22	64,64,64,64	0
58	MG	1B	208	1/1	0.81	0.14	60,60,60,60	0
58	MG	2A	3224	1/1	0.81	0.15	56,56,56,56	0
58	MG	1A	3330	1/1	0.81	0.19	55,55,55,55	0
58	MG	2A	3597	1/1	0.81	0.20	62,62,62,62	0
58	MG	1A	4010	1/1	0.81	0.10	73,73,73,73	0
58	MG	1a	1761	1/1	0.81	0.16	51,51,51,51	0
58	MG	2A	3860	1/1	0.81	0.23	56,56,56,56	0
58	MG	1A	3566	1/1	0.81	0.09	44,44,44,44	0
58	MG	1A	3199	1/1	0.81	0.25	44,44,44,44	0
58	MG	2A	3278	1/1	0.81	0.16	51,51,51,51	0
58	MG	1a	1814	1/1	0.81	0.29	64,64,64,64	0
58	MG	1A	4043	1/1	0.81	0.12	27,27,27,27	0
58	MG	2A	3708	1/1	0.81	0.11	29,29,29,29	0
58	MG	2a	1698	1/1	0.82	0.19	47,47,47,47	0
58	MG	2A	3268	1/1	0.82	0.20	56,56,56,56	0
58	MG	1a	1641	1/1	0.82	0.19	60,60,60,60	0
58	MG	1A	3665	1/1	0.82	0.14	47,47,47,47	0
58	MG	1A	3506	1/1	0.82	0.20	63,63,63,63	0
58	MG	1A	3548	1/1	0.82	0.50	52,52,52,52	0
58	MG	2A	3303	1/1	0.82	0.33	56,56,56,56	0
58	MG	1a	1733	1/1	0.82	0.17	50,50,50,50	0
58	MG	2A	3172	1/1	0.82	0.12	71,71,71,71	0
58	MG	1A	4034	1/1	0.82	0.13	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3358	1/1	0.82	0.23	58,58,58,58	0
58	MG	1A	3831	1/1	0.82	0.13	38,38,38,38	0
58	MG	2A	3385	1/1	0.82	0.14	61,61,61,61	0
58	MG	2E	301	1/1	0.82	0.22	57,57,57,57	0
58	MG	28	101	1/1	0.82	0.37	60,60,60,60	0
58	MG	1A	3924	1/1	0.82	0.17	68,68,68,68	0
58	MG	1A	3489	1/1	0.82	0.14	53,53,53,53	0
58	MG	2a	1625	1/1	0.82	0.15	63,63,63,63	0
58	MG	1t	201	1/1	0.82	0.14	51,51,51,51	0
58	MG	2a	1629	1/1	0.82	0.14	59,59,59,59	0
58	MG	1A	3955	1/1	0.82	0.13	53,53,53,53	0
58	MG	2A	3064	1/1	0.82	0.10	56,56,56,56	0
58	MG	2a	1696	1/1	0.82	0.20	64,64,64,64	0
58	MG	2a	1609	1/1	0.83	0.13	64,64,64,64	0
58	MG	1A	3549	1/1	0.83	0.16	53,53,53,53	0
58	MG	2A	3358	1/1	0.83	0.23	54,54,54,54	0
58	MG	1A	3957	1/1	0.83	0.22	69,69,69,69	0
58	MG	2A	3234	1/1	0.83	0.17	50,50,50,50	0
58	MG	1B	215	1/1	0.83	0.12	44,44,44,44	0
58	MG	2a	1632	1/1	0.83	0.39	71,71,71,71	0
58	MG	2A	3752	1/1	0.83	0.19	61,61,61,61	0
58	MG	2a	1655	1/1	0.83	0.15	66,66,66,66	0
58	MG	1A	3848	1/1	0.83	0.12	41,41,41,41	0
58	MG	1A	4046	1/1	0.83	0.10	44,44,44,44	0
58	MG	1A	4009	1/1	0.83	0.11	62,62,62,62	0
58	MG	2A	3432	1/1	0.83	0.28	60,60,60,60	0
58	MG	2a	1748	1/1	0.83	0.19	75,75,75,75	0
58	MG	2A	3477	1/1	0.83	0.26	68,68,68,68	0
58	MG	2A	3491	1/1	0.83	0.18	58,58,58,58	0
58	MG	2a	1762	1/1	0.83	0.11	76,76,76,76	0
58	MG	1A	3475	1/1	0.83	0.17	46,46,46,46	0
58	MG	2A	3100	1/1	0.83	0.18	62,62,62,62	0
58	MG	1U	211	1/1	0.83	0.69	64,64,64,64	0
58	MG	2A	3822	1/1	0.83	0.11	42,42,42,42	0
58	MG	1Y	202	1/1	0.83	0.10	57,57,57,57	0
58	MG	2a	1808	1/1	0.83	0.12	51,51,51,51	0
58	MG	1A	3725	1/1	0.83	0.19	48,48,48,48	0
58	MG	2A	3848	1/1	0.83	0.14	61,61,61,61	0
58	MG	2A	3616	1/1	0.83	0.14	31,31,31,31	0
58	MG	2a	1820	1/1	0.83	0.24	66,66,66,66	0
58	MG	2A	3645	1/1	0.83	0.20	46,46,46,46	0
58	MG	2A	3869	1/1	0.83	0.15	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3302	1/1	0.83	0.18	55,55,55,55	0
58	MG	2A	3670	1/1	0.83	0.22	55,55,55,55	0
58	MG	16	102	1/1	0.83	0.12	40,40,40,40	0
58	MG	2A	3191	1/1	0.83	0.14	52,52,52,52	0
58	MG	2U	202	1/1	0.83	0.09	40,40,40,40	0
58	MG	1a	1798	1/1	0.83	0.18	66,66,66,66	0
58	MG	2A	3342	1/1	0.83	0.33	68,68,68,68	0
58	MG	2a	1602	1/1	0.83	0.17	68,68,68,68	0
58	MG	2A	3697	1/1	0.84	0.14	57,57,57,57	0
58	MG	2A	3122	1/1	0.84	0.20	70,70,70,70	0
58	MG	1A	3837	1/1	0.84	0.11	30,30,30,30	0
58	MG	1W	208	1/1	0.84	0.18	33,33,33,33	0
58	MG	1Y	201	1/1	0.84	0.19	58,58,58,58	0
58	MG	2A	3718	1/1	0.84	0.17	50,50,50,50	0
58	MG	2A	3720	1/1	0.84	0.14	44,44,44,44	0
58	MG	2A	3195	1/1	0.84	0.18	62,62,62,62	0
58	MG	2a	1651	1/1	0.84	0.14	50,50,50,50	0
58	MG	1B	203	1/1	0.84	0.25	51,51,51,51	0
58	MG	2A	3212	1/1	0.84	0.14	64,64,64,64	0
58	MG	1a	1790	1/1	0.84	0.16	74,74,74,74	0
58	MG	2A	3767	1/1	0.84	0.16	48,48,48,48	0
58	MG	2A	3403	1/1	0.84	0.19	65,65,65,65	0
58	MG	1a	1797	1/1	0.84	0.13	55,55,55,55	0
58	MG	1A	3474	1/1	0.84	0.21	52,52,52,52	0
58	MG	1a	1809	1/1	0.84	0.12	63,63,63,63	0
58	MG	2A	3444	1/1	0.84	0.12	68,68,68,68	0
58	MG	2A	3465	1/1	0.84	0.17	62,62,62,62	0
58	MG	2A	3244	1/1	0.84	0.18	56,56,56,56	0
58	MG	2a	1793	1/1	0.84	0.17	56,56,56,56	0
58	MG	11	103	1/1	0.84	0.24	56,56,56,56	0
58	MG	2A	3519	1/1	0.84	0.18	57,57,57,57	0
58	MG	1A	3711	1/1	0.84	0.14	31,31,31,31	0
58	MG	1x	105	1/1	0.84	0.21	59,59,59,59	0
58	MG	1A	3589	1/1	0.84	0.48	54,54,54,54	0
58	MG	2A	3271	1/1	0.84	0.11	52,52,52,52	0
58	MG	1B	221	1/1	0.84	0.11	39,39,39,39	0
58	MG	1A	3505	1/1	0.84	0.15	49,49,49,49	0
58	MG	2A	3877	1/1	0.84	0.11	71,71,71,71	0
58	MG	2A	3879	1/1	0.84	0.16	49,49,49,49	0
58	MG	2A	3882	1/1	0.84	0.17	59,59,59,59	0
58	MG	1a	1687	1/1	0.84	0.19	62,62,62,62	0
58	MG	2A	3286	1/1	0.84	0.24	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3828	1/1	0.84	0.10	25,25,25,25	0
58	MG	1A	3568	1/1	0.84	0.37	48,48,48,48	0
58	MG	1A	3836	1/1	0.84	0.13	57,57,57,57	0
58	MG	1S	203	1/1	0.84	0.09	61,61,61,61	0
58	MG	2y	103	1/1	0.84	0.22	70,70,70,70	0
58	MG	2A	3334	1/1	0.84	0.15	60,60,60,60	0
58	MG	2a	1620	1/1	0.85	0.19	80,80,80,80	0
58	MG	2A	3384	1/1	0.85	0.14	50,50,50,50	0
58	MG	1s	101	1/1	0.85	0.17	54,54,54,54	0
58	MG	2A	3236	1/1	0.85	0.18	57,57,57,57	0
58	MG	2A	3237	1/1	0.85	0.22	53,53,53,53	0
58	MG	2A	3759	1/1	0.85	0.16	47,47,47,47	0
58	MG	1a	1605	1/1	0.85	0.13	62,62,62,62	0
58	MG	1A	3401	1/1	0.85	0.24	64,64,64,64	0
58	MG	2A	3250	1/1	0.85	0.15	57,57,57,57	0
58	MG	2a	1661	1/1	0.85	0.16	55,55,55,55	0
58	MG	2a	1666	1/1	0.85	0.22	53,53,53,53	0
58	MG	1A	3089	1/1	0.85	0.10	30,30,30,30	0
58	MG	1A	3511	1/1	0.85	0.12	59,59,59,59	0
58	MG	2a	1704	1/1	0.85	0.15	52,52,52,52	0
58	MG	1a	1688	1/1	0.85	0.20	52,52,52,52	0
58	MG	2a	1726	1/1	0.85	0.14	65,65,65,65	0
58	MG	2A	3488	1/1	0.85	0.18	63,63,63,63	0
58	MG	1A	3260	1/1	0.85	0.09	57,57,57,57	0
58	MG	1A	3839	1/1	0.85	0.15	45,45,45,45	0
58	MG	2a	1755	1/1	0.85	0.11	68,68,68,68	0
58	MG	2A	3817	1/1	0.85	0.14	51,51,51,51	0
58	MG	1A	3459	1/1	0.85	0.25	41,41,41,41	0
58	MG	1A	3274	1/1	0.85	0.26	62,62,62,62	0
58	MG	2A	3105	1/1	0.85	0.15	51,51,51,51	0
58	MG	2A	3283	1/1	0.85	0.30	54,54,54,54	0
58	MG	2a	1794	1/1	0.85	0.17	42,42,42,42	0
58	MG	2A	3114	1/1	0.85	0.18	57,57,57,57	0
58	MG	2A	3853	1/1	0.85	0.16	60,60,60,60	0
58	MG	2a	1799	1/1	0.85	0.16	51,51,51,51	0
58	MG	2a	1800	1/1	0.85	0.13	59,59,59,59	0
58	MG	1U	210	1/1	0.85	0.19	43,43,43,43	0
58	MG	2A	3626	1/1	0.85	0.16	55,55,55,55	0
58	MG	2a	1809	1/1	0.85	0.20	58,58,58,58	0
58	MG	2A	3293	1/1	0.85	0.12	53,53,53,53	0
58	MG	2A	3872	1/1	0.85	0.13	62,62,62,62	0
58	MG	1a	1747	1/1	0.85	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4058	1/1	0.85	0.11	13,13,13,13	0
58	MG	1A	4068	1/1	0.85	0.11	41,41,41,41	0
58	MG	1A	3943	1/1	0.85	0.14	51,51,51,51	0
58	MG	2g	201	1/1	0.85	0.15	63,63,63,63	0
58	MG	2A	3338	1/1	0.85	0.11	63,63,63,63	0
58	MG	1A	3303	1/1	0.85	0.31	52,52,52,52	0
58	MG	1A	3476	1/1	0.85	0.26	66,66,66,66	0
58	MG	2A	3209	1/1	0.85	0.21	57,57,57,57	0
58	MG	1A	3102	1/1	0.85	0.18	50,50,50,50	0
58	MG	1A	3970	1/1	0.85	0.15	34,34,34,34	0
58	MG	2x	105	1/1	0.85	0.42	58,58,58,58	0
58	MG	2A	3363	1/1	0.85	0.11	51,51,51,51	0
58	MG	1A	3074	1/1	0.85	0.26	54,54,54,54	0
58	MG	2a	1616	1/1	0.85	0.15	60,60,60,60	0
58	MG	2A	3504	1/1	0.86	0.20	57,57,57,57	0
58	MG	1a	1607	1/1	0.86	0.09	50,50,50,50	0
58	MG	2A	3310	1/1	0.86	0.26	53,53,53,53	0
58	MG	2A	3575	1/1	0.86	0.19	64,64,64,64	0
58	MG	2a	1701	1/1	0.86	0.29	66,66,66,66	0
58	MG	2A	3316	1/1	0.86	0.22	67,67,67,67	0
58	MG	2A	3320	1/1	0.86	0.17	65,65,65,65	0
58	MG	2a	1722	1/1	0.86	0.27	66,66,66,66	0
58	MG	2A	3324	1/1	0.86	0.18	59,59,59,59	0
58	MG	1A	3840	1/1	0.86	0.15	43,43,43,43	0
58	MG	1A	3841	1/1	0.86	0.17	50,50,50,50	0
58	MG	1a	1645	1/1	0.86	0.12	55,55,55,55	0
58	MG	2A	3629	1/1	0.86	0.12	52,52,52,52	0
58	MG	2A	3636	1/1	0.86	0.15	31,31,31,31	0
58	MG	2A	3243	1/1	0.86	0.16	59,59,59,59	0
58	MG	2A	3655	1/1	0.86	0.21	44,44,44,44	0
58	MG	1a	1663	1/1	0.86	0.15	53,53,53,53	0
58	MG	1a	1676	1/1	0.86	0.10	54,54,54,54	0
58	MG	2A	3113	1/1	0.86	0.18	44,44,44,44	0
58	MG	1a	1685	1/1	0.86	0.10	47,47,47,47	0
58	MG	1A	3842	1/1	0.86	0.12	42,42,42,42	0
58	MG	2A	3383	1/1	0.86	0.20	54,54,54,54	0
58	MG	2B	211	1/1	0.86	0.17	64,64,64,64	0
58	MG	1A	3554	1/1	0.86	0.18	60,60,60,60	0
58	MG	1A	3852	1/1	0.86	0.17	53,53,53,53	0
58	MG	2A	3704	1/1	0.86	0.09	65,65,65,65	0
58	MG	1A	3856	1/1	0.86	0.19	59,59,59,59	0
58	MG	2A	3275	1/1	0.86	0.11	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1v	101	1/1	0.86	0.23	65,65,65,65	0
58	MG	2a	1606	1/1	0.86	0.18	49,49,49,49	0
58	MG	2a	1827	1/1	0.86	0.27	66,66,66,66	0
58	MG	1A	3555	1/1	0.86	0.10	51,51,51,51	0
58	MG	2d	301	1/1	0.86	0.35	61,61,61,61	0
58	MG	1A	3805	1/1	0.86	0.12	47,47,47,47	0
58	MG	2A	3721	1/1	0.86	0.10	43,43,43,43	0
58	MG	2A	3207	1/1	0.86	0.22	65,65,65,65	0
58	MG	2A	3733	1/1	0.86	0.17	59,59,59,59	0
58	MG	2A	3058	1/1	0.86	0.15	60,60,60,60	0
58	MG	2A	3472	1/1	0.86	0.16	67,67,67,67	0
58	MG	2A	3473	1/1	0.86	0.11	52,52,52,52	0
58	MG	1A	3026	1/1	0.86	0.14	45,45,45,45	0
58	MG	2a	1633	1/1	0.86	0.23	60,60,60,60	0
58	MG	2A	3065	1/1	0.86	0.15	44,44,44,44	0
58	MG	2A	3070	1/1	0.86	0.25	47,47,47,47	0
58	MG	2A	3498	1/1	0.86	0.22	42,42,42,42	0
58	MG	1x	101	1/1	0.87	0.22	48,48,48,48	0
58	MG	2A	3214	1/1	0.87	0.23	60,60,60,60	0
58	MG	2A	3218	1/1	0.87	0.15	53,53,53,53	0
58	MG	1A	3172	1/1	0.87	0.17	48,48,48,48	0
58	MG	2a	1621	1/1	0.87	0.15	52,52,52,52	0
58	MG	1E	309	1/1	0.87	0.13	48,48,48,48	0
58	MG	2A	3054	1/1	0.87	0.29	53,53,53,53	0
58	MG	1A	4035	1/1	0.87	0.10	35,35,35,35	0
58	MG	1A	3816	1/1	0.87	0.14	54,54,54,54	0
58	MG	1A	3901	1/1	0.87	0.15	26,26,26,26	0
58	MG	1A	3906	1/1	0.87	0.13	49,49,49,49	0
58	MG	2a	1640	1/1	0.87	0.19	53,53,53,53	0
58	MG	2A	3393	1/1	0.87	0.22	61,61,61,61	0
58	MG	2A	3400	1/1	0.87	0.09	59,59,59,59	0
58	MG	2A	3401	1/1	0.87	0.13	57,57,57,57	0
58	MG	1A	3405	1/1	0.87	0.19	38,38,38,38	0
58	MG	2A	3082	1/1	0.87	0.13	50,50,50,50	0
58	MG	2A	3734	1/1	0.87	0.13	51,51,51,51	0
58	MG	2A	3745	1/1	0.87	0.13	39,39,39,39	0
58	MG	2A	3251	1/1	0.87	0.17	57,57,57,57	0
58	MG	2A	3406	1/1	0.87	0.14	52,52,52,52	0
58	MG	2A	3409	1/1	0.87	0.12	54,54,54,54	0
58	MG	2A	3411	1/1	0.87	0.12	49,49,49,49	0
58	MG	2A	3421	1/1	0.87	0.26	38,38,38,38	0
58	MG	2a	1733	1/1	0.87	0.14	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3830	1/1	0.87	0.14	40,40,40,40	0
58	MG	2A	3090	1/1	0.87	0.11	65,65,65,65	0
58	MG	2A	3096	1/1	0.87	0.15	61,61,61,61	0
58	MG	1A	3356	1/1	0.87	0.17	53,53,53,53	0
58	MG	1a	1758	1/1	0.87	0.11	40,40,40,40	0
58	MG	2A	3781	1/1	0.87	0.12	61,61,61,61	0
58	MG	1A	3726	1/1	0.87	0.09	33,33,33,33	0
58	MG	1A	3527	1/1	0.87	0.33	61,61,61,61	0
58	MG	2A	3277	1/1	0.87	0.18	58,58,58,58	0
58	MG	2A	3819	1/1	0.87	0.11	74,74,74,74	0
58	MG	2A	3493	1/1	0.87	0.12	44,44,44,44	0
58	MG	2A	3825	1/1	0.87	0.10	42,42,42,42	0
58	MG	1A	3540	1/1	0.87	0.21	46,46,46,46	0
58	MG	1A	3985	1/1	0.87	0.16	58,58,58,58	0
58	MG	2A	3116	1/1	0.87	0.15	48,48,48,48	0
58	MG	2A	3524	1/1	0.87	0.16	52,52,52,52	0
58	MG	1A	3987	1/1	0.87	0.20	58,58,58,58	0
58	MG	1B	214	1/1	0.87	0.26	56,56,56,56	0
58	MG	2A	3127	1/1	0.87	0.09	55,55,55,55	0
58	MG	1A	3544	1/1	0.87	0.36	56,56,56,56	0
58	MG	2A	3593	1/1	0.87	0.09	46,46,46,46	0
58	MG	2a	1822	1/1	0.87	0.21	55,55,55,55	0
58	MG	2a	1824	1/1	0.87	0.14	59,59,59,59	0
58	MG	2a	1825	1/1	0.87	0.14	62,62,62,62	0
58	MG	1A	3267	1/1	0.87	0.17	49,49,49,49	0
58	MG	1h	201	1/1	0.87	0.10	55,55,55,55	0
58	MG	2a	1841	1/1	0.87	0.21	60,60,60,60	0
58	MG	2A	3192	1/1	0.87	0.21	62,62,62,62	0
58	MG	2A	3883	1/1	0.87	0.17	59,59,59,59	0
58	MG	1l	201	1/1	0.87	0.15	64,64,64,64	0
58	MG	1A	3669	1/1	0.87	0.09	25,25,25,25	0
58	MG	2A	3206	1/1	0.87	0.12	45,45,45,45	0
58	MG	1B	226	1/1	0.87	0.13	49,49,49,49	0
58	MG	2v	102	1/1	0.87	0.12	42,42,42,42	0
58	MG	2A	3647	1/1	0.87	0.16	53,53,53,53	0
58	MG	2W	201	1/1	0.87	0.23	67,67,67,67	0
58	MG	2A	3336	1/1	0.87	0.30	52,52,52,52	0
58	MG	2x	102	1/1	0.87	0.22	40,40,40,40	0
58	MG	2A	3208	1/1	0.87	0.11	53,53,53,53	0
58	MG	1A	3359	1/1	0.87	0.20	64,64,64,64	0
58	MG	2A	3674	1/1	0.87	0.17	38,38,38,38	0
58	MG	2a	1607	1/1	0.87	0.28	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2y	105	1/1	0.87	0.24	68,68,68,68	0
58	MG	1A	3998	1/1	0.88	0.22	53,53,53,53	0
58	MG	1a	1670	1/1	0.88	0.27	60,60,60,60	0
58	MG	1a	1674	1/1	0.88	0.22	52,52,52,52	0
58	MG	2A	3581	1/1	0.88	0.10	48,48,48,48	0
58	MG	2I	101	1/1	0.88	0.12	59,59,59,59	0
58	MG	25	104	1/1	0.88	0.11	55,55,55,55	0
58	MG	1A	3368	1/1	0.88	0.10	42,42,42,42	0
58	MG	1A	3599	1/1	0.88	0.17	61,61,61,61	0
58	MG	1B	223	1/1	0.88	0.10	40,40,40,40	0
58	MG	2A	3292	1/1	0.88	0.32	63,63,63,63	0
58	MG	1A	3611	1/1	0.88	0.11	43,43,43,43	0
58	MG	2A	3295	1/1	0.88	0.18	56,56,56,56	0
58	MG	2A	3298	1/1	0.88	0.14	61,61,61,61	0
58	MG	2a	1615	1/1	0.88	0.21	62,62,62,62	0
58	MG	1a	1695	1/1	0.88	0.30	48,48,48,48	0
58	MG	1a	1702	1/1	0.88	0.16	52,52,52,52	0
58	MG	2A	3306	1/1	0.88	0.10	47,47,47,47	0
58	MG	1A	4027	1/1	0.88	0.11	53,53,53,53	0
58	MG	1a	1710	1/1	0.88	0.16	49,49,49,49	0
58	MG	2A	3660	1/1	0.88	0.12	62,62,62,62	0
58	MG	1B	234	1/1	0.88	0.12	63,63,63,63	0
58	MG	1A	3872	1/1	0.88	0.16	34,34,34,34	0
58	MG	2A	3675	1/1	0.88	0.15	46,46,46,46	0
58	MG	1A	3895	1/1	0.88	0.11	24,24,24,24	0
58	MG	2a	1646	1/1	0.88	0.27	56,56,56,56	0
58	MG	2A	3154	1/1	0.88	0.13	61,61,61,61	0
58	MG	2A	3170	1/1	0.88	0.10	60,60,60,60	0
58	MG	1a	1738	1/1	0.88	0.15	47,47,47,47	0
58	MG	1G	204	1/1	0.88	0.12	47,47,47,47	0
58	MG	2a	1662	1/1	0.88	0.23	56,56,56,56	0
58	MG	2A	3179	1/1	0.88	0.23	41,41,41,41	0
58	MG	2A	3703	1/1	0.88	0.13	59,59,59,59	0
58	MG	2A	3190	1/1	0.88	0.13	58,58,58,58	0
58	MG	2A	3351	1/1	0.88	0.21	52,52,52,52	0
58	MG	2A	3357	1/1	0.88	0.18	52,52,52,52	0
58	MG	1O	201	1/1	0.88	0.15	62,62,62,62	0
58	MG	1A	3470	1/1	0.88	0.14	53,53,53,53	0
58	MG	1A	3543	1/1	0.88	0.22	46,46,46,46	0
58	MG	2a	1730	1/1	0.88	0.35	60,60,60,60	0
58	MG	1A	3381	1/1	0.88	0.24	45,45,45,45	0
58	MG	2a	1741	1/1	0.88	0.23	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3375	1/1	0.88	0.32	62,62,62,62	0
58	MG	1A	4056	1/1	0.88	0.12	46,46,46,46	0
58	MG	1a	1782	1/1	0.88	0.12	49,49,49,49	0
58	MG	2a	1752	1/1	0.88	0.13	61,61,61,61	0
58	MG	2A	3742	1/1	0.88	0.13	32,32,32,32	0
58	MG	2A	3744	1/1	0.88	0.23	56,56,56,56	0
58	MG	1W	202	1/1	0.88	0.20	40,40,40,40	0
58	MG	2A	3746	1/1	0.88	0.10	62,62,62,62	0
58	MG	1A	3314	1/1	0.88	0.10	47,47,47,47	0
58	MG	2A	3391	1/1	0.88	0.14	53,53,53,53	0
58	MG	1A	4063	1/1	0.88	0.18	30,30,30,30	0
58	MG	2A	3760	1/1	0.88	0.22	40,40,40,40	0
58	MG	1a	1802	1/1	0.88	0.08	46,46,46,46	0
58	MG	2A	3216	1/1	0.88	0.13	52,52,52,52	0
58	MG	1A	3266	1/1	0.88	0.20	60,60,60,60	0
58	MG	1A	4090	1/1	0.88	0.27	46,46,46,46	0
58	MG	2a	1805	1/1	0.88	0.15	63,63,63,63	0
58	MG	2A	3222	1/1	0.88	0.27	55,55,55,55	0
58	MG	1A	3413	1/1	0.88	0.33	46,46,46,46	0
58	MG	11	105	1/1	0.88	0.08	59,59,59,59	0
58	MG	2a	1816	1/1	0.88	0.21	54,54,54,54	0
58	MG	1A	3334	1/1	0.88	0.09	41,41,41,41	0
58	MG	2A	3794	1/1	0.88	0.17	73,73,73,73	0
58	MG	2A	3797	1/1	0.88	0.12	56,56,56,56	0
58	MG	1A	3362	1/1	0.88	0.11	56,56,56,56	0
58	MG	2A	3809	1/1	0.88	0.12	63,63,63,63	0
58	MG	1a	1604	1/1	0.88	0.11	48,48,48,48	0
58	MG	1A	3455	1/1	0.88	0.24	51,51,51,51	0
58	MG	2A	3445	1/1	0.88	0.15	44,44,44,44	0
58	MG	2A	3451	1/1	0.88	0.23	47,47,47,47	0
58	MG	2A	3455	1/1	0.88	0.24	58,58,58,58	0
58	MG	2A	3464	1/1	0.88	0.14	43,43,43,43	0
58	MG	1A	3752	1/1	0.88	0.07	27,27,27,27	0
58	MG	1a	1612	1/1	0.88	0.12	58,58,58,58	0
58	MG	2A	3024	1/1	0.88	0.13	36,36,36,36	0
58	MG	2l	205	1/1	0.88	0.15	52,52,52,52	0
58	MG	2A	3252	1/1	0.88	0.20	62,62,62,62	0
58	MG	2t	201	1/1	0.88	0.11	52,52,52,52	0
58	MG	2A	3482	1/1	0.88	0.14	38,38,38,38	0
58	MG	2A	3484	1/1	0.88	0.13	51,51,51,51	0
58	MG	2A	3051	1/1	0.88	0.09	35,35,35,35	0
58	MG	1B	209	1/1	0.88	0.11	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2w	109	1/1	0.88	0.33	66,66,66,66	0
58	MG	1a	1635	1/1	0.88	0.15	48,48,48,48	0
58	MG	1a	1638	1/1	0.88	0.12	61,61,61,61	0
58	MG	1A	3457	1/1	0.88	0.29	41,41,41,41	0
58	MG	1a	1644	1/1	0.88	0.16	47,47,47,47	0
58	MG	1A	3995	1/1	0.88	0.08	25,25,25,25	0
58	MG	2A	3526	1/1	0.88	0.10	51,51,51,51	0
58	MG	1A	3973	1/1	0.89	0.13	34,34,34,34	0
58	MG	2A	3273	1/1	0.89	0.19	54,54,54,54	0
58	MG	2A	3420	1/1	0.89	0.20	45,45,45,45	0
58	MG	1A	3728	1/1	0.89	0.10	47,47,47,47	0
58	MG	1A	3412	1/1	0.89	0.16	53,53,53,53	0
58	MG	2A	3434	1/1	0.89	0.18	58,58,58,58	0
58	MG	2A	3437	1/1	0.89	0.20	42,42,42,42	0
58	MG	1A	3480	1/1	0.89	0.12	50,50,50,50	0
58	MG	2a	1639	1/1	0.89	0.13	48,48,48,48	0
58	MG	2A	3736	1/1	0.89	0.10	37,37,37,37	0
58	MG	1A	3603	1/1	0.89	0.09	31,31,31,31	0
58	MG	2a	1647	1/1	0.89	0.14	50,50,50,50	0
58	MG	1B	218	1/1	0.89	0.10	43,43,43,43	0
58	MG	2A	3454	1/1	0.89	0.19	48,48,48,48	0
58	MG	1A	3388	1/1	0.89	0.10	55,55,55,55	0
58	MG	2A	3750	1/1	0.89	0.13	67,67,67,67	0
58	MG	1A	3612	1/1	0.89	0.10	19,19,19,19	0
58	MG	2A	3174	1/1	0.89	0.16	63,63,63,63	0
58	MG	2A	3468	1/1	0.89	0.14	63,63,63,63	0
58	MG	1A	3496	1/1	0.89	0.09	39,39,39,39	0
58	MG	2a	1700	1/1	0.89	0.14	62,62,62,62	0
58	MG	1A	3861	1/1	0.89	0.13	53,53,53,53	0
58	MG	1A	3865	1/1	0.89	0.11	51,51,51,51	0
58	MG	1B	232	1/1	0.89	0.36	58,58,58,58	0
58	MG	1a	1651	1/1	0.89	0.17	55,55,55,55	0
58	MG	2a	1725	1/1	0.89	0.12	54,54,54,54	0
58	MG	2A	3487	1/1	0.89	0.11	51,51,51,51	0
58	MG	1a	1652	1/1	0.89	0.21	53,53,53,53	0
58	MG	2A	3777	1/1	0.89	0.15	60,60,60,60	0
58	MG	2a	1734	1/1	0.89	0.12	57,57,57,57	0
58	MG	2A	3202	1/1	0.89	0.20	50,50,50,50	0
58	MG	2A	3203	1/1	0.89	0.13	39,39,39,39	0
58	MG	2A	3314	1/1	0.89	0.15	49,49,49,49	0
58	MG	1a	1656	1/1	0.89	0.19	52,52,52,52	0
58	MG	2A	3799	1/1	0.89	0.12	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3516	1/1	0.89	0.17	49,49,49,49	0
58	MG	2A	3318	1/1	0.89	0.14	49,49,49,49	0
58	MG	1w	107	1/1	0.89	0.15	51,51,51,51	0
58	MG	2a	1764	1/1	0.89	0.13	67,67,67,67	0
58	MG	2A	3322	1/1	0.89	0.14	56,56,56,56	0
58	MG	2A	3542	1/1	0.89	0.18	45,45,45,45	0
58	MG	2a	1785	1/1	0.89	0.11	33,33,33,33	0
58	MG	1A	3666	1/1	0.89	0.13	36,36,36,36	0
58	MG	1A	3876	1/1	0.89	0.18	22,22,22,22	0
58	MG	1x	106	1/1	0.89	0.27	51,51,51,51	0
58	MG	1A	3259	1/1	0.89	0.14	55,55,55,55	0
58	MG	1G	203	1/1	0.89	0.11	51,51,51,51	0
58	MG	2A	3849	1/1	0.89	0.09	22,22,22,22	0
58	MG	2A	3215	1/1	0.89	0.16	56,56,56,56	0
58	MG	2A	3045	1/1	0.89	0.08	55,55,55,55	0
58	MG	2A	3347	1/1	0.89	0.13	58,58,58,58	0
58	MG	1A	4042	1/1	0.89	0.10	35,35,35,35	0
58	MG	2A	3870	1/1	0.89	0.10	52,52,52,52	0
58	MG	1A	3811	1/1	0.89	0.09	37,37,37,37	0
58	MG	1A	3298	1/1	0.89	0.20	57,57,57,57	0
58	MG	1a	1692	1/1	0.89	0.35	61,61,61,61	0
58	MG	1A	3913	1/1	0.89	0.18	48,48,48,48	0
58	MG	2A	3364	1/1	0.89	0.10	46,46,46,46	0
58	MG	2A	3369	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3067	1/1	0.89	0.14	52,52,52,52	0
58	MG	2B	204	1/1	0.89	0.17	62,62,62,62	0
58	MG	1A	3817	1/1	0.89	0.14	52,52,52,52	0
58	MG	1A	4062	1/1	0.89	0.11	49,49,49,49	0
58	MG	2A	3671	1/1	0.89	0.12	65,65,65,65	0
58	MG	2E	303	1/1	0.89	0.09	46,46,46,46	0
58	MG	2G	201	1/1	0.89	0.18	59,59,59,59	0
58	MG	2Q	202	1/1	0.89	0.14	38,38,38,38	0
58	MG	2A	3241	1/1	0.89	0.14	50,50,50,50	0
58	MG	1A	3932	1/1	0.89	0.09	40,40,40,40	0
58	MG	1A	3508	1/1	0.89	0.13	58,58,58,58	0
58	MG	1A	3438	1/1	0.89	0.09	40,40,40,40	0
58	MG	2A	3091	1/1	0.89	0.17	54,54,54,54	0
58	MG	1A	3714	1/1	0.89	0.12	40,40,40,40	0
58	MG	2A	3694	1/1	0.89	0.14	25,25,25,25	0
58	MG	2a	1604	1/1	0.89	0.16	56,56,56,56	0
58	MG	1A	3407	1/1	0.89	0.21	56,56,56,56	0
58	MG	2w	111	1/1	0.89	0.14	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2w	112	1/1	0.89	0.12	56,56,56,56	0
58	MG	1A	3966	1/1	0.89	0.13	38,38,38,38	0
58	MG	2A	3702	1/1	0.89	0.11	43,43,43,43	0
58	MG	1A	3537	1/1	0.89	0.15	51,51,51,51	0
58	MG	1a	1751	1/1	0.89	0.09	50,50,50,50	0
58	MG	15	109	1/1	0.89	0.11	42,42,42,42	0
58	MG	2a	1617	1/1	0.89	0.09	57,57,57,57	0
58	MG	2A	3490	1/1	0.90	0.08	44,44,44,44	0
58	MG	2A	3039	1/1	0.90	0.12	50,50,50,50	0
58	MG	1a	1614	1/1	0.90	0.10	48,48,48,48	0
58	MG	1A	4075	1/1	0.90	0.10	13,13,13,13	0
58	MG	1A	3349	1/1	0.90	0.26	65,65,65,65	0
58	MG	1A	3881	1/1	0.90	0.17	24,24,24,24	0
58	MG	1A	3265	1/1	0.90	0.13	50,50,50,50	0
58	MG	2B	207	1/1	0.90	0.12	53,53,53,53	0
58	MG	2B	210	1/1	0.90	0.07	56,56,56,56	0
58	MG	2A	3520	1/1	0.90	0.12	52,52,52,52	0
58	MG	2B	212	1/1	0.90	0.22	56,56,56,56	0
58	MG	1A	4095	1/1	0.90	0.14	50,50,50,50	0
58	MG	2D	307	1/1	0.90	0.23	44,44,44,44	0
58	MG	2A	3525	1/1	0.90	0.09	34,34,34,34	0
58	MG	1A	4099	1/1	0.90	0.10	41,41,41,41	0
58	MG	2E	309	1/1	0.90	0.10	38,38,38,38	0
58	MG	2E	311	1/1	0.90	0.14	57,57,57,57	0
58	MG	2F	301	1/1	0.90	0.13	37,37,37,37	0
58	MG	2F	306	1/1	0.90	0.09	44,44,44,44	0
58	MG	1A	3541	1/1	0.90	0.14	32,32,32,32	0
58	MG	2A	3073	1/1	0.90	0.12	46,46,46,46	0
58	MG	2Q	203	1/1	0.90	0.34	56,56,56,56	0
58	MG	2T	202	1/1	0.90	0.14	61,61,61,61	0
58	MG	1A	3448	1/1	0.90	0.14	35,35,35,35	0
58	MG	2A	3077	1/1	0.90	0.17	43,43,43,43	0
58	MG	2W	202	1/1	0.90	0.12	61,61,61,61	0
58	MG	1A	3191	1/1	0.90	0.11	43,43,43,43	0
58	MG	1A	3921	1/1	0.90	0.14	32,32,32,32	0
58	MG	2A	3592	1/1	0.90	0.09	58,58,58,58	0
58	MG	1a	1666	1/1	0.90	0.12	45,45,45,45	0
58	MG	2A	3300	1/1	0.90	0.09	44,44,44,44	0
58	MG	2A	3600	1/1	0.90	0.13	42,42,42,42	0
58	MG	1A	3115	1/1	0.90	0.19	32,32,32,32	0
58	MG	1A	3927	1/1	0.90	0.10	46,46,46,46	0
58	MG	2A	3624	1/1	0.90	0.07	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1675	1/1	0.90	0.25	56,56,56,56	0
58	MG	2a	1612	1/1	0.90	0.24	58,58,58,58	0
58	MG	2A	3627	1/1	0.90	0.15	42,42,42,42	0
58	MG	1A	3271	1/1	0.90	0.17	33,33,33,33	0
58	MG	1a	1678	1/1	0.90	0.22	51,51,51,51	0
58	MG	2A	3642	1/1	0.90	0.12	55,55,55,55	0
58	MG	2A	3102	1/1	0.90	0.23	50,50,50,50	0
58	MG	2a	1624	1/1	0.90	0.14	56,56,56,56	0
58	MG	1a	1679	1/1	0.90	0.23	48,48,48,48	0
58	MG	2A	3111	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3657	1/1	0.90	0.17	58,58,58,58	0
58	MG	1A	3552	1/1	0.90	0.19	45,45,45,45	0
58	MG	1A	3364	1/1	0.90	0.16	56,56,56,56	0
58	MG	2A	3664	1/1	0.90	0.14	55,55,55,55	0
58	MG	1A	3272	1/1	0.90	0.20	52,52,52,52	0
58	MG	2A	3326	1/1	0.90	0.11	58,58,58,58	0
58	MG	2a	1641	1/1	0.90	0.24	53,53,53,53	0
58	MG	1A	3378	1/1	0.90	0.16	41,41,41,41	0
58	MG	1a	1693	1/1	0.90	0.22	41,41,41,41	0
58	MG	2a	1648	1/1	0.90	0.14	56,56,56,56	0
58	MG	2A	3679	1/1	0.90	0.11	49,49,49,49	0
58	MG	2A	3337	1/1	0.90	0.18	60,60,60,60	0
58	MG	2a	1653	1/1	0.90	0.31	54,54,54,54	0
58	MG	1A	3804	1/1	0.90	0.09	27,27,27,27	0
58	MG	2A	3683	1/1	0.90	0.17	59,59,59,59	0
58	MG	2A	3146	1/1	0.90	0.23	60,60,60,60	0
58	MG	1A	3567	1/1	0.90	0.11	45,45,45,45	0
58	MG	2a	1679	1/1	0.90	0.17	43,43,43,43	0
58	MG	2a	1684	1/1	0.90	0.13	43,43,43,43	0
58	MG	2A	3691	1/1	0.90	0.13	49,49,49,49	0
58	MG	1A	3211	1/1	0.90	0.09	39,39,39,39	0
58	MG	1A	3167	1/1	0.90	0.14	39,39,39,39	0
58	MG	2A	3699	1/1	0.90	0.17	44,44,44,44	0
58	MG	2A	3349	1/1	0.90	0.20	52,52,52,52	0
58	MG	2A	3350	1/1	0.90	0.14	53,53,53,53	0
58	MG	2a	1715	1/1	0.90	0.15	53,53,53,53	0
58	MG	2a	1718	1/1	0.90	0.12	51,51,51,51	0
58	MG	1A	3235	1/1	0.90	0.16	43,43,43,43	0
58	MG	2A	3355	1/1	0.90	0.11	56,56,56,56	0
58	MG	1A	3594	1/1	0.90	0.14	30,30,30,30	0
58	MG	1E	312	1/1	0.90	0.15	44,44,44,44	0
58	MG	2A	3181	1/1	0.90	0.23	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3186	1/1	0.90	0.13	49,49,49,49	0
58	MG	2A	3719	1/1	0.90	0.08	38,38,38,38	0
58	MG	2a	1743	1/1	0.90	0.17	52,52,52,52	0
58	MG	1A	3488	1/1	0.90	0.20	24,24,24,24	0
58	MG	2A	3365	1/1	0.90	0.10	57,57,57,57	0
58	MG	2A	3723	1/1	0.90	0.10	46,46,46,46	0
58	MG	2A	3366	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1753	1/1	0.90	0.13	77,77,77,77	0
58	MG	1A	3313	1/1	0.90	0.17	61,61,61,61	0
58	MG	1A	4003	1/1	0.90	0.12	23,23,23,23	0
58	MG	1a	1750	1/1	0.90	0.12	45,45,45,45	0
58	MG	2A	3201	1/1	0.90	0.17	47,47,47,47	0
58	MG	1O	204	1/1	0.90	0.18	49,49,49,49	0
58	MG	1a	1757	1/1	0.90	0.09	47,47,47,47	0
58	MG	1A	3834	1/1	0.90	0.11	55,55,55,55	0
58	MG	1S	201	1/1	0.90	0.48	43,43,43,43	0
58	MG	1A	3491	1/1	0.90	0.09	33,33,33,33	0
58	MG	1A	3251	1/1	0.90	0.14	51,51,51,51	0
58	MG	1A	4024	1/1	0.90	0.11	51,51,51,51	0
58	MG	1V	207	1/1	0.90	0.12	43,43,43,43	0
58	MG	2A	3213	1/1	0.90	0.24	53,53,53,53	0
58	MG	2A	3763	1/1	0.90	0.12	47,47,47,47	0
58	MG	1A	3639	1/1	0.90	0.08	43,43,43,43	0
58	MG	1A	3644	1/1	0.90	0.14	53,53,53,53	0
58	MG	1A	3651	1/1	0.90	0.10	41,41,41,41	0
58	MG	1A	3659	1/1	0.90	0.12	45,45,45,45	0
58	MG	2A	3416	1/1	0.90	0.24	44,44,44,44	0
58	MG	2A	3776	1/1	0.90	0.19	63,63,63,63	0
58	MG	1A	3327	1/1	0.90	0.11	47,47,47,47	0
58	MG	1a	1817	1/1	0.90	0.11	47,47,47,47	0
58	MG	1e	201	1/1	0.90	0.12	54,54,54,54	0
58	MG	2A	3788	1/1	0.90	0.15	60,60,60,60	0
58	MG	2A	3792	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3433	1/1	0.90	0.24	50,50,50,50	0
58	MG	2a	1834	1/1	0.90	0.20	68,68,68,68	0
58	MG	1A	3850	1/1	0.90	0.09	49,49,49,49	0
58	MG	1A	4045	1/1	0.90	0.21	45,45,45,45	0
58	MG	1A	3069	1/1	0.90	0.09	36,36,36,36	0
58	MG	1A	4051	1/1	0.90	0.09	26,26,26,26	0
58	MG	2A	3449	1/1	0.90	0.16	52,52,52,52	0
58	MG	2A	3811	1/1	0.90	0.10	63,63,63,63	0
58	MG	17	103	1/1	0.90	0.09	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3452	1/1	0.90	0.32	50,50,50,50	0
58	MG	1A	3416	1/1	0.90	0.10	46,46,46,46	0
58	MG	1w	108	1/1	0.90	0.13	60,60,60,60	0
58	MG	2v	101	1/1	0.90	0.20	56,56,56,56	0
58	MG	2A	3826	1/1	0.90	0.09	31,31,31,31	0
58	MG	2A	3837	1/1	0.90	0.10	47,47,47,47	0
58	MG	1a	1602	1/1	0.90	0.18	57,57,57,57	0
58	MG	1x	103	1/1	0.90	0.13	46,46,46,46	0
58	MG	2w	107	1/1	0.90	0.20	60,60,60,60	0
58	MG	1A	3185	1/1	0.90	0.14	53,53,53,53	0
58	MG	1A	3523	1/1	0.90	0.15	55,55,55,55	0
58	MG	2A	3255	1/1	0.90	0.17	61,61,61,61	0
58	MG	2A	3256	1/1	0.90	0.25	49,49,49,49	0
58	MG	2x	104	1/1	0.90	0.14	49,49,49,49	0
58	MG	1A	3871	1/1	0.90	0.09	34,34,34,34	0
58	MG	2A	3868	1/1	0.90	0.12	39,39,39,39	0
58	MG	2y	102	1/1	0.90	0.13	62,62,62,62	0
58	MG	2A	3260	1/1	0.90	0.13	47,47,47,47	0
58	MG	1A	3424	1/1	0.90	0.10	39,39,39,39	0
58	MG	2A	3267	1/1	0.90	0.15	53,53,53,53	0
58	MG	2y	106	1/1	0.90	0.18	66,66,66,66	0
58	MG	2A	3559	1/1	0.91	0.15	25,25,25,25	0
58	MG	1A	3458	1/1	0.91	0.11	56,56,56,56	0
58	MG	2E	306	1/1	0.91	0.15	46,46,46,46	0
58	MG	1A	3316	1/1	0.91	0.18	47,47,47,47	0
58	MG	1a	1706	1/1	0.91	0.19	61,61,61,61	0
58	MG	1A	3757	1/1	0.91	0.08	18,18,18,18	0
58	MG	2A	3586	1/1	0.91	0.12	43,43,43,43	0
58	MG	2A	3589	1/1	0.91	0.08	25,25,25,25	0
58	MG	2A	3104	1/1	0.91	0.10	39,39,39,39	0
58	MG	2A	3301	1/1	0.91	0.20	40,40,40,40	0
58	MG	2S	201	1/1	0.91	0.22	64,64,64,64	0
58	MG	1A	3619	1/1	0.91	0.10	5,5,5,5	0
58	MG	1A	3628	1/1	0.91	0.08	31,31,31,31	0
58	MG	2V	201	1/1	0.91	0.35	44,44,44,44	0
58	MG	2A	3601	1/1	0.91	0.15	44,44,44,44	0
58	MG	1a	1716	1/1	0.91	0.27	48,48,48,48	0
58	MG	2A	3610	1/1	0.91	0.08	26,26,26,26	0
58	MG	1a	1722	1/1	0.91	0.27	52,52,52,52	0
58	MG	2A	3621	1/1	0.91	0.15	60,60,60,60	0
58	MG	28	104	1/1	0.91	0.15	44,44,44,44	0
58	MG	2A	3622	1/1	0.91	0.11	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3309	1/1	0.91	0.35	39,39,39,39	0
58	MG	1a	1726	1/1	0.91	0.24	56,56,56,56	0
58	MG	2A	3312	1/1	0.91	0.09	55,55,55,55	0
58	MG	1a	1729	1/1	0.91	0.11	53,53,53,53	0
58	MG	1A	3551	1/1	0.91	0.16	46,46,46,46	0
58	MG	1a	1734	1/1	0.91	0.10	53,53,53,53	0
58	MG	2A	3133	1/1	0.91	0.10	53,53,53,53	0
58	MG	2a	1613	1/1	0.91	0.26	61,61,61,61	0
58	MG	2a	1614	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3137	1/1	0.91	0.12	49,49,49,49	0
58	MG	1A	3904	1/1	0.91	0.10	37,37,37,37	0
58	MG	2A	3656	1/1	0.91	0.12	42,42,42,42	0
58	MG	2A	3147	1/1	0.91	0.15	47,47,47,47	0
58	MG	2A	3328	1/1	0.91	0.16	46,46,46,46	0
58	MG	2A	3332	1/1	0.91	0.33	59,59,59,59	0
58	MG	2A	3152	1/1	0.91	0.16	49,49,49,49	0
58	MG	1A	3029	1/1	0.91	0.09	30,30,30,30	0
58	MG	2A	3163	1/1	0.91	0.19	45,45,45,45	0
58	MG	2a	1630	1/1	0.91	0.19	43,43,43,43	0
58	MG	2A	3165	1/1	0.91	0.14	40,40,40,40	0
58	MG	2A	3166	1/1	0.91	0.26	65,65,65,65	0
58	MG	2A	3341	1/1	0.91	0.37	72,72,72,72	0
58	MG	10	106	1/1	0.91	0.10	48,48,48,48	0
58	MG	1A	3396	1/1	0.91	0.44	41,41,41,41	0
58	MG	10	109	1/1	0.91	0.08	42,42,42,42	0
58	MG	1A	3658	1/1	0.91	0.09	36,36,36,36	0
58	MG	2A	3687	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	4085	1/1	0.91	0.10	23,23,23,23	0
58	MG	1a	1759	1/1	0.91	0.14	55,55,55,55	0
58	MG	2A	3352	1/1	0.91	0.14	51,51,51,51	0
58	MG	2A	3182	1/1	0.91	0.16	38,38,38,38	0
58	MG	2a	1654	1/1	0.91	0.16	47,47,47,47	0
58	MG	11	106	1/1	0.91	0.11	45,45,45,45	0
58	MG	1A	3100	1/1	0.91	0.11	44,44,44,44	0
58	MG	1A	3429	1/1	0.91	0.17	41,41,41,41	0
58	MG	1A	3268	1/1	0.91	0.07	37,37,37,37	0
58	MG	2a	1678	1/1	0.91	0.17	50,50,50,50	0
58	MG	1a	1787	1/1	0.91	0.14	49,49,49,49	0
58	MG	2a	1682	1/1	0.91	0.12	51,51,51,51	0
58	MG	2A	3198	1/1	0.91	0.17	60,60,60,60	0
58	MG	1A	3933	1/1	0.91	0.07	25,25,25,25	0
58	MG	1A	3822	1/1	0.91	0.10	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3711	1/1	0.91	0.19	53,53,53,53	0
58	MG	2A	3372	1/1	0.91	0.19	46,46,46,46	0
58	MG	2a	1702	1/1	0.91	0.26	51,51,51,51	0
58	MG	1A	3531	1/1	0.91	0.33	50,50,50,50	0
58	MG	2a	1706	1/1	0.91	0.11	60,60,60,60	0
58	MG	1A	3574	1/1	0.91	0.15	46,46,46,46	0
58	MG	2a	1713	1/1	0.91	0.17	59,59,59,59	0
58	MG	1A	3582	1/1	0.91	0.09	28,28,28,28	0
58	MG	2a	1717	1/1	0.91	0.14	56,56,56,56	0
58	MG	1a	1811	1/1	0.91	0.11	53,53,53,53	0
58	MG	1A	3702	1/1	0.91	0.10	47,47,47,47	0
58	MG	2A	3388	1/1	0.91	0.31	56,56,56,56	0
58	MG	1A	3002	1/1	0.91	0.10	41,41,41,41	0
58	MG	2A	3210	1/1	0.91	0.11	64,64,64,64	0
58	MG	1b	301	1/1	0.91	0.09	53,53,53,53	0
58	MG	2A	3395	1/1	0.91	0.13	45,45,45,45	0
58	MG	2A	3397	1/1	0.91	0.16	53,53,53,53	0
58	MG	1a	1617	1/1	0.91	0.12	53,53,53,53	0
58	MG	1A	3713	1/1	0.91	0.10	45,45,45,45	0
58	MG	2A	3402	1/1	0.91	0.09	63,63,63,63	0
58	MG	1a	1627	1/1	0.91	0.16	42,42,42,42	0
58	MG	1a	1632	1/1	0.91	0.14	53,53,53,53	0
58	MG	1A	3979	1/1	0.91	0.11	62,62,62,62	0
58	MG	1A	3981	1/1	0.91	0.09	35,35,35,35	0
58	MG	2A	3407	1/1	0.91	0.10	44,44,44,44	0
58	MG	2A	3766	1/1	0.91	0.11	46,46,46,46	0
58	MG	1A	3454	1/1	0.91	0.11	31,31,31,31	0
58	MG	1A	3715	1/1	0.91	0.11	49,49,49,49	0
58	MG	2A	3225	1/1	0.91	0.11	47,47,47,47	0
58	MG	2a	1784	1/1	0.91	0.10	59,59,59,59	0
58	MG	2A	3228	1/1	0.91	0.14	52,52,52,52	0
58	MG	2a	1788	1/1	0.91	0.10	37,37,37,37	0
58	MG	2A	3230	1/1	0.91	0.16	40,40,40,40	0
58	MG	2A	3431	1/1	0.91	0.11	43,43,43,43	0
58	MG	1A	3716	1/1	0.91	0.19	44,44,44,44	0
58	MG	1a	1647	1/1	0.91	0.28	60,60,60,60	0
58	MG	1A	3236	1/1	0.91	0.24	42,42,42,42	0
58	MG	1B	229	1/1	0.91	0.10	44,44,44,44	0
58	MG	2A	3438	1/1	0.91	0.20	47,47,47,47	0
58	MG	2A	3240	1/1	0.91	0.13	34,34,34,34	0
58	MG	1A	3598	1/1	0.91	0.23	53,53,53,53	0
58	MG	2A	3005	1/1	0.91	0.27	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3379	1/1	0.91	0.10	41,41,41,41	0
58	MG	2A	3802	1/1	0.91	0.10	34,34,34,34	0
58	MG	2A	3032	1/1	0.91	0.10	30,30,30,30	0
58	MG	1A	3736	1/1	0.91	0.08	40,40,40,40	0
58	MG	1B	235	1/1	0.91	0.22	56,56,56,56	0
58	MG	2A	3812	1/1	0.91	0.10	60,60,60,60	0
58	MG	2A	3813	1/1	0.91	0.08	35,35,35,35	0
58	MG	1a	1671	1/1	0.91	0.14	50,50,50,50	0
58	MG	1a	1673	1/1	0.91	0.13	49,49,49,49	0
58	MG	2a	1828	1/1	0.91	0.16	50,50,50,50	0
58	MG	2a	1829	1/1	0.91	0.15	50,50,50,50	0
58	MG	2A	3057	1/1	0.91	0.13	43,43,43,43	0
58	MG	1A	3737	1/1	0.91	0.09	58,58,58,58	0
58	MG	2a	1839	1/1	0.91	0.17	50,50,50,50	0
58	MG	1E	306	1/1	0.91	0.10	38,38,38,38	0
58	MG	2A	3474	1/1	0.91	0.24	45,45,45,45	0
58	MG	2A	3475	1/1	0.91	0.15	53,53,53,53	0
58	MG	2A	3261	1/1	0.91	0.24	55,55,55,55	0
58	MG	2A	3479	1/1	0.91	0.13	54,54,54,54	0
58	MG	1A	3859	1/1	0.91	0.12	19,19,19,19	0
58	MG	2l	204	1/1	0.91	0.09	52,52,52,52	0
58	MG	1A	3860	1/1	0.91	0.07	24,24,24,24	0
58	MG	2A	3485	1/1	0.91	0.15	44,44,44,44	0
58	MG	1F	312	1/1	0.91	0.13	39,39,39,39	0
58	MG	2A	3071	1/1	0.91	0.14	46,46,46,46	0
58	MG	1a	1680	1/1	0.91	0.13	47,47,47,47	0
58	MG	2w	101	1/1	0.91	0.12	49,49,49,49	0
58	MG	1A	3494	1/1	0.91	0.10	45,45,45,45	0
58	MG	1A	3744	1/1	0.91	0.07	11,11,11,11	0
58	MG	2w	104	1/1	0.91	0.10	65,65,65,65	0
58	MG	2A	3276	1/1	0.91	0.14	54,54,54,54	0
58	MG	2A	3502	1/1	0.91	0.15	37,37,37,37	0
58	MG	2A	3079	1/1	0.91	0.11	37,37,37,37	0
58	MG	2w	110	1/1	0.91	0.10	58,58,58,58	0
58	MG	1A	3867	1/1	0.91	0.12	43,43,43,43	0
58	MG	2A	3280	1/1	0.91	0.15	59,59,59,59	0
58	MG	2B	201	1/1	0.91	0.14	56,56,56,56	0
58	MG	1a	1689	1/1	0.91	0.08	50,50,50,50	0
58	MG	1A	3868	1/1	0.91	0.17	65,65,65,65	0
58	MG	1A	4040	1/1	0.91	0.06	26,26,26,26	0
58	MG	2A	3289	1/1	0.91	0.19	57,57,57,57	0
58	MG	2A	3534	1/1	0.91	0.09	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3290	1/1	0.91	0.22	53,53,53,53	0
58	MG	2A	3552	1/1	0.91	0.08	33,33,33,33	0
58	MG	1A	3870	1/1	0.91	0.14	34,34,34,34	0
58	MG	1a	1665	1/1	0.92	0.09	56,56,56,56	0
58	MG	2E	308	1/1	0.92	0.07	54,54,54,54	0
58	MG	2A	3562	1/1	0.92	0.10	42,42,42,42	0
58	MG	1A	3900	1/1	0.92	0.07	20,20,20,20	0
58	MG	1A	3735	1/1	0.92	0.16	63,63,63,63	0
58	MG	2A	3299	1/1	0.92	0.15	64,64,64,64	0
58	MG	2F	309	1/1	0.92	0.10	47,47,47,47	0
58	MG	1A	3275	1/1	0.92	0.10	35,35,35,35	0
58	MG	2N	201	1/1	0.92	0.19	55,55,55,55	0
58	MG	2A	3584	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3363	1/1	0.92	0.12	49,49,49,49	0
58	MG	2R	201	1/1	0.92	0.13	57,57,57,57	0
58	MG	1A	3911	1/1	0.92	0.09	41,41,41,41	0
58	MG	1B	216	1/1	0.92	0.08	38,38,38,38	0
58	MG	1A	3066	1/1	0.92	0.12	36,36,36,36	0
58	MG	1A	3254	1/1	0.92	0.09	45,45,45,45	0
58	MG	1A	3747	1/1	0.92	0.06	12,12,12,12	0
58	MG	1A	3371	1/1	0.92	0.21	38,38,38,38	0
58	MG	2Z	301	1/1	0.92	0.10	58,58,58,58	0
58	MG	2A	3607	1/1	0.92	0.11	41,41,41,41	0
58	MG	2A	3311	1/1	0.92	0.15	60,60,60,60	0
58	MG	2A	3609	1/1	0.92	0.08	43,43,43,43	0
58	MG	1a	1682	1/1	0.92	0.10	63,63,63,63	0
58	MG	1a	1683	1/1	0.92	0.19	54,54,54,54	0
58	MG	1B	225	1/1	0.92	0.09	40,40,40,40	0
58	MG	2A	3317	1/1	0.92	0.09	37,37,37,37	0
58	MG	2a	1605	1/1	0.92	0.14	52,52,52,52	0
58	MG	1a	1686	1/1	0.92	0.26	46,46,46,46	0
58	MG	1A	3928	1/1	0.92	0.09	37,37,37,37	0
58	MG	2a	1608	1/1	0.92	0.20	47,47,47,47	0
58	MG	1A	3929	1/1	0.92	0.11	18,18,18,18	0
58	MG	1A	3377	1/1	0.92	0.13	43,43,43,43	0
58	MG	2A	3630	1/1	0.92	0.11	26,26,26,26	0
58	MG	1A	3473	1/1	0.92	0.17	47,47,47,47	0
58	MG	2A	3327	1/1	0.92	0.24	44,44,44,44	0
58	MG	2A	3644	1/1	0.92	0.11	36,36,36,36	0
58	MG	1A	3764	1/1	0.92	0.08	13,13,13,13	0
58	MG	1A	3948	1/1	0.92	0.15	54,54,54,54	0
58	MG	1A	3312	1/1	0.92	0.15	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3335	1/1	0.92	0.17	45,45,45,45	0
58	MG	1a	1704	1/1	0.92	0.13	41,41,41,41	0
58	MG	1A	3001	1/1	0.92	0.08	29,29,29,29	0
58	MG	2A	3659	1/1	0.92	0.08	53,53,53,53	0
58	MG	1A	3051	1/1	0.92	0.14	20,20,20,20	0
58	MG	2A	3663	1/1	0.92	0.08	55,55,55,55	0
58	MG	1A	3964	1/1	0.92	0.08	12,12,12,12	0
58	MG	2A	3669	1/1	0.92	0.11	47,47,47,47	0
58	MG	2A	3143	1/1	0.92	0.12	38,38,38,38	0
58	MG	2A	3144	1/1	0.92	0.14	29,29,29,29	0
58	MG	2A	3343	1/1	0.92	0.21	55,55,55,55	0
58	MG	1A	3795	1/1	0.92	0.12	38,38,38,38	0
58	MG	2a	1642	1/1	0.92	0.39	58,58,58,58	0
58	MG	2a	1644	1/1	0.92	0.11	54,54,54,54	0
58	MG	1A	3477	1/1	0.92	0.22	43,43,43,43	0
58	MG	1a	1715	1/1	0.92	0.17	37,37,37,37	0
58	MG	1A	3202	1/1	0.92	0.10	25,25,25,25	0
58	MG	2A	3161	1/1	0.92	0.11	44,44,44,44	0
58	MG	2a	1650	1/1	0.92	0.08	51,51,51,51	0
58	MG	1A	3978	1/1	0.92	0.12	51,51,51,51	0
58	MG	2A	3353	1/1	0.92	0.11	47,47,47,47	0
58	MG	1A	3321	1/1	0.92	0.19	49,49,49,49	0
58	MG	1A	3980	1/1	0.92	0.11	62,62,62,62	0
58	MG	2A	3168	1/1	0.92	0.14	35,35,35,35	0
58	MG	2A	3359	1/1	0.92	0.25	56,56,56,56	0
58	MG	1A	3483	1/1	0.92	0.06	32,32,32,32	0
58	MG	2A	3700	1/1	0.92	0.15	52,52,52,52	0
58	MG	1A	3815	1/1	0.92	0.09	42,42,42,42	0
58	MG	1T	201	1/1	0.92	0.17	46,46,46,46	0
58	MG	1T	203	1/1	0.92	0.22	44,44,44,44	0
58	MG	2a	1686	1/1	0.92	0.16	42,42,42,42	0
58	MG	2a	1691	1/1	0.92	0.26	49,49,49,49	0
58	MG	1a	1742	1/1	0.92	0.12	45,45,45,45	0
58	MG	1U	202	1/1	0.92	0.17	47,47,47,47	0
58	MG	2A	3371	1/1	0.92	0.12	48,48,48,48	0
58	MG	1U	204	1/1	0.92	0.11	27,27,27,27	0
58	MG	1A	3986	1/1	0.92	0.10	48,48,48,48	0
58	MG	2A	3717	1/1	0.92	0.17	57,57,57,57	0
58	MG	1a	1753	1/1	0.92	0.10	59,59,59,59	0
58	MG	2a	1707	1/1	0.92	0.13	45,45,45,45	0
58	MG	1A	3604	1/1	0.92	0.12	28,28,28,28	0
58	MG	1A	3027	1/1	0.92	0.10	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3171	1/1	0.92	0.21	27,27,27,27	0
58	MG	1A	3823	1/1	0.92	0.08	22,22,22,22	0
58	MG	1a	1766	1/1	0.92	0.18	45,45,45,45	0
58	MG	2a	1719	1/1	0.92	0.12	62,62,62,62	0
58	MG	1a	1768	1/1	0.92	0.11	54,54,54,54	0
58	MG	1A	3095	1/1	0.92	0.16	47,47,47,47	0
58	MG	2A	3394	1/1	0.92	0.26	64,64,64,64	0
58	MG	2a	1728	1/1	0.92	0.24	52,52,52,52	0
58	MG	1a	1773	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3335	1/1	0.92	0.12	47,47,47,47	0
58	MG	1A	3342	1/1	0.92	0.07	40,40,40,40	0
58	MG	2a	1737	1/1	0.92	0.21	40,40,40,40	0
58	MG	2a	1739	1/1	0.92	0.12	66,66,66,66	0
58	MG	1A	3641	1/1	0.92	0.15	42,42,42,42	0
58	MG	10	108	1/1	0.92	0.14	51,51,51,51	0
58	MG	1A	3835	1/1	0.92	0.08	39,39,39,39	0
58	MG	2A	3211	1/1	0.92	0.10	44,44,44,44	0
58	MG	1A	3642	1/1	0.92	0.07	8,8,8,8	0
58	MG	1A	4031	1/1	0.92	0.11	56,56,56,56	0
58	MG	1a	1804	1/1	0.92	0.08	62,62,62,62	0
58	MG	1A	4032	1/1	0.92	0.13	42,42,42,42	0
58	MG	1a	1810	1/1	0.92	0.16	48,48,48,48	0
58	MG	1A	3346	1/1	0.92	0.08	37,37,37,37	0
58	MG	1a	1812	1/1	0.92	0.14	42,42,42,42	0
58	MG	2a	1771	1/1	0.92	0.08	57,57,57,57	0
58	MG	2a	1772	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3645	1/1	0.92	0.10	69,69,69,69	0
58	MG	2A	3426	1/1	0.92	0.15	46,46,46,46	0
58	MG	2A	3223	1/1	0.92	0.37	52,52,52,52	0
58	MG	1A	3648	1/1	0.92	0.08	27,27,27,27	0
58	MG	1A	3269	1/1	0.92	0.11	45,45,45,45	0
58	MG	1A	3353	1/1	0.92	0.08	34,34,34,34	0
58	MG	2A	3780	1/1	0.92	0.09	39,39,39,39	0
58	MG	1A	3509	1/1	0.92	0.14	38,38,38,38	0
58	MG	1A	3425	1/1	0.92	0.14	34,34,34,34	0
58	MG	2A	3790	1/1	0.92	0.11	52,52,52,52	0
58	MG	2A	3441	1/1	0.92	0.17	43,43,43,43	0
58	MG	2a	1802	1/1	0.92	0.09	49,49,49,49	0
58	MG	2a	1803	1/1	0.92	0.23	53,53,53,53	0
58	MG	1l	202	1/1	0.92	0.07	49,49,49,49	0
58	MG	1A	3516	1/1	0.92	0.20	47,47,47,47	0
58	MG	1a	1608	1/1	0.92	0.23	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3176	1/1	0.92	0.11	28,28,28,28	0
58	MG	1w	101	1/1	0.92	0.11	43,43,43,43	0
58	MG	2a	1813	1/1	0.92	0.22	50,50,50,50	0
58	MG	2a	1815	1/1	0.92	0.10	43,43,43,43	0
58	MG	2A	3806	1/1	0.92	0.09	48,48,48,48	0
58	MG	1A	3682	1/1	0.92	0.10	47,47,47,47	0
58	MG	1a	1615	1/1	0.92	0.09	61,61,61,61	0
58	MG	1A	3428	1/1	0.92	0.28	41,41,41,41	0
58	MG	1x	102	1/1	0.92	0.22	51,51,51,51	0
58	MG	2A	3467	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3357	1/1	0.92	0.10	44,44,44,44	0
58	MG	1x	104	1/1	0.92	0.24	45,45,45,45	0
58	MG	1A	3533	1/1	0.92	0.08	41,41,41,41	0
58	MG	1a	1630	1/1	0.92	0.23	39,39,39,39	0
58	MG	1x	107	1/1	0.92	0.21	49,49,49,49	0
58	MG	2A	3258	1/1	0.92	0.14	44,44,44,44	0
58	MG	2a	1837	1/1	0.92	0.18	42,42,42,42	0
58	MG	1x	108	1/1	0.92	0.10	18,18,18,18	0
58	MG	2A	3841	1/1	0.92	0.09	41,41,41,41	0
58	MG	2a	1842	1/1	0.92	0.10	64,64,64,64	0
58	MG	2A	3481	1/1	0.92	0.27	51,51,51,51	0
58	MG	1A	3433	1/1	0.92	0.14	35,35,35,35	0
58	MG	2A	3262	1/1	0.92	0.12	52,52,52,52	0
58	MG	1A	3435	1/1	0.92	0.22	57,57,57,57	0
58	MG	2A	3007	1/1	0.92	0.10	44,44,44,44	0
58	MG	2l	202	1/1	0.92	0.10	48,48,48,48	0
58	MG	2A	3017	1/1	0.92	0.13	28,28,28,28	0
58	MG	2A	3867	1/1	0.92	0.09	49,49,49,49	0
58	MG	2p	101	1/1	0.92	0.24	57,57,57,57	0
58	MG	2A	3270	1/1	0.92	0.13	56,56,56,56	0
58	MG	1A	4076	1/1	0.92	0.10	55,55,55,55	0
58	MG	1a	1640	1/1	0.92	0.10	51,51,51,51	0
58	MG	2A	3036	1/1	0.92	0.16	51,51,51,51	0
58	MG	1A	3249	1/1	0.92	0.14	41,41,41,41	0
58	MG	1A	3442	1/1	0.92	0.32	51,51,51,51	0
58	MG	2A	3515	1/1	0.92	0.10	12,12,12,12	0
58	MG	2A	3047	1/1	0.92	0.15	53,53,53,53	0
58	MG	1A	3444	1/1	0.92	0.24	55,55,55,55	0
58	MG	2w	106	1/1	0.92	0.13	36,36,36,36	0
58	MG	2A	3052	1/1	0.92	0.09	44,44,44,44	0
58	MG	1A	3445	1/1	0.92	0.14	39,39,39,39	0
58	MG	2B	203	1/1	0.92	0.12	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3250	1/1	0.92	0.28	45,45,45,45	0
58	MG	1A	3885	1/1	0.92	0.09	33,33,33,33	0
58	MG	2B	209	1/1	0.92	0.11	43,43,43,43	0
58	MG	1A	3889	1/1	0.92	0.07	20,20,20,20	0
58	MG	2A	3535	1/1	0.92	0.12	45,45,45,45	0
58	MG	2A	3538	1/1	0.92	0.10	45,45,45,45	0
58	MG	2B	214	1/1	0.92	0.10	43,43,43,43	0
58	MG	1A	3452	1/1	0.92	0.11	32,32,32,32	0
58	MG	1a	1664	1/1	0.92	0.16	46,46,46,46	0
58	MG	2A	3068	1/1	0.92	0.07	36,36,36,36	0
58	MG	2A	3557	1/1	0.92	0.07	27,27,27,27	0
58	MG	2A	3511	1/1	0.93	0.13	42,42,42,42	0
58	MG	2A	3008	1/1	0.93	0.19	44,44,44,44	0
58	MG	2A	3010	1/1	0.93	0.13	41,41,41,41	0
58	MG	1A	3550	1/1	0.93	0.18	48,48,48,48	0
58	MG	2B	217	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3022	1/1	0.93	0.13	37,37,37,37	0
58	MG	1A	3024	1/1	0.93	0.10	39,39,39,39	0
58	MG	2A	3031	1/1	0.93	0.12	38,38,38,38	0
58	MG	1A	3888	1/1	0.93	0.06	15,15,15,15	0
58	MG	1A	3382	1/1	0.93	0.07	40,40,40,40	0
58	MG	1A	4096	1/1	0.93	0.12	45,45,45,45	0
58	MG	2A	3536	1/1	0.93	0.17	48,48,48,48	0
58	MG	2A	3042	1/1	0.93	0.12	38,38,38,38	0
58	MG	2A	3540	1/1	0.93	0.14	36,36,36,36	0
58	MG	2A	3043	1/1	0.93	0.12	52,52,52,52	0
58	MG	2A	3549	1/1	0.93	0.11	35,35,35,35	0
58	MG	1A	3890	1/1	0.93	0.13	27,27,27,27	0
58	MG	1a	1658	1/1	0.93	0.19	41,41,41,41	0
58	MG	1a	1659	1/1	0.93	0.22	47,47,47,47	0
58	MG	1a	1660	1/1	0.93	0.16	53,53,53,53	0
58	MG	1a	1661	1/1	0.93	0.12	46,46,46,46	0
58	MG	2A	3563	1/1	0.93	0.14	48,48,48,48	0
58	MG	2A	3572	1/1	0.93	0.15	46,46,46,46	0
58	MG	1A	3891	1/1	0.93	0.08	28,28,28,28	0
58	MG	1A	4103	1/1	0.93	0.10	40,40,40,40	0
58	MG	2V	202	1/1	0.93	0.09	54,54,54,54	0
58	MG	2A	3061	1/1	0.93	0.11	37,37,37,37	0
58	MG	2A	3063	1/1	0.93	0.09	69,69,69,69	0
58	MG	1A	3464	1/1	0.93	0.14	37,37,37,37	0
58	MG	1A	3467	1/1	0.93	0.07	51,51,51,51	0
58	MG	2A	3066	1/1	0.93	0.18	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	26	101	1/1	0.93	0.12	45,45,45,45	0
58	MG	1a	1669	1/1	0.93	0.16	42,42,42,42	0
58	MG	1A	3557	1/1	0.93	0.20	48,48,48,48	0
58	MG	1A	3560	1/1	0.93	0.13	41,41,41,41	0
58	MG	1A	3468	1/1	0.93	0.13	45,45,45,45	0
58	MG	1A	3385	1/1	0.93	0.12	43,43,43,43	0
58	MG	1A	3751	1/1	0.93	0.13	31,31,31,31	0
58	MG	2A	3313	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3919	1/1	0.93	0.06	15,15,15,15	0
58	MG	1A	3386	1/1	0.93	0.14	37,37,37,37	0
58	MG	1A	3328	1/1	0.93	0.09	29,29,29,29	0
58	MG	1A	3760	1/1	0.93	0.08	32,32,32,32	0
58	MG	2A	3319	1/1	0.93	0.30	64,64,64,64	0
58	MG	2A	3623	1/1	0.93	0.13	53,53,53,53	0
58	MG	1A	3053	1/1	0.93	0.27	48,48,48,48	0
58	MG	1A	3400	1/1	0.93	0.26	50,50,50,50	0
58	MG	1A	3195	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3325	1/1	0.93	0.09	60,60,60,60	0
58	MG	1A	3776	1/1	0.93	0.06	14,14,14,14	0
58	MG	1A	3784	1/1	0.93	0.14	42,42,42,42	0
58	MG	2A	3637	1/1	0.93	0.14	37,37,37,37	0
58	MG	1B	233	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3329	1/1	0.93	0.25	46,46,46,46	0
58	MG	2a	1628	1/1	0.93	0.10	53,53,53,53	0
58	MG	2A	3330	1/1	0.93	0.13	55,55,55,55	0
58	MG	2A	3646	1/1	0.93	0.09	28,28,28,28	0
58	MG	1A	3945	1/1	0.93	0.08	19,19,19,19	0
58	MG	2A	3649	1/1	0.93	0.10	43,43,43,43	0
58	MG	2A	3333	1/1	0.93	0.13	57,57,57,57	0
58	MG	2a	1635	1/1	0.93	0.19	40,40,40,40	0
58	MG	2a	1636	1/1	0.93	0.23	44,44,44,44	0
58	MG	1a	1690	1/1	0.93	0.21	39,39,39,39	0
58	MG	1A	3101	1/1	0.93	0.15	48,48,48,48	0
58	MG	1A	3597	1/1	0.93	0.13	38,38,38,38	0
58	MG	1A	3479	1/1	0.93	0.14	47,47,47,47	0
58	MG	1a	1696	1/1	0.93	0.21	38,38,38,38	0
58	MG	2a	1645	1/1	0.93	0.09	52,52,52,52	0
58	MG	2A	3662	1/1	0.93	0.14	43,43,43,43	0
58	MG	1A	3337	1/1	0.93	0.24	53,53,53,53	0
58	MG	1a	1703	1/1	0.93	0.12	36,36,36,36	0
58	MG	2A	3666	1/1	0.93	0.10	47,47,47,47	0
58	MG	1A	3961	1/1	0.93	0.06	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3125	1/1	0.93	0.13	37,37,37,37	0
58	MG	1F	310	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3409	1/1	0.93	0.13	39,39,39,39	0
58	MG	1a	1707	1/1	0.93	0.15	48,48,48,48	0
58	MG	2a	1658	1/1	0.93	0.11	55,55,55,55	0
58	MG	1a	1709	1/1	0.93	0.18	56,56,56,56	0
58	MG	1A	3005	1/1	0.93	0.09	36,36,36,36	0
58	MG	1A	3968	1/1	0.93	0.06	31,31,31,31	0
58	MG	2a	1670	1/1	0.93	0.20	51,51,51,51	0
58	MG	2a	1671	1/1	0.93	0.22	46,46,46,46	0
58	MG	2a	1677	1/1	0.93	0.16	50,50,50,50	0
58	MG	1N	203	1/1	0.93	0.13	40,40,40,40	0
58	MG	2A	3354	1/1	0.93	0.14	56,56,56,56	0
58	MG	1N	206	1/1	0.93	0.25	38,38,38,38	0
58	MG	2A	3688	1/1	0.93	0.14	51,51,51,51	0
58	MG	2A	3356	1/1	0.93	0.09	51,51,51,51	0
58	MG	2a	1687	1/1	0.93	0.11	38,38,38,38	0
58	MG	2a	1688	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3103	1/1	0.93	0.08	46,46,46,46	0
58	MG	2a	1695	1/1	0.93	0.09	56,56,56,56	0
58	MG	2A	3692	1/1	0.93	0.09	43,43,43,43	0
58	MG	1a	1720	1/1	0.93	0.10	48,48,48,48	0
58	MG	2a	1699	1/1	0.93	0.24	57,57,57,57	0
58	MG	1A	3106	1/1	0.93	0.30	40,40,40,40	0
58	MG	1A	3615	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3228	1/1	0.93	0.09	34,34,34,34	0
58	MG	1S	202	1/1	0.93	0.13	39,39,39,39	0
58	MG	2A	3169	1/1	0.93	0.08	43,43,43,43	0
58	MG	1A	3495	1/1	0.93	0.17	55,55,55,55	0
58	MG	1A	3825	1/1	0.93	0.10	24,24,24,24	0
58	MG	2A	3707	1/1	0.93	0.09	55,55,55,55	0
58	MG	1T	202	1/1	0.93	0.14	47,47,47,47	0
58	MG	1A	3019	1/1	0.93	0.10	30,30,30,30	0
58	MG	1a	1743	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3180	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3379	1/1	0.93	0.08	38,38,38,38	0
58	MG	2A	3380	1/1	0.93	0.08	51,51,51,51	0
58	MG	1A	3122	1/1	0.93	0.15	28,28,28,28	0
58	MG	1A	3297	1/1	0.93	0.20	37,37,37,37	0
58	MG	1A	3833	1/1	0.93	0.10	44,44,44,44	0
58	MG	2a	1731	1/1	0.93	0.27	48,48,48,48	0
58	MG	2A	3188	1/1	0.93	0.12	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1752	1/1	0.93	0.13	53,53,53,53	0
58	MG	2a	1736	1/1	0.93	0.28	47,47,47,47	0
58	MG	2A	3727	1/1	0.93	0.14	52,52,52,52	0
58	MG	2A	3730	1/1	0.93	0.08	40,40,40,40	0
58	MG	2a	1740	1/1	0.93	0.16	51,51,51,51	0
58	MG	1A	3140	1/1	0.93	0.23	36,36,36,36	0
58	MG	1V	206	1/1	0.93	0.11	39,39,39,39	0
58	MG	2A	3194	1/1	0.93	0.19	55,55,55,55	0
58	MG	2a	1746	1/1	0.93	0.30	50,50,50,50	0
58	MG	2A	3741	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3997	1/1	0.93	0.15	40,40,40,40	0
58	MG	1A	3020	1/1	0.93	0.08	37,37,37,37	0
58	MG	2A	3398	1/1	0.93	0.14	54,54,54,54	0
58	MG	2a	1754	1/1	0.93	0.11	50,50,50,50	0
58	MG	2A	3399	1/1	0.93	0.08	52,52,52,52	0
58	MG	2a	1756	1/1	0.93	0.12	64,64,64,64	0
58	MG	2A	3199	1/1	0.93	0.23	51,51,51,51	0
58	MG	2A	3200	1/1	0.93	0.16	46,46,46,46	0
58	MG	2A	3753	1/1	0.93	0.11	47,47,47,47	0
58	MG	1a	1760	1/1	0.93	0.10	47,47,47,47	0
58	MG	1A	3307	1/1	0.93	0.15	36,36,36,36	0
58	MG	2a	1777	1/1	0.93	0.09	59,59,59,59	0
58	MG	1A	3311	1/1	0.93	0.14	48,48,48,48	0
58	MG	1A	3654	1/1	0.93	0.10	34,34,34,34	0
58	MG	1Y	203	1/1	0.93	0.21	47,47,47,47	0
58	MG	1Z	3700	1/1	0.93	0.08	44,44,44,44	0
58	MG	1Z	3701	1/1	0.93	0.08	45,45,45,45	0
58	MG	1a	1781	1/1	0.93	0.09	48,48,48,48	0
58	MG	2A	3413	1/1	0.93	0.17	41,41,41,41	0
58	MG	10	102	1/1	0.93	0.14	39,39,39,39	0
58	MG	2A	3419	1/1	0.93	0.16	28,28,28,28	0
58	MG	2a	1798	1/1	0.93	0.13	36,36,36,36	0
58	MG	10	105	1/1	0.93	0.12	41,41,41,41	0
58	MG	1a	1788	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3423	1/1	0.93	0.22	52,52,52,52	0
58	MG	1A	4021	1/1	0.93	0.09	30,30,30,30	0
58	MG	2A	3429	1/1	0.93	0.23	53,53,53,53	0
58	MG	2A	3787	1/1	0.93	0.09	49,49,49,49	0
58	MG	1A	3517	1/1	0.93	0.08	54,54,54,54	0
58	MG	1A	3367	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	4026	1/1	0.93	0.11	43,43,43,43	0
58	MG	1A	3524	1/1	0.93	0.09	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3846	1/1	0.93	0.10	62,62,62,62	0
58	MG	1A	3049	1/1	0.93	0.06	8,8,8,8	0
58	MG	2A	3440	1/1	0.93	0.09	50,50,50,50	0
58	MG	15	103	1/1	0.93	0.28	37,37,37,37	0
58	MG	2A	3803	1/1	0.93	0.15	45,45,45,45	0
58	MG	2A	3804	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3529	1/1	0.93	0.07	37,37,37,37	0
58	MG	1A	3369	1/1	0.93	0.10	42,42,42,42	0
58	MG	2A	3447	1/1	0.93	0.14	49,49,49,49	0
58	MG	2A	3227	1/1	0.93	0.10	52,52,52,52	0
58	MG	1A	3370	1/1	0.93	0.18	39,39,39,39	0
58	MG	2a	1830	1/1	0.93	0.11	52,52,52,52	0
58	MG	1A	3252	1/1	0.93	0.08	37,37,37,37	0
58	MG	1A	3539	1/1	0.93	0.18	41,41,41,41	0
58	MG	1e	202	1/1	0.93	0.20	55,55,55,55	0
58	MG	2A	3461	1/1	0.93	0.23	32,32,32,32	0
58	MG	2A	3462	1/1	0.93	0.10	54,54,54,54	0
58	MG	1A	3449	1/1	0.93	0.16	34,34,34,34	0
58	MG	2A	3835	1/1	0.93	0.06	43,43,43,43	0
58	MG	1A	3863	1/1	0.93	0.12	36,36,36,36	0
58	MG	1A	3077	1/1	0.93	0.20	30,30,30,30	0
58	MG	2A	3839	1/1	0.93	0.07	47,47,47,47	0
58	MG	1A	4049	1/1	0.93	0.10	25,25,25,25	0
58	MG	2A	3844	1/1	0.93	0.13	61,61,61,61	0
58	MG	1A	3453	1/1	0.93	0.17	49,49,49,49	0
58	MG	1A	4052	1/1	0.93	0.07	40,40,40,40	0
58	MG	1A	3256	1/1	0.93	0.09	49,49,49,49	0
58	MG	1w	103	1/1	0.93	0.29	50,50,50,50	0
58	MG	1A	3050	1/1	0.93	0.10	40,40,40,40	0
58	MG	2A	3855	1/1	0.93	0.10	35,35,35,35	0
58	MG	1a	1619	1/1	0.93	0.10	36,36,36,36	0
58	MG	1a	1621	1/1	0.93	0.12	45,45,45,45	0
58	MG	1a	1622	1/1	0.93	0.10	41,41,41,41	0
58	MG	1A	3718	1/1	0.93	0.15	47,47,47,47	0
58	MG	1A	3723	1/1	0.93	0.11	28,28,28,28	0
58	MG	1a	1628	1/1	0.93	0.15	50,50,50,50	0
58	MG	1A	4067	1/1	0.93	0.08	35,35,35,35	0
58	MG	1A	3873	1/1	0.93	0.10	25,25,25,25	0
58	MG	2A	3878	1/1	0.93	0.14	52,52,52,52	0
58	MG	2A	3265	1/1	0.93	0.12	47,47,47,47	0
58	MG	1A	3875	1/1	0.93	0.04	27,27,27,27	0
58	MG	1A	3380	1/1	0.93	0.08	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3499	1/1	0.93	0.23	44,44,44,44	0
58	MG	2A	3500	1/1	0.93	0.11	39,39,39,39	0
58	MG	1A	4083	1/1	0.93	0.07	37,37,37,37	0
58	MG	1A	3878	1/1	0.93	0.24	27,27,27,27	0
58	MG	2B	205	1/1	0.93	0.15	51,51,51,51	0
58	MG	2B	206	1/1	0.93	0.16	53,53,53,53	0
58	MG	2A	3508	1/1	0.93	0.09	39,39,39,39	0
58	MG	2B	208	1/1	0.93	0.26	50,50,50,50	0
58	MG	2A	3509	1/1	0.93	0.11	38,38,38,38	0
60	ZN	24	501	1/1	0.93	0.10	113,113,113,113	0
58	MG	2A	3483	1/1	0.94	0.09	50,50,50,50	0
58	MG	2A	3876	1/1	0.94	0.14	36,36,36,36	0
58	MG	2A	3239	1/1	0.94	0.09	41,41,41,41	0
58	MG	1A	3117	1/1	0.94	0.17	28,28,28,28	0
58	MG	2A	3486	1/1	0.94	0.07	32,32,32,32	0
58	MG	1n	101	1/1	0.94	0.07	34,34,34,34	0
58	MG	1a	1609	1/1	0.94	0.25	56,56,56,56	0
58	MG	1A	3209	1/1	0.94	0.16	33,33,33,33	0
58	MG	2A	3246	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3668	1/1	0.94	0.07	17,17,17,17	0
58	MG	2A	3494	1/1	0.94	0.13	50,50,50,50	0
58	MG	1A	3092	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	4054	1/1	0.94	0.08	34,34,34,34	0
58	MG	1w	106	1/1	0.94	0.13	44,44,44,44	0
58	MG	1a	1618	1/1	0.94	0.09	43,43,43,43	0
58	MG	1A	3126	1/1	0.94	0.10	43,43,43,43	0
58	MG	2A	3505	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3437	1/1	0.94	0.06	36,36,36,36	0
58	MG	1A	4061	1/1	0.94	0.12	34,34,34,34	0
58	MG	1A	3530	1/1	0.94	0.28	55,55,55,55	0
58	MG	1a	1626	1/1	0.94	0.14	50,50,50,50	0
58	MG	1A	3693	1/1	0.94	0.08	15,15,15,15	0
58	MG	2D	304	1/1	0.94	0.06	39,39,39,39	0
58	MG	2A	3264	1/1	0.94	0.27	49,49,49,49	0
58	MG	1A	3699	1/1	0.94	0.07	20,20,20,20	0
58	MG	2E	302	1/1	0.94	0.14	47,47,47,47	0
58	MG	2A	3522	1/1	0.94	0.08	49,49,49,49	0
58	MG	1a	1629	1/1	0.94	0.31	45,45,45,45	0
58	MG	1A	3273	1/1	0.94	0.26	41,41,41,41	0
58	MG	1x	109	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3533	1/1	0.94	0.11	46,46,46,46	0
58	MG	1x	111	1/1	0.94	0.10	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2F	302	1/1	0.94	0.14	45,45,45,45	0
58	MG	2F	303	1/1	0.94	0.10	59,59,59,59	0
58	MG	2F	304	1/1	0.94	0.25	48,48,48,48	0
58	MG	1A	3709	1/1	0.94	0.10	39,39,39,39	0
58	MG	2A	3001	1/1	0.94	0.17	37,37,37,37	0
58	MG	2A	3003	1/1	0.94	0.15	44,44,44,44	0
58	MG	2A	3539	1/1	0.94	0.13	41,41,41,41	0
58	MG	2O	201	1/1	0.94	0.20	43,43,43,43	0
58	MG	2Q	201	1/1	0.94	0.18	48,48,48,48	0
58	MG	1a	1634	1/1	0.94	0.19	53,53,53,53	0
58	MG	1A	3441	1/1	0.94	0.15	31,31,31,31	0
58	MG	2A	3544	1/1	0.94	0.08	28,28,28,28	0
58	MG	2R	202	1/1	0.94	0.19	38,38,38,38	0
58	MG	1A	4079	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	4082	1/1	0.94	0.09	36,36,36,36	0
58	MG	2U	201	1/1	0.94	0.28	41,41,41,41	0
58	MG	2A	3279	1/1	0.94	0.19	56,56,56,56	0
58	MG	1A	3535	1/1	0.94	0.29	28,28,28,28	0
58	MG	2A	3018	1/1	0.94	0.18	48,48,48,48	0
58	MG	1a	1642	1/1	0.94	0.24	54,54,54,54	0
58	MG	2A	3023	1/1	0.94	0.09	51,51,51,51	0
58	MG	2A	3569	1/1	0.94	0.15	22,22,22,22	0
58	MG	1A	3536	1/1	0.94	0.16	25,25,25,25	0
58	MG	2A	3029	1/1	0.94	0.17	49,49,49,49	0
58	MG	1A	3221	1/1	0.94	0.08	40,40,40,40	0
58	MG	27	103	1/1	0.94	0.12	44,44,44,44	0
58	MG	1A	3443	1/1	0.94	0.15	52,52,52,52	0
58	MG	2A	3033	1/1	0.94	0.13	32,32,32,32	0
58	MG	2A	3294	1/1	0.94	0.15	49,49,49,49	0
58	MG	2a	1601	1/1	0.94	0.12	54,54,54,54	0
58	MG	1a	1650	1/1	0.94	0.12	45,45,45,45	0
58	MG	2A	3588	1/1	0.94	0.13	49,49,49,49	0
58	MG	2A	3297	1/1	0.94	0.30	52,52,52,52	0
58	MG	1A	3227	1/1	0.94	0.12	31,31,31,31	0
58	MG	1A	3882	1/1	0.94	0.12	23,23,23,23	0
58	MG	2A	3594	1/1	0.94	0.12	43,43,43,43	0
58	MG	1A	3719	1/1	0.94	0.09	26,26,26,26	0
58	MG	2A	3598	1/1	0.94	0.13	49,49,49,49	0
58	MG	2a	1611	1/1	0.94	0.17	55,55,55,55	0
58	MG	1A	3720	1/1	0.94	0.13	47,47,47,47	0
58	MG	2A	3046	1/1	0.94	0.07	38,38,38,38	0
58	MG	2A	3604	1/1	0.94	0.10	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3605	1/1	0.94	0.16	47,47,47,47	0
58	MG	1A	3722	1/1	0.94	0.08	35,35,35,35	0
58	MG	2A	3304	1/1	0.94	0.12	46,46,46,46	0
58	MG	2a	1618	1/1	0.94	0.18	58,58,58,58	0
58	MG	2A	3048	1/1	0.94	0.14	39,39,39,39	0
58	MG	2A	3050	1/1	0.94	0.26	53,53,53,53	0
58	MG	2A	3611	1/1	0.94	0.08	45,45,45,45	0
58	MG	2A	3615	1/1	0.94	0.10	24,24,24,24	0
58	MG	2A	3308	1/1	0.94	0.08	47,47,47,47	0
58	MG	1A	4101	1/1	0.94	0.07	41,41,41,41	0
58	MG	1A	3292	1/1	0.94	0.13	33,33,33,33	0
58	MG	1a	1662	1/1	0.94	0.23	44,44,44,44	0
58	MG	1A	3447	1/1	0.94	0.16	43,43,43,43	0
58	MG	1B	204	1/1	0.94	0.07	34,34,34,34	0
58	MG	1A	3366	1/1	0.94	0.10	39,39,39,39	0
58	MG	2A	3315	1/1	0.94	0.09	59,59,59,59	0
58	MG	1A	3547	1/1	0.94	0.15	34,34,34,34	0
58	MG	2a	1637	1/1	0.94	0.15	52,52,52,52	0
58	MG	1A	3004	1/1	0.94	0.11	18,18,18,18	0
58	MG	1B	213	1/1	0.94	0.20	43,43,43,43	0
58	MG	1A	3230	1/1	0.94	0.14	51,51,51,51	0
58	MG	1A	3300	1/1	0.94	0.07	39,39,39,39	0
58	MG	2a	1643	1/1	0.94	0.20	54,54,54,54	0
58	MG	1A	3908	1/1	0.94	0.09	24,24,24,24	0
58	MG	1A	3302	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3741	1/1	0.94	0.09	40,40,40,40	0
58	MG	1a	1677	1/1	0.94	0.10	52,52,52,52	0
58	MG	1A	3234	1/1	0.94	0.12	34,34,34,34	0
58	MG	2A	3075	1/1	0.94	0.16	40,40,40,40	0
58	MG	1A	3920	1/1	0.94	0.08	18,18,18,18	0
58	MG	1A	3456	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3749	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3375	1/1	0.94	0.07	37,37,37,37	0
58	MG	2A	3089	1/1	0.94	0.11	44,44,44,44	0
58	MG	2a	1656	1/1	0.94	0.08	64,64,64,64	0
58	MG	2a	1657	1/1	0.94	0.08	46,46,46,46	0
58	MG	1a	1684	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3304	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3146	1/1	0.94	0.14	34,34,34,34	0
58	MG	2a	1664	1/1	0.94	0.11	55,55,55,55	0
58	MG	2A	3668	1/1	0.94	0.06	37,37,37,37	0
58	MG	1A	3931	1/1	0.94	0.09	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3339	1/1	0.94	0.08	52,52,52,52	0
58	MG	2a	1672	1/1	0.94	0.16	45,45,45,45	0
58	MG	1A	3755	1/1	0.94	0.10	28,28,28,28	0
58	MG	1A	3166	1/1	0.94	0.16	44,44,44,44	0
58	MG	1A	3759	1/1	0.94	0.09	33,33,33,33	0
58	MG	2A	3676	1/1	0.94	0.17	53,53,53,53	0
58	MG	2A	3677	1/1	0.94	0.15	26,26,26,26	0
58	MG	1A	3944	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3248	1/1	0.94	0.11	35,35,35,35	0
58	MG	2A	3106	1/1	0.94	0.21	57,57,57,57	0
58	MG	2a	1689	1/1	0.94	0.13	47,47,47,47	0
58	MG	2a	1690	1/1	0.94	0.19	33,33,33,33	0
58	MG	2A	3108	1/1	0.94	0.26	40,40,40,40	0
58	MG	2a	1692	1/1	0.94	0.16	48,48,48,48	0
58	MG	2A	3110	1/1	0.94	0.08	58,58,58,58	0
58	MG	1E	310	1/1	0.94	0.07	21,21,21,21	0
58	MG	2A	3112	1/1	0.94	0.14	28,28,28,28	0
58	MG	1A	3946	1/1	0.94	0.08	17,17,17,17	0
58	MG	1a	1698	1/1	0.94	0.11	56,56,56,56	0
58	MG	1a	1701	1/1	0.94	0.17	44,44,44,44	0
58	MG	1F	307	1/1	0.94	0.10	19,19,19,19	0
58	MG	2A	3695	1/1	0.94	0.08	51,51,51,51	0
58	MG	1A	3096	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3123	1/1	0.94	0.07	43,43,43,43	0
58	MG	1A	3765	1/1	0.94	0.06	19,19,19,19	0
58	MG	1F	313	1/1	0.94	0.14	42,42,42,42	0
58	MG	2a	1714	1/1	0.94	0.19	58,58,58,58	0
58	MG	2A	3362	1/1	0.94	0.19	56,56,56,56	0
58	MG	2a	1716	1/1	0.94	0.19	49,49,49,49	0
58	MG	1A	3169	1/1	0.94	0.18	30,30,30,30	0
58	MG	1A	3047	1/1	0.94	0.06	27,27,27,27	0
58	MG	2A	3705	1/1	0.94	0.12	54,54,54,54	0
58	MG	2a	1720	1/1	0.94	0.21	34,34,34,34	0
58	MG	2a	1721	1/1	0.94	0.16	43,43,43,43	0
58	MG	2A	3140	1/1	0.94	0.08	54,54,54,54	0
58	MG	1G	205	1/1	0.94	0.11	44,44,44,44	0
58	MG	1A	3319	1/1	0.94	0.07	28,28,28,28	0
58	MG	2A	3145	1/1	0.94	0.14	37,37,37,37	0
58	MG	1A	3962	1/1	0.94	0.07	36,36,36,36	0
58	MG	2A	3712	1/1	0.94	0.11	40,40,40,40	0
58	MG	1A	3052	1/1	0.94	0.15	21,21,21,21	0
58	MG	1O	203	1/1	0.94	0.11	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3376	1/1	0.94	0.11	38,38,38,38	0
58	MG	1A	3786	1/1	0.94	0.08	47,47,47,47	0
58	MG	2a	1738	1/1	0.94	0.11	59,59,59,59	0
58	MG	2A	3155	1/1	0.94	0.11	43,43,43,43	0
58	MG	2A	3382	1/1	0.94	0.27	42,42,42,42	0
58	MG	2A	3157	1/1	0.94	0.15	38,38,38,38	0
58	MG	2A	3158	1/1	0.94	0.15	32,32,32,32	0
58	MG	2A	3159	1/1	0.94	0.14	42,42,42,42	0
58	MG	1A	3787	1/1	0.94	0.11	33,33,33,33	0
58	MG	2a	1747	1/1	0.94	0.20	51,51,51,51	0
58	MG	2A	3162	1/1	0.94	0.29	56,56,56,56	0
58	MG	2A	3735	1/1	0.94	0.11	49,49,49,49	0
58	MG	1P	201	1/1	0.94	0.35	30,30,30,30	0
58	MG	2A	3737	1/1	0.94	0.11	53,53,53,53	0
58	MG	1Q	207	1/1	0.94	0.09	30,30,30,30	0
58	MG	1a	1728	1/1	0.94	0.09	49,49,49,49	0
58	MG	2A	3743	1/1	0.94	0.10	47,47,47,47	0
58	MG	2A	3167	1/1	0.94	0.13	44,44,44,44	0
58	MG	2a	1759	1/1	0.94	0.10	52,52,52,52	0
58	MG	1R	201	1/1	0.94	0.07	38,38,38,38	0
58	MG	1A	3322	1/1	0.94	0.24	25,25,25,25	0
58	MG	1A	3972	1/1	0.94	0.09	42,42,42,42	0
58	MG	1a	1737	1/1	0.94	0.15	53,53,53,53	0
58	MG	2a	1776	1/1	0.94	0.17	43,43,43,43	0
58	MG	1A	3595	1/1	0.94	0.06	31,31,31,31	0
58	MG	2A	3754	1/1	0.94	0.14	49,49,49,49	0
58	MG	1A	3976	1/1	0.94	0.10	44,44,44,44	0
58	MG	2a	1782	1/1	0.94	0.12	57,57,57,57	0
58	MG	2A	3756	1/1	0.94	0.07	40,40,40,40	0
58	MG	2A	3758	1/1	0.94	0.09	20,20,20,20	0
58	MG	2A	3177	1/1	0.94	0.13	52,52,52,52	0
58	MG	2a	1790	1/1	0.94	0.23	54,54,54,54	0
58	MG	1A	3398	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3326	1/1	0.94	0.07	34,34,34,34	0
58	MG	2A	3762	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	3175	1/1	0.94	0.14	30,30,30,30	0
58	MG	1A	3601	1/1	0.94	0.14	36,36,36,36	0
58	MG	2A	3183	1/1	0.94	0.10	44,44,44,44	0
58	MG	1U	207	1/1	0.94	0.33	27,27,27,27	0
58	MG	1A	3983	1/1	0.94	0.23	62,62,62,62	0
58	MG	2A	3770	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3772	1/1	0.94	0.06	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3402	1/1	0.94	0.26	30,30,30,30	0
58	MG	2a	1807	1/1	0.94	0.18	54,54,54,54	0
58	MG	2A	3417	1/1	0.94	0.17	40,40,40,40	0
58	MG	1a	1756	1/1	0.94	0.14	41,41,41,41	0
58	MG	1A	3255	1/1	0.94	0.10	46,46,46,46	0
58	MG	2a	1811	1/1	0.94	0.14	48,48,48,48	0
58	MG	1A	3607	1/1	0.94	0.09	39,39,39,39	0
58	MG	2A	3779	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	3487	1/1	0.94	0.10	29,29,29,29	0
58	MG	1A	3025	1/1	0.94	0.26	35,35,35,35	0
58	MG	2A	3427	1/1	0.94	0.19	45,45,45,45	0
58	MG	1A	3996	1/1	0.94	0.10	41,41,41,41	0
58	MG	2A	3789	1/1	0.94	0.07	55,55,55,55	0
58	MG	1a	1763	1/1	0.94	0.07	49,49,49,49	0
58	MG	1A	3184	1/1	0.94	0.14	37,37,37,37	0
58	MG	2a	1826	1/1	0.94	0.11	55,55,55,55	0
58	MG	1A	3410	1/1	0.94	0.10	37,37,37,37	0
58	MG	1A	4000	1/1	0.94	0.11	38,38,38,38	0
58	MG	2A	3435	1/1	0.94	0.28	55,55,55,55	0
58	MG	1A	3829	1/1	0.94	0.14	27,27,27,27	0
58	MG	2A	3801	1/1	0.94	0.09	38,38,38,38	0
58	MG	1A	4008	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3439	1/1	0.94	0.19	52,52,52,52	0
58	MG	1A	3624	1/1	0.94	0.07	24,24,24,24	0
58	MG	2a	1840	1/1	0.94	0.12	69,69,69,69	0
58	MG	2A	3805	1/1	0.94	0.09	56,56,56,56	0
58	MG	1A	3492	1/1	0.94	0.30	38,38,38,38	0
58	MG	2A	3442	1/1	0.94	0.19	49,49,49,49	0
58	MG	1A	3060	1/1	0.94	0.16	41,41,41,41	0
58	MG	1A	3640	1/1	0.94	0.10	30,30,30,30	0
58	MG	1A	3263	1/1	0.94	0.10	29,29,29,29	0
58	MG	1A	4025	1/1	0.94	0.16	44,44,44,44	0
58	MG	2A	3815	1/1	0.94	0.08	57,57,57,57	0
58	MG	1A	3340	1/1	0.94	0.16	41,41,41,41	0
58	MG	1a	1801	1/1	0.94	0.09	62,62,62,62	0
58	MG	2A	3820	1/1	0.94	0.11	32,32,32,32	0
58	MG	2A	3453	1/1	0.94	0.23	40,40,40,40	0
58	MG	1A	3502	1/1	0.94	0.21	25,25,25,25	0
58	MG	1A	3838	1/1	0.94	0.06	22,22,22,22	0
58	MG	2A	3827	1/1	0.94	0.09	36,36,36,36	0
58	MG	2A	3832	1/1	0.94	0.07	56,56,56,56	0
58	MG	2A	3456	1/1	0.94	0.22	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3459	1/1	0.94	0.09	32,32,32,32	0
58	MG	1a	1807	1/1	0.94	0.16	38,38,38,38	0
58	MG	2A	3219	1/1	0.94	0.15	44,44,44,44	0
58	MG	2A	3840	1/1	0.94	0.07	31,31,31,31	0
58	MG	2A	3463	1/1	0.94	0.16	57,57,57,57	0
58	MG	2w	108	1/1	0.94	0.08	53,53,53,53	0
58	MG	2A	3842	1/1	0.94	0.10	32,32,32,32	0
58	MG	15	106	1/1	0.94	0.16	37,37,37,37	0
58	MG	15	108	1/1	0.94	0.15	34,34,34,34	0
58	MG	1A	3419	1/1	0.94	0.09	42,42,42,42	0
58	MG	1A	3088	1/1	0.94	0.22	29,29,29,29	0
58	MG	2x	103	1/1	0.94	0.34	65,65,65,65	0
58	MG	2A	3470	1/1	0.94	0.09	34,34,34,34	0
58	MG	1a	1813	1/1	0.94	0.10	52,52,52,52	0
58	MG	2x	106	1/1	0.94	0.15	43,43,43,43	0
58	MG	1A	3423	1/1	0.94	0.09	38,38,38,38	0
58	MG	1A	3109	1/1	0.94	0.20	37,37,37,37	0
58	MG	1A	3844	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3656	1/1	0.94	0.06	17,17,17,17	0
58	MG	1A	3348	1/1	0.94	0.12	43,43,43,43	0
58	MG	1a	1606	1/1	0.94	0.11	60,60,60,60	0
58	MG	1A	3061	1/1	0.94	0.12	25,25,25,25	0
58	MG	2A	3862	1/1	0.95	0.13	47,47,47,47	0
58	MG	2A	3863	1/1	0.95	0.09	36,36,36,36	0
58	MG	1A	3977	1/1	0.95	0.13	55,55,55,55	0
58	MG	1A	3247	1/1	0.95	0.19	38,38,38,38	0
58	MG	1A	3779	1/1	0.95	0.06	31,31,31,31	0
58	MG	1A	3484	1/1	0.95	0.08	36,36,36,36	0
58	MG	1a	1793	1/1	0.95	0.11	55,55,55,55	0
58	MG	1W	207	1/1	0.95	0.14	14,14,14,14	0
58	MG	2A	3873	1/1	0.95	0.06	37,37,37,37	0
58	MG	2A	3874	1/1	0.95	0.17	45,45,45,45	0
58	MG	1A	3188	1/1	0.95	0.06	28,28,28,28	0
58	MG	1a	1799	1/1	0.95	0.07	62,62,62,62	0
58	MG	2A	3220	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3982	1/1	0.95	0.05	45,45,45,45	0
58	MG	2A	3880	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3881	1/1	0.95	0.08	48,48,48,48	0
58	MG	1A	3602	1/1	0.95	0.13	48,48,48,48	0
58	MG	1a	1803	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3417	1/1	0.95	0.17	32,32,32,32	0
58	MG	2A	3489	1/1	0.95	0.07	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3299	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3800	1/1	0.95	0.07	11,11,11,11	0
58	MG	1A	3490	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3991	1/1	0.95	0.06	23,23,23,23	0
58	MG	2A	3495	1/1	0.95	0.12	29,29,29,29	0
58	MG	2A	3231	1/1	0.95	0.16	46,46,46,46	0
58	MG	1A	3610	1/1	0.95	0.06	23,23,23,23	0
58	MG	2A	3235	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3189	1/1	0.95	0.09	24,24,24,24	0
58	MG	2A	3503	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3422	1/1	0.95	0.06	35,35,35,35	0
58	MG	2B	216	1/1	0.95	0.13	54,54,54,54	0
58	MG	1a	1815	1/1	0.95	0.09	44,44,44,44	0
58	MG	1a	1816	1/1	0.95	0.10	43,43,43,43	0
58	MG	2D	301	1/1	0.95	0.11	35,35,35,35	0
58	MG	2D	303	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3812	1/1	0.95	0.10	35,35,35,35	0
58	MG	1a	1818	1/1	0.95	0.13	42,42,42,42	0
58	MG	2A	3512	1/1	0.95	0.08	50,50,50,50	0
58	MG	2A	3242	1/1	0.95	0.28	32,32,32,32	0
58	MG	11	102	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	3999	1/1	0.95	0.08	35,35,35,35	0
58	MG	1A	3814	1/1	0.95	0.07	35,35,35,35	0
58	MG	2A	3249	1/1	0.95	0.10	54,54,54,54	0
58	MG	1f	202	1/1	0.95	0.14	44,44,44,44	0
58	MG	1A	3613	1/1	0.95	0.10	41,41,41,41	0
58	MG	12	101	1/1	0.95	0.07	43,43,43,43	0
58	MG	2A	3529	1/1	0.95	0.07	28,28,28,28	0
58	MG	12	102	1/1	0.95	0.12	33,33,33,33	0
58	MG	2F	305	1/1	0.95	0.12	40,40,40,40	0
58	MG	1m	3001	1/1	0.95	0.07	38,38,38,38	0
58	MG	15	102	1/1	0.95	0.12	23,23,23,23	0
58	MG	1A	4005	1/1	0.95	0.23	22,22,22,22	0
58	MG	2A	3537	1/1	0.95	0.09	50,50,50,50	0
58	MG	1A	3150	1/1	0.95	0.08	27,27,27,27	0
58	MG	1A	3151	1/1	0.95	0.33	32,32,32,32	0
58	MG	1A	3622	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	4012	1/1	0.95	0.06	23,23,23,23	0
58	MG	2A	3543	1/1	0.95	0.08	43,43,43,43	0
58	MG	1A	4018	1/1	0.95	0.05	27,27,27,27	0
58	MG	2R	203	1/1	0.95	0.14	42,42,42,42	0
58	MG	1A	3623	1/1	0.95	0.12	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2T	201	1/1	0.95	0.11	52,52,52,52	0
58	MG	2A	3550	1/1	0.95	0.07	34,34,34,34	0
58	MG	19	101	1/1	0.95	0.11	38,38,38,38	0
58	MG	1a	1601	1/1	0.95	0.27	48,48,48,48	0
58	MG	1A	4022	1/1	0.95	0.06	40,40,40,40	0
58	MG	1a	1603	1/1	0.95	0.09	38,38,38,38	0
58	MG	2A	3560	1/1	0.95	0.09	42,42,42,42	0
58	MG	2A	3561	1/1	0.95	0.06	24,24,24,24	0
58	MG	2X	101	1/1	0.95	0.09	51,51,51,51	0
58	MG	1A	3360	1/1	0.95	0.10	32,32,32,32	0
58	MG	1A	3361	1/1	0.95	0.05	41,41,41,41	0
58	MG	23	101	1/1	0.95	0.17	47,47,47,47	0
58	MG	25	103	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3636	1/1	0.95	0.11	44,44,44,44	0
58	MG	2A	3571	1/1	0.95	0.06	28,28,28,28	0
58	MG	27	102	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3503	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3153	1/1	0.95	0.18	31,31,31,31	0
58	MG	28	103	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3083	1/1	0.95	0.14	34,34,34,34	0
58	MG	2A	3577	1/1	0.95	0.12	36,36,36,36	0
58	MG	2A	3579	1/1	0.95	0.06	26,26,26,26	0
58	MG	2A	3580	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3507	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3432	1/1	0.95	0.07	32,32,32,32	0
58	MG	2A	3583	1/1	0.95	0.08	20,20,20,20	0
58	MG	1A	3308	1/1	0.95	0.15	36,36,36,36	0
58	MG	1a	1616	1/1	0.95	0.15	41,41,41,41	0
58	MG	2A	3282	1/1	0.95	0.16	46,46,46,46	0
58	MG	1A	3203	1/1	0.95	0.18	18,18,18,18	0
58	MG	2A	3284	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3006	1/1	0.95	0.13	51,51,51,51	0
58	MG	2A	3287	1/1	0.95	0.05	55,55,55,55	0
58	MG	1A	3512	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	3121	1/1	0.95	0.14	35,35,35,35	0
58	MG	1A	3655	1/1	0.95	0.07	22,22,22,22	0
58	MG	2A	3016	1/1	0.95	0.15	51,51,51,51	0
58	MG	2A	3603	1/1	0.95	0.11	49,49,49,49	0
58	MG	2a	1619	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	4044	1/1	0.95	0.06	24,24,24,24	0
58	MG	1A	3210	1/1	0.95	0.08	29,29,29,29	0
58	MG	2a	1623	1/1	0.95	0.08	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3606	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3657	1/1	0.95	0.06	28,28,28,28	0
58	MG	1A	3843	1/1	0.95	0.05	31,31,31,31	0
58	MG	1A	3520	1/1	0.95	0.39	34,34,34,34	0
58	MG	2A	3028	1/1	0.95	0.19	45,45,45,45	0
58	MG	1A	3439	1/1	0.95	0.25	28,28,28,28	0
58	MG	2A	3612	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3847	1/1	0.95	0.06	50,50,50,50	0
58	MG	1A	3660	1/1	0.95	0.06	20,20,20,20	0
58	MG	2a	1634	1/1	0.95	0.18	37,37,37,37	0
58	MG	2A	3619	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3663	1/1	0.95	0.07	19,19,19,19	0
58	MG	2A	3035	1/1	0.95	0.12	23,23,23,23	0
58	MG	1A	4059	1/1	0.95	0.12	55,55,55,55	0
58	MG	1A	3440	1/1	0.95	0.19	32,32,32,32	0
58	MG	2A	3040	1/1	0.95	0.08	42,42,42,42	0
58	MG	2A	3041	1/1	0.95	0.27	43,43,43,43	0
58	MG	1A	3853	1/1	0.95	0.19	39,39,39,39	0
58	MG	1A	3526	1/1	0.95	0.26	54,54,54,54	0
58	MG	1A	4064	1/1	0.95	0.09	44,44,44,44	0
58	MG	1a	1643	1/1	0.95	0.14	41,41,41,41	0
58	MG	2A	3641	1/1	0.95	0.08	37,37,37,37	0
58	MG	1A	3857	1/1	0.95	0.06	42,42,42,42	0
58	MG	1A	3858	1/1	0.95	0.09	13,13,13,13	0
58	MG	1A	3084	1/1	0.95	0.12	22,22,22,22	0
58	MG	1a	1649	1/1	0.95	0.10	47,47,47,47	0
58	MG	1A	3528	1/1	0.95	0.11	66,66,66,66	0
58	MG	2A	3053	1/1	0.95	0.12	49,49,49,49	0
58	MG	2A	3650	1/1	0.95	0.15	46,46,46,46	0
58	MG	2A	3654	1/1	0.95	0.17	49,49,49,49	0
58	MG	1A	4077	1/1	0.95	0.08	34,34,34,34	0
58	MG	2A	3321	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3672	1/1	0.95	0.07	20,20,20,20	0
58	MG	1A	4081	1/1	0.95	0.10	31,31,31,31	0
58	MG	2A	3060	1/1	0.95	0.18	44,44,44,44	0
58	MG	1A	3676	1/1	0.95	0.06	11,11,11,11	0
58	MG	2a	1667	1/1	0.95	0.15	28,28,28,28	0
58	MG	2a	1668	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3062	1/1	0.95	0.25	52,52,52,52	0
58	MG	1A	3681	1/1	0.95	0.13	37,37,37,37	0
58	MG	1A	4084	1/1	0.95	0.10	22,22,22,22	0
58	MG	2a	1673	1/1	0.95	0.07	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3665	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3866	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3315	1/1	0.95	0.10	32,32,32,32	0
58	MG	1A	3015	1/1	0.95	0.08	23,23,23,23	0
58	MG	1A	3374	1/1	0.95	0.09	39,39,39,39	0
58	MG	2a	1685	1/1	0.95	0.09	47,47,47,47	0
58	MG	1A	3264	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3694	1/1	0.95	0.06	22,22,22,22	0
58	MG	2A	3072	1/1	0.95	0.06	42,42,42,42	0
58	MG	1a	1668	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3446	1/1	0.95	0.16	26,26,26,26	0
58	MG	1A	3874	1/1	0.95	0.13	23,23,23,23	0
58	MG	1A	3214	1/1	0.95	0.15	34,34,34,34	0
58	MG	2a	1693	1/1	0.95	0.15	37,37,37,37	0
58	MG	1a	1672	1/1	0.95	0.12	37,37,37,37	0
58	MG	1A	4102	1/1	0.95	0.12	39,39,39,39	0
58	MG	2a	1697	1/1	0.95	0.18	30,30,30,30	0
58	MG	2A	3685	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3084	1/1	0.95	0.11	42,42,42,42	0
58	MG	2A	3345	1/1	0.95	0.06	35,35,35,35	0
58	MG	2A	3346	1/1	0.95	0.08	54,54,54,54	0
58	MG	2A	3086	1/1	0.95	0.12	40,40,40,40	0
58	MG	1A	3131	1/1	0.95	0.12	52,52,52,52	0
58	MG	1A	4104	1/1	0.95	0.28	44,44,44,44	0
58	MG	1A	3710	1/1	0.95	0.10	28,28,28,28	0
58	MG	1A	3174	1/1	0.95	0.16	41,41,41,41	0
58	MG	2A	3092	1/1	0.95	0.29	36,36,36,36	0
58	MG	1A	3712	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3883	1/1	0.95	0.10	57,57,57,57	0
58	MG	2A	3099	1/1	0.95	0.16	44,44,44,44	0
58	MG	1A	3137	1/1	0.95	0.15	26,26,26,26	0
58	MG	1A	3138	1/1	0.95	0.09	41,41,41,41	0
58	MG	1A	3329	1/1	0.95	0.14	35,35,35,35	0
58	MG	2A	3360	1/1	0.95	0.10	53,53,53,53	0
58	MG	1A	3016	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3331	1/1	0.95	0.24	36,36,36,36	0
58	MG	2a	1723	1/1	0.95	0.08	38,38,38,38	0
58	MG	2a	1724	1/1	0.95	0.25	45,45,45,45	0
58	MG	1A	3091	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3896	1/1	0.95	0.07	16,16,16,16	0
58	MG	1A	3897	1/1	0.95	0.06	12,12,12,12	0
58	MG	1A	3899	1/1	0.95	0.15	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2A	3716	1/1	0.95	0.07	34,34,34,34	0
58	MG	2a	1732	1/1	0.95	0.11	42,42,42,42	0
58	MG	1A	3391	1/1	0.95	0.08	39,39,39,39	0
58	MG	2A	3370	1/1	0.95	0.09	57,57,57,57	0
58	MG	2a	1735	1/1	0.95	0.21	48,48,48,48	0
58	MG	1a	1691	1/1	0.95	0.18	33,33,33,33	0
58	MG	1A	3393	1/1	0.95	0.16	15,15,15,15	0
58	MG	1A	3461	1/1	0.95	0.08	51,51,51,51	0
58	MG	2A	3374	1/1	0.95	0.23	67,67,67,67	0
58	MG	1a	1694	1/1	0.95	0.17	30,30,30,30	0
58	MG	2A	3119	1/1	0.95	0.17	53,53,53,53	0
58	MG	2a	1742	1/1	0.95	0.18	53,53,53,53	0
58	MG	2A	3378	1/1	0.95	0.20	48,48,48,48	0
58	MG	2a	1744	1/1	0.95	0.24	48,48,48,48	0
58	MG	1A	3395	1/1	0.95	0.10	48,48,48,48	0
58	MG	1A	3553	1/1	0.95	0.11	38,38,38,38	0
58	MG	1a	1697	1/1	0.95	0.16	45,45,45,45	0
58	MG	1A	3909	1/1	0.95	0.29	15,15,15,15	0
58	MG	2A	3128	1/1	0.95	0.10	54,54,54,54	0
58	MG	2A	3738	1/1	0.95	0.21	64,64,64,64	0
58	MG	2A	3131	1/1	0.95	0.10	39,39,39,39	0
58	MG	2A	3386	1/1	0.95	0.10	51,51,51,51	0
58	MG	2A	3387	1/1	0.95	0.09	58,58,58,58	0
58	MG	2A	3132	1/1	0.95	0.09	42,42,42,42	0
58	MG	2A	3389	1/1	0.95	0.07	36,36,36,36	0
58	MG	1a	1700	1/1	0.95	0.12	48,48,48,48	0
58	MG	2a	1761	1/1	0.95	0.08	71,71,71,71	0
58	MG	2A	3748	1/1	0.95	0.07	47,47,47,47	0
58	MG	2a	1763	1/1	0.95	0.09	59,59,59,59	0
58	MG	2A	3749	1/1	0.95	0.25	41,41,41,41	0
58	MG	2A	3134	1/1	0.95	0.10	45,45,45,45	0
58	MG	2A	3392	1/1	0.95	0.15	39,39,39,39	0
58	MG	2a	1773	1/1	0.95	0.06	66,66,66,66	0
58	MG	1A	3727	1/1	0.95	0.08	42,42,42,42	0
58	MG	1A	3466	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3187	1/1	0.95	0.12	49,49,49,49	0
58	MG	1D	312	1/1	0.95	0.14	23,23,23,23	0
58	MG	2a	1781	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3757	1/1	0.95	0.08	43,43,43,43	0
58	MG	1A	3237	1/1	0.95	0.32	39,39,39,39	0
58	MG	1E	307	1/1	0.95	0.07	24,24,24,24	0
58	MG	2a	1787	1/1	0.95	0.16	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3399	1/1	0.95	0.09	52,52,52,52	0
58	MG	2a	1789	1/1	0.95	0.14	52,52,52,52	0
58	MG	2A	3148	1/1	0.95	0.16	34,34,34,34	0
58	MG	2A	3151	1/1	0.95	0.15	34,34,34,34	0
58	MG	1A	3923	1/1	0.95	0.06	17,17,17,17	0
58	MG	1E	311	1/1	0.95	0.07	16,16,16,16	0
58	MG	1a	1712	1/1	0.95	0.26	45,45,45,45	0
58	MG	2a	1797	1/1	0.95	0.08	55,55,55,55	0
58	MG	1A	3738	1/1	0.95	0.07	51,51,51,51	0
58	MG	1E	314	1/1	0.95	0.20	45,45,45,45	0
58	MG	2A	3408	1/1	0.95	0.22	38,38,38,38	0
58	MG	1A	3563	1/1	0.95	0.19	34,34,34,34	0
58	MG	2A	3410	1/1	0.95	0.06	42,42,42,42	0
58	MG	1A	3338	1/1	0.95	0.22	42,42,42,42	0
58	MG	1a	1718	1/1	0.95	0.15	32,32,32,32	0
58	MG	2A	3414	1/1	0.95	0.20	35,35,35,35	0
58	MG	1F	311	1/1	0.95	0.17	20,20,20,20	0
58	MG	1a	1721	1/1	0.95	0.14	48,48,48,48	0
58	MG	2A	3418	1/1	0.95	0.17	34,34,34,34	0
58	MG	1A	3339	1/1	0.95	0.08	39,39,39,39	0
58	MG	2a	1812	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3783	1/1	0.95	0.07	61,61,61,61	0
58	MG	2A	3785	1/1	0.95	0.13	50,50,50,50	0
58	MG	1a	1725	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3745	1/1	0.95	0.12	24,24,24,24	0
58	MG	2A	3422	1/1	0.95	0.30	40,40,40,40	0
58	MG	2a	1819	1/1	0.95	0.14	51,51,51,51	0
58	MG	1A	3238	1/1	0.95	0.11	47,47,47,47	0
58	MG	1A	3748	1/1	0.95	0.12	39,39,39,39	0
58	MG	2A	3793	1/1	0.95	0.11	58,58,58,58	0
58	MG	2A	3171	1/1	0.95	0.06	50,50,50,50	0
58	MG	2A	3795	1/1	0.95	0.06	32,32,32,32	0
58	MG	1A	3570	1/1	0.95	0.07	30,30,30,30	0
58	MG	2A	3798	1/1	0.95	0.07	38,38,38,38	0
58	MG	2A	3430	1/1	0.95	0.13	40,40,40,40	0
58	MG	2A	3173	1/1	0.95	0.08	41,41,41,41	0
58	MG	2a	1831	1/1	0.95	0.10	49,49,49,49	0
58	MG	1N	201	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3572	1/1	0.95	0.06	12,12,12,12	0
58	MG	2a	1836	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3280	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3580	1/1	0.95	0.26	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3436	1/1	0.95	0.22	39,39,39,39	0
58	MG	1O	202	1/1	0.95	0.10	42,42,42,42	0
58	MG	2A	3807	1/1	0.95	0.12	49,49,49,49	0
58	MG	1A	3753	1/1	0.95	0.07	44,44,44,44	0
58	MG	1a	1746	1/1	0.95	0.08	37,37,37,37	0
58	MG	1A	3343	1/1	0.95	0.18	42,42,42,42	0
58	MG	2A	3184	1/1	0.95	0.09	39,39,39,39	0
58	MG	1A	3246	1/1	0.95	0.23	31,31,31,31	0
58	MG	2A	3443	1/1	0.95	0.15	42,42,42,42	0
58	MG	2l	203	1/1	0.95	0.08	42,42,42,42	0
58	MG	1A	3956	1/1	0.95	0.07	30,30,30,30	0
58	MG	2A	3818	1/1	0.95	0.09	44,44,44,44	0
58	MG	1Q	201	1/1	0.95	0.09	29,29,29,29	0
58	MG	2q	202	1/1	0.95	0.11	49,49,49,49	0
58	MG	2A	3446	1/1	0.95	0.07	33,33,33,33	0
58	MG	1A	3347	1/1	0.95	0.13	26,26,26,26	0
58	MG	1A	3959	1/1	0.95	0.07	36,36,36,36	0
58	MG	1R	202	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3960	1/1	0.95	0.11	46,46,46,46	0
58	MG	2A	3196	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3834	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3590	1/1	0.95	0.09	41,41,41,41	0
58	MG	1A	3762	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3592	1/1	0.95	0.24	37,37,37,37	0
58	MG	2A	3457	1/1	0.95	0.22	50,50,50,50	0
58	MG	2A	3458	1/1	0.95	0.19	50,50,50,50	0
58	MG	1A	3293	1/1	0.95	0.11	38,38,38,38	0
58	MG	1A	3766	1/1	0.95	0.06	22,22,22,22	0
58	MG	1A	3768	1/1	0.95	0.07	18,18,18,18	0
58	MG	2A	3845	1/1	0.95	0.07	52,52,52,52	0
58	MG	1U	203	1/1	0.95	0.14	21,21,21,21	0
58	MG	2A	3847	1/1	0.95	0.07	51,51,51,51	0
58	MG	2A	3205	1/1	0.95	0.10	53,53,53,53	0
58	MG	1A	3770	1/1	0.95	0.06	29,29,29,29	0
58	MG	1a	1774	1/1	0.95	0.07	48,48,48,48	0
58	MG	1a	1778	1/1	0.95	0.08	33,33,33,33	0
58	MG	2A	3854	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3481	1/1	0.95	0.15	32,32,32,32	0
58	MG	2A	3857	1/1	0.95	0.08	30,30,30,30	0
58	MG	2A	3859	1/1	0.95	0.05	46,46,46,46	0
58	MG	1A	3482	1/1	0.95	0.09	40,40,40,40	0
58	MG	2A	3861	1/1	0.95	0.16	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3802	1/1	0.96	0.11	30,30,30,30	0
58	MG	1A	3521	1/1	0.96	0.16	27,27,27,27	0
58	MG	1a	1699	1/1	0.96	0.20	44,44,44,44	0
58	MG	2T	203	1/1	0.96	0.14	46,46,46,46	0
58	MG	2A	3633	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3634	1/1	0.96	0.08	43,43,43,43	0
58	MG	1A	3132	1/1	0.96	0.05	25,25,25,25	0
58	MG	1A	3647	1/1	0.96	0.06	24,24,24,24	0
58	MG	2A	3639	1/1	0.96	0.06	44,44,44,44	0
58	MG	2A	3107	1/1	0.96	0.04	35,35,35,35	0
58	MG	1A	3963	1/1	0.96	0.06	39,39,39,39	0
58	MG	2A	3643	1/1	0.96	0.08	20,20,20,20	0
58	MG	1A	3807	1/1	0.96	0.06	10,10,10,10	0
58	MG	1A	3186	1/1	0.96	0.05	46,46,46,46	0
58	MG	25	101	1/1	0.96	0.13	37,37,37,37	0
58	MG	25	102	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3525	1/1	0.96	0.07	35,35,35,35	0
58	MG	1G	201	1/1	0.96	0.10	30,30,30,30	0
58	MG	1G	202	1/1	0.96	0.15	43,43,43,43	0
58	MG	1a	1708	1/1	0.96	0.11	45,45,45,45	0
58	MG	2A	3651	1/1	0.96	0.24	37,37,37,37	0
58	MG	2A	3652	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	3813	1/1	0.96	0.05	34,34,34,34	0
58	MG	1A	3133	1/1	0.96	0.12	48,48,48,48	0
58	MG	1A	3310	1/1	0.96	0.07	25,25,25,25	0
58	MG	1A	3974	1/1	0.96	0.10	36,36,36,36	0
58	MG	1N	202	1/1	0.96	0.12	31,31,31,31	0
58	MG	2a	1603	1/1	0.96	0.08	56,56,56,56	0
58	MG	1A	3975	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3134	1/1	0.96	0.09	25,25,25,25	0
58	MG	2A	3661	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3367	1/1	0.96	0.16	41,41,41,41	0
58	MG	1N	207	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3043	1/1	0.96	0.23	29,29,29,29	0
58	MG	1A	3818	1/1	0.96	0.08	22,22,22,22	0
58	MG	1A	3819	1/1	0.96	0.07	46,46,46,46	0
58	MG	2A	3135	1/1	0.96	0.20	37,37,37,37	0
58	MG	1A	3820	1/1	0.96	0.32	26,26,26,26	0
58	MG	1A	3372	1/1	0.96	0.10	45,45,45,45	0
58	MG	1A	3054	1/1	0.96	0.07	38,38,38,38	0
58	MG	1P	203	1/1	0.96	0.30	24,24,24,24	0
58	MG	1a	1732	1/1	0.96	0.08	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3067	1/1	0.96	0.09	30,30,30,30	0
58	MG	1Q	204	1/1	0.96	0.08	43,43,43,43	0
58	MG	1a	1735	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3680	1/1	0.96	0.13	50,50,50,50	0
58	MG	1Q	205	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3826	1/1	0.96	0.06	24,24,24,24	0
58	MG	1a	1739	1/1	0.96	0.05	22,22,22,22	0
58	MG	1A	3661	1/1	0.96	0.06	18,18,18,18	0
58	MG	2a	1627	1/1	0.96	0.21	54,54,54,54	0
58	MG	1A	3534	1/1	0.96	0.25	31,31,31,31	0
58	MG	1R	203	1/1	0.96	0.15	27,27,27,27	0
58	MG	1a	1744	1/1	0.96	0.07	38,38,38,38	0
58	MG	1R	204	1/1	0.96	0.17	29,29,29,29	0
58	MG	1A	3142	1/1	0.96	0.20	38,38,38,38	0
58	MG	1a	1748	1/1	0.96	0.17	38,38,38,38	0
58	MG	2A	3164	1/1	0.96	0.09	43,43,43,43	0
58	MG	1A	3989	1/1	0.96	0.11	47,47,47,47	0
58	MG	2A	3396	1/1	0.96	0.15	50,50,50,50	0
58	MG	2A	3698	1/1	0.96	0.07	48,48,48,48	0
58	MG	2a	1638	1/1	0.96	0.14	53,53,53,53	0
58	MG	1A	3201	1/1	0.96	0.14	30,30,30,30	0
58	MG	1A	3993	1/1	0.96	0.06	11,11,11,11	0
58	MG	1A	3832	1/1	0.96	0.10	31,31,31,31	0
58	MG	1a	1755	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3451	1/1	0.96	0.19	33,33,33,33	0
58	MG	1A	3317	1/1	0.96	0.12	40,40,40,40	0
58	MG	1A	3318	1/1	0.96	0.18	43,43,43,43	0
58	MG	2A	3706	1/1	0.96	0.07	49,49,49,49	0
58	MG	1A	3257	1/1	0.96	0.22	36,36,36,36	0
58	MG	1U	205	1/1	0.96	0.20	27,27,27,27	0
58	MG	1A	3320	1/1	0.96	0.07	42,42,42,42	0
58	MG	1A	4002	1/1	0.96	0.08	48,48,48,48	0
58	MG	1A	3384	1/1	0.96	0.07	34,34,34,34	0
58	MG	2a	1652	1/1	0.96	0.07	57,57,57,57	0
58	MG	1a	1767	1/1	0.96	0.14	60,60,60,60	0
58	MG	1V	203	1/1	0.96	0.18	24,24,24,24	0
58	MG	1A	4004	1/1	0.96	0.05	9,9,9,9	0
58	MG	1A	3683	1/1	0.96	0.05	16,16,16,16	0
58	MG	1A	3545	1/1	0.96	0.12	27,27,27,27	0
58	MG	2A	3415	1/1	0.96	0.15	38,38,38,38	0
58	MG	2A	3185	1/1	0.96	0.09	24,24,24,24	0
58	MG	1W	203	1/1	0.96	0.09	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	2a	1663	1/1	0.96	0.09	55,55,55,55	0
58	MG	1W	205	1/1	0.96	0.09	35,35,35,35	0
58	MG	1A	3686	1/1	0.96	0.08	27,27,27,27	0
58	MG	1A	3546	1/1	0.96	0.06	18,18,18,18	0
58	MG	1a	1783	1/1	0.96	0.05	36,36,36,36	0
58	MG	2A	3193	1/1	0.96	0.09	46,46,46,46	0
58	MG	1X	101	1/1	0.96	0.13	28,28,28,28	0
58	MG	1X	103	1/1	0.96	0.17	29,29,29,29	0
58	MG	1A	3691	1/1	0.96	0.09	29,29,29,29	0
58	MG	2A	3428	1/1	0.96	0.15	41,41,41,41	0
58	MG	2A	3197	1/1	0.96	0.27	43,43,43,43	0
58	MG	1A	4013	1/1	0.96	0.05	17,17,17,17	0
58	MG	2a	1681	1/1	0.96	0.08	41,41,41,41	0
58	MG	1a	1795	1/1	0.96	0.13	67,67,67,67	0
58	MG	1A	4015	1/1	0.96	0.07	20,20,20,20	0
58	MG	1A	4017	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3258	1/1	0.96	0.09	21,21,21,21	0
58	MG	1Z	3702	1/1	0.96	0.08	34,34,34,34	0
58	MG	1A	3845	1/1	0.96	0.08	27,27,27,27	0
58	MG	10	104	1/1	0.96	0.16	39,39,39,39	0
58	MG	1A	3059	1/1	0.96	0.07	32,32,32,32	0
58	MG	1a	1806	1/1	0.96	0.14	35,35,35,35	0
58	MG	1A	3695	1/1	0.96	0.07	56,56,56,56	0
58	MG	1A	3697	1/1	0.96	0.08	35,35,35,35	0
58	MG	1A	3698	1/1	0.96	0.10	34,34,34,34	0
58	MG	1A	3323	1/1	0.96	0.15	23,23,23,23	0
58	MG	1A	3389	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	4028	1/1	0.96	0.08	48,48,48,48	0
58	MG	1A	4029	1/1	0.96	0.05	33,33,33,33	0
58	MG	1A	4030	1/1	0.96	0.08	62,62,62,62	0
58	MG	1A	3704	1/1	0.96	0.06	14,14,14,14	0
58	MG	1A	3708	1/1	0.96	0.10	19,19,19,19	0
58	MG	2a	1703	1/1	0.96	0.13	42,42,42,42	0
58	MG	1A	3462	1/1	0.96	0.10	53,53,53,53	0
58	MG	1A	3390	1/1	0.96	0.12	42,42,42,42	0
58	MG	1d	301	1/1	0.96	0.28	49,49,49,49	0
58	MG	1A	3465	1/1	0.96	0.06	34,34,34,34	0
58	MG	2a	1709	1/1	0.96	0.07	50,50,50,50	0
58	MG	2a	1710	1/1	0.96	0.06	38,38,38,38	0
58	MG	2a	1711	1/1	0.96	0.08	45,45,45,45	0
58	MG	2a	1712	1/1	0.96	0.09	49,49,49,49	0
58	MG	1A	3090	1/1	0.96	0.14	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1f	201	1/1	0.96	0.16	34,34,34,34	0
58	MG	1A	3262	1/1	0.96	0.05	33,33,33,33	0
58	MG	2A	3774	1/1	0.96	0.07	50,50,50,50	0
58	MG	16	101	1/1	0.96	0.06	32,32,32,32	0
58	MG	2A	3460	1/1	0.96	0.11	47,47,47,47	0
58	MG	1A	3556	1/1	0.96	0.09	48,48,48,48	0
58	MG	2A	3229	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3206	1/1	0.96	0.10	42,42,42,42	0
58	MG	18	101	1/1	0.96	0.38	49,49,49,49	0
58	MG	2A	3232	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3469	1/1	0.96	0.16	27,27,27,27	0
58	MG	2A	3784	1/1	0.96	0.19	46,46,46,46	0
58	MG	1A	3207	1/1	0.96	0.07	13,13,13,13	0
58	MG	1A	4048	1/1	0.96	0.08	25,25,25,25	0
58	MG	2A	3471	1/1	0.96	0.13	45,45,45,45	0
58	MG	1A	3108	1/1	0.96	0.06	23,23,23,23	0
58	MG	1A	4050	1/1	0.96	0.06	14,14,14,14	0
58	MG	2A	3791	1/1	0.96	0.07	21,21,21,21	0
58	MG	1A	3012	1/1	0.96	0.07	23,23,23,23	0
58	MG	1A	3332	1/1	0.96	0.08	41,41,41,41	0
58	MG	1A	3160	1/1	0.96	0.09	29,29,29,29	0
58	MG	1A	3161	1/1	0.96	0.05	43,43,43,43	0
58	MG	1A	3404	1/1	0.96	0.16	25,25,25,25	0
58	MG	1A	3575	1/1	0.96	0.20	34,34,34,34	0
58	MG	1A	3165	1/1	0.96	0.26	26,26,26,26	0
58	MG	2A	3247	1/1	0.96	0.10	47,47,47,47	0
58	MG	1A	3880	1/1	0.96	0.11	35,35,35,35	0
58	MG	1A	3406	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3076	1/1	0.96	0.06	25,25,25,25	0
58	MG	1A	4065	1/1	0.96	0.04	26,26,26,26	0
58	MG	1A	3222	1/1	0.96	0.09	31,31,31,31	0
58	MG	2A	3254	1/1	0.96	0.09	45,45,45,45	0
58	MG	1A	3884	1/1	0.96	0.06	28,28,28,28	0
58	MG	1a	1620	1/1	0.96	0.06	38,38,38,38	0
58	MG	1x	112	1/1	0.96	0.15	39,39,39,39	0
58	MG	1x	113	1/1	0.96	0.18	45,45,45,45	0
58	MG	1A	4072	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3225	1/1	0.96	0.09	22,22,22,22	0
58	MG	2A	3814	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3341	1/1	0.96	0.04	34,34,34,34	0
58	MG	2A	3816	1/1	0.96	0.05	41,41,41,41	0
58	MG	2A	3004	1/1	0.96	0.15	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3116	1/1	0.96	0.06	30,30,30,30	0
58	MG	1A	3093	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3277	1/1	0.96	0.14	21,21,21,21	0
58	MG	2a	1765	1/1	0.96	0.06	55,55,55,55	0
58	MG	2A	3507	1/1	0.96	0.08	50,50,50,50	0
58	MG	1A	3893	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	3894	1/1	0.96	0.09	12,12,12,12	0
58	MG	2A	3510	1/1	0.96	0.09	22,22,22,22	0
58	MG	2A	3011	1/1	0.96	0.07	36,36,36,36	0
58	MG	1a	1631	1/1	0.96	0.15	42,42,42,42	0
58	MG	1A	3418	1/1	0.96	0.11	23,23,23,23	0
58	MG	1A	3170	1/1	0.96	0.08	31,31,31,31	0
58	MG	2A	3518	1/1	0.96	0.07	31,31,31,31	0
58	MG	2A	3020	1/1	0.96	0.27	47,47,47,47	0
58	MG	1A	4088	1/1	0.96	0.10	34,34,34,34	0
58	MG	2a	1786	1/1	0.96	0.05	45,45,45,45	0
58	MG	1A	4089	1/1	0.96	0.08	33,33,33,33	0
58	MG	1a	1639	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3025	1/1	0.96	0.07	35,35,35,35	0
58	MG	2A	3026	1/1	0.96	0.13	36,36,36,36	0
58	MG	2A	3528	1/1	0.96	0.05	47,47,47,47	0
58	MG	1A	3600	1/1	0.96	0.13	37,37,37,37	0
58	MG	2A	3531	1/1	0.96	0.06	22,22,22,22	0
58	MG	1A	4092	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3281	1/1	0.96	0.09	25,25,25,25	0
58	MG	1A	3283	1/1	0.96	0.12	22,22,22,22	0
58	MG	1A	3289	1/1	0.96	0.11	37,37,37,37	0
58	MG	2A	3288	1/1	0.96	0.18	54,54,54,54	0
58	MG	2a	1801	1/1	0.96	0.14	53,53,53,53	0
58	MG	1A	3355	1/1	0.96	0.18	29,29,29,29	0
58	MG	2A	3858	1/1	0.96	0.14	43,43,43,43	0
58	MG	1A	4097	1/1	0.96	0.10	53,53,53,53	0
58	MG	1a	1648	1/1	0.96	0.11	41,41,41,41	0
58	MG	1A	4098	1/1	0.96	0.13	44,44,44,44	0
58	MG	1A	3905	1/1	0.96	0.11	33,33,33,33	0
58	MG	1A	3606	1/1	0.96	0.05	23,23,23,23	0
58	MG	2A	3864	1/1	0.96	0.09	45,45,45,45	0
58	MG	2A	3865	1/1	0.96	0.08	40,40,40,40	0
58	MG	2A	3866	1/1	0.96	0.13	43,43,43,43	0
58	MG	2A	3546	1/1	0.96	0.06	32,32,32,32	0
58	MG	1A	3498	1/1	0.96	0.12	37,37,37,37	0
58	MG	2A	3296	1/1	0.96	0.12	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3758	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3499	1/1	0.96	0.09	38,38,38,38	0
58	MG	1A	3500	1/1	0.96	0.09	31,31,31,31	0
58	MG	1A	3290	1/1	0.96	0.11	26,26,26,26	0
58	MG	2a	1821	1/1	0.96	0.06	58,58,58,58	0
58	MG	1A	3232	1/1	0.96	0.19	25,25,25,25	0
58	MG	2a	1823	1/1	0.96	0.10	50,50,50,50	0
58	MG	2A	3875	1/1	0.96	0.18	53,53,53,53	0
58	MG	1B	205	1/1	0.96	0.25	47,47,47,47	0
58	MG	1B	206	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3427	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3305	1/1	0.96	0.09	48,48,48,48	0
58	MG	1A	3616	1/1	0.96	0.16	37,37,37,37	0
58	MG	2A	3056	1/1	0.96	0.11	60,60,60,60	0
58	MG	2A	3573	1/1	0.96	0.14	52,52,52,52	0
58	MG	2a	1832	1/1	0.96	0.16	44,44,44,44	0
58	MG	2a	1833	1/1	0.96	0.11	57,57,57,57	0
58	MG	2A	3574	1/1	0.96	0.05	37,37,37,37	0
58	MG	1B	210	1/1	0.96	0.09	38,38,38,38	0
58	MG	1a	1667	1/1	0.96	0.11	38,38,38,38	0
58	MG	1A	3618	1/1	0.96	0.05	26,26,26,26	0
58	MG	1A	3925	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3926	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3094	1/1	0.96	0.08	17,17,17,17	0
58	MG	1A	3011	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3430	1/1	0.96	0.13	32,32,32,32	0
58	MG	1A	3930	1/1	0.96	0.06	35,35,35,35	0
58	MG	2f	202	1/1	0.96	0.09	51,51,51,51	0
58	MG	1A	3775	1/1	0.96	0.07	23,23,23,23	0
58	MG	2i	201	1/1	0.96	0.06	41,41,41,41	0
58	MG	2A	3587	1/1	0.96	0.14	40,40,40,40	0
58	MG	1A	3431	1/1	0.96	0.11	24,24,24,24	0
58	MG	1A	3123	1/1	0.96	0.20	37,37,37,37	0
58	MG	1A	3934	1/1	0.96	0.05	5,5,5,5	0
58	MG	1A	3940	1/1	0.96	0.07	41,41,41,41	0
58	MG	2B	218	1/1	0.96	0.11	53,53,53,53	0
58	MG	1A	3782	1/1	0.96	0.08	22,22,22,22	0
58	MG	2q	201	1/1	0.96	0.07	55,55,55,55	0
58	MG	2A	3323	1/1	0.96	0.06	35,35,35,35	0
58	MG	1a	1681	1/1	0.96	0.09	55,55,55,55	0
58	MG	1B	231	1/1	0.96	0.08	57,57,57,57	0
58	MG	1A	3783	1/1	0.96	0.06	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3602	1/1	0.96	0.07	26,26,26,26	0
58	MG	2v	103	1/1	0.96	0.14	41,41,41,41	0
58	MG	1A	3630	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3080	1/1	0.96	0.09	41,41,41,41	0
58	MG	2E	304	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3081	1/1	0.96	0.16	35,35,35,35	0
58	MG	2E	307	1/1	0.96	0.08	29,29,29,29	0
58	MG	1A	3081	1/1	0.96	0.10	23,23,23,23	0
58	MG	1A	3947	1/1	0.96	0.11	37,37,37,37	0
58	MG	2A	3085	1/1	0.96	0.17	40,40,40,40	0
58	MG	1D	305	1/1	0.96	0.09	33,33,33,33	0
58	MG	2A	3087	1/1	0.96	0.06	36,36,36,36	0
58	MG	1D	307	1/1	0.96	0.08	23,23,23,23	0
58	MG	1D	309	1/1	0.96	0.12	37,37,37,37	0
58	MG	2A	3613	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3614	1/1	0.96	0.07	18,18,18,18	0
58	MG	1A	3515	1/1	0.96	0.35	34,34,34,34	0
58	MG	1A	3127	1/1	0.96	0.19	26,26,26,26	0
58	MG	2A	3617	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3952	1/1	0.96	0.06	53,53,53,53	0
58	MG	2A	3620	1/1	0.96	0.08	37,37,37,37	0
58	MG	2A	3095	1/1	0.96	0.08	31,31,31,31	0
58	MG	1A	3240	1/1	0.96	0.11	22,22,22,22	0
58	MG	1E	308	1/1	0.96	0.09	43,43,43,43	0
58	MG	1A	3796	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3098	1/1	0.96	0.07	25,25,25,25	0
58	MG	2A	3014	1/1	0.97	0.06	30,30,30,30	0
58	MG	2E	310	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3700	1/1	0.97	0.11	16,16,16,16	0
58	MG	2A	3585	1/1	0.97	0.15	37,37,37,37	0
58	MG	1A	3701	1/1	0.97	0.06	12,12,12,12	0
58	MG	1A	4066	1/1	0.97	0.05	13,13,13,13	0
58	MG	2A	3019	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3065	1/1	0.97	0.07	30,30,30,30	0
58	MG	2A	3590	1/1	0.97	0.09	40,40,40,40	0
58	MG	2F	307	1/1	0.97	0.22	35,35,35,35	0
58	MG	1a	1623	1/1	0.97	0.05	37,37,37,37	0
58	MG	1a	1624	1/1	0.97	0.15	42,42,42,42	0
58	MG	1A	3703	1/1	0.97	0.09	19,19,19,19	0
58	MG	1A	3205	1/1	0.97	0.16	30,30,30,30	0
58	MG	1A	3044	1/1	0.97	0.14	25,25,25,25	0
58	MG	1A	3139	1/1	0.97	0.16	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3877	1/1	0.97	0.17	21,21,21,21	0
58	MG	1A	3450	1/1	0.97	0.17	27,27,27,27	0
58	MG	1A	4080	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3879	1/1	0.97	0.23	25,25,25,25	0
58	MG	1a	1633	1/1	0.97	0.10	45,45,45,45	0
58	MG	1A	3365	1/1	0.97	0.07	37,37,37,37	0
58	MG	2A	3037	1/1	0.97	0.06	31,31,31,31	0
58	MG	2A	3038	1/1	0.97	0.11	13,13,13,13	0
58	MG	1A	3284	1/1	0.97	0.25	37,37,37,37	0
58	MG	1a	1637	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3208	1/1	0.97	0.13	23,23,23,23	0
58	MG	1A	3097	1/1	0.97	0.10	28,28,28,28	0
58	MG	1A	4087	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3291	1/1	0.97	0.11	30,30,30,30	0
58	MG	1A	3141	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3886	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	4091	1/1	0.97	0.06	30,30,30,30	0
58	MG	2A	3618	1/1	0.97	0.12	28,28,28,28	0
58	MG	1A	3887	1/1	0.97	0.05	11,11,11,11	0
58	MG	1a	1646	1/1	0.97	0.11	60,60,60,60	0
58	MG	1A	3008	1/1	0.97	0.05	13,13,13,13	0
58	MG	1A	3294	1/1	0.97	0.08	45,45,45,45	0
58	MG	1A	3373	1/1	0.97	0.17	35,35,35,35	0
58	MG	27	101	1/1	0.97	0.14	28,28,28,28	0
58	MG	2A	3055	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3721	1/1	0.97	0.08	36,36,36,36	0
58	MG	1A	3558	1/1	0.97	0.13	26,26,26,26	0
58	MG	28	102	1/1	0.97	0.13	39,39,39,39	0
58	MG	1A	3295	1/1	0.97	0.15	15,15,15,15	0
58	MG	2A	3059	1/1	0.97	0.11	35,35,35,35	0
58	MG	2A	3632	1/1	0.97	0.08	26,26,26,26	0
58	MG	1A	3562	1/1	0.97	0.18	18,18,18,18	0
58	MG	1a	1657	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3144	1/1	0.97	0.04	5,5,5,5	0
58	MG	1A	3463	1/1	0.97	0.12	30,30,30,30	0
58	MG	1A	3898	1/1	0.97	0.07	11,11,11,11	0
58	MG	1A	3376	1/1	0.97	0.07	31,31,31,31	0
58	MG	1A	3729	1/1	0.97	0.04	24,24,24,24	0
58	MG	1A	4105	1/1	0.97	0.20	41,41,41,41	0
58	MG	1A	3730	1/1	0.97	0.12	45,45,45,45	0
58	MG	1A	3903	1/1	0.97	0.06	15,15,15,15	0
58	MG	1A	3731	1/1	0.97	0.07	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3732	1/1	0.97	0.06	25,25,25,25	0
58	MG	1B	207	1/1	0.97	0.21	33,33,33,33	0
58	MG	1A	3733	1/1	0.97	0.06	16,16,16,16	0
58	MG	1A	3022	1/1	0.97	0.18	27,27,27,27	0
58	MG	1A	3220	1/1	0.97	0.13	20,20,20,20	0
58	MG	2A	3653	1/1	0.97	0.10	44,44,44,44	0
58	MG	1B	211	1/1	0.97	0.26	34,34,34,34	0
58	MG	1A	3910	1/1	0.97	0.06	46,46,46,46	0
58	MG	2A	3348	1/1	0.97	0.08	44,44,44,44	0
58	MG	1A	3571	1/1	0.97	0.13	21,21,21,21	0
58	MG	2a	1622	1/1	0.97	0.06	60,60,60,60	0
58	MG	1A	3147	1/1	0.97	0.12	37,37,37,37	0
58	MG	1A	3914	1/1	0.97	0.06	31,31,31,31	0
58	MG	1A	3915	1/1	0.97	0.20	21,21,21,21	0
58	MG	1B	217	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3916	1/1	0.97	0.14	15,15,15,15	0
58	MG	1A	3739	1/1	0.97	0.08	30,30,30,30	0
58	MG	1A	3071	1/1	0.97	0.04	6,6,6,6	0
58	MG	1A	3223	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3577	1/1	0.97	0.14	32,32,32,32	0
58	MG	2A	3667	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3028	1/1	0.97	0.17	15,15,15,15	0
58	MG	2A	3093	1/1	0.97	0.19	36,36,36,36	0
58	MG	2A	3094	1/1	0.97	0.13	33,33,33,33	0
58	MG	1B	228	1/1	0.97	0.05	30,30,30,30	0
58	MG	2A	3673	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3581	1/1	0.97	0.08	27,27,27,27	0
58	MG	1A	3471	1/1	0.97	0.38	35,35,35,35	0
58	MG	2A	3098	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3472	1/1	0.97	0.13	33,33,33,33	0
58	MG	2A	3678	1/1	0.97	0.08	25,25,25,25	0
58	MG	1A	3588	1/1	0.97	0.09	37,37,37,37	0
58	MG	2A	3368	1/1	0.97	0.08	43,43,43,43	0
58	MG	1A	3017	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3155	1/1	0.97	0.12	23,23,23,23	0
58	MG	2A	3103	1/1	0.97	0.09	22,22,22,22	0
58	MG	2A	3684	1/1	0.97	0.08	32,32,32,32	0
58	MG	1A	3591	1/1	0.97	0.07	35,35,35,35	0
58	MG	1B	236	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3158	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3593	1/1	0.97	0.25	27,27,27,27	0
58	MG	2A	3689	1/1	0.97	0.07	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3387	1/1	0.97	0.20	18,18,18,18	0
58	MG	2A	3109	1/1	0.97	0.12	32,32,32,32	0
58	MG	1D	310	1/1	0.97	0.25	19,19,19,19	0
58	MG	1A	3935	1/1	0.97	0.06	21,21,21,21	0
58	MG	2A	3381	1/1	0.97	0.17	31,31,31,31	0
58	MG	2a	1659	1/1	0.97	0.30	44,44,44,44	0
58	MG	1A	3936	1/1	0.97	0.08	57,57,57,57	0
58	MG	1A	3938	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3159	1/1	0.97	0.34	31,31,31,31	0
58	MG	2A	3115	1/1	0.97	0.12	36,36,36,36	0
58	MG	2a	1665	1/1	0.97	0.07	54,54,54,54	0
58	MG	1A	3104	1/1	0.97	0.08	15,15,15,15	0
58	MG	1A	3761	1/1	0.97	0.09	8,8,8,8	0
58	MG	1A	3030	1/1	0.97	0.17	14,14,14,14	0
58	MG	2a	1669	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3121	1/1	0.97	0.17	39,39,39,39	0
58	MG	1A	3162	1/1	0.97	0.17	20,20,20,20	0
58	MG	1A	3392	1/1	0.97	0.21	18,18,18,18	0
58	MG	2A	3124	1/1	0.97	0.14	45,45,45,45	0
58	MG	2a	1676	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3107	1/1	0.97	0.12	23,23,23,23	0
58	MG	2A	3126	1/1	0.97	0.04	36,36,36,36	0
58	MG	1F	304	1/1	0.97	0.05	43,43,43,43	0
58	MG	2a	1680	1/1	0.97	0.10	37,37,37,37	0
58	MG	1F	305	1/1	0.97	0.08	25,25,25,25	0
58	MG	2A	3129	1/1	0.97	0.15	47,47,47,47	0
58	MG	2a	1683	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3713	1/1	0.97	0.09	38,38,38,38	0
58	MG	2A	3715	1/1	0.97	0.07	20,20,20,20	0
58	MG	2A	3130	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	3949	1/1	0.97	0.07	45,45,45,45	0
58	MG	1F	309	1/1	0.97	0.05	32,32,32,32	0
58	MG	1A	3767	1/1	0.97	0.06	25,25,25,25	0
58	MG	1A	3394	1/1	0.97	0.13	16,16,16,16	0
58	MG	1A	3953	1/1	0.97	0.05	48,48,48,48	0
58	MG	1A	3954	1/1	0.97	0.07	37,37,37,37	0
58	MG	2A	3138	1/1	0.97	0.22	34,34,34,34	0
58	MG	2a	1694	1/1	0.97	0.26	35,35,35,35	0
58	MG	2A	3725	1/1	0.97	0.10	29,29,29,29	0
58	MG	1a	1717	1/1	0.97	0.15	40,40,40,40	0
58	MG	2A	3141	1/1	0.97	0.16	31,31,31,31	0
58	MG	2A	3142	1/1	0.97	0.13	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3079	1/1	0.97	0.05	18,18,18,18	0
58	MG	1A	3485	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3605	1/1	0.97	0.05	16,16,16,16	0
58	MG	1A	3958	1/1	0.97	0.10	43,43,43,43	0
58	MG	1a	1724	1/1	0.97	0.12	49,49,49,49	0
58	MG	1A	3239	1/1	0.97	0.13	21,21,21,21	0
58	MG	2A	3150	1/1	0.97	0.05	27,27,27,27	0
58	MG	1I	201	1/1	0.97	0.05	48,48,48,48	0
58	MG	1a	1727	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3153	1/1	0.97	0.17	53,53,53,53	0
58	MG	1A	3080	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3608	1/1	0.97	0.08	17,17,17,17	0
58	MG	2A	3156	1/1	0.97	0.05	43,43,43,43	0
58	MG	1A	3781	1/1	0.97	0.04	15,15,15,15	0
58	MG	1N	204	1/1	0.97	0.04	27,27,27,27	0
58	MG	1N	205	1/1	0.97	0.27	41,41,41,41	0
58	MG	1A	3241	1/1	0.97	0.09	31,31,31,31	0
58	MG	1a	1736	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3242	1/1	0.97	0.08	22,22,22,22	0
58	MG	1A	3965	1/1	0.97	0.10	51,51,51,51	0
58	MG	1A	3243	1/1	0.97	0.05	23,23,23,23	0
58	MG	1A	3245	1/1	0.97	0.14	18,18,18,18	0
58	MG	1A	3493	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3789	1/1	0.97	0.04	28,28,28,28	0
58	MG	1A	3791	1/1	0.97	0.05	35,35,35,35	0
58	MG	1A	3110	1/1	0.97	0.31	27,27,27,27	0
58	MG	2A	3764	1/1	0.97	0.06	46,46,46,46	0
58	MG	2a	1727	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3794	1/1	0.97	0.10	38,38,38,38	0
58	MG	1Q	203	1/1	0.97	0.11	26,26,26,26	0
58	MG	1A	3617	1/1	0.97	0.05	13,13,13,13	0
58	MG	1A	3324	1/1	0.97	0.07	50,50,50,50	0
58	MG	2A	3175	1/1	0.97	0.12	43,43,43,43	0
58	MG	2A	3771	1/1	0.97	0.08	30,30,30,30	0
58	MG	1Q	206	1/1	0.97	0.10	45,45,45,45	0
58	MG	1A	3797	1/1	0.97	0.05	15,15,15,15	0
58	MG	1A	3798	1/1	0.97	0.04	17,17,17,17	0
58	MG	1A	3325	1/1	0.97	0.17	25,25,25,25	0
58	MG	1A	3497	1/1	0.97	0.15	35,35,35,35	0
58	MG	2A	3448	1/1	0.97	0.20	40,40,40,40	0
58	MG	1A	3032	1/1	0.97	0.21	20,20,20,20	0
58	MG	1A	3034	1/1	0.97	0.20	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3625	1/1	0.97	0.05	18,18,18,18	0
58	MG	1A	3806	1/1	0.97	0.04	13,13,13,13	0
58	MG	2A	3782	1/1	0.97	0.09	33,33,33,33	0
58	MG	1A	3626	1/1	0.97	0.05	29,29,29,29	0
58	MG	1a	1764	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3808	1/1	0.97	0.04	33,33,33,33	0
58	MG	2A	3786	1/1	0.97	0.05	30,30,30,30	0
58	MG	2a	1750	1/1	0.97	0.06	42,42,42,42	0
58	MG	2a	1751	1/1	0.97	0.05	58,58,58,58	0
58	MG	1A	3055	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3501	1/1	0.97	0.12	24,24,24,24	0
58	MG	1A	3631	1/1	0.97	0.04	19,19,19,19	0
58	MG	1a	1770	1/1	0.97	0.07	49,49,49,49	0
58	MG	1a	1772	1/1	0.97	0.06	58,58,58,58	0
58	MG	1A	3994	1/1	0.97	0.04	16,16,16,16	0
58	MG	1A	3634	1/1	0.97	0.04	20,20,20,20	0
58	MG	1a	1776	1/1	0.97	0.06	56,56,56,56	0
58	MG	1A	3635	1/1	0.97	0.04	13,13,13,13	0
58	MG	1A	3411	1/1	0.97	0.13	49,49,49,49	0
58	MG	1A	3637	1/1	0.97	0.05	20,20,20,20	0
58	MG	2A	3469	1/1	0.97	0.25	36,36,36,36	0
58	MG	2a	1766	1/1	0.97	0.12	32,32,32,32	0
58	MG	2a	1770	1/1	0.97	0.05	46,46,46,46	0
58	MG	1V	201	1/1	0.97	0.14	15,15,15,15	0
58	MG	1A	3118	1/1	0.97	0.28	31,31,31,31	0
58	MG	1a	1784	1/1	0.97	0.05	57,57,57,57	0
58	MG	2a	1774	1/1	0.97	0.10	43,43,43,43	0
58	MG	2a	1775	1/1	0.97	0.05	56,56,56,56	0
58	MG	1a	1786	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3504	1/1	0.97	0.14	31,31,31,31	0
58	MG	1A	4001	1/1	0.97	0.04	31,31,31,31	0
58	MG	1a	1789	1/1	0.97	0.05	36,36,36,36	0
58	MG	1W	201	1/1	0.97	0.06	41,41,41,41	0
58	MG	2A	3808	1/1	0.97	0.09	48,48,48,48	0
58	MG	2a	1783	1/1	0.97	0.07	39,39,39,39	0
58	MG	2A	3480	1/1	0.97	0.09	35,35,35,35	0
58	MG	1a	1792	1/1	0.97	0.04	33,33,33,33	0
58	MG	1A	3119	1/1	0.97	0.16	22,22,22,22	0
58	MG	1A	3821	1/1	0.97	0.07	35,35,35,35	0
58	MG	1W	204	1/1	0.97	0.10	22,22,22,22	0
58	MG	1A	3415	1/1	0.97	0.10	33,33,33,33	0
58	MG	1A	3086	1/1	0.97	0.39	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1791	1/1	0.97	0.15	47,47,47,47	0
58	MG	1A	3178	1/1	0.97	0.22	25,25,25,25	0
58	MG	1A	3333	1/1	0.97	0.06	31,31,31,31	0
58	MG	1X	102	1/1	0.97	0.08	27,27,27,27	0
58	MG	1A	3827	1/1	0.97	0.05	29,29,29,29	0
58	MG	1X	106	1/1	0.97	0.07	57,57,57,57	0
58	MG	2A	3492	1/1	0.97	0.14	45,45,45,45	0
58	MG	2A	3824	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	4011	1/1	0.97	0.11	31,31,31,31	0
58	MG	1a	1808	1/1	0.97	0.16	51,51,51,51	0
58	MG	1A	3181	1/1	0.97	0.11	16,16,16,16	0
58	MG	2A	3828	1/1	0.97	0.10	45,45,45,45	0
58	MG	2A	3829	1/1	0.97	0.07	28,28,28,28	0
58	MG	2A	3497	1/1	0.97	0.11	32,32,32,32	0
58	MG	2a	1806	1/1	0.97	0.07	43,43,43,43	0
58	MG	1A	3649	1/1	0.97	0.06	10,10,10,10	0
58	MG	2A	3226	1/1	0.97	0.20	30,30,30,30	0
58	MG	2A	3836	1/1	0.97	0.05	54,54,54,54	0
58	MG	1A	3183	1/1	0.97	0.10	29,29,29,29	0
58	MG	2A	3501	1/1	0.97	0.05	61,61,61,61	0
58	MG	1A	3513	1/1	0.97	0.16	22,22,22,22	0
58	MG	1A	3514	1/1	0.97	0.12	37,37,37,37	0
58	MG	2a	1814	1/1	0.97	0.06	46,46,46,46	0
58	MG	10	101	1/1	0.97	0.09	28,28,28,28	0
58	MG	1A	4019	1/1	0.97	0.05	30,30,30,30	0
58	MG	2A	3506	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3336	1/1	0.97	0.18	38,38,38,38	0
58	MG	1A	3087	1/1	0.97	0.22	30,30,30,30	0
58	MG	1A	3057	1/1	0.97	0.08	31,31,31,31	0
58	MG	1A	3518	1/1	0.97	0.36	21,21,21,21	0
58	MG	1A	3035	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3040	1/1	0.97	0.12	43,43,43,43	0
58	MG	2A	3852	1/1	0.97	0.07	21,21,21,21	0
58	MG	2A	3514	1/1	0.97	0.08	36,36,36,36	0
58	MG	11	101	1/1	0.97	0.25	23,23,23,23	0
58	MG	1A	3261	1/1	0.97	0.12	16,16,16,16	0
58	MG	2A	3517	1/1	0.97	0.13	34,34,34,34	0
58	MG	1A	3664	1/1	0.97	0.04	12,12,12,12	0
58	MG	1A	3128	1/1	0.97	0.10	25,25,25,25	0
58	MG	1A	3130	1/1	0.97	0.32	25,25,25,25	0
58	MG	1A	3344	1/1	0.97	0.17	48,48,48,48	0
58	MG	1A	3041	1/1	0.97	0.06	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	13	102	1/1	0.97	0.12	32,32,32,32	0
58	MG	2A	3248	1/1	0.97	0.07	47,47,47,47	0
58	MG	1p	101	1/1	0.97	0.11	54,54,54,54	0
58	MG	1A	3192	1/1	0.97	0.15	30,30,30,30	0
58	MG	1A	3193	1/1	0.97	0.09	28,28,28,28	0
58	MG	15	104	1/1	0.97	0.15	20,20,20,20	0
58	MG	15	105	1/1	0.97	0.27	41,41,41,41	0
58	MG	1w	102	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	4037	1/1	0.97	0.05	38,38,38,38	0
58	MG	1w	105	1/1	0.97	0.06	41,41,41,41	0
58	MG	2f	201	1/1	0.97	0.18	35,35,35,35	0
58	MG	1A	3677	1/1	0.97	0.07	12,12,12,12	0
58	MG	1A	4039	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3678	1/1	0.97	0.04	12,12,12,12	0
58	MG	2A	3541	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	4041	1/1	0.97	0.08	36,36,36,36	0
58	MG	1A	3849	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3194	1/1	0.97	0.21	20,20,20,20	0
58	MG	2A	3545	1/1	0.97	0.05	41,41,41,41	0
58	MG	1A	3851	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3547	1/1	0.97	0.06	31,31,31,31	0
58	MG	2A	3548	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3436	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3350	1/1	0.97	0.14	33,33,33,33	0
58	MG	1A	4047	1/1	0.97	0.05	27,27,27,27	0
58	MG	2A	3553	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3855	1/1	0.97	0.11	30,30,30,30	0
58	MG	1A	3352	1/1	0.97	0.18	28,28,28,28	0
58	MG	1x	110	1/1	0.97	0.12	43,43,43,43	0
58	MG	1A	3685	1/1	0.97	0.06	11,11,11,11	0
58	MG	2A	3274	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3006	1/1	0.97	0.08	31,31,31,31	0
58	MG	1A	3196	1/1	0.97	0.26	27,27,27,27	0
58	MG	2A	3564	1/1	0.97	0.06	41,41,41,41	0
58	MG	2B	213	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3566	1/1	0.97	0.04	38,38,38,38	0
58	MG	2A	3568	1/1	0.97	0.06	26,26,26,26	0
58	MG	1A	4053	1/1	0.97	0.04	25,25,25,25	0
58	MG	2A	3570	1/1	0.97	0.05	26,26,26,26	0
58	MG	1A	3197	1/1	0.97	0.32	18,18,18,18	0
58	MG	1a	1611	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3538	1/1	0.97	0.21	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1613	1/1	0.97	0.12	21,21,21,21	0
58	MG	2D	306	1/1	0.97	0.25	30,30,30,30	0
58	MG	1A	3063	1/1	0.97	0.27	44,44,44,44	0
58	MG	1A	3200	1/1	0.97	0.08	25,25,25,25	0
58	MG	1A	3064	1/1	0.97	0.10	33,33,33,33	0
58	MG	2A	3578	1/1	0.97	0.07	26,26,26,26	0
58	MG	1A	3542	1/1	0.97	0.18	33,33,33,33	0
58	MG	1A	3135	1/1	0.97	0.11	20,20,20,20	0
58	MG	2A	3012	1/1	0.97	0.06	30,30,30,30	0
59	K	2x	101	1/1	0.97	0.05	41,41,41,41	0
58	MG	2A	3013	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3296	1/1	0.98	0.07	23,23,23,23	0
58	MG	2A	3747	1/1	0.98	0.05	33,33,33,33	0
58	MG	1B	201	1/1	0.98	0.07	36,36,36,36	0
58	MG	1B	202	1/1	0.98	0.12	34,34,34,34	0
58	MG	1a	1749	1/1	0.98	0.06	37,37,37,37	0
58	MG	2A	3751	1/1	0.98	0.11	40,40,40,40	0
58	MG	1A	3967	1/1	0.98	0.07	30,30,30,30	0
58	MG	13	101	1/1	0.98	0.11	18,18,18,18	0
58	MG	1A	3734	1/1	0.98	0.04	13,13,13,13	0
58	MG	13	103	1/1	0.98	0.07	33,33,33,33	0
58	MG	1a	1754	1/1	0.98	0.04	41,41,41,41	0
58	MG	15	101	1/1	0.98	0.24	28,28,28,28	0
58	MG	1A	3969	1/1	0.98	0.08	17,17,17,17	0
58	MG	1A	3629	1/1	0.98	0.04	11,11,11,11	0
58	MG	2A	3513	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3414	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3354	1/1	0.98	0.22	19,19,19,19	0
58	MG	1A	3632	1/1	0.98	0.03	25,25,25,25	0
58	MG	15	107	1/1	0.98	0.04	18,18,18,18	0
58	MG	2A	3765	1/1	0.98	0.04	39,39,39,39	0
58	MG	1a	1762	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	3633	1/1	0.98	0.05	13,13,13,13	0
58	MG	1A	3198	1/1	0.98	0.15	28,28,28,28	0
58	MG	2A	3521	1/1	0.98	0.06	39,39,39,39	0
58	MG	1a	1765	1/1	0.98	0.10	40,40,40,40	0
58	MG	2A	3523	1/1	0.98	0.05	25,25,25,25	0
58	MG	1A	3163	1/1	0.98	0.15	25,25,25,25	0
58	MG	1A	3854	1/1	0.98	0.10	14,14,14,14	0
58	MG	17	101	1/1	0.98	0.12	23,23,23,23	0
58	MG	2a	1660	1/1	0.98	0.06	52,52,52,52	0
58	MG	1A	3742	1/1	0.98	0.06	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3164	1/1	0.98	0.17	21,21,21,21	0
58	MG	1a	1771	1/1	0.98	0.04	49,49,49,49	0
58	MG	2A	3532	1/1	0.98	0.07	39,39,39,39	0
58	MG	18	103	1/1	0.98	0.10	33,33,33,33	0
58	MG	18	104	1/1	0.98	0.04	28,28,28,28	0
58	MG	1A	3113	1/1	0.98	0.14	25,25,25,25	0
58	MG	1A	3746	1/1	0.98	0.06	10,10,10,10	0
58	MG	1a	1777	1/1	0.98	0.05	56,56,56,56	0
58	MG	1A	3420	1/1	0.98	0.06	34,34,34,34	0
58	MG	1B	219	1/1	0.98	0.09	21,21,21,21	0
58	MG	1a	1780	1/1	0.98	0.05	40,40,40,40	0
58	MG	2A	3117	1/1	0.98	0.06	39,39,39,39	0
58	MG	2a	1674	1/1	0.98	0.05	29,29,29,29	0
58	MG	2a	1675	1/1	0.98	0.14	35,35,35,35	0
58	MG	1B	220	1/1	0.98	0.04	24,24,24,24	0
58	MG	1A	3301	1/1	0.98	0.11	28,28,28,28	0
58	MG	1A	3114	1/1	0.98	0.15	21,21,21,21	0
58	MG	1A	3862	1/1	0.98	0.19	29,29,29,29	0
58	MG	1a	1785	1/1	0.98	0.06	40,40,40,40	0
58	MG	1B	224	1/1	0.98	0.06	45,45,45,45	0
58	MG	1A	3486	1/1	0.98	0.06	21,21,21,21	0
58	MG	1A	3864	1/1	0.98	0.05	35,35,35,35	0
58	MG	2A	3796	1/1	0.98	0.04	37,37,37,37	0
58	MG	2A	3331	1/1	0.98	0.08	38,38,38,38	0
58	MG	2A	3551	1/1	0.98	0.03	25,25,25,25	0
58	MG	1a	1610	1/1	0.98	0.05	34,34,34,34	0
58	MG	1B	227	1/1	0.98	0.04	26,26,26,26	0
58	MG	2A	3554	1/1	0.98	0.06	22,22,22,22	0
58	MG	2A	3555	1/1	0.98	0.07	35,35,35,35	0
58	MG	1a	1791	1/1	0.98	0.04	53,53,53,53	0
58	MG	1A	3643	1/1	0.98	0.06	9,9,9,9	0
58	MG	2A	3558	1/1	0.98	0.08	20,20,20,20	0
58	MG	1A	3136	1/1	0.98	0.07	32,32,32,32	0
58	MG	1a	1794	1/1	0.98	0.03	51,51,51,51	0
58	MG	1A	3168	1/1	0.98	0.12	26,26,26,26	0
58	MG	1a	1796	1/1	0.98	0.04	54,54,54,54	0
58	MG	1A	3754	1/1	0.98	0.04	25,25,25,25	0
58	MG	2A	3136	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3869	1/1	0.98	0.12	19,19,19,19	0
58	MG	2A	3567	1/1	0.98	0.05	24,24,24,24	0
58	MG	1A	3646	1/1	0.98	0.07	12,12,12,12	0
58	MG	2A	3139	1/1	0.98	0.10	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1800	1/1	0.98	0.08	52,52,52,52	0
58	MG	2a	1705	1/1	0.98	0.05	49,49,49,49	0
58	MG	1A	3085	1/1	0.98	0.10	22,22,22,22	0
58	MG	1A	3253	1/1	0.98	0.26	31,31,31,31	0
58	MG	1A	3309	1/1	0.98	0.12	41,41,41,41	0
58	MG	1B	237	1/1	0.98	0.04	25,25,25,25	0
58	MG	2A	3821	1/1	0.98	0.06	22,22,22,22	0
58	MG	1a	1805	1/1	0.98	0.06	47,47,47,47	0
58	MG	1D	301	1/1	0.98	0.17	22,22,22,22	0
58	MG	1A	3650	1/1	0.98	0.04	18,18,18,18	0
58	MG	1A	3018	1/1	0.98	0.10	20,20,20,20	0
58	MG	2A	3149	1/1	0.98	0.12	27,27,27,27	0
58	MG	1D	308	1/1	0.98	0.14	38,38,38,38	0
58	MG	1A	3652	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3763	1/1	0.98	0.04	20,20,20,20	0
58	MG	1A	3561	1/1	0.98	0.12	21,21,21,21	0
58	MG	1A	4006	1/1	0.98	0.05	13,13,13,13	0
58	MG	1E	303	1/1	0.98	0.08	18,18,18,18	0
58	MG	1E	304	1/1	0.98	0.14	22,22,22,22	0
58	MG	1A	3099	1/1	0.98	0.12	10,10,10,10	0
58	MG	1A	3010	1/1	0.98	0.05	18,18,18,18	0
58	MG	1A	3564	1/1	0.98	0.23	26,26,26,26	0
58	MG	2A	3160	1/1	0.98	0.12	37,37,37,37	0
58	MG	2A	3591	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3565	1/1	0.98	0.14	23,23,23,23	0
58	MG	2a	1729	1/1	0.98	0.13	33,33,33,33	0
58	MG	1a	1636	1/1	0.98	0.08	23,23,23,23	0
58	MG	1A	3769	1/1	0.98	0.06	17,17,17,17	0
58	MG	1A	3173	1/1	0.98	0.10	6,6,6,6	0
58	MG	1A	4014	1/1	0.98	0.03	15,15,15,15	0
58	MG	2A	3599	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3771	1/1	0.98	0.07	17,17,17,17	0
58	MG	2A	3851	1/1	0.98	0.04	36,36,36,36	0
58	MG	1F	301	1/1	0.98	0.08	27,27,27,27	0
58	MG	1F	302	1/1	0.98	0.09	13,13,13,13	0
58	MG	1F	303	1/1	0.98	0.17	26,26,26,26	0
58	MG	1A	4016	1/1	0.98	0.08	15,15,15,15	0
58	MG	2A	3856	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3772	1/1	0.98	0.04	21,21,21,21	0
58	MG	2A	3377	1/1	0.98	0.03	39,39,39,39	0
58	MG	1A	3075	1/1	0.98	0.04	23,23,23,23	0
58	MG	1F	308	1/1	0.98	0.17	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3046	1/1	0.98	0.03	18,18,18,18	0
58	MG	1A	3213	1/1	0.98	0.06	32,32,32,32	0
58	MG	1v	102	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3036	1/1	0.98	0.09	21,21,21,21	0
58	MG	2A	3178	1/1	0.98	0.08	19,19,19,19	0
58	MG	1A	3778	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	3892	1/1	0.98	0.08	43,43,43,43	0
58	MG	1w	104	1/1	0.98	0.05	51,51,51,51	0
58	MG	1a	1653	1/1	0.98	0.03	36,36,36,36	0
58	MG	1a	1654	1/1	0.98	0.13	33,33,33,33	0
58	MG	1a	1655	1/1	0.98	0.09	39,39,39,39	0
58	MG	1A	3216	1/1	0.98	0.03	20,20,20,20	0
58	MG	2a	1758	1/1	0.98	0.06	50,50,50,50	0
58	MG	1A	3217	1/1	0.98	0.12	36,36,36,36	0
58	MG	2A	3187	1/1	0.98	0.10	40,40,40,40	0
58	MG	1A	3218	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3219	1/1	0.98	0.14	32,32,32,32	0
58	MG	2A	3625	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3671	1/1	0.98	0.06	19,19,19,19	0
58	MG	1A	3785	1/1	0.98	0.04	17,17,17,17	0
58	MG	2a	1768	1/1	0.98	0.12	44,44,44,44	0
58	MG	2A	3628	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3578	1/1	0.98	0.11	24,24,24,24	0
58	MG	1A	3675	1/1	0.98	0.07	16,16,16,16	0
58	MG	2A	3631	1/1	0.98	0.07	39,39,39,39	0
58	MG	1A	4033	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3788	1/1	0.98	0.05	27,27,27,27	0
58	MG	1A	3902	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3579	1/1	0.98	0.16	23,23,23,23	0
58	MG	2a	1778	1/1	0.98	0.05	54,54,54,54	0
58	MG	1A	3145	1/1	0.98	0.05	38,38,38,38	0
58	MG	2A	3638	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3792	1/1	0.98	0.05	14,14,14,14	0
58	MG	1A	3179	1/1	0.98	0.07	19,19,19,19	0
58	MG	1A	3907	1/1	0.98	0.06	35,35,35,35	0
58	MG	2A	3002	1/1	0.98	0.23	35,35,35,35	0
58	MG	1A	3680	1/1	0.98	0.05	21,21,21,21	0
58	MG	1A	3056	1/1	0.98	0.04	24,24,24,24	0
58	MG	1A	3584	1/1	0.98	0.35	30,30,30,30	0
58	MG	1P	202	1/1	0.98	0.23	20,20,20,20	0
58	MG	2B	215	1/1	0.98	0.11	44,44,44,44	0
58	MG	2A	3648	1/1	0.98	0.08	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3182	1/1	0.98	0.08	28,28,28,28	0
58	MG	2a	1792	1/1	0.98	0.11	43,43,43,43	0
58	MG	1A	3586	1/1	0.98	0.05	28,28,28,28	0
58	MG	2A	3009	1/1	0.98	0.05	29,29,29,29	0
58	MG	1A	3799	1/1	0.98	0.07	10,10,10,10	0
58	MG	2D	302	1/1	0.98	0.15	38,38,38,38	0
58	MG	1A	3587	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3801	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	3224	1/1	0.98	0.08	25,25,25,25	0
58	MG	1A	3383	1/1	0.98	0.15	21,21,21,21	0
58	MG	2A	3015	1/1	0.98	0.11	38,38,38,38	0
58	MG	2A	3217	1/1	0.98	0.14	37,37,37,37	0
58	MG	2A	3425	1/1	0.98	0.10	27,27,27,27	0
58	MG	1A	3124	1/1	0.98	0.14	26,26,26,26	0
58	MG	2E	305	1/1	0.98	0.09	35,35,35,35	0
58	MG	1A	3922	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3692	1/1	0.98	0.09	9,9,9,9	0
58	MG	1A	4055	1/1	0.98	0.04	19,19,19,19	0
58	MG	1A	3226	1/1	0.98	0.07	30,30,30,30	0
58	MG	2A	3021	1/1	0.98	0.07	16,16,16,16	0
58	MG	1A	4057	1/1	0.98	0.08	43,43,43,43	0
58	MG	1A	3149	1/1	0.98	0.23	18,18,18,18	0
58	MG	1A	3125	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	4060	1/1	0.98	0.12	44,44,44,44	0
58	MG	1A	3810	1/1	0.98	0.22	18,18,18,18	0
58	MG	2A	3027	1/1	0.98	0.12	24,24,24,24	0
58	MG	2A	3672	1/1	0.98	0.12	37,37,37,37	0
58	MG	1A	3276	1/1	0.98	0.04	31,31,31,31	0
58	MG	2F	308	1/1	0.98	0.11	35,35,35,35	0
58	MG	1A	3105	1/1	0.98	0.11	31,31,31,31	0
58	MG	2A	3030	1/1	0.98	0.12	33,33,33,33	0
58	MG	2A	3233	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3596	1/1	0.98	0.13	23,23,23,23	0
58	MG	1A	3278	1/1	0.98	0.07	31,31,31,31	0
58	MG	1U	206	1/1	0.98	0.13	29,29,29,29	0
58	MG	2A	3034	1/1	0.98	0.10	32,32,32,32	0
58	MG	1A	3279	1/1	0.98	0.09	28,28,28,28	0
58	MG	1U	208	1/1	0.98	0.12	21,21,21,21	0
58	MG	1A	3519	1/1	0.98	0.20	27,27,27,27	0
58	MG	1A	3152	1/1	0.98	0.24	23,23,23,23	0
58	MG	2A	3450	1/1	0.98	0.20	28,28,28,28	0
58	MG	1A	4071	1/1	0.98	0.07	6,6,6,6	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1V	202	1/1	0.98	0.19	30,30,30,30	0
58	MG	1A	3038	1/1	0.98	0.11	28,28,28,28	0
58	MG	2A	3245	1/1	0.98	0.19	37,37,37,37	0
58	MG	1V	204	1/1	0.98	0.25	22,22,22,22	0
58	MG	1A	4074	1/1	0.98	0.11	27,27,27,27	0
58	MG	2a	1838	1/1	0.98	0.07	49,49,49,49	0
58	MG	2A	3044	1/1	0.98	0.04	35,35,35,35	0
58	MG	2A	3693	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3707	1/1	0.98	0.07	18,18,18,18	0
58	MG	1A	3522	1/1	0.98	0.19	26,26,26,26	0
58	MG	1A	3939	1/1	0.98	0.07	18,18,18,18	0
58	MG	1A	4078	1/1	0.98	0.04	19,19,19,19	0
58	MG	2A	3049	1/1	0.98	0.11	14,14,14,14	0
58	MG	1A	3282	1/1	0.98	0.14	21,21,21,21	0
58	MG	1A	3942	1/1	0.98	0.03	48,48,48,48	0
58	MG	1A	3154	1/1	0.98	0.27	20,20,20,20	0
58	MG	1A	3190	1/1	0.98	0.14	23,23,23,23	0
58	MG	1A	3460	1/1	0.98	0.14	32,32,32,32	0
58	MG	2A	3259	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3285	1/1	0.98	0.11	16,16,16,16	0
58	MG	1A	3286	1/1	0.98	0.25	25,25,25,25	0
58	MG	1a	1719	1/1	0.98	0.07	30,30,30,30	0
58	MG	2A	3263	1/1	0.98	0.06	50,50,50,50	0
58	MG	1X	104	1/1	0.98	0.16	33,33,33,33	0
58	MG	1X	105	1/1	0.98	0.03	25,25,25,25	0
58	MG	2A	3476	1/1	0.98	0.06	39,39,39,39	0
58	MG	1A	3287	1/1	0.98	0.30	20,20,20,20	0
58	MG	2A	3478	1/1	0.98	0.08	16,16,16,16	0
58	MG	1A	3288	1/1	0.98	0.21	31,31,31,31	0
58	MG	1A	3950	1/1	0.98	0.04	33,33,33,33	0
58	MG	2A	3269	1/1	0.98	0.07	35,35,35,35	0
58	MG	1A	3717	1/1	0.98	0.05	7,7,7,7	0
58	MG	1A	3009	1/1	0.98	0.03	18,18,18,18	0
58	MG	1A	3532	1/1	0.98	0.09	39,39,39,39	0
58	MG	2A	3722	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3614	1/1	0.98	0.08	25,25,25,25	0
58	MG	1A	3403	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3345	1/1	0.98	0.09	31,31,31,31	0
58	MG	2A	3069	1/1	0.98	0.04	23,23,23,23	0
58	MG	2A	3728	1/1	0.98	0.05	28,28,28,28	0
58	MG	2A	3729	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3156	1/1	0.98	0.04	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3732	1/1	0.98	0.11	37,37,37,37	0
58	MG	1A	3129	1/1	0.98	0.26	29,29,29,29	0
58	MG	1A	3082	1/1	0.98	0.16	22,22,22,22	0
58	MG	1A	3620	1/1	0.98	0.04	18,18,18,18	0
58	MG	1A	3408	1/1	0.98	0.13	36,36,36,36	0
58	MG	1A	3033	1/1	0.98	0.24	20,20,20,20	0
58	MG	1A	3070	1/1	0.98	0.08	14,14,14,14	0
58	MG	2A	3740	1/1	0.98	0.05	36,36,36,36	0
58	MG	2A	3496	1/1	0.98	0.12	35,35,35,35	0
58	MG	1A	3351	1/1	0.98	0.30	26,26,26,26	0
58	MG	2A	3285	1/1	0.98	0.10	44,44,44,44	0
59	K	1A	3569	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3111	1/1	0.98	0.22	22,22,22,22	0
60	ZN	14	501	1/1	0.98	0.05	79,79,79,79	0
60	ZN	2Y	501	1/1	0.98	0.04	70,70,70,70	0
58	MG	11	104	1/1	0.98	0.06	30,30,30,30	0
58	MG	1W	206	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	3689	1/1	0.99	0.03	11,11,11,11	0
58	MG	1a	1740	1/1	0.99	0.06	23,23,23,23	0
58	MG	1E	301	1/1	0.99	0.26	20,20,20,20	0
58	MG	1E	302	1/1	0.99	0.09	31,31,31,31	0
58	MG	2a	1767	1/1	0.99	0.05	28,28,28,28	0
58	MG	1A	3809	1/1	0.99	0.04	14,14,14,14	0
58	MG	2a	1769	1/1	0.99	0.04	46,46,46,46	0
58	MG	1A	3690	1/1	0.99	0.04	16,16,16,16	0
58	MG	2A	3635	1/1	0.99	0.04	27,27,27,27	0
58	MG	2A	3412	1/1	0.99	0.06	24,24,24,24	0
58	MG	1a	1745	1/1	0.99	0.03	44,44,44,44	0
58	MG	1E	305	1/1	0.99	0.14	21,21,21,21	0
58	MG	1A	3638	1/1	0.99	0.03	12,12,12,12	0
58	MG	2A	3640	1/1	0.99	0.06	26,26,26,26	0
58	MG	1A	3204	1/1	0.99	0.08	24,24,24,24	0
58	MG	1A	3231	1/1	0.99	0.15	19,19,19,19	0
58	MG	2A	3527	1/1	0.99	0.03	20,20,20,20	0
58	MG	1A	3937	1/1	0.99	0.03	16,16,16,16	0
58	MG	1A	4007	1/1	0.99	0.03	22,22,22,22	0
58	MG	2A	3530	1/1	0.99	0.06	30,30,30,30	0
58	MG	1A	3013	1/1	0.99	0.06	12,12,12,12	0
58	MG	1A	3559	1/1	0.99	0.17	22,22,22,22	0
58	MG	1E	313	1/1	0.99	0.08	25,25,25,25	0
58	MG	1A	3696	1/1	0.99	0.06	12,12,12,12	0
58	MG	2A	3424	1/1	0.99	0.06	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4086	1/1	0.99	0.04	16,16,16,16	0
58	MG	10	103	1/1	0.99	0.15	28,28,28,28	0
58	MG	1A	3941	1/1	0.99	0.05	18,18,18,18	0
58	MG	1A	3233	1/1	0.99	0.22	24,24,24,24	0
58	MG	1A	3120	1/1	0.99	0.17	25,25,25,25	0
58	MG	1A	3058	1/1	0.99	0.02	16,16,16,16	0
58	MG	1F	306	1/1	0.99	0.03	28,28,28,28	0
58	MG	1A	3072	1/1	0.99	0.22	21,21,21,21	0
58	MG	1A	3073	1/1	0.99	0.05	8,8,8,8	0
58	MG	2D	305	1/1	0.99	0.07	26,26,26,26	0
58	MG	1A	3037	1/1	0.99	0.09	15,15,15,15	0
58	MG	1A	3143	1/1	0.99	0.10	20,20,20,20	0
58	MG	1A	3824	1/1	0.99	0.05	25,25,25,25	0
58	MG	1A	4020	1/1	0.99	0.02	21,21,21,21	0
58	MG	1A	3048	1/1	0.99	0.16	25,25,25,25	0
58	MG	1A	3705	1/1	0.99	0.03	5,5,5,5	0
58	MG	2A	3120	1/1	0.99	0.04	16,16,16,16	0
58	MG	1A	3706	1/1	0.99	0.04	32,32,32,32	0
58	MG	1A	3270	1/1	0.99	0.05	30,30,30,30	0
58	MG	1A	3609	1/1	0.99	0.09	31,31,31,31	0
58	MG	1A	3653	1/1	0.99	0.04	23,23,23,23	0
58	MG	1a	1775	1/1	0.99	0.03	42,42,42,42	0
58	MG	1A	3397	1/1	0.99	0.10	22,22,22,22	0
58	MG	1A	3031	1/1	0.99	0.13	20,20,20,20	0
58	MG	1A	3039	1/1	0.99	0.28	22,22,22,22	0
58	MG	1A	4106	1/1	0.99	0.04	42,42,42,42	0
58	MG	1A	3573	1/1	0.99	0.14	31,31,31,31	0
58	MG	1A	3215	1/1	0.99	0.22	23,23,23,23	0
58	MG	1A	3434	1/1	0.99	0.06	34,34,34,34	0
58	MG	1A	3576	1/1	0.99	0.19	32,32,32,32	0
58	MG	2A	3565	1/1	0.99	0.06	24,24,24,24	0
58	MG	1A	3244	1/1	0.99	0.24	23,23,23,23	0
58	MG	1A	3662	1/1	0.99	0.05	14,14,14,14	0
58	MG	1A	3305	1/1	0.99	0.05	19,19,19,19	0
58	MG	1A	3306	1/1	0.99	0.06	18,18,18,18	0
58	MG	17	102	1/1	0.99	0.21	31,31,31,31	0
58	MG	1A	3078	1/1	0.99	0.17	24,24,24,24	0
58	MG	1A	3621	1/1	0.99	0.03	19,19,19,19	0
58	MG	18	102	1/1	0.99	0.11	24,24,24,24	0
58	MG	1A	3667	1/1	0.99	0.06	21,21,21,21	0
58	MG	1A	3148	1/1	0.99	0.14	14,14,14,14	0
58	MG	1P	204	1/1	0.99	0.05	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3971	1/1	0.99	0.05	22,22,22,22	0
58	MG	2A	3466	1/1	0.99	0.07	14,14,14,14	0
58	MG	1Q	202	1/1	0.99	0.07	22,22,22,22	0
58	MG	2A	3696	1/1	0.99	0.10	21,21,21,21	0
58	MG	1A	3021	1/1	0.99	0.11	15,15,15,15	0
58	MG	1A	3670	1/1	0.99	0.03	10,10,10,10	0
58	MG	1A	3583	1/1	0.99	0.22	24,24,24,24	0
58	MG	1A	3112	1/1	0.99	0.05	29,29,29,29	0
58	MG	1A	3790	1/1	0.99	0.03	22,22,22,22	0
58	MG	2A	3823	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3673	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3912	1/1	0.99	0.04	32,32,32,32	0
58	MG	1A	3674	1/1	0.99	0.05	12,12,12,12	0
58	MG	1A	3510	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3627	1/1	0.99	0.12	39,39,39,39	0
58	MG	1A	3007	1/1	0.99	0.04	29,29,29,29	0
58	MG	2A	3830	1/1	0.99	0.07	25,25,25,25	0
58	MG	2A	3831	1/1	0.99	0.04	36,36,36,36	0
58	MG	1A	3917	1/1	0.99	0.03	26,26,26,26	0
58	MG	2A	3833	1/1	0.99	0.03	43,43,43,43	0
58	MG	1A	3984	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	3918	1/1	0.99	0.03	20,20,20,20	0
58	MG	1A	3042	1/1	0.99	0.13	13,13,13,13	0
58	MG	2A	3595	1/1	0.99	0.06	29,29,29,29	0
58	MG	2A	3596	1/1	0.99	0.03	27,27,27,27	0
58	MG	1a	1711	1/1	0.99	0.08	29,29,29,29	0
58	MG	1U	201	1/1	0.99	0.20	16,16,16,16	0
58	MG	1A	3679	1/1	0.99	0.03	11,11,11,11	0
58	MG	1A	3023	1/1	0.99	0.06	6,6,6,6	0
58	MG	2A	3843	1/1	0.99	0.04	21,21,21,21	0
58	MG	1A	3003	1/1	0.99	0.06	19,19,19,19	0
58	MG	1A	3990	1/1	0.99	0.05	14,14,14,14	0
58	MG	1A	3068	1/1	0.99	0.03	19,19,19,19	0
58	MG	1A	3992	1/1	0.99	0.08	24,24,24,24	0
58	MG	1A	3177	1/1	0.99	0.14	21,21,21,21	0
58	MG	1U	209	1/1	0.99	0.23	24,24,24,24	0
58	MG	1A	3045	1/1	0.99	0.06	23,23,23,23	0
58	MG	2A	3726	1/1	0.99	0.11	26,26,26,26	0
58	MG	1A	3157	1/1	0.99	0.13	22,22,22,22	0
58	MG	1a	1723	1/1	0.99	0.04	42,42,42,42	0
58	MG	1A	3743	1/1	0.99	0.03	39,39,39,39	0
58	MG	1D	302	1/1	0.99	0.06	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3731	1/1	0.99	0.03	24,24,24,24	0
58	MG	1D	303	1/1	0.99	0.05	25,25,25,25	0
58	MG	1D	304	1/1	0.99	0.04	7,7,7,7	0
58	MG	1V	205	1/1	0.99	0.10	17,17,17,17	0
58	MG	1A	4069	1/1	0.99	0.03	27,27,27,27	0
58	MG	2A	3076	1/1	0.99	0.16	28,28,28,28	0
58	MG	1a	1730	1/1	0.99	0.04	22,22,22,22	0
58	MG	2A	3078	1/1	0.99	0.11	20,20,20,20	0
58	MG	2A	3739	1/1	0.99	0.06	38,38,38,38	0
58	MG	1a	1731	1/1	0.99	0.10	25,25,25,25	0
58	MG	1D	306	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	4070	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3180	1/1	0.99	0.06	21,21,21,21	0
58	MG	2A	3083	1/1	0.99	0.05	44,44,44,44	0
58	MG	2A	3189	1/1	0.99	0.09	37,37,37,37	0
58	MG	1A	3687	1/1	0.99	0.04	17,17,17,17	0
60	ZN	1Y	204	1/1	0.99	0.03	54,54,54,54	0
58	MG	1A	4073	1/1	0.99	0.04	12,12,12,12	0
60	ZN	19	102	1/1	0.99	0.03	31,31,31,31	0
60	ZN	1n	102	1/1	0.99	0.03	47,47,47,47	0
58	MG	2a	1760	1/1	0.99	0.03	62,62,62,62	0
58	MG	1A	3229	1/1	0.99	0.12	30,30,30,30	0
60	ZN	25	105	1/1	0.99	0.06	50,50,50,50	0
60	ZN	29	102	1/1	0.99	0.03	62,62,62,62	0
60	ZN	2n	501	1/1	0.99	0.03	68,68,68,68	0
61	SF4	1d	302	8/8	0.99	0.04	45,51,56,57	0
61	SF4	2d	302	8/8	0.99	0.03	45,53,60,64	0
58	MG	1A	3724	1/1	1.00	0.04	5,5,5,5	0
58	MG	1A	3780	1/1	1.00	0.02	21,21,21,21	0
58	MG	1A	4036	1/1	1.00	0.02	13,13,13,13	0
58	MG	1A	3014	1/1	1.00	0.08	16,16,16,16	0
58	MG	1A	3777	1/1	1.00	0.02	23,23,23,23	0
60	ZN	26	102	1/1	1.00	0.02	43,43,43,43	0
58	MG	2A	3714	1/1	1.00	0.04	13,13,13,13	0
58	MG	1A	3756	1/1	1.00	0.04	10,10,10,10	0
60	ZN	15	110	1/1	1.00	0.04	28,28,28,28	0
60	ZN	16	103	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers i

There are no such residues in this entry.