



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:08 AM UTC

PDB ID : 8UD8 / pdb_00008ud8
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with cresomycin, mRNA, deacylated A-site tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.70Å resolution
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Wu, K.J.Y.; Tresco, B.I.C.; Ramkissoon, A.; See, D.N.Y.; Liow, P.; Dittamore, G.A.; Yu, M.; Testolin, G.; Mitcheltree, M.J.; Liu, R.Y.; Svetlov, M.S.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-09-28
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	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12

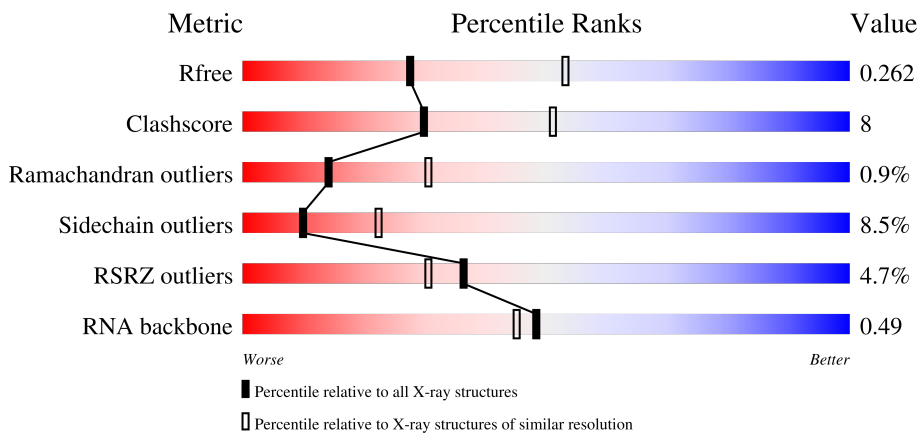
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	

Continued on next page...

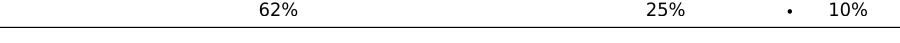
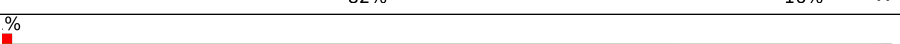
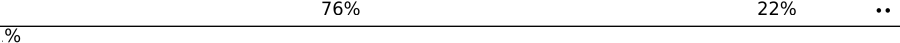
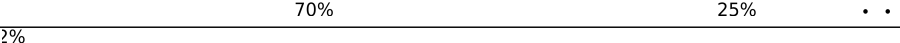
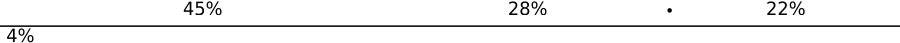
Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	2A	2915	
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
26	24	71	
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	1h	138	
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	2y	55	-	-	X	-
60	SF4	1d	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	11284	19390	2800			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	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
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called A- and E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-tRNA^{met}.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1096	Total	Mg	0	0
			1096	1096		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	15	Total	Mg	0	0
			15	15		
56	1F	15	Total	Mg	0	0
			15	15		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1I	1	Total 1	Mg 1	0	0
56	1N	6	Total 6	Mg 6	0	0
56	1O	5	Total 5	Mg 5	0	0
56	1P	5	Total 5	Mg 5	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	9	Total 9	Mg 9	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	7	Total 7	Mg 7	0	0
56	1Y	5	Total 5	Mg 5	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	10	8	Total 8	Mg 8	0	0
56	11	6	Total 6	Mg 6	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	3	Total 3	Mg 3	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	10	Total 10	Mg 10	0	0
56	16	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	17	6	Total 6	Mg 6	0	0
56	18	6	Total 6	Mg 6	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	210	Total 210	Mg 210	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1w	8	Total 8	Mg 8	0	0
56	1x	15	Total 15	Mg 15	0	0
56	1y	1	Total 1	Mg 1	0	0
56	2A	844	Total 844	Mg 844	0	0
56	2B	19	Total 19	Mg 19	0	0
56	2D	8	Total 8	Mg 8	0	0
56	2E	9	Total 9	Mg 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2F	8	Total 8	Mg 8	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	4	Total 4	Mg 4	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	4	Total 4	Mg 4	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	6	Total 6	Mg 6	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	3	Total 3	Mg 3	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	225	Total 225	Mg 225	0	0

Continued on next page...

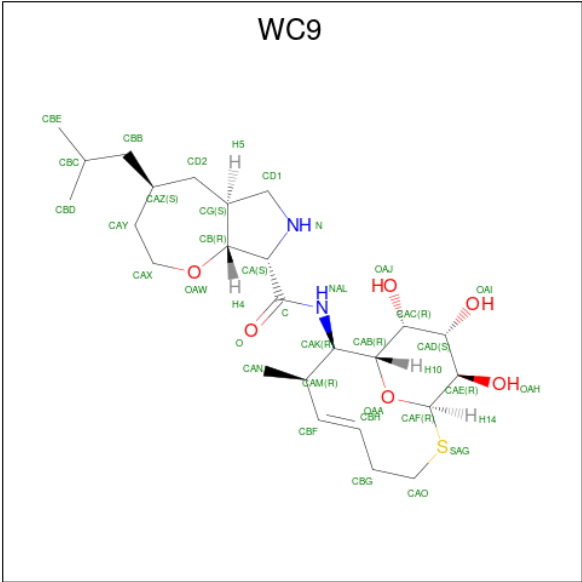
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2d	2	Total	Mg	0	0
			2	2		
56	2e	1	Total	Mg	0	0
			1	1		
56	2f	2	Total	Mg	0	0
			2	2		
56	2g	1	Total	Mg	0	0
			1	1		
56	2j	1	Total	Mg	0	0
			1	1		
56	2l	5	Total	Mg	0	0
			5	5		
56	2m	1	Total	Mg	0	0
			1	1		
56	2q	3	Total	Mg	0	0
			3	3		
56	2t	1	Total	Mg	0	0
			1	1		
56	2v	3	Total	Mg	0	0
			3	3		
56	2w	6	Total	Mg	0	0
			6	6		
56	2x	7	Total	Mg	0	0
			7	7		
56	2y	7	Total	Mg	0	0
			7	7		

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

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

- Molecule 58 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1R,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-13-oxa-2-thiabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: WC9) (formula: C₂₅H₄₂N₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	1A	1	Total	C	N	O	S	0	0
			34	25	2	6	1		
58	2A	1	Total	C	N	O	S	0	0
			34	25	2	6	1		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

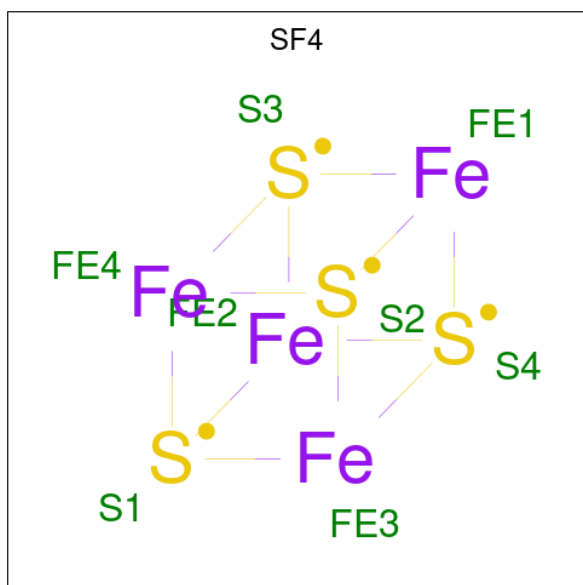
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1907	Total	O	0	0
			1907	1907		
61	1B	59	Total	O	0	0
			59	59		
61	1D	26	Total	O	0	0
			26	26		
61	1E	28	Total	O	0	0
			28	28		
61	1F	17	Total	O	0	0
			17	17		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	2	Total	O	0	0
			2	2		
61	1H	2	Total	O	0	0
			2	2		
61	1N	4	Total	O	0	0
			4	4		
61	1O	4	Total	O	0	0
			4	4		
61	1P	23	Total	O	0	0
			23	23		
61	1Q	5	Total	O	0	0
			5	5		
61	1R	10	Total	O	0	0
			10	10		
61	1S	3	Total	O	0	0
			3	3		
61	1T	8	Total	O	0	0
			8	8		
61	1U	14	Total	O	0	0
			14	14		
61	1V	7	Total	O	0	0
			7	7		
61	1W	7	Total	O	0	0
			7	7		
61	1X	6	Total	O	0	0
			6	6		
61	1Y	2	Total	O	0	0
			2	2		
61	1Z	1	Total	O	0	0
			1	1		
61	10	11	Total	O	0	0
			11	11		
61	11	9	Total	O	0	0
			9	9		
61	12	3	Total	O	0	0
			3	3		
61	13	5	Total	O	0	0
			5	5		
61	14	1	Total	O	0	0
			1	1		
61	15	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	3	Total 3	O 3	0	0
61	17	8	Total 8	O 8	0	0
61	18	7	Total 7	O 7	0	0
61	1a	267	Total 267	O 267	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	3	Total 3	O 3	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1v	4	Total 4	O 4	0	0
61	1w	15	Total 15	O 15	0	0
61	1x	10	Total 10	O 10	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1000	Total 1000	O 1000	0	0
61	2B	18	Total 18	O 18	0	0
61	2D	17	Total 17	O 17	0	0
61	2E	10	Total 10	O 10	0	0
61	2F	12	Total 12	O 12	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	8	Total 8	O 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	4	Total 4	O 4	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	2	Total 2	O 2	0	0
61	20	3	Total 3	O 3	0	0
61	21	8	Total 8	O 8	0	0
61	23	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	172	Total 172	O 172	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2p	1	Total 1	O 1	0	0

Continued on next page...

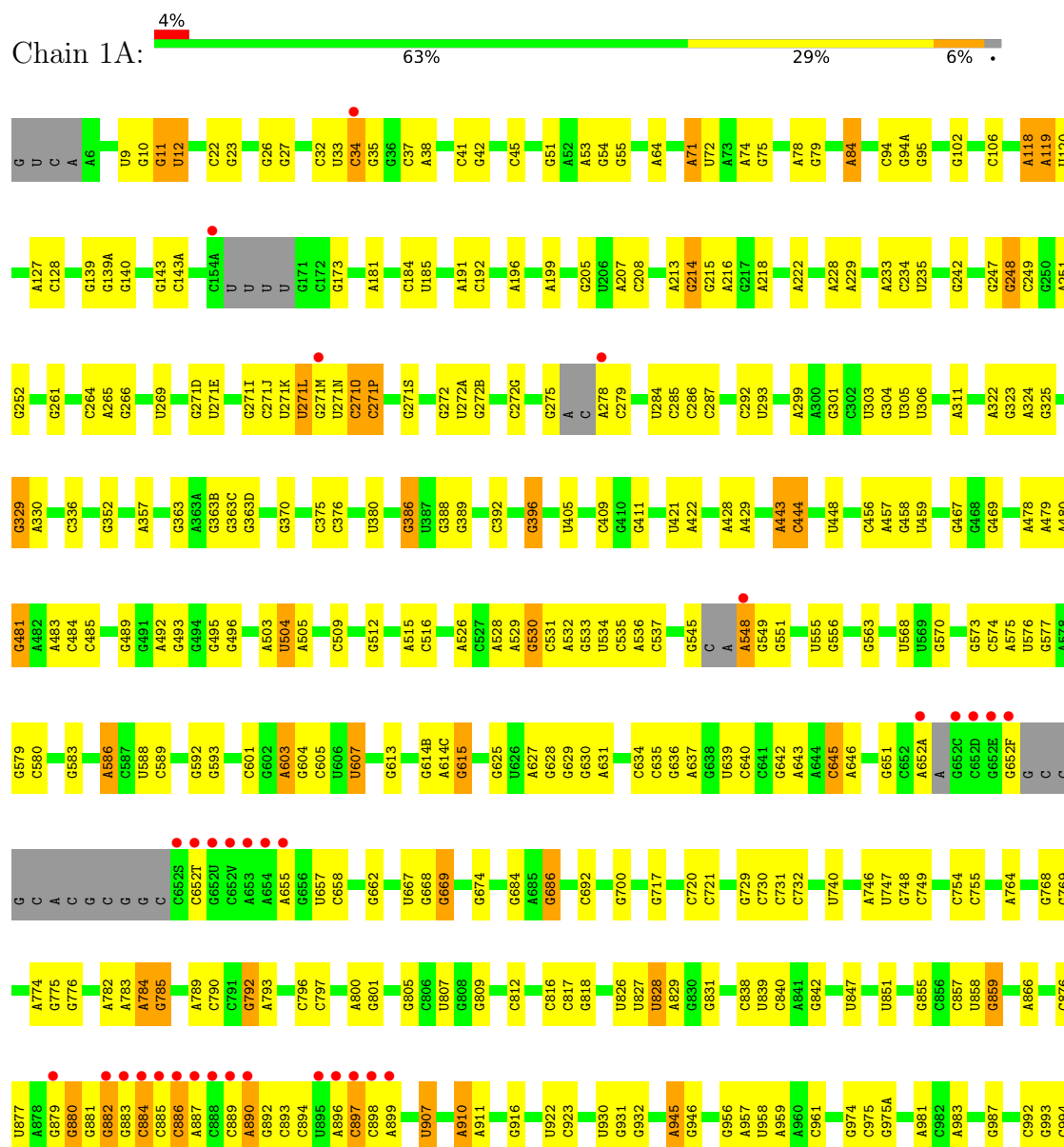
Continued from previous page...

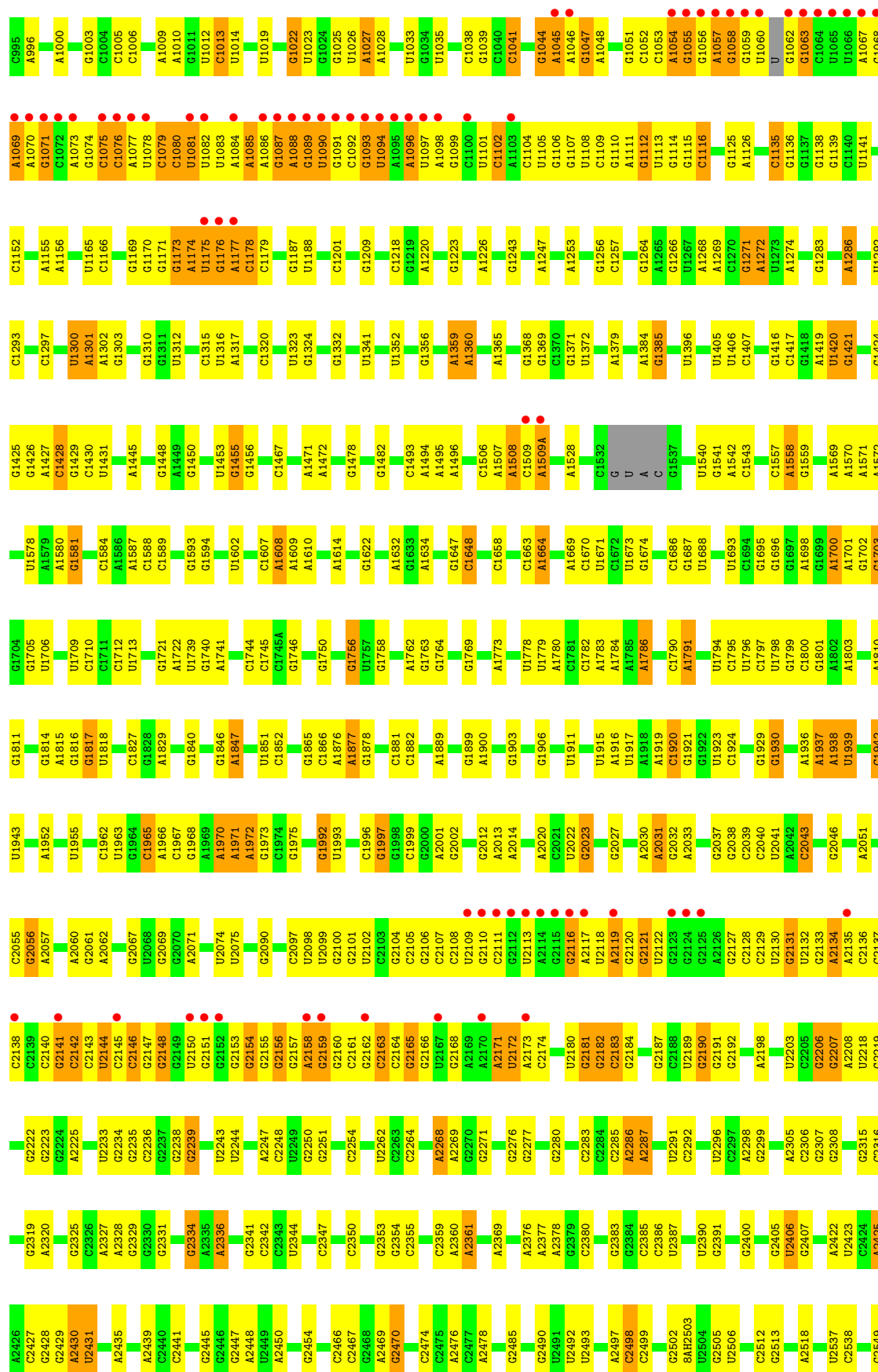
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2q	1	Total	O	0	0
			1	1		
61	2r	1	Total	O	0	0
			1	1		
61	2t	2	Total	O	0	0
			2	2		
61	2v	3	Total	O	0	0
			3	3		
61	2w	3	Total	O	0	0
			3	3		
61	2x	4	Total	O	0	0
			4	4		
61	2y	4	Total	O	0	0
			4	4		

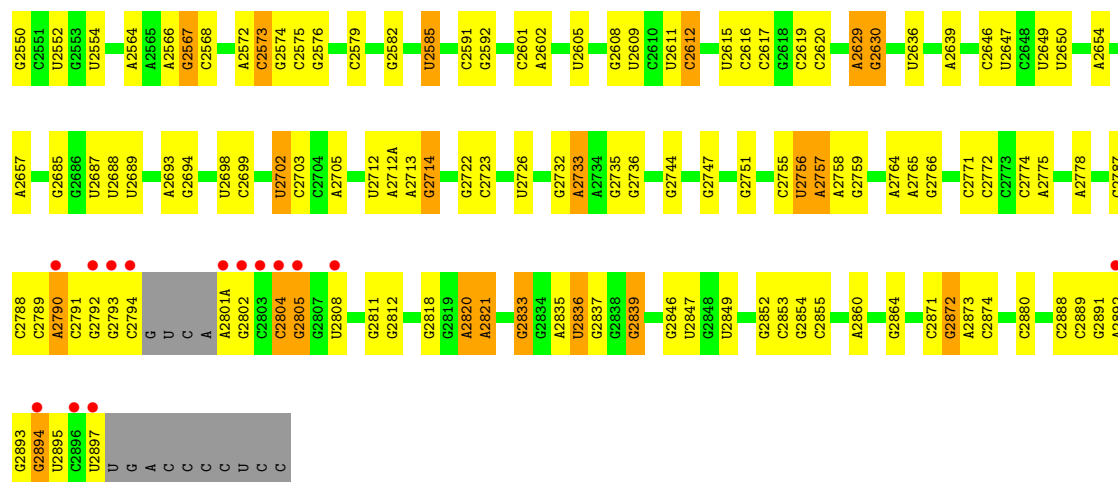
3 Residue-property plots

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

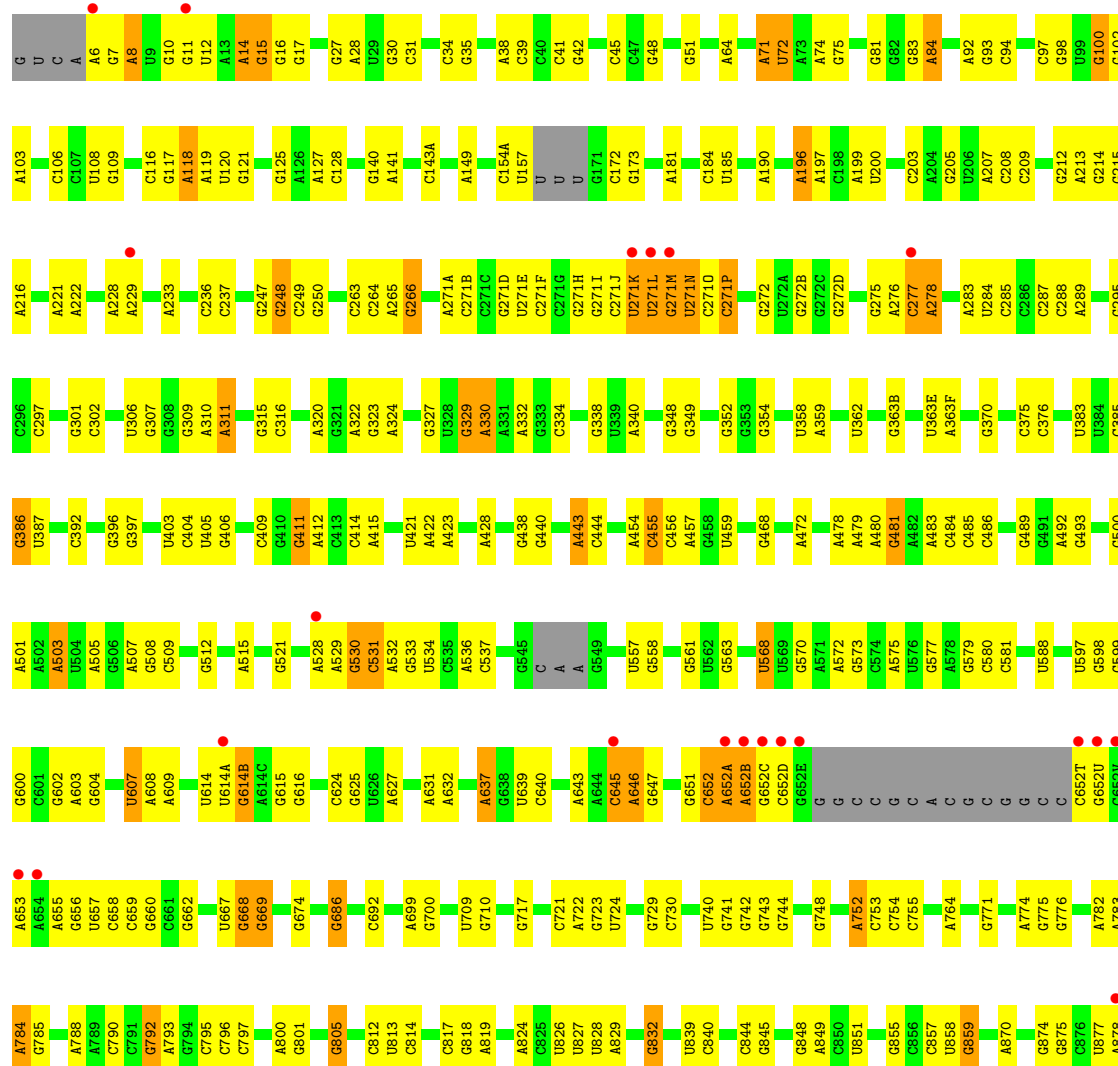
• Molecule 1: 23S Ribosomal RNA



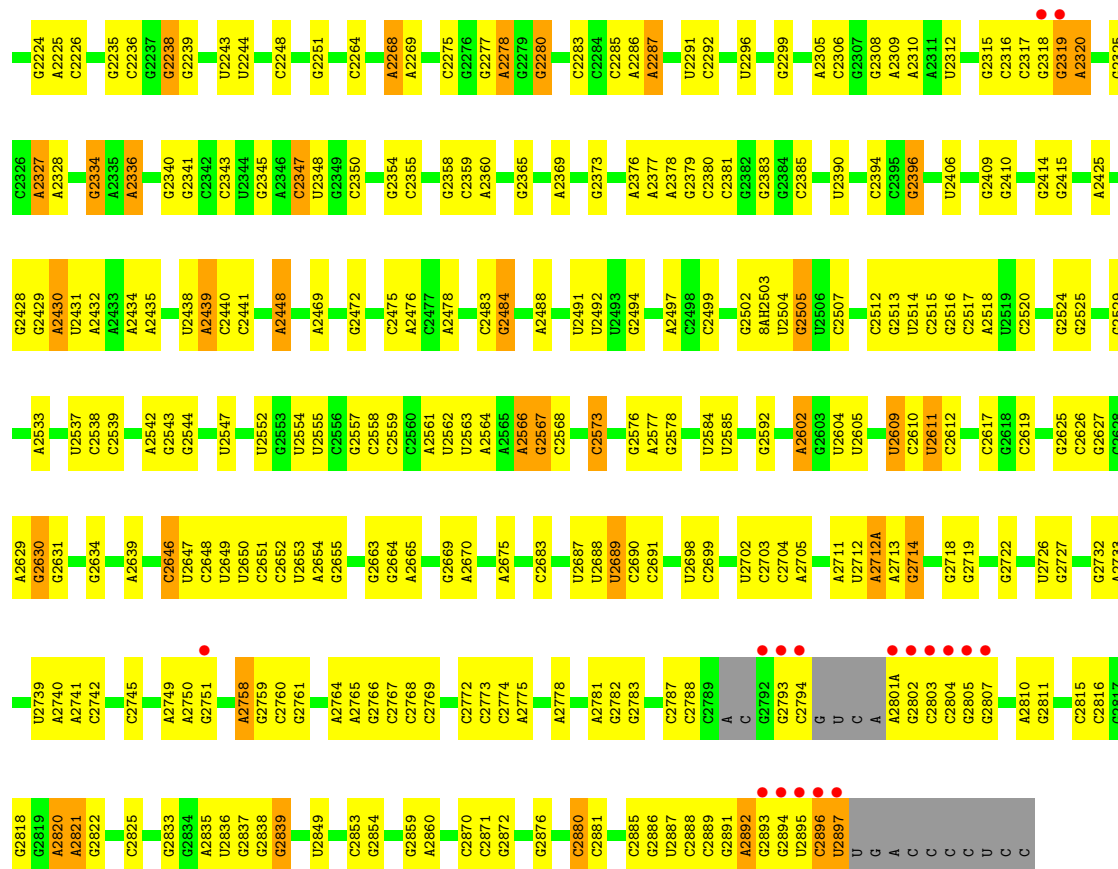




● Molecule 1: 23S Ribosomal RNA

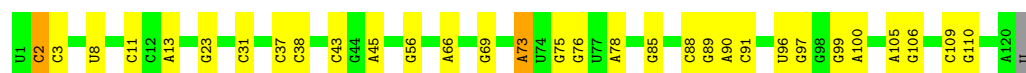


C2139	G2056	C1838	G1750	G1630	G1515	U1420	C1315	A1204	C1116	A	G962	G879
C2140	A2060	G1839	G1751	G1631	C1516	G1421	U1316	U1205	G1117	G	U963	G880
G2141	G2061	C1843	C1754	A1631A	G1519	G1426	A1317	G1206	G1122	A	G974	G881
C2142	C2062	C1947	A1755	A1632	G1529	C1428	A1321	U1210	C1123	G	C975	G882
U2144	C2063	A1847	G1756	C1636	C1530	G1429	A1322	U1211	G1124	G	A880	G883
C2145	C2064	A1848	A1759	A1637	C1531	C1430	G1325	C1218	G1125	U	A891	G884
C2146	C2065	U1851	A1762	G1647	C1532	A1434	A1336	G1219	A1127	U	C982	C885
G2147	C2069	C1852	G1763	C1648	U	C1437	G1337	A1220	G1128	G	A883	C886
C2148	G2070	G1857	G1764	G1649	A	G1442	G1338	G1225	A1129	C	G887	C887
C2149	A2071	A1858	G1769	G1650	C1536	G1443	G1339	G1226	U1130	U	A890	C888
U2150	U2079	A1859	G1777	G1651	G1537	C1444	U1340	G1227	G1131	A	G892	C889
C2151	U2086	C1866	A1773	A1652	G1538	A1445	U1341	G1231	C1135	A	C994	C893
C2152	G2087	A1876	C1774	A1654	G1539	A1448	A1342	G1232	G1136	G	C995	C894
G2153	A2086	A1877	U1777	A1664	U1540	G1449	C1345	G1236	U1139	G	U999	C895
C2154	C2087	G1878	U1778	A1665	G1541	G1450	A1349	G1244	C1140	C	A1000	C896
C2155	U2098	C1882	U1779	G1666	C1542	G1455	U1352	G1239	U1141	A	C1005	C897
C2156	U2099	G1883	A1780	G1667	C1548	G1456	A1353	U1240	A1142	C	C1006	C898
C2157	A1971	A1889	C1781	A1668	C1549	G1461	G1354	A1241	A1143	C	A1009	C899
C2158	A1972	A1890	C1782	A1669	A1554	A1460	A1355	G1244	G1144	A	U1019	A900
C2159	G1973	A1891	A1783	C1670	A1557	G1466	G1356	G1252	U1145	G	A1021	A901
C2160	G1984	G1896	A1784	U1671	C1558	C1467	U1357	U1254	A1146	C	A1022	C902
C2161	U1991	C1899	A1785	G1674	A1559	G1471	G1358	G1255	C1147	A	U1023	C903
C2162	G1992	G1899	A1786	G1674	C1561	A1472	A1359	C1257	U1148	A	U1012	A909
C2163	U1993	A1900	C1687	U1688	A1562	A1477	A1360	G1257	A1149	A	C1013	A910
G2166	C2111	G1906	U1688	A1586	G1566	A1477	G1364	C1257	C1153	A	U1019	A911
U2167	G2112	U1911	C1688	A1567	A1567	G1478	A1365	G1264	G1163	A	A1029	A917
C2168	A2013	A1912	U1795	U1693	C1568	G1479	A1366	G1265	U1023	A	G1030	U922
C2169	A2014	A1913	U1796	G1696	A1569	G1479	G1368	U1266	G1024	A	U1026	C923
C2170	A2015	C1914	C1797	G1697	A1572	G1482	G1369	U1267	A1027	G	A1028	G928
C2171	A2016	U1915	U1798	G1698	U1578	A1490	C1370	A1268	U1028	C	A1029	G932
C2172	A2017	A1916	G1799	A1698	A1579	A1490	U1372	C1270	G1031	G	G1030	G932
C2173	A2018	U1917	C1800	G1699	A1580	C1493	A1373	G1271	A1032	A	U1033	G938
C2174	U2022	A1918	G1801	A1700	A1580	A1494	C1374	A1272	G1034	U	A1035	A941
C2175	G2023	A1919	A1802	A1701	A1583	A1495	C1375	U1273	U1035	A	G	G942
C2176	G2027	C1920	A1803	G1702	C1584	A1496	A1379	A1274	A1035	A	C1038	A945
C2177	A2030	C1924	A1810	G1704	C1584	U1497	G1380	A1278	G1181	G	G1039	G946
C2178	A2031	C1925	G1811	U1709	C1599	C1498	A1384	A1287	G1182	C	C1043	G947
C2179	G2032	A1926	A1812	C1710	C1599	G1500	G1385	U1288	G1183	U	A	G948
U2180	A2033	A1927	G1816	C1711	A1603	U1503	U1405	C1297	G1187	A	G	G952
C2181	G2038	G1928	A1819	U1713	C1607	C1504	U1406	U1300	U1188	C	A	G953
C2182	C2039	G1930	U1820	G1714	A1608	C1505	A1412	A1301	A1189	U	A	G954
C2183	C2040	U1931	G1721	G1714	A1609	C1506	A1413	A1302	G1190	G	C	G955
C2184	U2041	A1932	A1722	G1721	A1610	A1507	G1413	G1303	G1191	U	A	G956
C2185	A2042	G1933	A1729	A1722	A1614	C1508	G1416	G1311	G1192	G	A	A959
C2186	C2043	A1936	G1740	A1741	C1615	C1509	C1417	C1314	G1193	C	C	A960
C2187	A2051	A1937	G1835	A1741	A1616	A1509A	G1418	G1112	G1194	A	G	C961
C2188	C2055	A1938	C1836	G1746	G1622	U1514	A1419	G1112	G1195	G	C	
U2189		U1939	C1837						C1201			
G2192												
C2193												
C2194												
C2195												
C2196												
C2197												
C2198												
C2199												
C2200												
C2201												
C2202												
C2203												
C2204												
C2205												
C2206												
C2207												
C2208												
C2209												
C2210												
C2211												
C2212												
C2213												
C2214												
C2215												
C2216												
C2217												
C2218												
C2219												
C2220												
C2221												
C2222												
C2223												
C2224												
C2225												
C2226												
C2227												
C2228												
C2229												
C2230												
C2231												
C2232												
C2233												
C2234												
C2235												
C2236												
C2237												
C2238												
C2239												
C2240												
C2241												
C2242												
C2243												
C2244												
C2245												
C2246												
C2247												
C2248												
C2249												
C2250												
C2251												
C2252												
C2253												
C2254												
C2255												
C2256												
C2257												
C2258												
C2259												
C2260												
C2261												
C2262												
C2263												
C2264												
C2265												
C2266												
C2267												
C2268												
C2269												
C2270												
C2271												
C2272												
C2273												
C2274												
C2275												
C2276												
C2277												
C2278												
C2279												
C2280												
C2281												
C2282												
C2283												
C2284												
C2285												
C2286												
C2287												
C2288												
C2289												
C2290												
C2291												
C2292												
C2293												
C2294												
C2295												
C2296												
C2297												
C2298												
C2299												



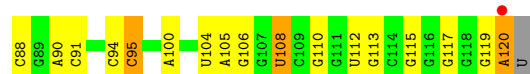
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 74% 24% ..



• Molecule 2: 5S Ribosomal RNA

Chain 2B: 52% 38% 9% .



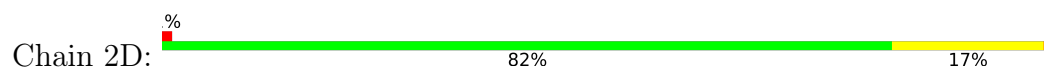
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 77% 21% .

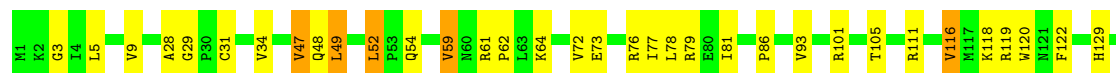
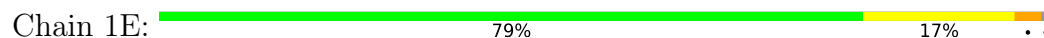




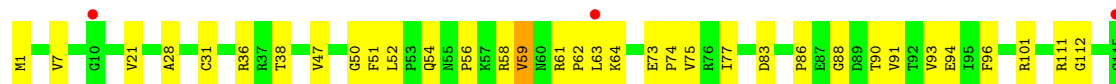
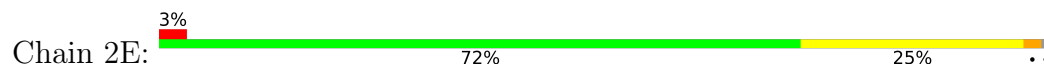
- Molecule 3: 50S ribosomal protein L2



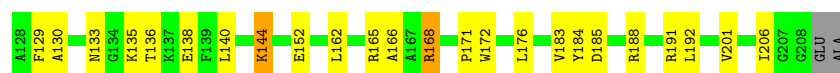
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3

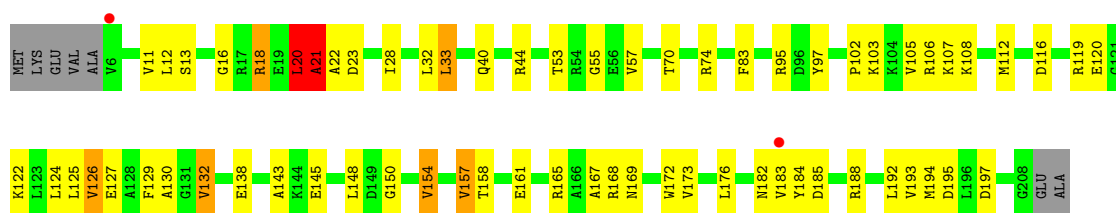


- Molecule 5: 50S ribosomal protein L4

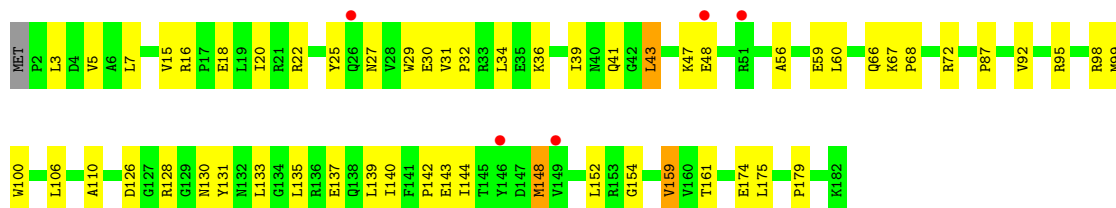


- Molecule 5: 50S ribosomal protein L4

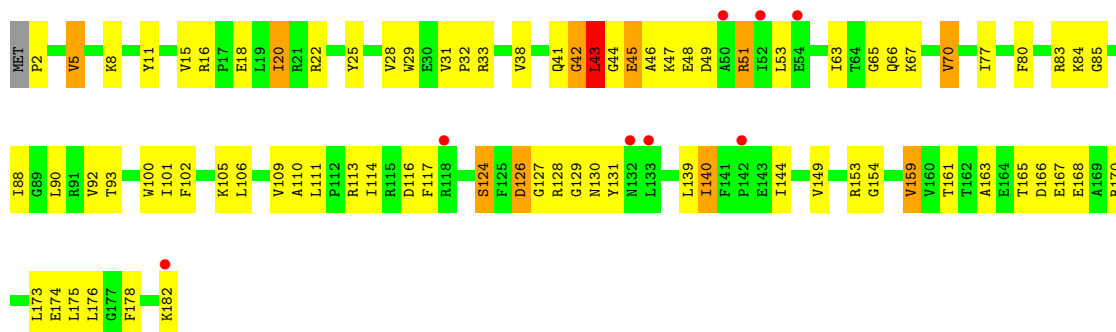




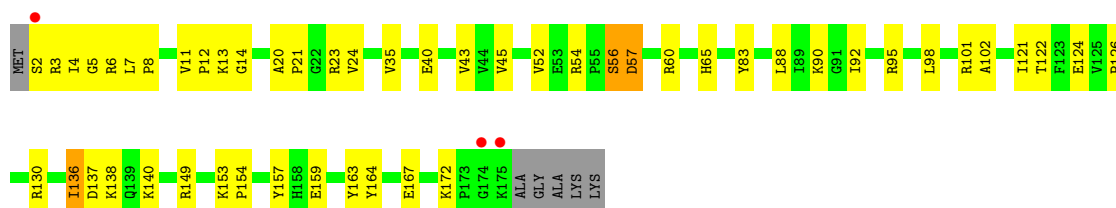
• Molecule 6: 50S ribosomal protein L5



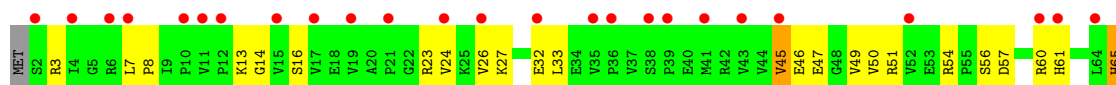
• Molecule 6: 50S ribosomal protein L5

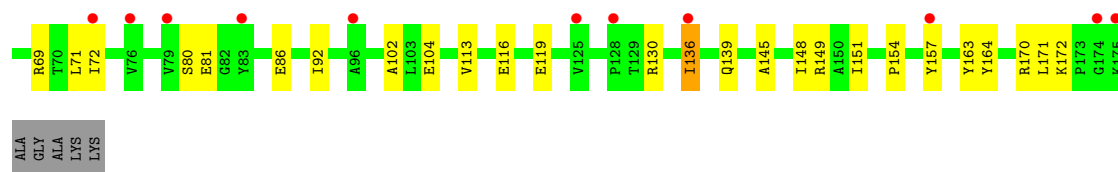


• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

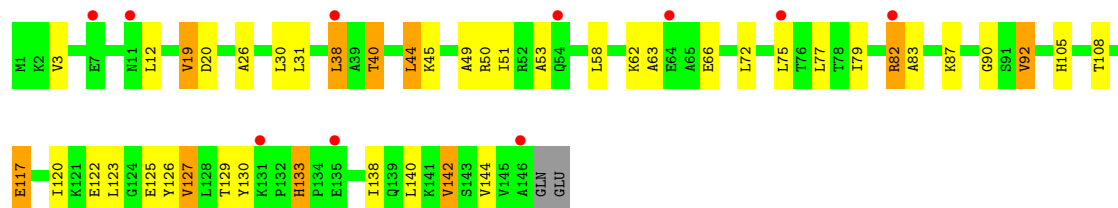




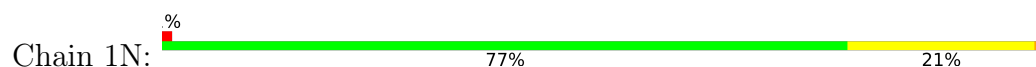
- Molecule 8: 50S ribosomal protein L9



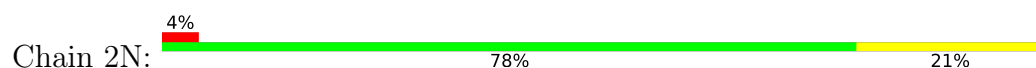
- Molecule 8: 50S ribosomal protein L9



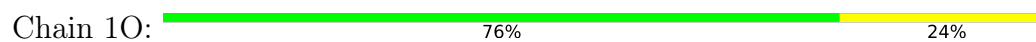
- Molecule 9: 50S ribosomal protein L13



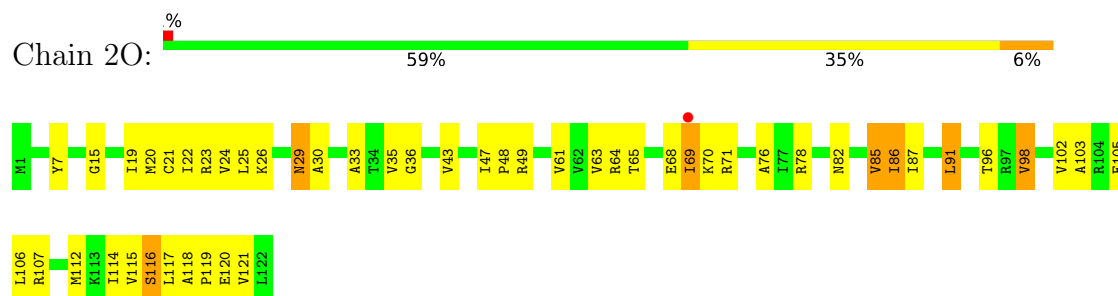
- Molecule 9: 50S ribosomal protein L13



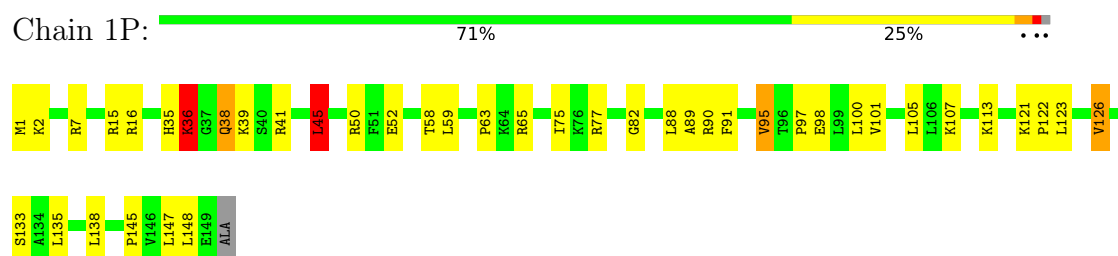
- Molecule 10: 50S ribosomal protein L14



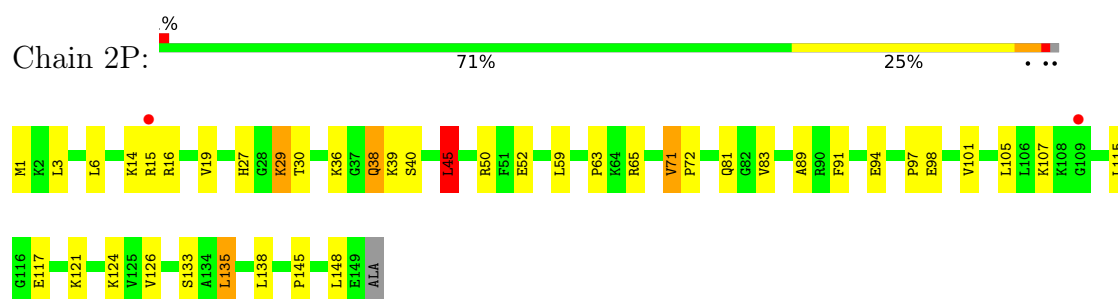
- Molecule 10: 50S ribosomal protein L14



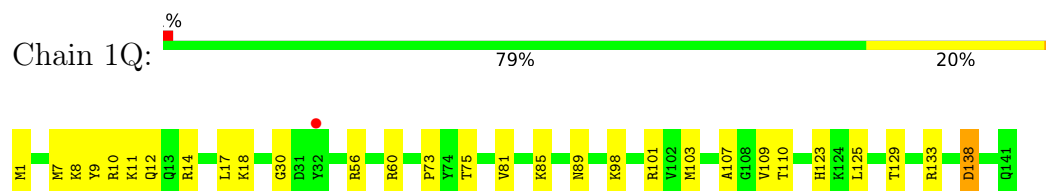
- Molecule 11: 50S ribosomal protein L15



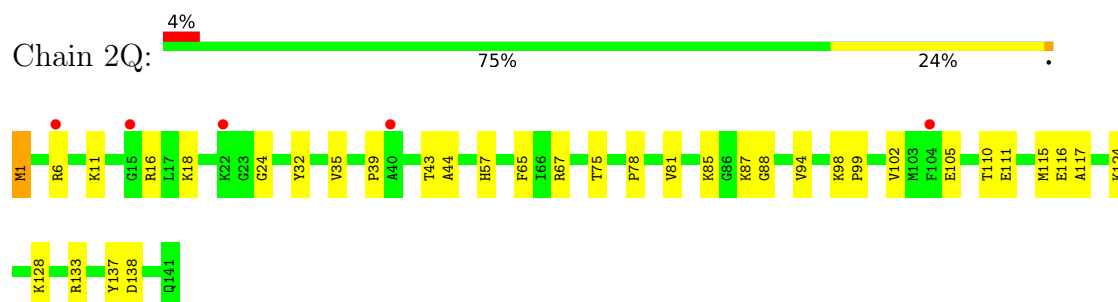
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  78% 20% .



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  76% 19% .



- Molecule 14: 50S ribosomal protein L18

Chain 1S:  73% 23% . .



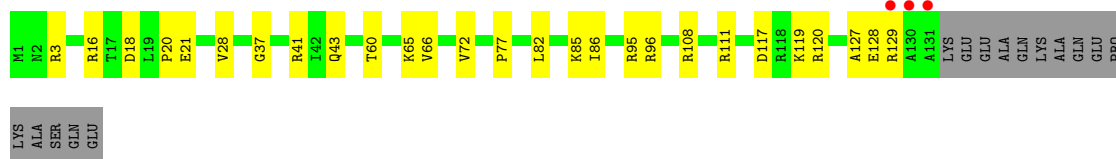
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  63% 28% 7% .



- Molecule 15: 50S ribosomal protein L19

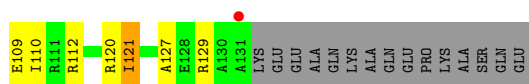
Chain 1T:  71% 18% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T:  62% 25% 10%





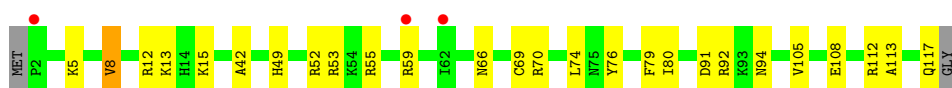
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 81% 15% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U: 3% 76% 21% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V: 82% 16% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V: % 76% 22% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W: % 82% 15% ..



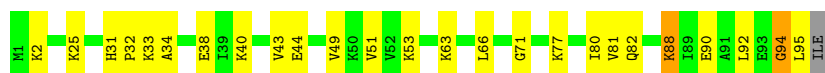
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 76% 21% ..

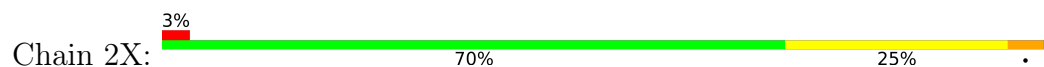


- Molecule 19: 50S ribosomal protein L23

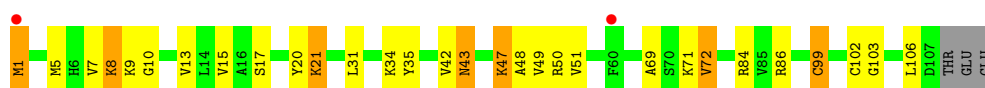
Chain 1X: 73% 24% ..



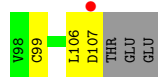
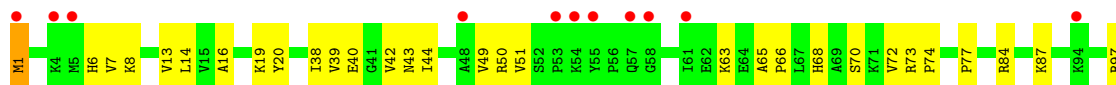
- Molecule 19: 50S ribosomal protein L23



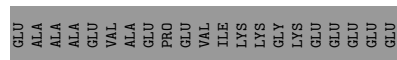
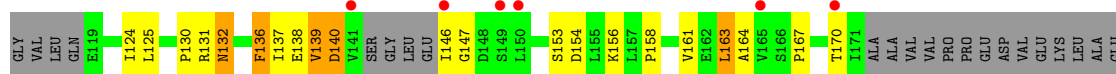
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

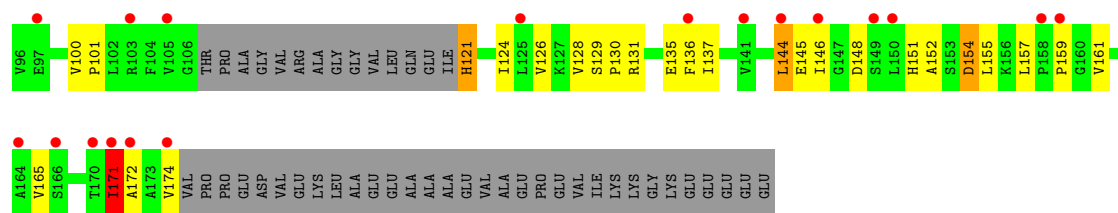


- Molecule 21: 50S ribosomal protein L25

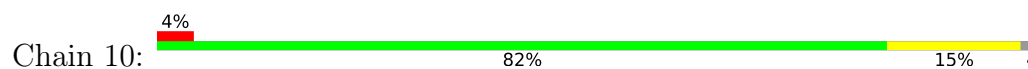


- Molecule 21: 50S ribosomal protein L25

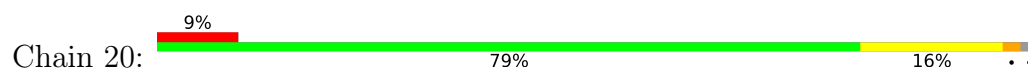




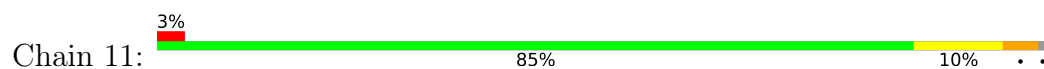
- Molecule 22: 50S ribosomal protein L27



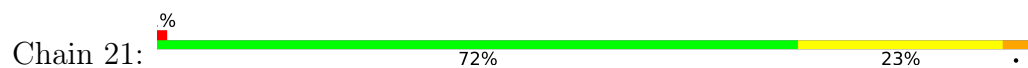
- Molecule 22: 50S ribosomal protein L27



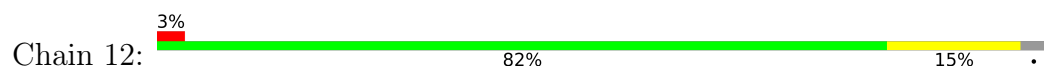
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

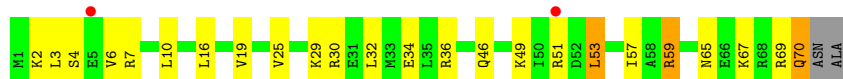


- Molecule 24: 50S ribosomal protein L29

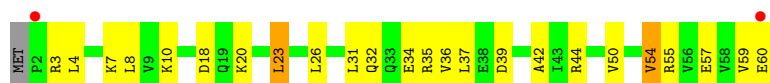


- Molecule 24: 50S ribosomal protein L29





- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



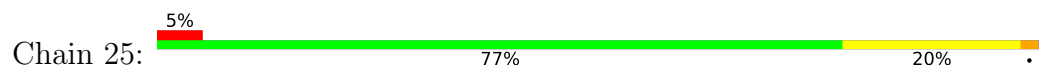
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

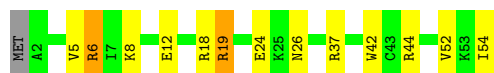


- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  74% 20% . .



- Molecule 28: 50S ribosomal protein L33

Chain 26:  85% 13% .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  6% 73% 20% . .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  6% 69% 24% . .



- Molecule 30: 50S ribosomal protein L35

Chain 18:  68% 31% .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  2% 75% 23% .



- Molecule 31: 50S ribosomal protein L36

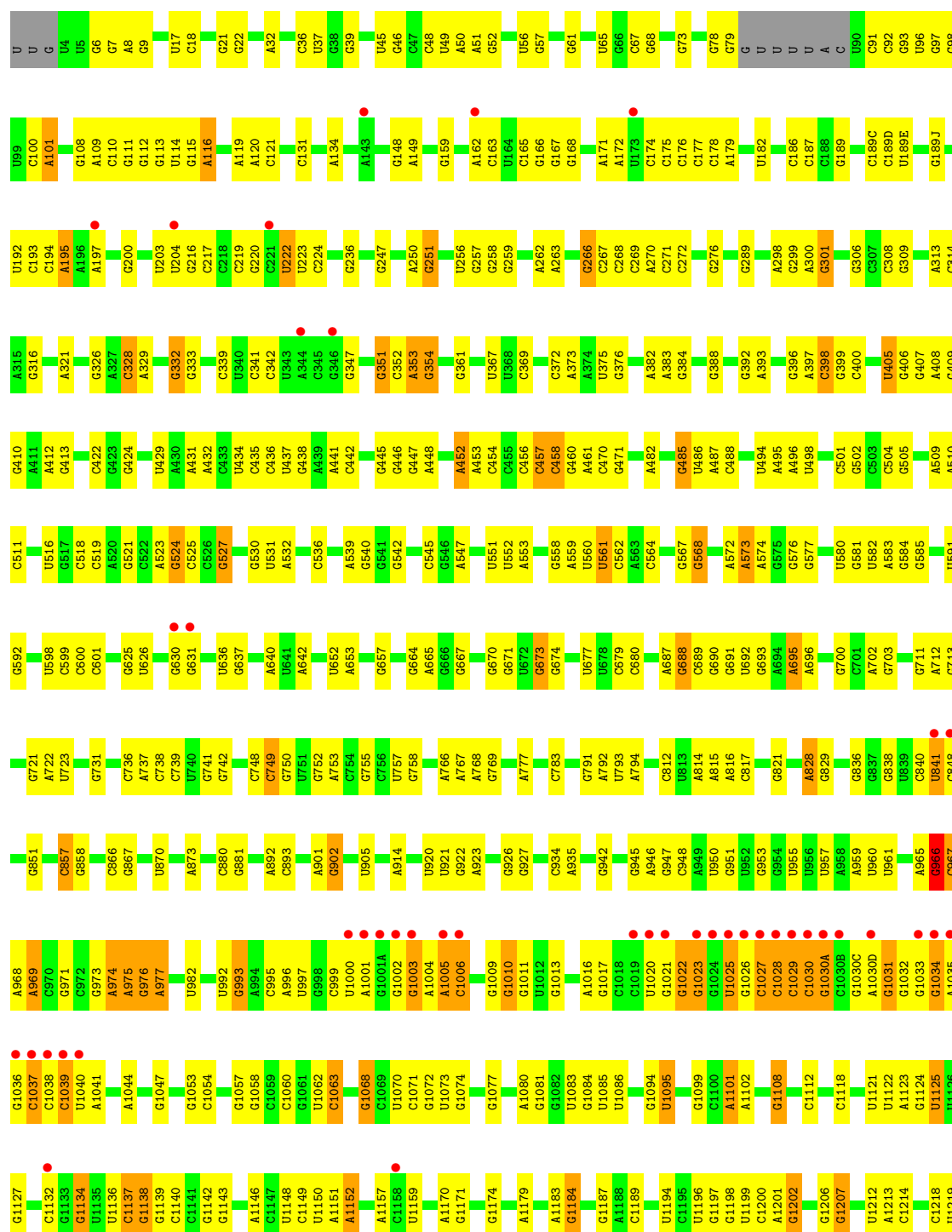
Chain 19:  86% 14%



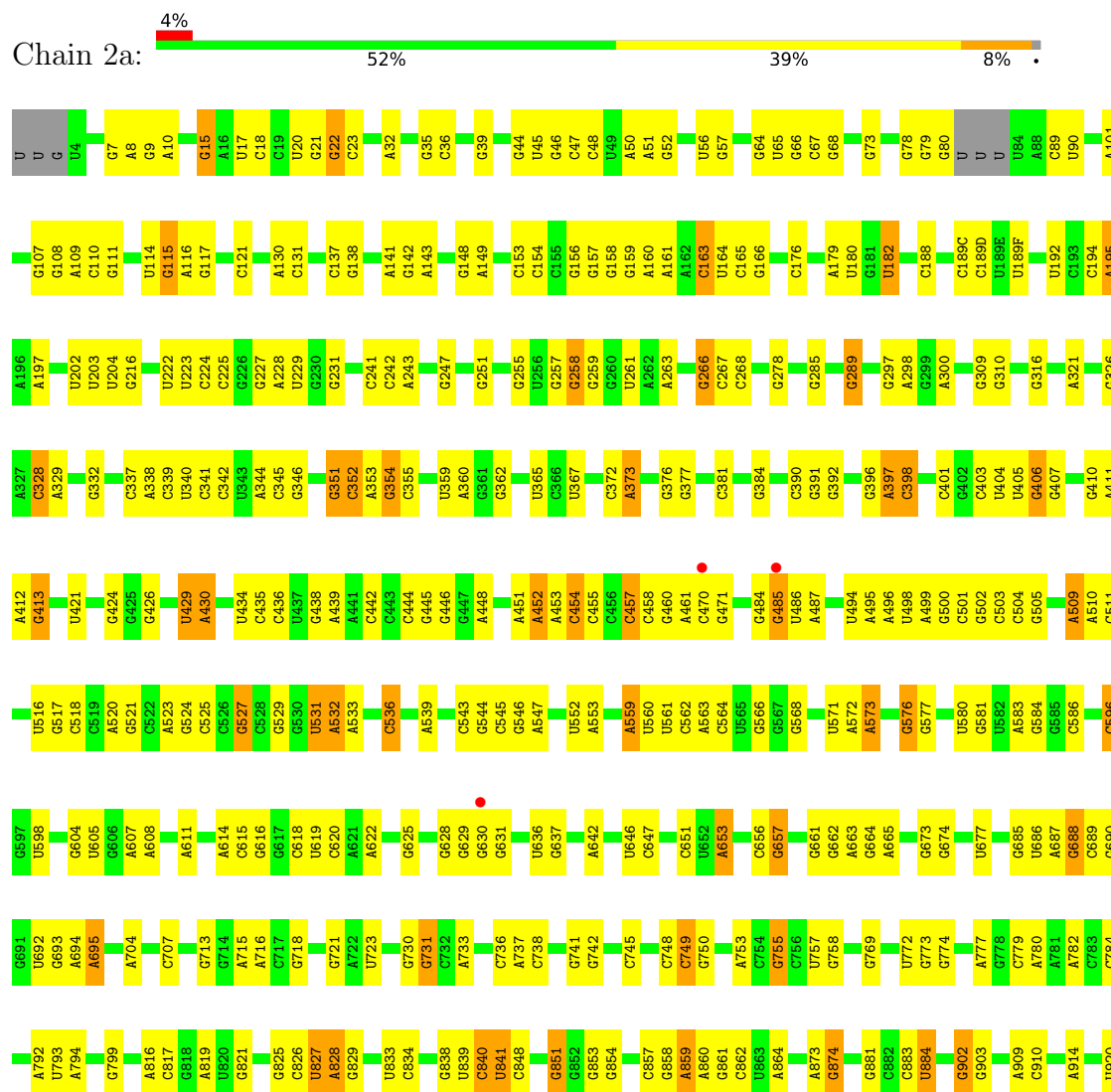
- Molecule 31: 50S ribosomal protein L36

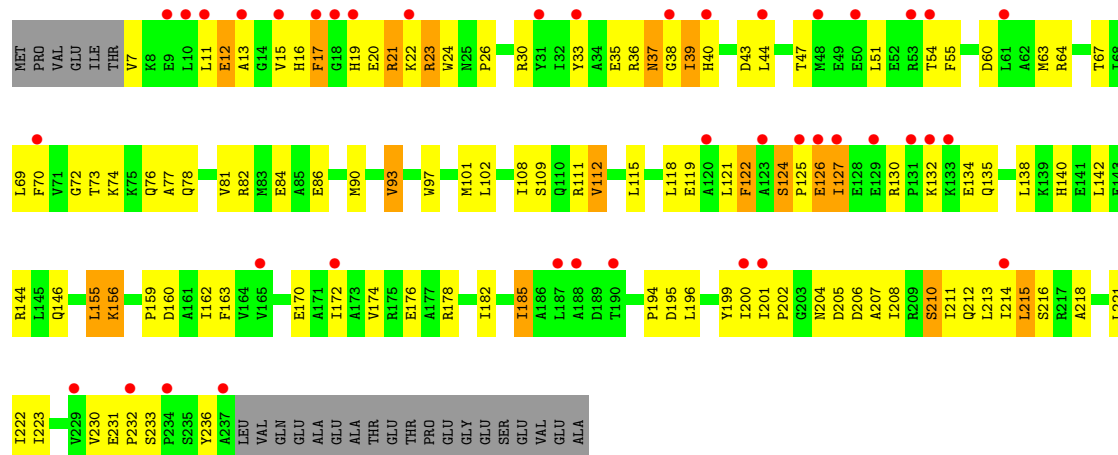


• Molecule 32: 16S Ribosomal RNA

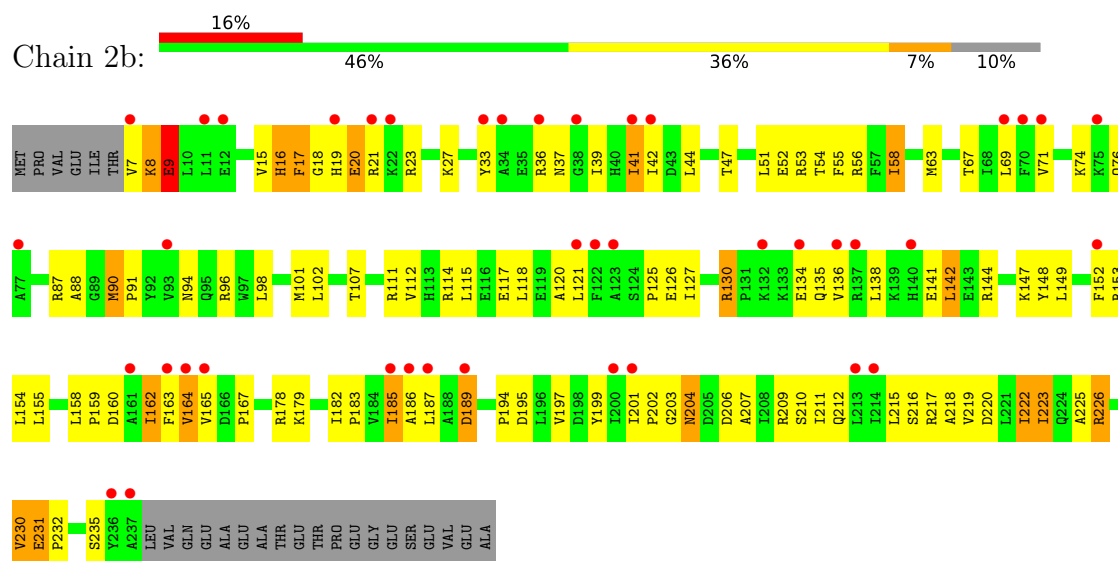


- Molecule 32: 16S Ribosomal RNA

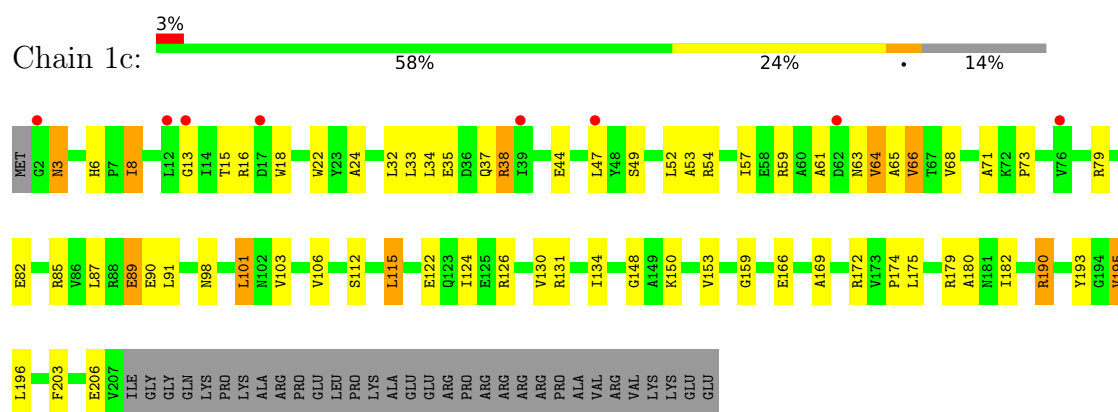




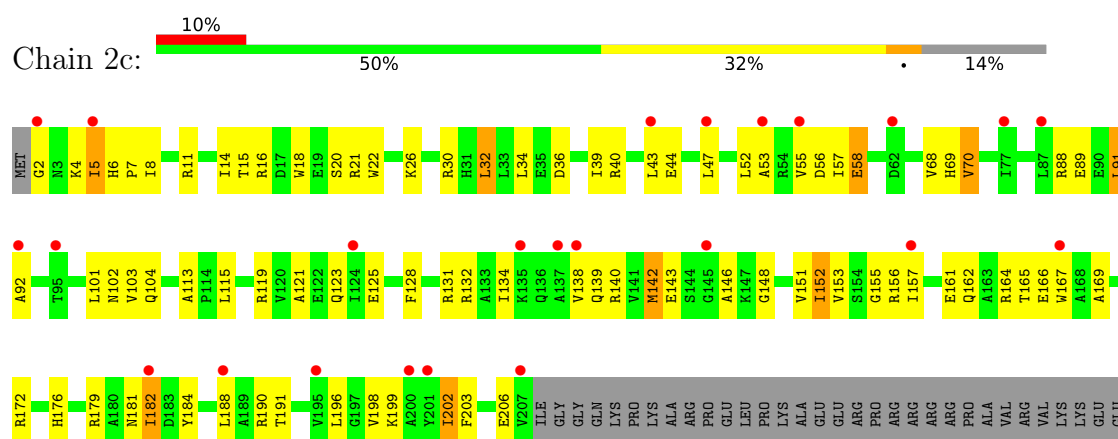
- Molecule 33: 30S ribosomal protein S2



- Molecule 34: 30S ribosomal protein S3

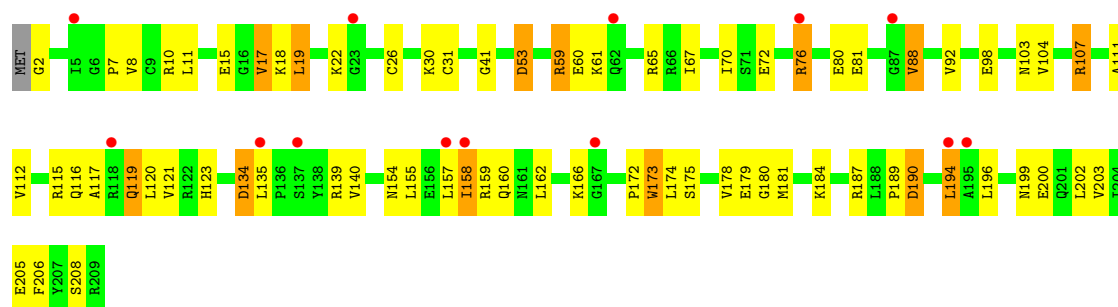


- Molecule 34: 30S ribosomal protein S3

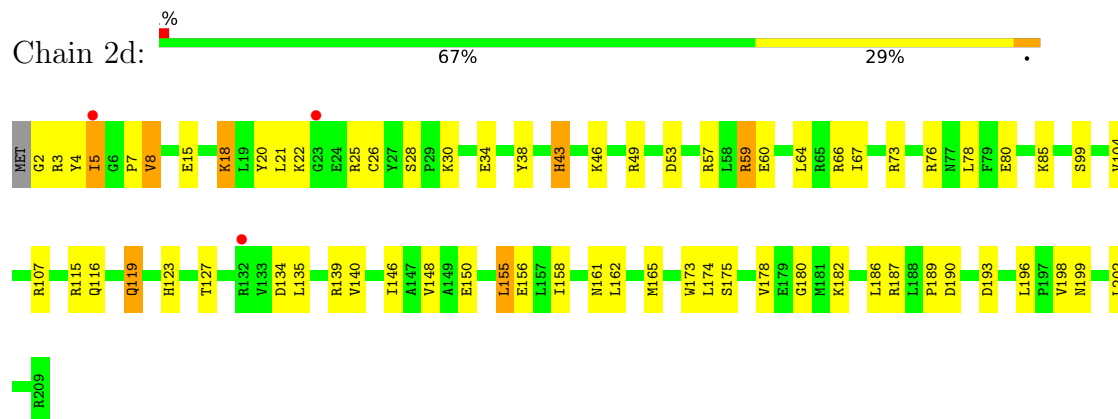


- Molecule 35: 30S ribosomal protein S4

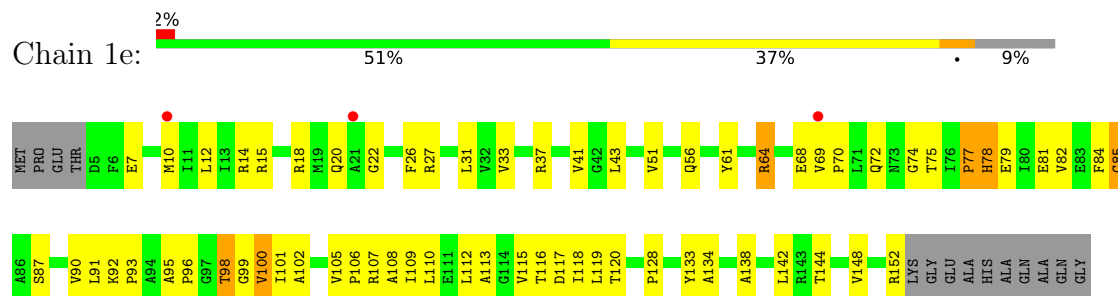




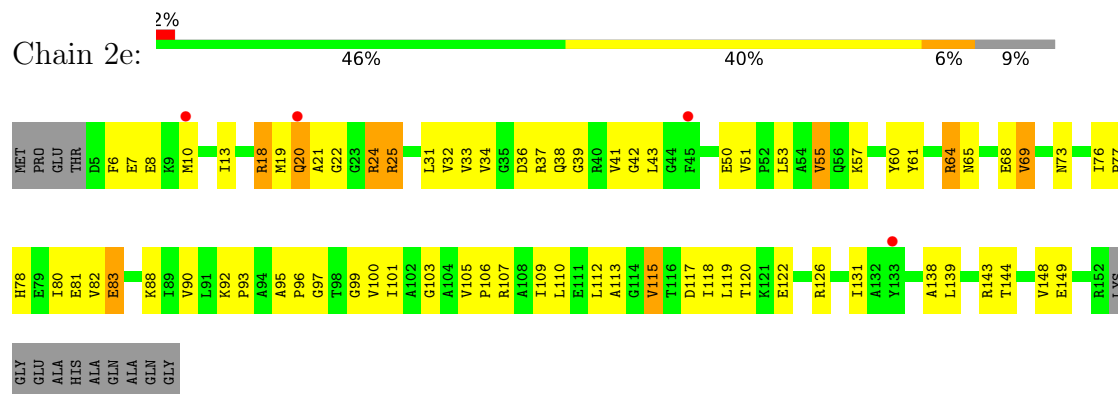
- Molecule 35: 30S ribosomal protein S4



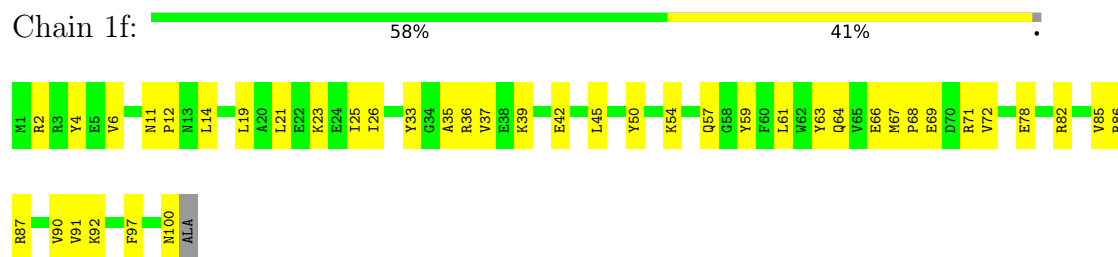
- Molecule 36: 30S ribosomal protein S5



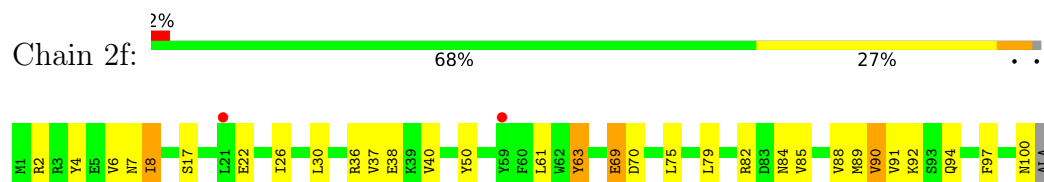
- Molecule 36: 30S ribosomal protein S5



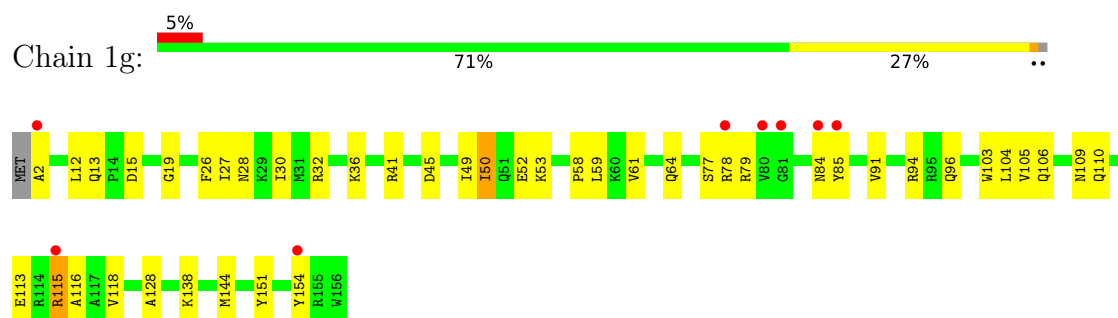
- Molecule 37: 30S ribosomal protein S6



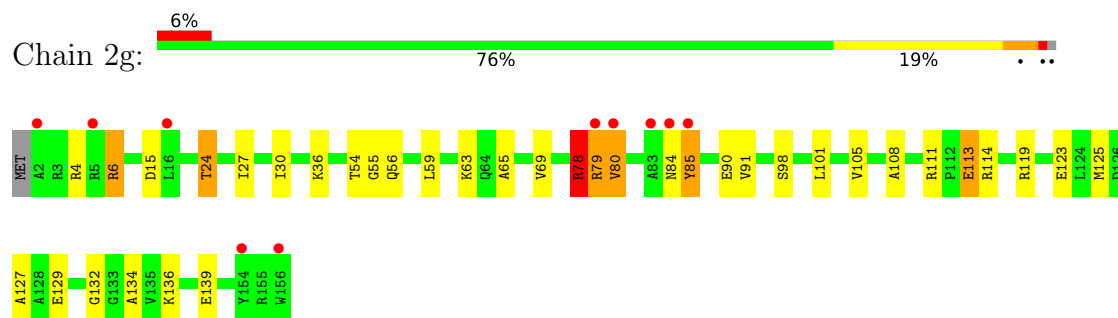
- Molecule 37: 30S ribosomal protein S6



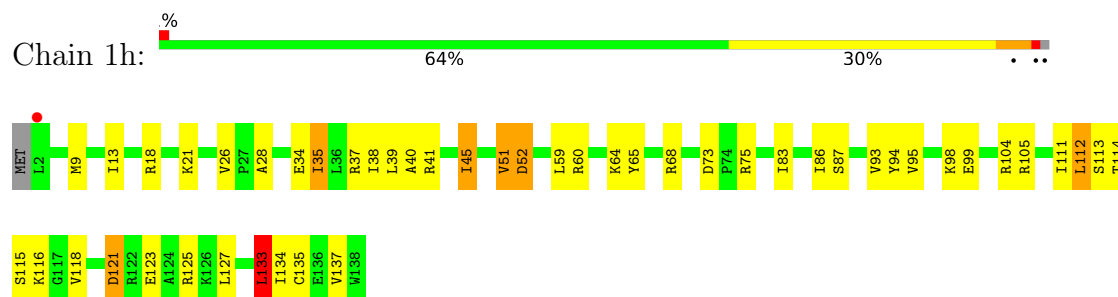
- Molecule 38: 30S ribosomal protein S7



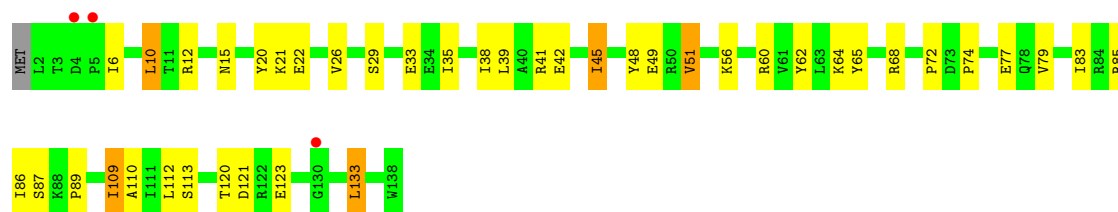
- Molecule 38: 30S ribosomal protein S7



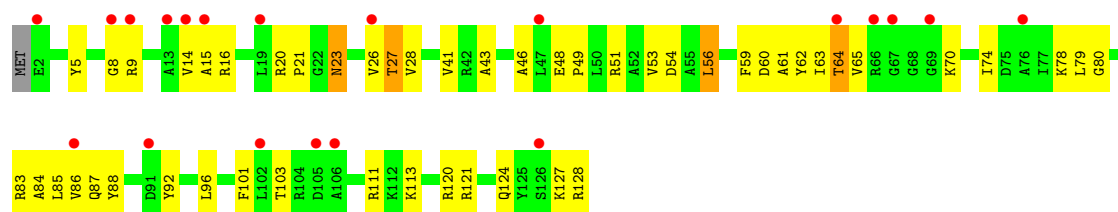
- Molecule 39: 30S ribosomal protein S8



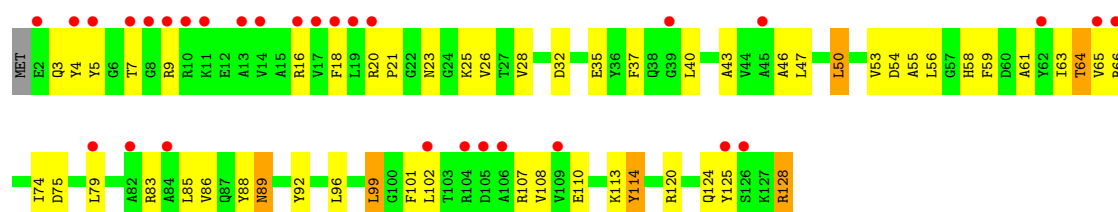
- Molecule 39: 30S ribosomal protein S8



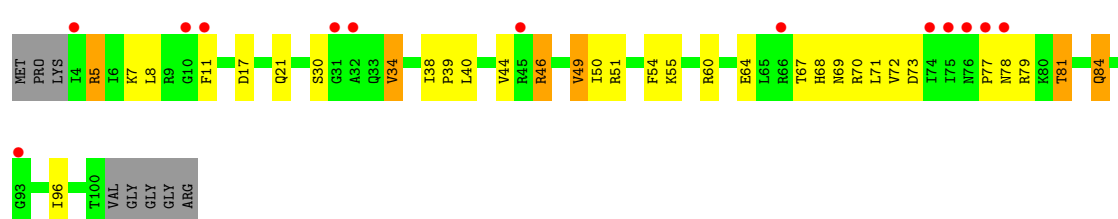
• Molecule 40: 30S ribosomal protein S9



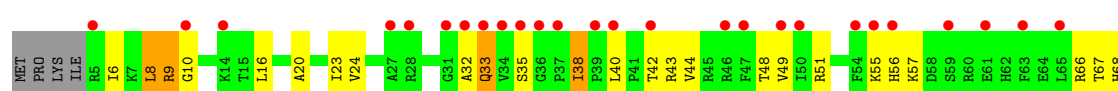
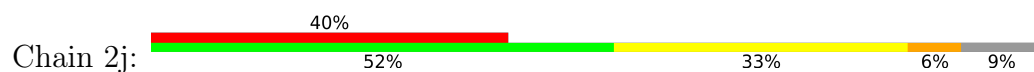
• Molecule 40: 30S ribosomal protein S9

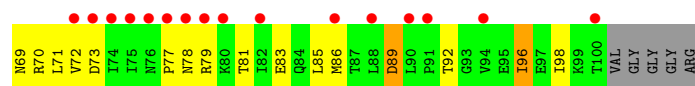


• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10

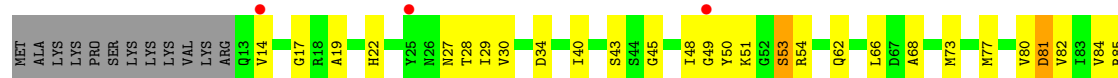




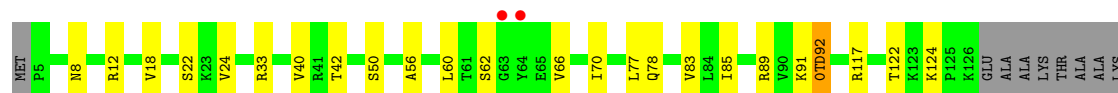
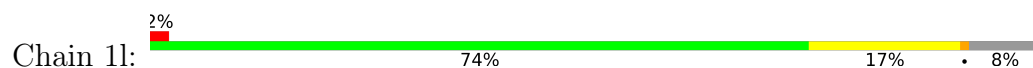
- Molecule 42: 30S ribosomal protein S11



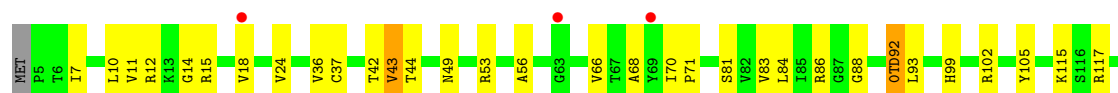
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

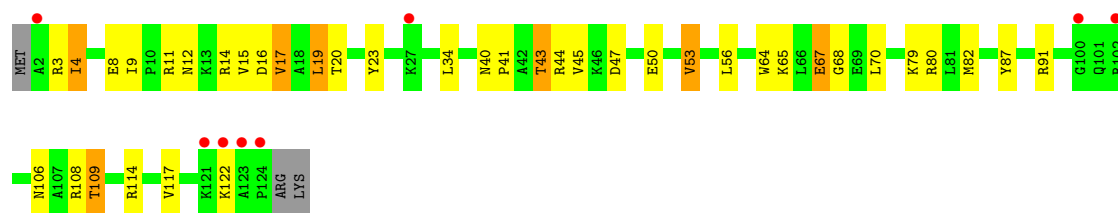


- Molecule 43: 30S ribosomal protein S12

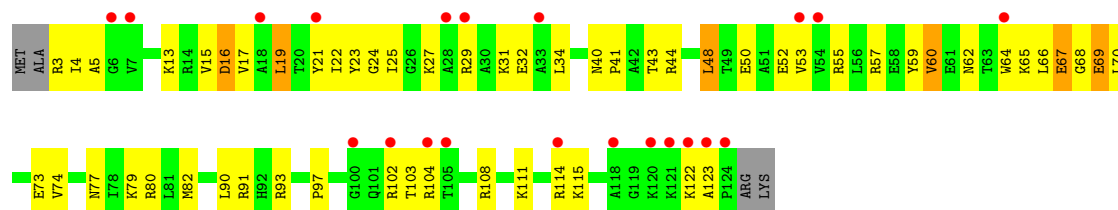


- Molecule 44: 30S ribosomal protein S13





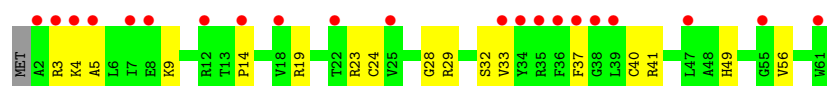
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



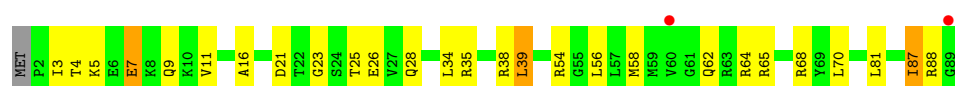
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



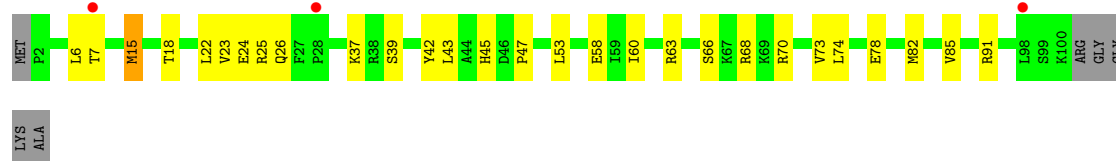
- Molecule 47: 30S ribosomal protein S16



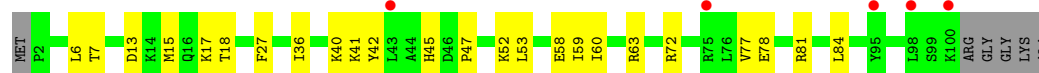
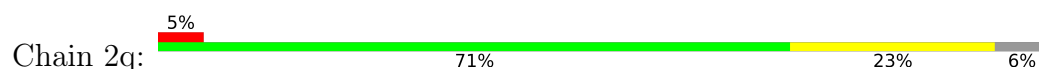
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



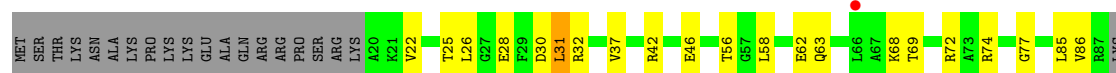
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

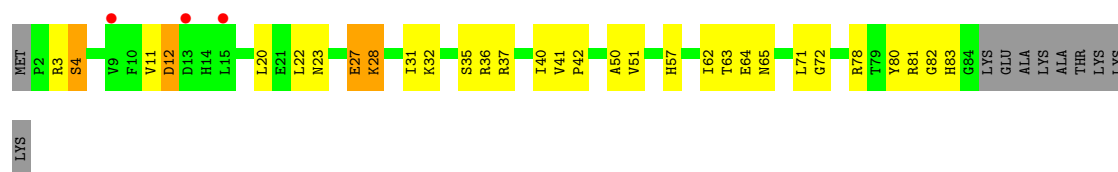


- Molecule 49: 30S ribosomal protein S18

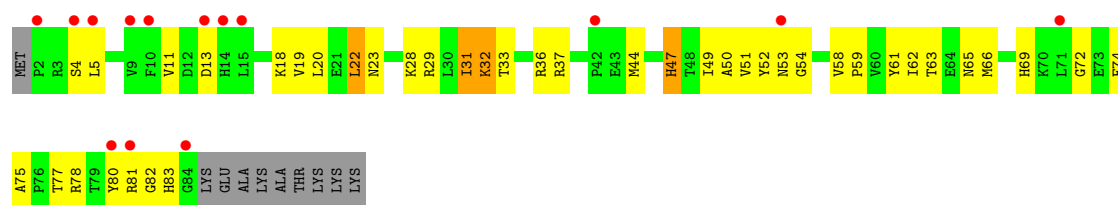


- Molecule 50: 30S ribosomal protein S19

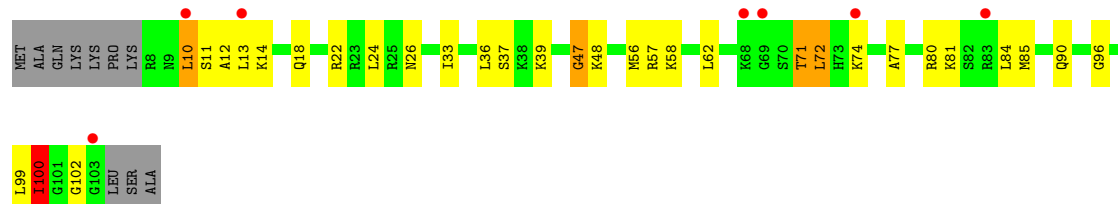




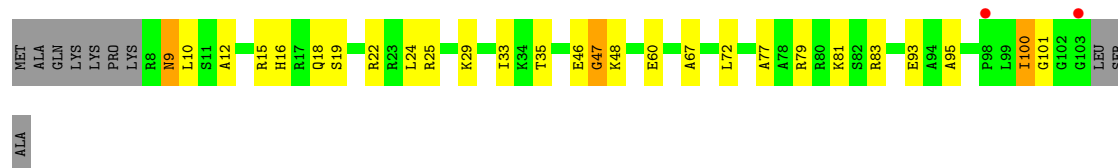
- Molecule 50: 30S ribosomal protein S19



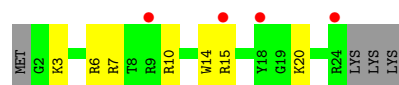
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

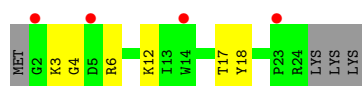


- Molecule 52: 30S ribosomal protein Thx

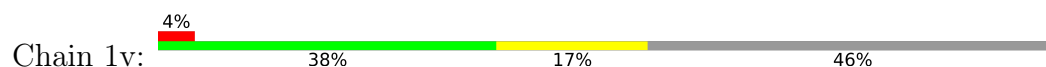


- Molecule 52: 30S ribosomal protein Thx





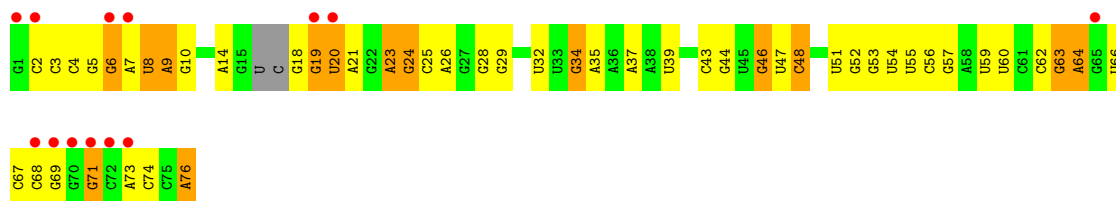
• Molecule 53: MF-mRNA



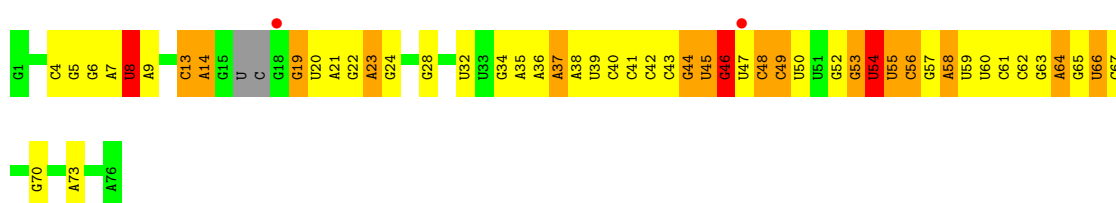
• Molecule 53: MF-mRNA



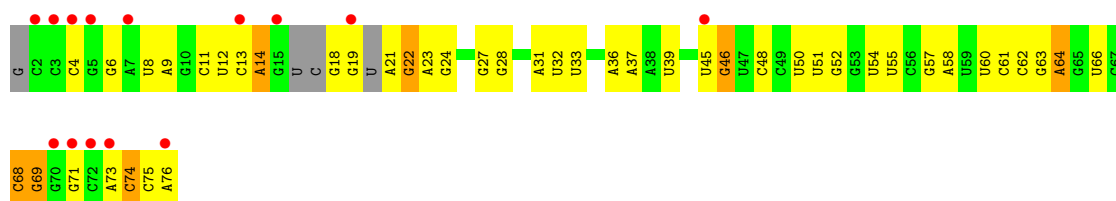
• Molecule 54: A- and E-site Deacylated tRNAphe



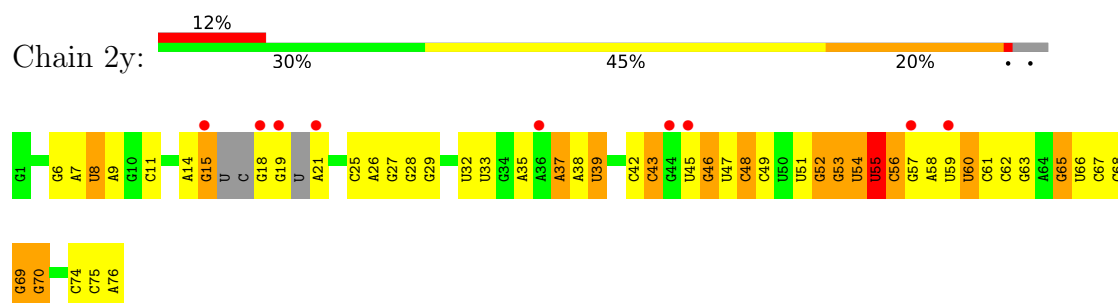
• Molecule 54: A- and E-site Deacylated tRNAphe



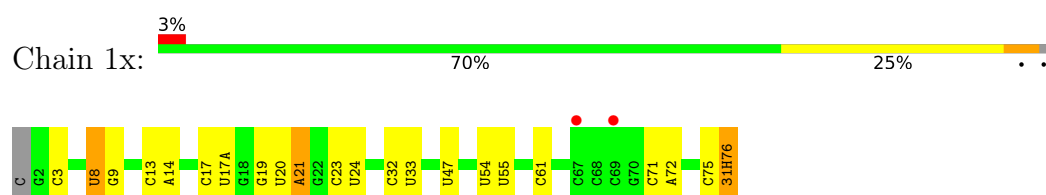
• Molecule 54: A- and E-site Deacylated tRNAphe



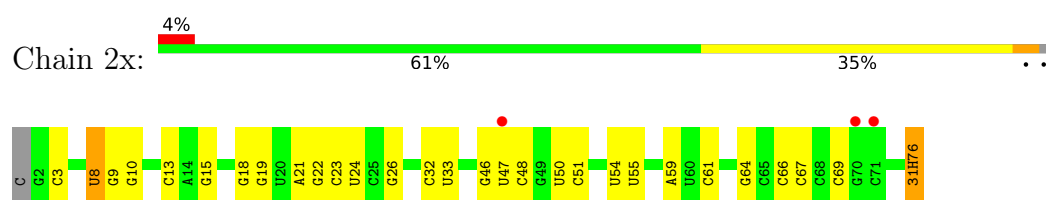
- Molecule 54: A- and E-site Deacylated tRNA^{phe}



- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNA^{met}



- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNA^{met}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.01Å 449.04Å 621.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.89 – 2.60 121.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (121.89-2.60) 97.0 (121.89-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.216 , 0.261 0.218 , 0.262	Depositor DCC
R_{free} test set	86389 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299649	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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: 31H, MA6, ZN, G7M, OMG, 5MU, 4SU, MIA, OMC, WC9, 5MC, MG, 4OC, 8AH, UR3, PSU, OMU, 0TD, M2G, K, SF4, 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	0.28	0/69011	0.45	1/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.18	0/2879	0.36	0/4487
3	1D	0.26	0/2186	0.49	0/2944
3	2D	0.22	0/2186	0.43	0/2944
4	1E	0.27	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.25	0/1619	0.48	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.22	0/1453	0.42	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.24	0/1112	0.42	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.47	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.25	0/1152	0.52	0/1533
11	2P	0.21	0/1152	0.45	0/1533
12	1Q	0.28	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.40	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.22	0/982	0.48	0/1312
14	1S	0.22	0/883	0.46	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.42	0/1468
16	1U	0.29	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.19	0/782	0.39	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.26	0/764	0.50	0/1025
19	2X	0.22	0/764	0.49	2/1025 (0.2%)
20	1Y	0.23	0/819	0.48	0/1095
20	2Y	0.20	0/819	0.49	0/1095
21	1Z	0.21	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.45	0/1763
22	10	0.26	0/662	0.49	0/881
22	20	0.21	0/662	0.43	0/881
23	11	0.23	0/762	0.40	0/1014
23	21	0.22	0/762	0.42	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.18	0/590	0.38	0/781
25	13	0.25	0/474	0.46	0/635
25	23	0.18	0/469	0.43	0/630
26	14	0.26	0/565	0.57	0/761
26	24	0.24	0/545	0.55	0/737
27	15	0.29	0/469	0.50	0/635
27	25	0.22	0/469	0.48	0/635
28	16	0.25	0/460	0.44	0/613
28	26	0.23	0/456	0.45	0/608
29	17	0.29	0/426	0.52	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.26	0/525	0.48	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.28	0/310	0.52	0/407
31	29	0.19	0/310	0.42	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.38	4/56005 (0.0%)
33	1b	0.21	0/1881	0.52	0/2542
33	2b	0.22	0/1860	0.47	0/2518
34	1c	0.20	0/1572	0.45	0/2126
34	2c	0.25	0/1566	0.41	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.20	0/1704	0.43	0/2284
36	1e	0.21	0/1145	0.46	0/1543
36	2e	0.27	0/1149	0.47	0/1548
37	1f	0.19	0/823	0.40	0/1115
37	2f	0.20	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.47	0/1346
40	2i	0.22	0/997	0.52	0/1343
41	1j	0.26	0/722	0.46	0/982
41	2j	0.23	0/727	0.51	0/988
42	1k	0.18	0/844	0.42	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.22	0/937	0.44	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.20	0/969	0.48	1/1302 (0.1%)
44	2m	0.20	0/961	0.45	0/1291
45	1n	0.20	0/501	0.44	0/664
45	2n	0.20	0/501	0.42	0/664
46	1o	0.20	0/739	0.38	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.19	0/697	0.44	0/939
47	2p	0.20	0/693	0.46	0/935
48	1q	0.19	0/836	0.39	0/1117
48	2q	0.18	0/836	0.38	0/1117
49	1r	0.20	0/560	0.40	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.24	0/661	0.55	0/893
51	1t	0.20	0/730	0.51	0/965
51	2t	0.21	0/729	0.46	0/965
52	1u	0.20	0/203	0.46	0/266
52	2u	0.27	0/203	0.56	0/266
53	1v	0.21	0/310	0.33	0/480
53	2v	0.19	0/310	0.34	0/480
54	1w	0.28	1/1606 (0.1%)	0.40	0/2497
54	1y	0.28	2/1606 (0.1%)	0.38	0/2497
54	2w	0.31	2/1556 (0.1%)	0.41	0/2418
54	2y	0.28	2/1583 (0.1%)	0.40	0/2459
55	1x	0.27	0/1700	0.40	0/2650
55	2x	0.25	0/1700	0.39	0/2650
All	All	0.23	8/316640 (0.0%)	0.42	11/474051 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
33	1b	0	2
38	2g	0	1
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	O3'-P	5.62	1.61	1.56
54	2w	46	G7M	O3'-P	5.57	1.61	1.56
54	1y	8	4SU	O3'-P	5.36	1.61	1.56
54	2w	8	4SU	O3'-P	5.30	1.61	1.56
54	2y	46	G7M	O3'-P	5.30	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.70	119.54	109.50
32	2a	1272	G	N1-C2-N2	-5.92	98.45	116.20
32	2a	1263	C	N1-C2-O2	5.49	135.36	118.90
5	2F	21	ALA	CA-C-N	5.37	131.36	121.70
5	2F	21	ALA	C-N-CA	5.37	131.36	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide
33	1b	124	SER	Peptide
5	2F	20	LEU	Peptide
38	2g	78	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61853	0	31183	617	0
1	2A	60323	0	30413	682	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	33	0
3	1D	2136	0	2217	56	0
3	2D	2136	0	2218	33	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	34	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	38	0
6	1G	1423	0	1436	37	0
6	2G	1428	0	1438	57	0
7	1H	1330	0	1407	31	0
7	2H	1330	0	1407	26	0
8	1I	1097	0	1140	34	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	16	0
10	1O	933	0	996	21	0
10	2O	933	0	996	35	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	23	0
14	1S	873	0	927	16	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	28	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	17	0
17	1V	771	0	830	14	0
17	2V	771	0	830	16	0
18	1W	886	0	940	12	0
18	2W	886	0	940	19	0
19	1X	750	0	814	21	0
19	2X	750	0	814	22	0
20	1Y	806	0	881	23	0
20	2Y	806	0	881	17	0
21	1Z	1240	0	1240	37	0
21	2Z	1271	0	1273	43	0
22	10	653	0	674	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	11	0
23	11	755	0	826	7	0
23	21	755	0	826	18	0
24	12	588	0	643	5	0
24	22	588	0	643	18	0
25	13	469	0	518	12	0
25	23	464	0	514	12	0
26	14	552	0	533	36	0
26	24	532	0	503	29	0
27	15	455	0	465	4	0
27	25	455	0	465	9	0
28	16	453	0	473	9	0
28	26	449	0	469	3	0
29	17	418	0	467	9	0
29	27	418	0	467	11	0
30	18	517	0	582	16	0
30	28	517	0	582	12	0
31	19	307	0	335	2	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	374	0
32	2a	32327	0	16338	457	0
33	1b	1846	0	1867	72	0
33	2b	1825	0	1828	83	0
34	1c	1548	0	1535	42	0
34	2c	1542	0	1517	54	0
35	1d	1655	0	1672	57	0
35	2d	1674	0	1714	43	0
36	1e	1129	0	1185	38	0
36	2e	1133	0	1191	49	0
37	1f	810	0	804	24	0
37	2f	816	0	808	16	0
38	1g	1231	0	1238	20	0
38	2g	1235	0	1249	23	0
39	1h	1088	0	1126	32	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	32	0
40	2i	978	0	966	38	0
41	1j	709	0	650	24	0
41	2j	714	0	672	37	0
42	1k	829	0	825	15	0
42	2k	833	0	836	23	0
43	1l	932	0	981	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	20	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	43	0
45	1n	492	0	528	12	0
45	2n	492	0	529	14	0
46	1o	728	0	760	16	0
46	2o	728	0	760	20	0
47	1p	681	0	697	19	0
47	2p	677	0	686	22	0
48	1q	823	0	891	13	0
48	2q	823	0	891	14	0
49	1r	555	0	618	9	0
49	2r	555	0	618	11	0
50	1s	652	0	662	27	0
50	2s	646	0	644	34	0
51	1t	728	0	798	21	0
51	2t	727	0	796	20	0
52	1u	199	0	208	5	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	2	0
54	1w	1592	0	818	31	0
54	1y	1585	0	803	25	0
54	2w	1544	0	787	20	0
54	2y	1565	0	794	37	0
55	1x	1635	0	839	7	0
55	2x	1635	0	839	12	0
56	10	8	0	0	0	0
56	11	6	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	10	0	0	0	0
56	16	1	0	0	0	0
56	17	6	0	0	0	0
56	18	6	0	0	0	0
56	19	1	0	0	0	0
56	1A	1096	0	0	0	0
56	1B	36	0	0	0	0
56	1D	14	0	0	0	0
56	1E	15	0	0	0	0
56	1F	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	9	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	5	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	210	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1t	1	0	0	0	0
56	1w	8	0	0	0	0
56	1x	15	0	0	0	0
56	1y	1	0	0	0	0
56	20	4	0	0	0	0
56	21	1	0	0	0	0
56	23	2	0	0	0	0
56	25	6	0	0	0	0
56	26	1	0	0	0	0
56	27	3	0	0	0	0
56	28	3	0	0	0	0
56	2A	844	0	0	0	0
56	2B	19	0	0	0	0
56	2D	8	0	0	0	0
56	2E	9	0	0	0	0
56	2F	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	225	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	1	0	0	0	0
56	2l	5	0	0	0	0
56	2m	1	0	0	0	0
56	2q	3	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	6	0	0	0	0
56	2x	7	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	34	0	0	1	0
58	2A	34	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1d	8	0	0	2	0
60	2d	8	0	0	0	0
61	10	11	0	0	0	0
61	11	9	0	0	0	0
61	12	3	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	5	0	0	0	0
61	16	3	0	0	0	0
61	17	8	0	0	0	0
61	18	7	0	0	0	0
61	1A	1907	0	0	82	0
61	1B	59	0	0	3	0
61	1D	26	0	0	0	0
61	1E	28	0	0	2	0
61	1F	17	0	0	0	0
61	1G	2	0	0	0	0
61	1H	2	0	0	1	0
61	1N	4	0	0	0	0
61	1O	4	0	0	1	0
61	1P	23	0	0	1	0
61	1Q	5	0	0	0	0
61	1R	10	0	0	2	0
61	1S	3	0	0	1	0
61	1T	8	0	0	0	0
61	1U	14	0	0	0	0
61	1V	7	0	0	0	0
61	1W	7	0	0	2	0
61	1X	6	0	0	0	0
61	1Y	2	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	267	0	0	18	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	0	0
61	1n	1	0	0	0	0
61	1q	2	0	0	0	0
61	1v	4	0	0	0	0
61	1w	15	0	0	0	0
61	1x	10	0	0	0	0
61	1y	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	20	3	0	0	0	0
61	21	8	0	0	1	0
61	23	1	0	0	0	0
61	27	4	0	0	0	0
61	28	3	0	0	0	0
61	29	1	0	0	0	0
61	2A	1000	0	0	74	0
61	2B	18	0	0	0	0
61	2D	17	0	0	0	0
61	2E	10	0	0	0	0
61	2F	12	0	0	0	0
61	2O	2	0	0	0	0
61	2P	8	0	0	0	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	4	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	1	0	0	0	0
61	2Y	2	0	0	0	0
61	2a	172	0	0	13	0
61	2d	2	0	0	0	0
61	2e	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	2	0	0	0	0
61	2l	4	0	0	1	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	1	0
61	2v	3	0	0	0	0
61	2w	3	0	0	0	0
61	2x	4	0	0	1	0
61	2y	4	0	0	0	0
All	All	299649	0	196683	4079	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 4079 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.32	1.26
1:1A:1082:U:O4	1:1A:1086:A:N1	1.99	0.95
54:2y:55:PSU:HN1	54:2y:57:G:H5"	1.32	0.93
1:1A:1062:G:H1	1:1A:1077:A:H61	1.02	0.93
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.49	0.93

There are no symmetry-related clashes.

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%)	255 (93%)	18 (7%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	46
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24	46
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	46
5	2F	201/210 (96%)	196 (98%)	1 (0%)	4 (2%)	6	12
6	1G	179/182 (98%)	167 (93%)	12 (7%)	0	100	100
6	2G	179/182 (98%)	153 (86%)	23 (13%)	3 (2%)	7	15
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	152 (88%)	20 (12%)	0	100	100
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18	38
9	1N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	18	38
9	2N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9	19
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	128 (87%)	15 (10%)	4 (3%)	4	7
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	7
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	13
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	34
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	12
17	2V	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	12
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	25
19	2X	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	19
21	2Z	156/206 (76%)	128 (82%)	23 (15%)	5 (3%)	3	5
22	10	81/85 (95%)	81 (100%)	0	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	11	25
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
26	14	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	3	5
33	2b	229/256 (90%)	182 (80%)	39 (17%)	8 (4%)	3	4
34	1c	204/239 (85%)	182 (89%)	22 (11%)	0	100	100
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	6	12
35	1d	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12	28
35	2d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	28
36	1e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	11
36	2e	146/162 (90%)	131 (90%)	12 (8%)	3 (2%)	5	11
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	38
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	21
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	38
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	34
40	2i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	3	5
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2	2
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	14
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	6	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	16	34
44	2m	120/126 (95%)	104 (87%)	15 (12%)	1 (1%)	16	34
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	15
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
49	2r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	8
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	2
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	11
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10431 (92%)	836 (7%)	103 (1%)	14	30

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	36	LYS
21	1Z	53	ILE
26	14	62	ARG
33	1b	17	PHE
33	1b	125	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	207 (96%)	8 (4%)	30	57
3	2D	215/218 (99%)	207 (96%)	8 (4%)	30	57
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26	51
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17	37
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	12
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	12
6	1G	143/156 (92%)	133 (93%)	10 (7%)	14	31
6	2G	143/156 (92%)	128 (90%)	15 (10%)	6	14
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	27
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	32
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	5
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	4
9	1N	118/119 (99%)	113 (96%)	5 (4%)	26	52
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	38
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	64
10	2O	100/100 (100%)	90 (90%)	10 (10%)	7	16
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	17
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	51
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	24
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	39	67
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22	46
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	38
14	1S	86/88 (98%)	78 (91%)	8 (9%)	8	18
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	14
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	51
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	43
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	35
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	51
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	76 (95%)	4 (5%)	22	46
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	61
18	2W	90/92 (98%)	88 (98%)	2 (2%)	45	72
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	82
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	55
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	10
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	24
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3	6
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	36
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	28
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	28
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	36
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	25
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	3
26	24	53/63 (84%)	41 (77%)	12 (23%)	1	1
27	15	50/52 (96%)	49 (98%)	1 (2%)	48	74
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	25
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	26
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	37
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	38
33	1b	192/220 (87%)	162 (84%)	30 (16%)	2	4
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	14
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2	4
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5	10
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19
36	1e	113/123 (92%)	102 (90%)	11 (10%)	8	17
36	2e	114/123 (93%)	98 (86%)	16 (14%)	3	6
37	1f	84/90 (93%)	81 (96%)	3 (4%)	31	58
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	14
38	1g	119/127 (94%)	108 (91%)	11 (9%)	8	19
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7	16
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	21
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	26
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	4
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	5
41	2j	69/92 (75%)	63 (91%)	6 (9%)	9	21
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	13
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	23
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	29
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	13
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	8
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	10
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	74
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	56
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	45
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	8
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	29
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	51
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	10
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	39
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17	37
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	11
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	22
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	40
All	All	9303/10064 (92%)	8516 (92%)	787 (8%)	10	22

5 of 787 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	2N	138	LEU
26	24	59	PHE
11	2P	71	VAL
9	2N	83	LYS
20	2Y	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
38	2g	13	GLN
51	2t	75	ASN
38	2g	109	ASN
43	2l	80	HIS
41	1j	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	24 (0%)
1	2A	2791/2915 (95%)	476 (17%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	273 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	1 (8%)	0
54	1w	72/76 (94%)	26 (36%)	0
54	1y	72/76 (94%)	29 (40%)	0
54	2w	69/76 (90%)	18 (26%)	0
54	2y	70/76 (92%)	19 (27%)	0
55	1x	74/77 (96%)	9 (12%)	0
55	2x	74/77 (96%)	10 (13%)	0
All	All	9345/9620 (97%)	1574 (16%)	49 (0%)

5 of 1574 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	271(K)	U
1	2A	1026	U
1	2A	271(M)	G
1	2A	752	A
1	2A	1379	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.90	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	4SU	2w	8	54	18,21,22	1.73	5 (27%)	25,30,33	2.11	5 (20%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	1.97	4 (19%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
54	MIA	2w	37	54	24,27,32	2.00	6 (25%)	32,39,47	2.62	10 (31%)
54	PSU	2y	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.69	3 (14%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.93	4 (19%)
55	5MC	2x	32	55	19,22,23	1.59	3 (15%)	26,32,35	1.31	4 (15%)
54	G7M	2w	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.59	4 (11%)
54	G7M	1y	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.70	4 (11%)
32	5MC	2a	1407	32,56	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
55	5MC	1x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.20	3 (11%)
1	PSU	1A	2605	56,1	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
55	4SU	2x	8	55	18,21,22	2.02	5 (27%)	25,30,33	1.29	4 (16%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.12	5 (23%)
1	PSU	2A	1917	56,1	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.97	1 (4%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	21,30,33	1.95	3 (14%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.18	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
55	31H	1x	76	55,56	31,34,35	1.21	3 (9%)	35,47,50	2.37	11 (31%)
1	5MC	1A	1942	56,1	19,22,23	1.60	3 (15%)	26,32,35	1.26	2 (7%)
55	5MU	1x	54	55,56	19,22,23	1.48	6 (31%)	27,32,35	1.87	8 (29%)
32	UR3	1a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.79	4 (15%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.95	1 (4%)
1	5MC	2A	1962	56,1	19,22,23	1.67	3 (15%)	26,32,35	1.18	2 (7%)
54	4SU	2y	8	54	18,21,22	1.69	4 (22%)	25,30,33	2.26	5 (20%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
32	2MG	1a	1207	32,56	23,26,27	1.24	2 (8%)	33,38,41	2.25	8 (24%)
54	G7M	1w	46	54	23,26,27	1.59	3 (13%)	34,39,42	1.74	4 (11%)
54	MIA	2y	37	54	21,24,32	1.59	3 (14%)	30,35,47	2.00	7 (23%)
1	5MU	1A	1939	56,1	19,22,23	1.43	6 (31%)	27,32,35	2.20	6 (22%)
1	OMU	2A	2552	56,1	19,22,23	1.20	3 (15%)	25,31,34	1.76	5 (20%)
55	PSU	1x	55	55,56	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.91	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1400	32	19,22,23	1.53	3 (15%)	26,32,35	1.10	2 (7%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	27,32,35	1.86	6 (22%)
54	PSU	1w	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
54	G7M	2y	46	54	23,26,27	1.60	3 (13%)	34,39,42	1.89	5 (14%)
54	5MU	2w	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.72	6 (22%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.25	8 (24%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.88	1 (4%)
1	5MC	1A	1962	56,1	19,22,23	1.81	3 (15%)	26,32,35	1.13	4 (15%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	3 (14%)
54	5MU	2y	54	54	19,22,23	1.46	5 (26%)	27,32,35	1.90	6 (22%)
32	5MC	1a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
1	8AH	1A	2503	56,1	22,26,27	1.61	5 (22%)	29,39,42	2.14	5 (17%)
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.84	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.16	9 (27%)
1	OMG	2A	2251	55,56,1	23,26,27	1.22	3 (13%)	32,38,41	2.05	7 (21%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.11	2 (7%)
54	4SU	1y	8	54	18,21,22	1.84	5 (27%)	25,30,33	1.88	4 (16%)
54	PSU	1w	32	56,54	18,21,22	1.33	2 (11%)	21,30,33	1.90	3 (14%)
32	PSU	1a	516	32,56	18,21,22	1.42	2 (11%)	21,30,33	2.06	5 (23%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
43	0TD	1l	92	43	8,9,10	4.53	1 (12%)	6,11,13	1.79	2 (33%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
54	MIA	1y	37	54	21,24,32	1.65	4 (19%)	30,35,47	2.01	7 (23%)
54	MIA	1w	37	54	28,31,32	2.33	6 (21%)	38,44,47	2.78	12 (31%)
32	G7M	2a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.70	5 (14%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.03	9 (27%)
1	5MU	2A	1939	56,1	19,22,23	1.45	6 (31%)	27,32,35	2.20	6 (22%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.84	6 (18%)
54	5MU	1y	54	54	19,22,23	1.48	5 (26%)	27,32,35	1.77	5 (18%)
32	5MC	1a	1404	32	19,22,23	1.78	3 (15%)	26,32,35	1.27	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.82	3 (11%)
55	5MU	2x	54	55	19,22,23	1.44	5 (26%)	27,32,35	1.94	6 (22%)
54	PSU	2y	55	54	18,21,22	1.44	3 (16%)	21,30,33	1.95	5 (23%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.06	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	55,56,1	23,26,27	1.24	3 (13%)	32,38,41	1.89	5 (15%)
1	OMU	1A	2552	56,1	19,22,23	1.29	4 (21%)	25,31,34	1.82	5 (20%)
55	31H	2x	76	55,57,56,1	31,34,35	1.21	3 (9%)	35,47,50	1.95	9 (25%)
32	G7M	1a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.62	5 (14%)
32	5MC	1a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.15	2 (7%)
55	4SU	1x	8	55	18,21,22	2.43	5 (27%)	25,30,33	1.83	6 (24%)
1	5MU	2A	1915	56,1	19,22,23	1.46	5 (26%)	27,32,35	2.09	6 (22%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	2 (7%)
54	PSU	2w	55	54	18,21,22	1.42	2 (11%)	21,30,33	1.97	3 (14%)
32	5MC	2a	967	32	19,22,23	1.68	3 (15%)	26,32,35	1.06	2 (7%)
43	0TD	2l	92	43	8,9,10	4.62	1 (12%)	6,11,13	2.31	3 (50%)
54	4SU	1w	8	54	18,21,22	1.85	5 (27%)	25,30,33	1.97	4 (16%)
1	8AH	2A	2503	56,1	22,26,27	1.68	5 (22%)	29,39,42	2.19	5 (17%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.87	6 (18%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.03	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	56,1	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,56	-	5/22/40/41	0/3/3/3
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,56	-	2/9/27/28	0/3/3/3
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	8AH	1A	2503	56,1	-	1/7/25/26	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMG	2A	2251	55,56,1	-	0/9/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	1/7/25/34	0/3/3/3
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
55	31H	2x	76	55,57,56,1	-	6/22/40/41	0/3/3/3
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	56,1	-	1/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	56,1	-	0/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2

The worst 5 of 258 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.64	1.69	1.82
43	1l	92	0TD	CB-SB	-12.37	1.69	1.82
54	1w	37	MIA	C2-S10	-7.07	1.69	1.75
1	1A	1962	5MC	C5-C4	6.82	1.49	1.44
54	1w	37	MIA	C13-C14	6.78	1.52	1.32

The worst 5 of 404 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C12-C13-C14	-9.44	110.07	127.01
54	2w	37	MIA	C5-C4-N3	-9.22	117.47	127.18
1	2A	2503	8AH	C5-C4-N3	-8.19	118.56	127.18
54	1w	37	MIA	C5-C4-N3	-7.94	118.81	127.18
1	1A	2503	8AH	C5-C4-N3	-7.67	119.10	127.18

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	31H	CB-CA-N-CN

There are no ring outliers.

33 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1518	MA6	1	0
54	2y	39	PSU	1	0
54	1y	46	G7M	1	0
55	2x	8	4SU	2	0
1	1A	1920	OMC	1	0
55	1x	76	31H	1	0
1	1A	1942	5MC	1	0
32	1a	1402	4OC	1	0
54	2y	8	4SU	3	0
32	1a	1207	2MG	1	0
54	2y	37	MIA	1	0
1	1A	1939	5MU	1	0
54	2y	46	G7M	2	0
32	2a	1207	2MG	1	0
54	2y	54	5MU	1	0
32	1a	967	5MC	1	0
32	1a	1519	MA6	1	0
54	1y	8	4SU	1	0
43	1l	92	0TD	1	0
54	1y	37	MIA	3	0
32	1a	1518	MA6	1	0
1	2A	1939	5MU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	966	M2G	2	0
54	1y	54	5MU	1	0
54	2y	55	PSU	7	0
32	2a	1519	MA6	1	0
55	2x	76	31H	1	0
55	1x	8	4SU	2	0
1	2A	1915	5MU	1	0
32	2a	967	5MC	2	0
43	2l	92	0TD	1	0
32	2a	966	M2G	1	0
54	1y	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2763 ligands modelled in this entry, 2759 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	WC9	1A	4098	1	34,37,37	1.68	6 (17%)	31,53,53	1.10	2 (6%)
60	SF4	1d	302	35	0,12,12	-	-	-	-	-
58	WC9	2A	3846	-	34,37,37	1.32	4 (11%)	31,53,53	1.01	2 (6%)
60	SF4	2d	303	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	WC9	1A	4098	1	-	2/28/71/71	0/3/4/4
60	SF4	1d	302	35	-	-	0/6/5/5
58	WC9	2A	3846	-	-	0/28/71/71	0/3/4/4
60	SF4	2d	303	35	-	-	0/6/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4098	WC9	CAM-CBF	-4.79	1.39	1.51
58	1A	4098	WC9	OAW-CB	4.63	1.47	1.42
58	2A	3846	WC9	CAM-CBF	-4.48	1.40	1.51
58	1A	4098	WC9	OAW-CAX	3.41	1.48	1.43
58	2A	3846	WC9	OAW-CB	3.04	1.45	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3846	WC9	CBC-CBB-CAZ	-3.13	110.61	116.68
58	1A	4098	WC9	CBC-CBB-CAZ	-2.91	111.02	116.68
58	1A	4098	WC9	CD2-CAZ-CAY	-2.59	109.91	113.78
58	2A	3846	WC9	CAF-OAA-CAB	-2.46	110.94	114.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4098	WC9	CAB-CAK-NAL-C
58	1A	4098	WC9	CAM-CAK-NAL-C

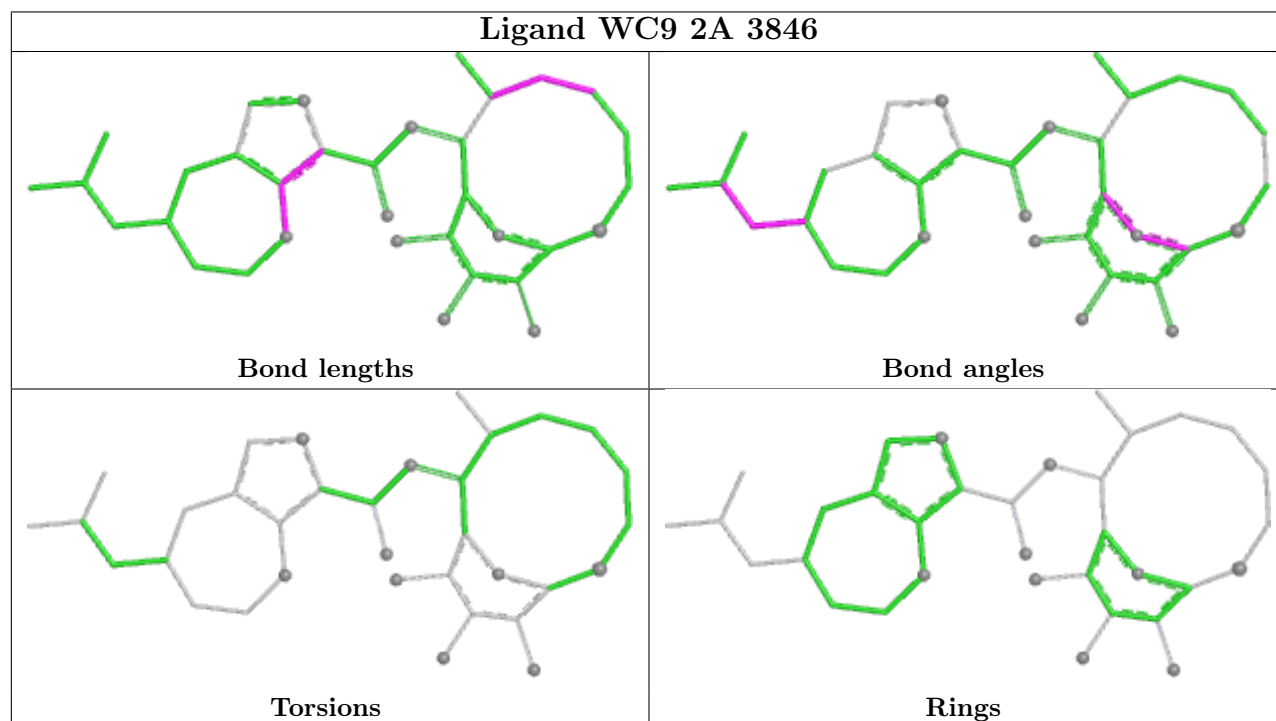
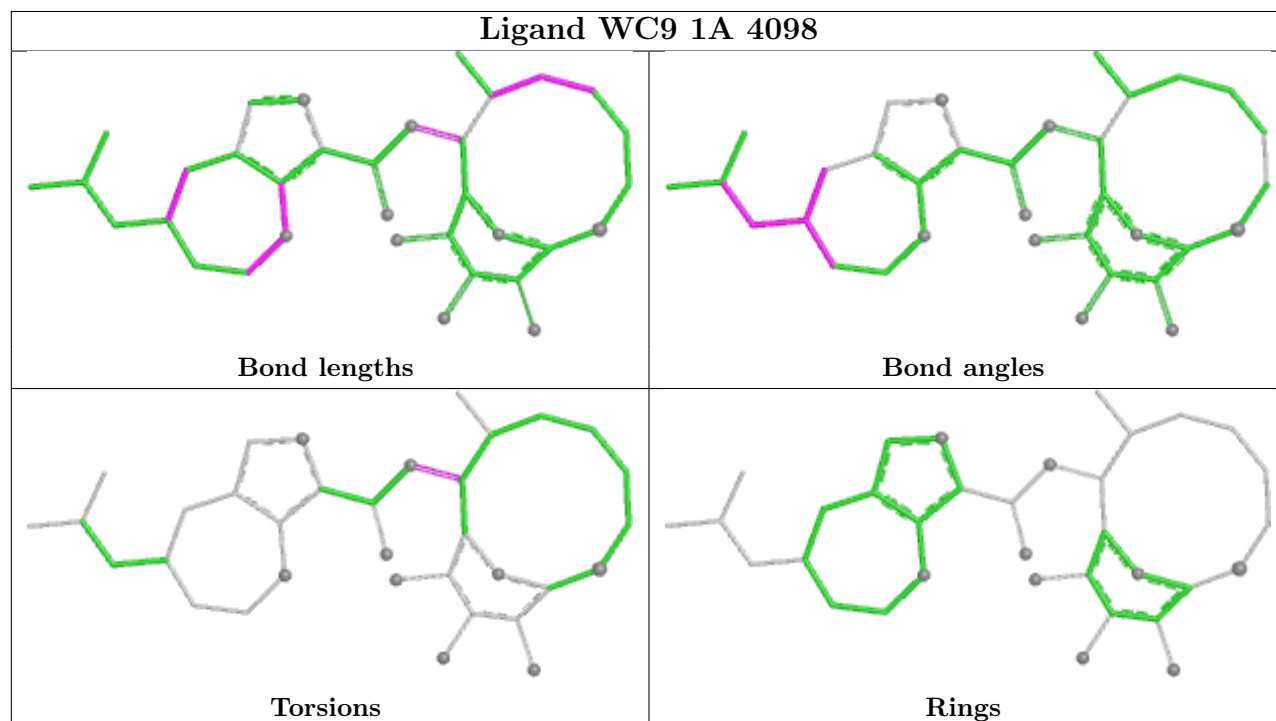
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4098	WC9	1	0
60	1d	302	SF4	2	0
58	2A	3846	WC9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.52	120 (4%) 40 35	21, 38, 95, 108	0
1	2A	2789/2915 (95%)	-0.05	104 (3%) 45 39	34, 57, 93, 107	0
2	1B	120/121 (99%)	-0.33	0 100 100	33, 52, 67, 88	0
2	2B	120/121 (99%)	0.39	1 (0%) 82 80	61, 73, 82, 93	0
3	1D	275/276 (99%)	-0.25	2 (0%) 84 82	21, 39, 52, 79	0
3	2D	275/276 (99%)	0.10	2 (0%) 84 82	30, 50, 62, 82	0
4	1E	204/206 (99%)	-0.27	0 100 100	21, 39, 61, 72	0
4	2E	204/206 (99%)	0.39	6 (2%) 53 48	39, 60, 72, 83	0
5	1F	203/210 (96%)	-0.07	1 (0%) 87 85	22, 45, 68, 84	0
5	2F	203/210 (96%)	0.38	2 (0%) 79 76	36, 64, 76, 84	0
6	1G	181/182 (99%)	0.30	5 (2%) 55 49	46, 60, 74, 83	0
6	2G	181/182 (99%)	0.73	8 (4%) 39 33	62, 74, 82, 86	0
7	1H	174/180 (96%)	0.08	3 (1%) 69 64	39, 54, 66, 73	0
7	2H	174/180 (96%)	1.31	36 (20%) 2 2	71, 84, 91, 95	0
8	1I	146/148 (98%)	0.67	4 (2%) 56 50	49, 72, 81, 84	0
8	2I	146/148 (98%)	0.81	10 (6%) 23 19	50, 71, 82, 88	0
9	1N	140/140 (100%)	-0.24	1 (0%) 84 82	25, 38, 62, 75	0
9	2N	140/140 (100%)	0.55	5 (3%) 46 40	48, 66, 79, 84	0
10	1O	122/122 (100%)	-0.23	0 100 100	29, 41, 59, 63	0
10	2O	122/122 (100%)	0.35	1 (0%) 82 80	50, 61, 71, 76	0
11	1P	149/150 (99%)	0.02	0 100 100	23, 50, 70, 75	0
11	2P	149/150 (99%)	0.40	2 (1%) 75 71	41, 63, 80, 87	0
12	1Q	141/141 (100%)	-0.06	1 (0%) 84 82	28, 43, 61, 77	0
12	2Q	141/141 (100%)	0.64	5 (3%) 47 41	52, 67, 76, 83	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%)	-0.33	0 100 100	27, 36, 47, 59	0
13	2R	118/118 (100%)	0.28	1 (0%) 82 80	44, 54, 65, 73	0
14	1S	110/112 (98%)	0.10	0 100 100	41, 52, 64, 70	0
14	2S	110/112 (98%)	0.80	6 (5%) 30 25	58, 68, 77, 80	0
15	1T	131/146 (89%)	0.14	3 (2%) 61 55	36, 48, 73, 81	0
15	2T	131/146 (89%)	0.50	2 (1%) 72 68	53, 65, 75, 81	0
16	1U	116/118 (98%)	-0.47	0 100 100	20, 30, 46, 66	0
16	2U	116/118 (98%)	0.47	3 (2%) 57 51	41, 63, 75, 81	0
17	1V	101/101 (100%)	-0.39	0 100 100	23, 38, 57, 65	0
17	2V	101/101 (100%)	0.44	1 (0%) 79 76	44, 71, 79, 82	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 78	23, 32, 51, 77	0
18	2W	112/113 (99%)	0.19	0 100 100	42, 51, 67, 83	0
19	1X	95/96 (98%)	-0.23	0 100 100	29, 39, 61, 72	0
19	2X	95/96 (98%)	0.35	3 (3%) 50 44	45, 58, 74, 86	0
20	1Y	107/110 (97%)	0.24	2 (1%) 66 61	37, 52, 69, 78	0
20	2Y	107/110 (97%)	0.96	12 (11%) 10 8	56, 69, 81, 87	0
21	1Z	154/206 (74%)	0.60	6 (3%) 43 38	38, 66, 84, 91	0
21	2Z	160/206 (77%)	1.12	20 (12%) 8 6	69, 80, 89, 92	0
22	10	83/85 (97%)	0.03	3 (3%) 46 40	30, 40, 60, 76	0
22	20	83/85 (97%)	0.79	8 (9%) 13 10	45, 62, 74, 83	0
23	11	97/98 (98%)	0.20	3 (3%) 51 45	31, 46, 72, 77	0
23	21	97/98 (98%)	0.22	1 (1%) 79 76	38, 53, 72, 81	0
24	12	70/72 (97%)	-0.00	2 (2%) 53 48	38, 50, 59, 71	0
24	22	70/72 (97%)	0.50	2 (2%) 53 48	57, 67, 75, 76	0
25	13	59/60 (98%)	-0.24	2 (3%) 48 42	26, 38, 61, 82	0
25	23	59/60 (98%)	0.38	1 (1%) 69 64	54, 65, 78, 81	0
26	14	69/71 (97%)	0.96	10 (14%) 6 4	56, 76, 87, 90	0
26	24	69/71 (97%)	1.06	7 (10%) 12 9	71, 83, 92, 101	0
27	15	59/60 (98%)	-0.48	0 100 100	20, 33, 52, 59	0
27	25	59/60 (98%)	0.32	3 (5%) 33 28	39, 54, 69, 76	0
28	16	53/54 (98%)	-0.24	0 100 100	35, 47, 60, 65	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%)	0.40	0 100 100	47, 59, 66, 75	0
29	17	48/49 (97%)	-0.18	3 (6%) 26 20	23, 29, 59, 69	0
29	27	48/49 (97%)	0.04	3 (6%) 26 20	35, 42, 68, 73	0
30	18	64/65 (98%)	-0.25	0 100 100	28, 38, 44, 58	0
30	28	64/65 (98%)	0.26	1 (1%) 70 66	46, 53, 60, 68	0
31	19	37/37 (100%)	-0.19	0 100 100	34, 42, 55, 66	0
31	29	37/37 (100%)	1.04	3 (8%) 18 14	63, 69, 78, 84	0
32	1a	1488/1521 (97%)	0.19	49 (3%) 49 43	36, 66, 93, 109	0
32	2a	1491/1521 (98%)	0.41	65 (4%) 39 33	45, 73, 93, 106	0
33	1b	231/256 (90%)	1.11	41 (17%) 4 3	64, 78, 87, 93	0
33	2b	231/256 (90%)	1.23	41 (17%) 4 3	68, 82, 88, 93	0
34	1c	206/239 (86%)	0.68	8 (3%) 43 38	60, 72, 82, 91	0
34	2c	206/239 (86%)	1.17	24 (11%) 9 7	71, 79, 86, 90	0
35	1d	208/209 (99%)	0.77	13 (6%) 26 20	56, 69, 78, 85	0
35	2d	208/209 (99%)	0.51	3 (1%) 73 69	54, 66, 74, 79	0
36	1e	148/162 (91%)	0.42	3 (2%) 65 60	51, 64, 74, 85	0
36	2e	148/162 (91%)	0.74	4 (2%) 56 50	57, 71, 79, 88	0
37	1f	100/101 (99%)	0.48	0 100 100	56, 68, 74, 77	0
37	2f	100/101 (99%)	0.51	2 (2%) 65 60	55, 67, 75, 77	0
38	1g	155/156 (99%)	0.58	8 (5%) 33 27	59, 70, 80, 88	0
38	2g	155/156 (99%)	0.70	10 (6%) 25 19	67, 74, 81, 88	0
39	1h	137/138 (99%)	0.39	1 (0%) 84 82	55, 67, 73, 78	0
39	2h	137/138 (99%)	0.83	3 (2%) 62 57	65, 73, 78, 82	0
40	1i	127/128 (99%)	1.21	20 (15%) 5 4	56, 77, 83, 88	0
40	2i	127/128 (99%)	1.42	30 (23%) 2 1	64, 81, 87, 90	0
41	1j	97/105 (92%)	1.12	13 (13%) 7 5	58, 77, 87, 92	0
41	2j	96/105 (91%)	1.89	42 (43%) 0 0	71, 82, 90, 91	0
42	1k	114/129 (88%)	0.53	4 (3%) 47 41	43, 64, 76, 81	0
42	2k	114/129 (88%)	0.57	4 (3%) 47 41	53, 70, 79, 81	0
43	1l	121/132 (91%)	0.13	2 (1%) 69 64	44, 53, 67, 74	0
43	2l	121/132 (91%)	0.51	4 (3%) 49 43	55, 63, 74, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.77	8 (6%) 25 19	52, 70, 78, 90	0
44	2m	122/126 (96%)	1.38	21 (17%) 4 3	66, 79, 85, 90	0
45	1n	60/61 (98%)	1.03	7 (11%) 9 7	60, 68, 77, 81	0
45	2n	60/61 (98%)	1.85	21 (35%) 1 1	73, 80, 85, 89	0
46	1o	88/89 (98%)	0.55	1 (1%) 78 74	50, 65, 75, 82	0
46	2o	88/89 (98%)	0.61	2 (2%) 61 55	57, 68, 79, 81	0
47	1p	82/88 (93%)	0.90	2 (2%) 59 54	55, 69, 77, 85	0
47	2p	82/88 (93%)	0.85	5 (6%) 27 22	57, 67, 75, 79	0
48	1q	99/105 (94%)	0.72	3 (3%) 52 47	53, 66, 74, 77	0
48	2q	99/105 (94%)	0.71	5 (5%) 33 28	61, 70, 77, 80	0
49	1r	68/88 (77%)	0.36	1 (1%) 72 68	53, 66, 76, 78	0
49	2r	68/88 (77%)	0.45	1 (1%) 72 68	57, 68, 75, 80	0
50	1s	83/93 (89%)	0.67	3 (3%) 46 40	62, 74, 79, 82	0
50	2s	83/93 (89%)	1.31	14 (16%) 4 3	74, 82, 87, 93	0
51	1t	96/106 (90%)	0.81	7 (7%) 21 17	58, 70, 80, 83	0
51	2t	96/106 (90%)	0.65	2 (2%) 63 58	57, 68, 80, 86	0
52	1u	23/27 (85%)	1.05	4 (17%) 4 3	63, 68, 71, 79	0
52	2u	23/27 (85%)	1.32	4 (17%) 4 3	69, 76, 79, 85	0
53	1v	13/24 (54%)	0.22	1 (7%) 19 15	48, 58, 84, 92	0
53	2v	13/24 (54%)	0.79	3 (23%) 2 1	62, 72, 87, 98	0
54	1w	67/76 (88%)	1.09	13 (19%) 3 2	49, 86, 99, 101	0
54	1y	67/76 (88%)	0.83	2 (2%) 52 47	38, 90, 97, 101	0
54	2w	65/76 (85%)	1.37	14 (21%) 2 2	69, 94, 102, 108	0
54	2y	66/76 (86%)	1.06	9 (13%) 7 5	50, 92, 98, 102	0
55	1x	71/77 (92%)	0.21	2 (2%) 55 49	33, 63, 80, 86	0
55	2x	71/77 (92%)	0.42	3 (4%) 40 35	46, 75, 86, 97	0
All	All	20873/21748 (95%)	0.25	983 (4%) 36 30	20, 63, 88, 109	0

The worst 5 of 983 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	10.6
1	1A	653	A	10.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	10.5
1	2A	652(U)	G	10.5
1	1A	652(U)	G	9.6

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
54	PSU	2y	55	20/21	0.60	0.15	91,95,108,119	0
54	4SU	2y	8	20/21	0.68	0.16	85,95,101,110	0
54	4SU	2w	8	20/21	0.70	0.15	91,95,111,121	0
54	PSU	1y	55	20/21	0.71	0.13	93,96,110,114	0
54	G7M	2w	46	24/25	0.72	0.15	84,94,106,115	0
54	G7M	2y	46	24/25	0.74	0.15	86,94,102,115	0
54	G7M	1w	46	24/25	0.74	0.15	81,90,102,115	0
54	MIA	2y	37	22/30	0.75	0.14	83,90,101,107	0
54	G7M	1y	46	24/25	0.76	0.16	84,92,106,114	0
54	5MU	1y	54	21/22	0.76	0.16	81,92,102,108	0
54	4SU	1y	8	20/21	0.76	0.12	88,92,100,101	0
54	5MU	2y	54	21/22	0.78	0.15	85,93,105,118	0
54	PSU	2y	32	20/21	0.80	0.12	84,90,96,103	0
54	MIA	1y	37	22/30	0.81	0.12	77,84,90,93	0
54	PSU	2w	55	20/21	0.81	0.10	82,87,96,99	0
54	PSU	1w	55	20/21	0.83	0.11	65,80,88,89	0
54	PSU	1y	39	20/21	0.84	0.11	77,82,86,92	0
54	4SU	1w	8	20/21	0.86	0.12	78,86,98,98	0
54	PSU	1y	32	20/21	0.86	0.10	78,84,89,90	0
54	PSU	2y	39	20/21	0.87	0.10	81,89,98,99	0
55	4SU	2x	8	20/21	0.88	0.12	77,80,85,87	0
54	5MU	2w	54	21/22	0.89	0.10	77,80,85,89	0
55	5MU	2x	54	21/22	0.90	0.11	72,76,81,84	0
54	PSU	2w	32	20/21	0.90	0.13	67,77,87,91	0
54	MIA	2w	37	25/30	0.90	0.13	58,71,83,101	0
43	0TD	2l	92	10/11	0.90	0.11	59,61,67,70	0
32	PSU	2a	516	20/21	0.91	0.10	63,69,75,81	0
55	PSU	2x	55	20/21	0.91	0.09	66,74,79,86	0
32	G7M	2a	527	24/25	0.91	0.12	58,64,70,75	0
54	PSU	1w	32	20/21	0.92	0.12	59,66,73,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	5MU	1x	54	21/22	0.92	0.09	53,64,77,81	0
55	5MC	2x	32	21/22	0.92	0.12	68,71,74,81	0
55	PSU	1x	55	20/21	0.92	0.09	54,61,75,85	0
1	PSU	2A	1917	20/21	0.92	0.09	53,63,68,69	0
32	2MG	2a	1207	24/25	0.93	0.09	70,79,82,83	0
55	4SU	1x	8	20/21	0.93	0.10	54,66,73,75	0
54	5MU	1w	54	21/22	0.93	0.09	47,66,73,75	0
1	5MU	2A	1915	21/22	0.93	0.09	57,63,68,70	0
32	M2G	2a	966	25/26	0.93	0.15	58,65,77,83	0
32	5MC	2a	967	21/22	0.94	0.12	59,65,73,80	0
43	0TD	1l	92	10/11	0.94	0.09	48,54,56,71	0
32	5MC	2a	1400	21/22	0.94	0.12	65,70,73,83	0
32	5MC	2a	1404	21/22	0.94	0.10	52,56,60,65	0
54	MIA	1w	37	29/30	0.94	0.13	45,57,69,81	0
55	5MC	1x	32	21/22	0.94	0.11	56,59,62,72	0
32	4OC	2a	1402	22/23	0.95	0.10	51,60,64,65	0
32	G7M	1a	527	24/25	0.95	0.09	44,51,57,63	0
32	MA6	2a	1518	24/25	0.95	0.11	51,62,66,70	0
32	M2G	1a	966	25/26	0.95	0.11	46,53,62,64	0
32	5MC	1a	967	21/22	0.95	0.09	46,53,61,62	0
32	2MG	1a	1207	24/25	0.95	0.09	61,70,73,75	0
54	PSU	1w	39	20/21	0.95	0.09	54,64,74,76	0
1	PSU	1A	1917	20/21	0.95	0.08	47,52,56,58	0
54	PSU	2w	39	20/21	0.95	0.09	60,74,83,83	0
1	OMC	2A	1920	21/22	0.95	0.10	48,59,62,68	0
1	5MC	2A	1942	21/22	0.95	0.09	50,56,60,64	0
32	MA6	2a	1519	24/25	0.96	0.11	45,56,65,67	0
55	31H	2x	76	32/33	0.96	0.09	39,51,61,69	0
1	PSU	2A	1911	20/21	0.96	0.07	56,58,63,63	0
1	5MU	1A	1915	21/22	0.96	0.09	46,52,57,57	0
32	MA6	1a	1519	24/25	0.96	0.09	36,43,48,52	0
55	31H	1x	76	32/33	0.96	0.10	26,37,45,60	10
32	5MC	2a	1407	21/22	0.96	0.08	48,53,59,61	0
32	UR3	2a	1498	21/22	0.96	0.10	48,53,59,60	0
1	5MC	1A	1942	21/22	0.96	0.08	32,37,41,42	0
32	PSU	1a	516	20/21	0.96	0.08	44,56,61,64	0
1	OMU	2A	2552	21/22	0.96	0.09	43,47,50,62	0
32	4OC	1a	1402	22/23	0.97	0.07	42,46,53,60	0
32	5MC	1a	1404	21/22	0.97	0.07	33,38,42,44	0
32	5MC	1a	1407	21/22	0.97	0.08	36,45,46,49	0
32	UR3	1a	1498	21/22	0.97	0.08	37,40,43,55	0
1	5MU	2A	1939	21/22	0.97	0.07	34,40,46,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	1A	1911	20/21	0.97	0.07	36,46,54,54	0
32	MA6	1a	1518	24/25	0.97	0.09	34,43,47,49	0
1	5MC	2A	1962	21/22	0.97	0.08	36,49,53,62	0
1	8AH	2A	2503	24/25	0.97	0.08	35,41,45,50	0
32	5MC	1a	1400	21/22	0.97	0.09	46,53,57,63	0
1	PSU	1A	2605	20/21	0.97	0.06	25,29,32,33	0
1	PSU	2A	2605	20/21	0.97	0.07	33,40,46,47	0
1	OMG	2A	2251	24/25	0.98	0.07	37,43,49,57	0
1	OMC	1A	1920	21/22	0.98	0.06	38,47,50,54	0
1	OMU	1A	2552	21/22	0.98	0.06	27,30,35,37	0
1	5MC	1A	1962	21/22	0.98	0.06	28,36,41,47	0
1	5MU	1A	1939	21/22	0.98	0.06	26,32,34,39	0
1	OMG	1A	2251	24/25	0.98	0.06	22,26,30,32	0
1	8AH	1A	2503	24/25	0.99	0.06	14,24,29,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
56	MG	2w	104	1/1	0.63	0.20	79,79,79,79	0
56	MG	2A	3083	1/1	0.64	0.15	61,61,61,61	0
56	MG	1A	3985	1/1	0.66	0.18	37,37,37,37	0
56	MG	1A	3992	1/1	0.68	0.16	70,70,70,70	0
56	MG	2v	102	1/1	0.69	0.29	82,82,82,82	0
56	MG	2W	202	1/1	0.69	0.14	76,76,76,76	0
56	MG	1a	1771	1/1	0.70	0.15	78,78,78,78	0
56	MG	2a	1748	1/1	0.70	0.19	96,96,96,96	0
56	MG	2A	3100	1/1	0.70	0.17	78,78,78,78	0
56	MG	2A	3585	1/1	0.70	0.18	73,73,73,73	0
56	MG	2A	3689	1/1	0.71	0.22	66,66,66,66	0
56	MG	1B	207	1/1	0.71	0.25	73,73,73,73	0
56	MG	2A	3217	1/1	0.71	0.18	69,69,69,69	0
56	MG	1Z	302	1/1	0.71	0.13	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3593	1/1	0.71	0.18	74,74,74,74	0
56	MG	1A	3587	1/1	0.72	0.36	54,54,54,54	0
56	MG	1A	3674	1/1	0.72	0.14	59,59,59,59	0
56	MG	2a	1720	1/1	0.72	0.28	78,78,78,78	0
56	MG	20	101	1/1	0.73	0.30	64,64,64,64	0
56	MG	1A	3966	1/1	0.73	0.14	70,70,70,70	0
56	MG	2A	3650	1/1	0.73	0.14	72,72,72,72	0
56	MG	2a	1821	1/1	0.73	0.25	81,81,81,81	0
56	MG	2A	3227	1/1	0.73	0.24	69,69,69,69	0
56	MG	1A	3724	1/1	0.73	0.14	63,63,63,63	0
56	MG	2A	3336	1/1	0.74	0.14	78,78,78,78	0
56	MG	2A	3368	1/1	0.74	0.31	83,83,83,83	0
56	MG	1A	4015	1/1	0.74	0.24	51,51,51,51	0
56	MG	1A	3459	1/1	0.74	0.13	63,63,63,63	0
56	MG	1a	1807	1/1	0.74	0.23	85,85,85,85	0
56	MG	1w	105	1/1	0.74	0.26	86,86,86,86	0
56	MG	2A	3699	1/1	0.74	0.14	62,62,62,62	0
56	MG	1A	3761	1/1	0.75	0.09	21,21,21,21	0
56	MG	1A	3823	1/1	0.75	0.14	62,62,62,62	0
56	MG	1A	3585	1/1	0.75	0.26	64,64,64,64	0
56	MG	2A	3442	1/1	0.75	0.19	72,72,72,72	0
56	MG	2A	3815	1/1	0.75	0.14	63,63,63,63	0
56	MG	1A	4087	1/1	0.75	0.21	62,62,62,62	0
56	MG	2a	1672	1/1	0.76	0.12	63,63,63,63	0
56	MG	1A	3596	1/1	0.76	0.13	36,36,36,36	0
56	MG	2A	3712	1/1	0.76	0.18	68,68,68,68	0
56	MG	2A	3006	1/1	0.76	0.14	78,78,78,78	0
56	MG	1a	1711	1/1	0.76	0.28	60,60,60,60	0
56	MG	2w	101	1/1	0.76	0.14	79,79,79,79	0
56	MG	2A	3483	1/1	0.76	0.20	62,62,62,62	0
56	MG	2w	106	1/1	0.76	0.22	77,77,77,77	0
56	MG	1A	3738	1/1	0.77	0.18	63,63,63,63	0
56	MG	1a	1797	1/1	0.77	0.17	76,76,76,76	0
56	MG	2a	1794	1/1	0.77	0.30	65,65,65,65	0
56	MG	2a	1796	1/1	0.77	0.16	70,70,70,70	0
56	MG	2a	1814	1/1	0.77	0.38	80,80,80,80	0
56	MG	1A	3715	1/1	0.77	0.21	62,62,62,62	0
56	MG	2B	201	1/1	0.77	0.38	82,82,82,82	0
56	MG	1A	3781	1/1	0.77	0.18	75,75,75,75	0
56	MG	1A	3516	1/1	0.77	0.18	79,79,79,79	0
56	MG	2A	3069	1/1	0.77	0.30	69,69,69,69	0
56	MG	2a	1730	1/1	0.78	0.23	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4072	1/1	0.78	0.14	60,60,60,60	0
56	MG	2A	3391	1/1	0.78	0.17	65,65,65,65	0
56	MG	1Z	304	1/1	0.78	0.11	62,62,62,62	0
56	MG	1a	1660	1/1	0.78	0.20	71,71,71,71	0
56	MG	1A	3700	1/1	0.78	0.18	52,52,52,52	0
56	MG	2A	3233	1/1	0.78	0.30	61,61,61,61	0
56	MG	2a	1607	1/1	0.78	0.33	69,69,69,69	0
56	MG	2A	3299	1/1	0.78	0.15	70,70,70,70	0
56	MG	1A	3828	1/1	0.78	0.18	63,63,63,63	0
56	MG	1A	4071	1/1	0.79	0.17	69,69,69,69	0
56	MG	2a	1778	1/1	0.79	0.22	67,67,67,67	0
56	MG	2A	3833	1/1	0.79	0.17	65,65,65,65	0
56	MG	1A	3745	1/1	0.79	0.12	46,46,46,46	0
56	MG	2A	3239	1/1	0.79	0.16	57,57,57,57	0
56	MG	2A	3243	1/1	0.79	0.15	72,72,72,72	0
56	MG	1B	226	1/1	0.79	0.19	65,65,65,65	0
56	MG	1D	312	1/1	0.79	0.17	66,66,66,66	0
56	MG	2A	3184	1/1	0.79	0.22	82,82,82,82	0
56	MG	1w	107	1/1	0.79	0.20	70,70,70,70	0
56	MG	2A	3289	1/1	0.80	0.13	66,66,66,66	0
56	MG	2A	3606	1/1	0.80	0.26	70,70,70,70	0
56	MG	2A	3110	1/1	0.80	0.17	71,71,71,71	0
56	MG	2A	3319	1/1	0.80	0.19	61,61,61,61	0
56	MG	1A	3526	1/1	0.80	0.12	51,51,51,51	0
56	MG	2A	3340	1/1	0.80	0.22	76,76,76,76	0
56	MG	1x	113	1/1	0.80	0.16	71,71,71,71	0
56	MG	2A	3821	1/1	0.80	0.15	45,45,45,45	0
56	MG	1B	221	1/1	0.80	0.16	67,67,67,67	0
56	MG	1A	3532	1/1	0.80	0.24	59,59,59,59	0
56	MG	1B	229	1/1	0.80	0.22	72,72,72,72	0
56	MG	2A	3544	1/1	0.80	0.18	40,40,40,40	0
56	MG	1a	1663	1/1	0.80	0.13	57,57,57,57	0
56	MG	2x	106	1/1	0.80	0.29	71,71,71,71	0
56	MG	2A	3724	1/1	0.81	0.17	62,62,62,62	0
56	MG	2A	3043	1/1	0.81	0.19	66,66,66,66	0
56	MG	1A	3978	1/1	0.81	0.13	38,38,38,38	0
56	MG	1A	3075	1/1	0.81	0.30	65,65,65,65	0
56	MG	2A	3835	1/1	0.81	0.13	65,65,65,65	0
56	MG	1A	3529	1/1	0.81	0.28	57,57,57,57	0
56	MG	2A	3365	1/1	0.81	0.18	74,74,74,74	0
56	MG	1a	1712	1/1	0.81	0.36	58,58,58,58	0
56	MG	2a	1603	1/1	0.81	0.17	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3112	1/1	0.81	0.26	73,73,73,73	0
56	MG	2a	1653	1/1	0.81	0.31	74,74,74,74	0
56	MG	2A	3182	1/1	0.81	0.20	76,76,76,76	0
56	MG	2A	3473	1/1	0.81	0.17	63,63,63,63	0
56	MG	2A	3480	1/1	0.81	0.14	67,67,67,67	0
56	MG	1A	3705	1/1	0.81	0.22	64,64,64,64	0
56	MG	2A	3215	1/1	0.81	0.12	65,65,65,65	0
56	MG	1A	3873	1/1	0.81	0.12	26,26,26,26	0
56	MG	1E	309	1/1	0.81	0.38	79,79,79,79	0
56	MG	1S	202	1/1	0.81	0.27	62,62,62,62	0
56	MG	2A	3234	1/1	0.81	0.19	63,63,63,63	0
56	MG	2A	3685	1/1	0.81	0.19	70,70,70,70	0
56	MG	1A	3931	1/1	0.81	0.20	37,37,37,37	0
56	MG	2A	3690	1/1	0.81	0.23	72,72,72,72	0
56	MG	1A	3095	1/1	0.81	0.12	71,71,71,71	0
56	MG	1a	1623	1/1	0.81	0.12	68,68,68,68	0
56	MG	1A	3897	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3474	1/1	0.82	0.17	71,71,71,71	0
56	MG	2E	302	1/1	0.82	0.08	69,69,69,69	0
56	MG	1a	1714	1/1	0.82	0.23	64,64,64,64	0
56	MG	2A	3013	1/1	0.82	0.13	59,59,59,59	0
56	MG	1a	1739	1/1	0.82	0.16	53,53,53,53	0
56	MG	1a	1740	1/1	0.82	0.24	81,81,81,81	0
56	MG	2a	1641	1/1	0.82	0.22	70,70,70,70	0
56	MG	2a	1646	1/1	0.82	0.17	63,63,63,63	0
56	MG	2a	1650	1/1	0.82	0.34	79,79,79,79	0
56	MG	1A	4008	1/1	0.82	0.19	65,65,65,65	0
56	MG	2A	3600	1/1	0.82	0.13	44,44,44,44	0
56	MG	2a	1701	1/1	0.82	0.16	69,69,69,69	0
56	MG	2a	1703	1/1	0.82	0.30	61,61,61,61	0
56	MG	1a	1789	1/1	0.82	0.20	61,61,61,61	0
56	MG	2A	3648	1/1	0.82	0.17	60,60,60,60	0
56	MG	2A	3304	1/1	0.82	0.14	62,62,62,62	0
56	MG	2a	1777	1/1	0.82	0.29	78,78,78,78	0
56	MG	1a	1658	1/1	0.82	0.13	63,63,63,63	0
56	MG	1A	3704	1/1	0.82	0.13	63,63,63,63	0
56	MG	1n	101	1/1	0.82	0.37	73,73,73,73	0
56	MG	2A	3354	1/1	0.82	0.38	66,66,66,66	0
56	MG	1w	104	1/1	0.82	0.16	67,67,67,67	0
56	MG	2a	1825	1/1	0.82	0.30	72,72,72,72	0
56	MG	2l	202	1/1	0.82	0.17	65,65,65,65	0
56	MG	2A	3213	1/1	0.82	0.11	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3744	1/1	0.82	0.15	50,50,50,50	0
56	MG	1A	4069	1/1	0.82	0.22	71,71,71,71	0
56	MG	2A	3414	1/1	0.82	0.19	58,58,58,58	0
56	MG	1A	3932	1/1	0.82	0.14	32,32,32,32	0
56	MG	2A	3292	1/1	0.83	0.41	75,75,75,75	0
56	MG	2a	1605	1/1	0.83	0.20	67,67,67,67	0
56	MG	1a	1689	1/1	0.83	0.34	56,56,56,56	0
56	MG	2a	1611	1/1	0.83	0.39	75,75,75,75	0
56	MG	2a	1618	1/1	0.83	0.19	69,69,69,69	0
56	MG	2a	1636	1/1	0.83	0.25	61,61,61,61	0
56	MG	1Y	203	1/1	0.83	0.11	73,73,73,73	0
56	MG	1A	4059	1/1	0.83	0.11	48,48,48,48	0
56	MG	2A	3142	1/1	0.83	0.22	71,71,71,71	0
56	MG	1A	3819	1/1	0.83	0.13	39,39,39,39	0
56	MG	2A	3659	1/1	0.83	0.18	58,58,58,58	0
56	MG	2a	1677	1/1	0.83	0.31	59,59,59,59	0
56	MG	2A	3669	1/1	0.83	0.17	64,64,64,64	0
56	MG	1x	104	1/1	0.83	0.14	60,60,60,60	0
56	MG	2a	1713	1/1	0.83	0.19	67,67,67,67	0
56	MG	1a	1604	1/1	0.83	0.21	64,64,64,64	0
56	MG	2A	3005	1/1	0.83	0.18	69,69,69,69	0
56	MG	1A	3230	1/1	0.83	0.15	54,54,54,54	0
56	MG	2a	1775	1/1	0.83	0.23	73,73,73,73	0
56	MG	1A	3339	1/1	0.83	0.14	48,48,48,48	0
56	MG	1A	3956	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3470	1/1	0.83	0.16	66,66,66,66	0
56	MG	2A	3781	1/1	0.83	0.14	77,77,77,77	0
56	MG	2a	1804	1/1	0.83	0.18	60,60,60,60	0
56	MG	2A	3784	1/1	0.83	0.11	52,52,52,52	0
56	MG	2A	3045	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3358	1/1	0.83	0.12	72,72,72,72	0
56	MG	2j	201	1/1	0.83	0.25	80,80,80,80	0
56	MG	2A	3477	1/1	0.83	0.15	63,63,63,63	0
56	MG	2v	101	1/1	0.83	0.35	73,73,73,73	0
56	MG	2A	3078	1/1	0.83	0.37	62,62,62,62	0
56	MG	1a	1668	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3491	1/1	0.83	0.17	66,66,66,66	0
56	MG	2A	3523	1/1	0.83	0.38	76,76,76,76	0
56	MG	2A	3291	1/1	0.83	0.16	68,68,68,68	0
56	MG	2A	3315	1/1	0.84	0.26	78,78,78,78	0
56	MG	1y	4301	1/1	0.84	0.11	63,63,63,63	0
56	MG	1a	1640	1/1	0.84	0.29	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3338	1/1	0.84	0.11	67,67,67,67	0
56	MG	2A	3209	1/1	0.84	0.21	74,74,74,74	0
56	MG	1a	1764	1/1	0.84	0.26	58,58,58,58	0
56	MG	2A	3684	1/1	0.84	0.12	79,79,79,79	0
56	MG	1A	3837	1/1	0.84	0.16	67,67,67,67	0
56	MG	1W	207	1/1	0.84	0.26	43,43,43,43	0
56	MG	2A	3371	1/1	0.84	0.19	67,67,67,67	0
56	MG	2A	3697	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3225	1/1	0.84	0.24	62,62,62,62	0
56	MG	2A	3701	1/1	0.84	0.14	58,58,58,58	0
56	MG	1A	3435	1/1	0.84	0.10	70,70,70,70	0
56	MG	2A	3718	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3719	1/1	0.84	0.11	66,66,66,66	0
56	MG	1A	3649	1/1	0.84	0.17	57,57,57,57	0
56	MG	1a	1673	1/1	0.84	0.15	67,67,67,67	0
56	MG	2A	3778	1/1	0.84	0.28	73,73,73,73	0
56	MG	1A	3971	1/1	0.84	0.11	59,59,59,59	0
56	MG	14	101	1/1	0.84	0.16	70,70,70,70	0
56	MG	2A	3791	1/1	0.84	0.14	48,48,48,48	0
56	MG	2A	3266	1/1	0.84	0.15	72,72,72,72	0
56	MG	2a	1815	1/1	0.84	0.22	58,58,58,58	0
56	MG	2A	3267	1/1	0.84	0.16	58,58,58,58	0
56	MG	2a	1824	1/1	0.84	0.22	65,65,65,65	0
56	MG	2A	3273	1/1	0.84	0.25	72,72,72,72	0
56	MG	1a	1603	1/1	0.84	0.15	66,66,66,66	0
56	MG	2A	3111	1/1	0.84	0.22	68,68,68,68	0
56	MG	2A	3541	1/1	0.84	0.13	70,70,70,70	0
56	MG	2F	304	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3245	1/1	0.84	0.18	56,56,56,56	0
56	MG	2A	3547	1/1	0.84	0.19	53,53,53,53	0
56	MG	1E	312	1/1	0.84	0.21	61,61,61,61	0
56	MG	2A	3176	1/1	0.84	0.34	74,74,74,74	0
56	MG	2y	102	1/1	0.84	0.18	79,79,79,79	0
56	MG	2A	3524	1/1	0.85	0.18	63,63,63,63	0
56	MG	1A	4070	1/1	0.85	0.15	70,70,70,70	0
56	MG	1A	3518	1/1	0.85	0.15	90,90,90,90	0
56	MG	1A	3313	1/1	0.85	0.21	51,51,51,51	0
56	MG	25	101	1/1	0.85	0.20	63,63,63,63	0
56	MG	1A	3447	1/1	0.85	0.09	64,64,64,64	0
56	MG	1A	3385	1/1	0.85	0.16	64,64,64,64	0
56	MG	1B	215	1/1	0.85	0.13	68,68,68,68	0
56	MG	2a	1609	1/1	0.85	0.21	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3602	1/1	0.85	0.18	52,52,52,52	0
56	MG	2a	1617	1/1	0.85	0.21	70,70,70,70	0
56	MG	1A	3494	1/1	0.85	0.21	69,69,69,69	0
56	MG	2A	3120	1/1	0.85	0.18	60,60,60,60	0
56	MG	2a	1638	1/1	0.85	0.38	72,72,72,72	0
56	MG	2A	3124	1/1	0.85	0.29	59,59,59,59	0
56	MG	2A	3331	1/1	0.85	0.14	66,66,66,66	0
56	MG	2a	1648	1/1	0.85	0.28	64,64,64,64	0
56	MG	1B	222	1/1	0.85	0.13	68,68,68,68	0
56	MG	1A	3586	1/1	0.85	0.22	60,60,60,60	0
56	MG	2a	1670	1/1	0.85	0.20	60,60,60,60	0
56	MG	1A	3506	1/1	0.85	0.17	75,75,75,75	0
56	MG	2A	3341	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	4006	1/1	0.85	0.13	47,47,47,47	0
56	MG	2a	1702	1/1	0.85	0.20	62,62,62,62	0
56	MG	2A	3363	1/1	0.85	0.18	61,61,61,61	0
56	MG	2A	3698	1/1	0.85	0.19	65,65,65,65	0
56	MG	2A	3208	1/1	0.85	0.22	59,59,59,59	0
56	MG	1A	3876	1/1	0.85	0.14	28,28,28,28	0
56	MG	2a	1738	1/1	0.85	0.14	71,71,71,71	0
56	MG	1A	3590	1/1	0.85	0.36	60,60,60,60	0
56	MG	2a	1749	1/1	0.85	0.13	69,69,69,69	0
56	MG	2A	3389	1/1	0.85	0.43	70,70,70,70	0
56	MG	2a	1776	1/1	0.85	0.15	61,61,61,61	0
56	MG	1x	115	1/1	0.85	0.29	71,71,71,71	0
56	MG	1A	4045	1/1	0.85	0.12	44,44,44,44	0
56	MG	2a	1785	1/1	0.85	0.25	62,62,62,62	0
56	MG	2A	3728	1/1	0.85	0.23	60,60,60,60	0
56	MG	2A	3422	1/1	0.85	0.29	64,64,64,64	0
56	MG	2A	3753	1/1	0.85	0.23	60,60,60,60	0
56	MG	2a	1807	1/1	0.85	0.32	74,74,74,74	0
56	MG	2A	3756	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3222	1/1	0.85	0.39	69,69,69,69	0
56	MG	1A	3899	1/1	0.85	0.11	58,58,58,58	0
56	MG	1A	3428	1/1	0.85	0.24	58,58,58,58	0
56	MG	2A	3231	1/1	0.85	0.25	70,70,70,70	0
56	MG	2A	3805	1/1	0.85	0.13	66,66,66,66	0
56	MG	1a	1720	1/1	0.85	0.29	73,73,73,73	0
56	MG	2A	3030	1/1	0.85	0.24	61,61,61,61	0
56	MG	1a	1722	1/1	0.85	0.27	71,71,71,71	0
56	MG	1a	1737	1/1	0.85	0.14	59,59,59,59	0
56	MG	2A	3058	1/1	0.85	0.12	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2B	206	1/1	0.85	0.26	65,65,65,65	0
56	MG	2B	210	1/1	0.85	0.17	72,72,72,72	0
56	MG	2B	211	1/1	0.85	0.22	68,68,68,68	0
56	MG	2A	3510	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3230	1/1	0.86	0.13	63,63,63,63	0
56	MG	1A	3410	1/1	0.86	0.24	70,70,70,70	0
56	MG	1B	218	1/1	0.86	0.14	59,59,59,59	0
56	MG	2a	1604	1/1	0.86	0.21	56,56,56,56	0
56	MG	2A	3003	1/1	0.86	0.29	64,64,64,64	0
56	MG	1A	3800	1/1	0.86	0.10	33,33,33,33	0
56	MG	2A	3561	1/1	0.86	0.18	60,60,60,60	0
56	MG	1A	3813	1/1	0.86	0.13	37,37,37,37	0
56	MG	2a	1615	1/1	0.86	0.24	73,73,73,73	0
56	MG	2A	3255	1/1	0.86	0.33	56,56,56,56	0
56	MG	1a	1683	1/1	0.86	0.17	66,66,66,66	0
56	MG	2a	1620	1/1	0.86	0.12	65,65,65,65	0
56	MG	2a	1629	1/1	0.86	0.32	76,76,76,76	0
56	MG	2a	1635	1/1	0.86	0.25	69,69,69,69	0
56	MG	1A	3414	1/1	0.86	0.24	47,47,47,47	0
56	MG	2A	3272	1/1	0.86	0.20	73,73,73,73	0
56	MG	2A	3611	1/1	0.86	0.13	53,53,53,53	0
56	MG	1a	1691	1/1	0.86	0.26	62,62,62,62	0
56	MG	2A	3275	1/1	0.86	0.12	70,70,70,70	0
56	MG	2A	3280	1/1	0.86	0.14	63,63,63,63	0
56	MG	2A	3666	1/1	0.86	0.12	72,72,72,72	0
56	MG	2A	3286	1/1	0.86	0.27	65,65,65,65	0
56	MG	1A	3420	1/1	0.86	0.32	61,61,61,61	0
56	MG	1A	3091	1/1	0.86	0.23	54,54,54,54	0
56	MG	2a	1690	1/1	0.86	0.11	79,79,79,79	0
56	MG	2a	1695	1/1	0.86	0.24	57,57,57,57	0
56	MG	1D	313	1/1	0.86	0.18	44,44,44,44	0
56	MG	1A	3195	1/1	0.86	0.23	50,50,50,50	0
56	MG	1A	3360	1/1	0.86	0.33	65,65,65,65	0
56	MG	2A	3084	1/1	0.86	0.15	58,58,58,58	0
56	MG	2A	3097	1/1	0.86	0.17	61,61,61,61	0
56	MG	1a	1729	1/1	0.86	0.20	65,65,65,65	0
56	MG	1G	205	1/1	0.86	0.16	62,62,62,62	0
56	MG	2a	1740	1/1	0.86	0.25	62,62,62,62	0
56	MG	1A	4022	1/1	0.86	0.12	45,45,45,45	0
56	MG	1S	203	1/1	0.86	0.12	73,73,73,73	0
56	MG	1a	1745	1/1	0.86	0.16	62,62,62,62	0
56	MG	1a	1749	1/1	0.86	0.22	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4023	1/1	0.86	0.10	40,40,40,40	0
56	MG	2A	3149	1/1	0.86	0.14	67,67,67,67	0
56	MG	2a	1784	1/1	0.86	0.23	71,71,71,71	0
56	MG	1A	4043	1/1	0.86	0.17	39,39,39,39	0
56	MG	2A	3768	1/1	0.86	0.26	80,80,80,80	0
56	MG	2A	3181	1/1	0.86	0.17	67,67,67,67	0
56	MG	2a	1802	1/1	0.86	0.10	62,62,62,62	0
56	MG	1a	1781	1/1	0.86	0.14	59,59,59,59	0
56	MG	1A	3544	1/1	0.86	0.13	64,64,64,64	0
56	MG	2a	1813	1/1	0.86	0.15	71,71,71,71	0
56	MG	1A	3371	1/1	0.86	0.22	50,50,50,50	0
56	MG	1A	3476	1/1	0.86	0.13	61,61,61,61	0
56	MG	2A	3436	1/1	0.86	0.30	58,58,58,58	0
56	MG	2A	3210	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	3905	1/1	0.86	0.12	23,23,23,23	0
56	MG	1A	3208	1/1	0.86	0.15	63,63,63,63	0
56	MG	1A	3500	1/1	0.86	0.17	63,63,63,63	0
56	MG	2A	3218	1/1	0.86	0.20	64,64,64,64	0
56	MG	1A	3951	1/1	0.86	0.12	56,56,56,56	0
56	MG	1a	1656	1/1	0.86	0.23	57,57,57,57	0
56	MG	2w	103	1/1	0.86	0.16	83,83,83,83	0
56	MG	2B	215	1/1	0.86	0.23	61,61,61,61	0
56	MG	2D	307	1/1	0.86	0.30	49,49,49,49	0
56	MG	2x	102	1/1	0.86	0.24	67,67,67,67	0
56	MG	2A	3485	1/1	0.86	0.23	48,48,48,48	0
56	MG	2x	107	1/1	0.86	0.14	55,55,55,55	0
56	MG	2y	101	1/1	0.86	0.15	74,74,74,74	0
56	MG	1A	3779	1/1	0.86	0.10	46,46,46,46	0
56	MG	2A	3503	1/1	0.87	0.22	59,59,59,59	0
56	MG	2A	3012	1/1	0.87	0.23	55,55,55,55	0
56	MG	1A	3187	1/1	0.87	0.12	47,47,47,47	0
56	MG	2A	3253	1/1	0.87	0.24	77,77,77,77	0
56	MG	1F	310	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3261	1/1	0.87	0.32	63,63,63,63	0
56	MG	1A	3326	1/1	0.87	0.15	57,57,57,57	0
56	MG	2A	3548	1/1	0.87	0.14	61,61,61,61	0
56	MG	1A	3957	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3268	1/1	0.87	0.33	78,78,78,78	0
56	MG	1A	3965	1/1	0.87	0.11	64,64,64,64	0
56	MG	1A	3592	1/1	0.87	0.31	70,70,70,70	0
56	MG	2A	3076	1/1	0.87	0.30	58,58,58,58	0
56	MG	1A	3250	1/1	0.87	0.13	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1738	1/1	0.87	0.16	60,60,60,60	0
56	MG	2A	3630	1/1	0.87	0.18	55,55,55,55	0
56	MG	2A	3640	1/1	0.87	0.17	62,62,62,62	0
56	MG	1A	4075	1/1	0.87	0.15	61,61,61,61	0
56	MG	2A	3089	1/1	0.87	0.21	60,60,60,60	0
56	MG	1A	3613	1/1	0.87	0.11	33,33,33,33	0
56	MG	1a	1744	1/1	0.87	0.11	60,60,60,60	0
56	MG	1A	4092	1/1	0.87	0.31	45,45,45,45	0
56	MG	2A	3680	1/1	0.87	0.15	56,56,56,56	0
56	MG	18	104	1/1	0.87	0.19	53,53,53,53	0
56	MG	1A	3625	1/1	0.87	0.08	25,25,25,25	0
56	MG	2A	3320	1/1	0.87	0.17	66,66,66,66	0
56	MG	2A	3325	1/1	0.87	0.18	76,76,76,76	0
56	MG	1a	1770	1/1	0.87	0.09	71,71,71,71	0
56	MG	2A	3122	1/1	0.87	0.24	65,65,65,65	0
56	MG	2a	1707	1/1	0.87	0.19	72,72,72,72	0
56	MG	1A	3991	1/1	0.87	0.12	72,72,72,72	0
56	MG	2a	1717	1/1	0.87	0.14	76,76,76,76	0
56	MG	1a	1605	1/1	0.87	0.11	67,67,67,67	0
56	MG	1a	1788	1/1	0.87	0.13	86,86,86,86	0
56	MG	1A	3887	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3361	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3556	1/1	0.87	0.29	52,52,52,52	0
56	MG	1a	1798	1/1	0.87	0.18	53,53,53,53	0
56	MG	2a	1763	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3739	1/1	0.87	0.13	61,61,61,61	0
56	MG	1a	1800	1/1	0.87	0.10	58,58,58,58	0
56	MG	2A	3206	1/1	0.87	0.25	63,63,63,63	0
56	MG	2A	3372	1/1	0.87	0.17	60,60,60,60	0
56	MG	2a	1781	1/1	0.87	0.25	71,71,71,71	0
56	MG	1A	3492	1/1	0.87	0.12	48,48,48,48	0
56	MG	1a	1808	1/1	0.87	0.10	55,55,55,55	0
56	MG	2a	1792	1/1	0.87	0.25	68,68,68,68	0
56	MG	1A	4009	1/1	0.87	0.10	75,75,75,75	0
56	MG	1A	3678	1/1	0.87	0.13	67,67,67,67	0
56	MG	1B	232	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3801	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3804	1/1	0.87	0.09	53,53,53,53	0
56	MG	1B	233	1/1	0.87	0.15	69,69,69,69	0
56	MG	2A	3806	1/1	0.87	0.10	66,66,66,66	0
56	MG	2A	3811	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3444	1/1	0.87	0.24	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3448	1/1	0.87	0.27	69,69,69,69	0
56	MG	2A	3458	1/1	0.87	0.12	62,62,62,62	0
56	MG	1w	108	1/1	0.87	0.10	71,71,71,71	0
56	MG	2A	3836	1/1	0.87	0.12	66,66,66,66	0
56	MG	1a	1672	1/1	0.87	0.19	62,62,62,62	0
56	MG	1A	3921	1/1	0.87	0.13	54,54,54,54	0
56	MG	1a	1681	1/1	0.87	0.14	62,62,62,62	0
56	MG	1A	3689	1/1	0.87	0.09	33,33,33,33	0
56	MG	2A	3481	1/1	0.87	0.12	77,77,77,77	0
56	MG	1D	314	1/1	0.87	0.22	44,44,44,44	0
56	MG	1A	3300	1/1	0.87	0.20	56,56,56,56	0
56	MG	2E	309	1/1	0.87	0.11	59,59,59,59	0
56	MG	1a	1698	1/1	0.87	0.23	66,66,66,66	0
56	MG	2V	201	1/1	0.87	0.24	60,60,60,60	0
56	MG	2A	3495	1/1	0.87	0.12	62,62,62,62	0
56	MG	2y	107	1/1	0.87	0.18	72,72,72,72	0
56	MG	28	103	1/1	0.88	0.26	54,54,54,54	0
56	MG	2A	3567	1/1	0.88	0.17	68,68,68,68	0
56	MG	2A	3308	1/1	0.88	0.29	61,61,61,61	0
56	MG	2A	3312	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3163	1/1	0.88	0.16	67,67,67,67	0
56	MG	2A	3316	1/1	0.88	0.14	61,61,61,61	0
56	MG	2A	3164	1/1	0.88	0.18	65,65,65,65	0
56	MG	1a	1709	1/1	0.88	0.46	70,70,70,70	0
56	MG	2A	3615	1/1	0.88	0.21	42,42,42,42	0
56	MG	2A	3324	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3638	1/1	0.88	0.24	66,66,66,66	0
56	MG	2a	1627	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	4080	1/1	0.88	0.28	43,43,43,43	0
56	MG	2A	3327	1/1	0.88	0.12	52,52,52,52	0
56	MG	1x	111	1/1	0.88	0.09	55,55,55,55	0
56	MG	1A	3732	1/1	0.88	0.11	24,24,24,24	0
56	MG	2A	3661	1/1	0.88	0.16	44,44,44,44	0
56	MG	2a	1643	1/1	0.88	0.16	70,70,70,70	0
56	MG	2A	3665	1/1	0.88	0.28	71,71,71,71	0
56	MG	2A	3189	1/1	0.88	0.20	52,52,52,52	0
56	MG	1A	3455	1/1	0.88	0.16	53,53,53,53	0
56	MG	1A	3182	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3352	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	4004	1/1	0.88	0.12	73,73,73,73	0
56	MG	2A	3355	1/1	0.88	0.23	64,64,64,64	0
56	MG	2a	1686	1/1	0.88	0.29	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3676	1/1	0.88	0.12	52,52,52,52	0
56	MG	2a	1692	1/1	0.88	0.27	68,68,68,68	0
56	MG	1A	3289	1/1	0.88	0.19	66,66,66,66	0
56	MG	18	106	1/1	0.88	0.10	74,74,74,74	0
56	MG	1A	3545	1/1	0.88	0.26	61,61,61,61	0
56	MG	2A	3022	1/1	0.88	0.31	62,62,62,62	0
56	MG	2A	3025	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3713	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3374	1/1	0.88	0.26	65,65,65,65	0
56	MG	2A	3388	1/1	0.88	0.20	55,55,55,55	0
56	MG	1B	225	1/1	0.88	0.11	58,58,58,58	0
56	MG	2a	1733	1/1	0.88	0.35	68,68,68,68	0
56	MG	2A	3042	1/1	0.88	0.33	60,60,60,60	0
56	MG	2A	3738	1/1	0.88	0.15	61,61,61,61	0
56	MG	2A	3400	1/1	0.88	0.13	68,68,68,68	0
56	MG	2A	3403	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	3788	1/1	0.88	0.09	17,17,17,17	0
56	MG	2a	1769	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3054	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3764	1/1	0.88	0.18	69,69,69,69	0
56	MG	2A	3767	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3425	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3433	1/1	0.88	0.26	61,61,61,61	0
56	MG	2A	3050	1/1	0.88	0.25	57,57,57,57	0
56	MG	2A	3053	1/1	0.88	0.18	61,61,61,61	0
56	MG	2a	1786	1/1	0.88	0.15	71,71,71,71	0
56	MG	2a	1789	1/1	0.88	0.20	78,78,78,78	0
56	MG	1A	3579	1/1	0.88	0.14	42,42,42,42	0
56	MG	1a	1641	1/1	0.88	0.24	63,63,63,63	0
56	MG	2A	3450	1/1	0.88	0.18	58,58,58,58	0
56	MG	1A	3948	1/1	0.88	0.07	41,41,41,41	0
56	MG	2A	3254	1/1	0.88	0.18	71,71,71,71	0
56	MG	2A	3807	1/1	0.88	0.14	45,45,45,45	0
56	MG	1A	3618	1/1	0.88	0.15	66,66,66,66	0
56	MG	1A	3163	1/1	0.88	0.20	56,56,56,56	0
56	MG	1a	1661	1/1	0.88	0.17	63,63,63,63	0
56	MG	2a	1816	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3822	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3827	1/1	0.88	0.10	51,51,51,51	0
56	MG	1A	3631	1/1	0.88	0.14	54,54,54,54	0
56	MG	2f	202	1/1	0.88	0.20	71,71,71,71	0
56	MG	2A	3098	1/1	0.88	0.10	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1670	1/1	0.88	0.11	59,59,59,59	0
56	MG	2A	3489	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	3835	1/1	0.88	0.12	54,54,54,54	0
56	MG	1A	3725	1/1	0.88	0.13	60,60,60,60	0
56	MG	2A	3282	1/1	0.88	0.21	63,63,63,63	0
56	MG	1A	3848	1/1	0.88	0.13	51,51,51,51	0
56	MG	1I	201	1/1	0.88	0.10	67,67,67,67	0
56	MG	1w	101	1/1	0.88	0.18	55,55,55,55	0
56	MG	2x	104	1/1	0.88	0.31	66,66,66,66	0
56	MG	1O	201	1/1	0.88	0.09	56,56,56,56	0
56	MG	2A	3296	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3297	1/1	0.88	0.16	62,62,62,62	0
56	MG	1Q	206	1/1	0.88	0.13	47,47,47,47	0
56	MG	2y	105	1/1	0.88	0.23	85,85,85,85	0
56	MG	1A	4076	1/1	0.88	0.24	76,76,76,76	0
56	MG	1a	1768	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	3770	1/1	0.89	0.10	35,35,35,35	0
56	MG	1A	3259	1/1	0.89	0.17	51,51,51,51	0
56	MG	1a	1772	1/1	0.89	0.21	71,71,71,71	0
56	MG	2A	3187	1/1	0.89	0.08	55,55,55,55	0
56	MG	2A	3407	1/1	0.89	0.22	56,56,56,56	0
56	MG	2A	3819	1/1	0.89	0.11	78,78,78,78	0
56	MG	2A	3410	1/1	0.89	0.21	54,54,54,54	0
56	MG	2A	3411	1/1	0.89	0.24	56,56,56,56	0
56	MG	1a	1780	1/1	0.89	0.14	51,51,51,51	0
56	MG	2A	3200	1/1	0.89	0.15	70,70,70,70	0
56	MG	2A	3204	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3842	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3426	1/1	0.89	0.12	62,62,62,62	0
56	MG	2B	202	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3430	1/1	0.89	0.34	61,61,61,61	0
56	MG	15	102	1/1	0.89	0.18	33,33,33,33	0
56	MG	1A	3682	1/1	0.89	0.11	24,24,24,24	0
56	MG	1A	3942	1/1	0.89	0.10	46,46,46,46	0
56	MG	2B	219	1/1	0.89	0.21	71,71,71,71	0
56	MG	19	101	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3943	1/1	0.89	0.14	70,70,70,70	0
56	MG	1A	3683	1/1	0.89	0.08	19,19,19,19	0
56	MG	2A	3457	1/1	0.89	0.14	53,53,53,53	0
56	MG	1A	4090	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3467	1/1	0.89	0.30	68,68,68,68	0
56	MG	2A	3469	1/1	0.89	0.10	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1612	1/1	0.89	0.09	63,63,63,63	0
56	MG	1l	201	1/1	0.89	0.15	59,59,59,59	0
56	MG	1a	1622	1/1	0.89	0.25	65,65,65,65	0
56	MG	1n	102	1/1	0.89	0.17	60,60,60,60	0
56	MG	1t	201	1/1	0.89	0.26	58,58,58,58	0
56	MG	1A	3262	1/1	0.89	0.18	60,60,60,60	0
56	MG	1a	1637	1/1	0.89	0.20	65,65,65,65	0
56	MG	1A	4096	1/1	0.89	0.26	59,59,59,59	0
56	MG	2a	1613	1/1	0.89	0.27	72,72,72,72	0
56	MG	2A	3238	1/1	0.89	0.16	53,53,53,53	0
56	MG	1B	202	1/1	0.89	0.16	45,45,45,45	0
56	MG	2A	3242	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3502	1/1	0.89	0.13	29,29,29,29	0
56	MG	2a	1622	1/1	0.89	0.16	73,73,73,73	0
56	MG	1a	1642	1/1	0.89	0.15	65,65,65,65	0
56	MG	2A	3250	1/1	0.89	0.11	65,65,65,65	0
56	MG	2a	1633	1/1	0.89	0.26	67,67,67,67	0
56	MG	2a	1634	1/1	0.89	0.32	67,67,67,67	0
56	MG	2A	3517	1/1	0.89	0.08	40,40,40,40	0
56	MG	2A	3252	1/1	0.89	0.34	64,64,64,64	0
56	MG	1a	1649	1/1	0.89	0.21	61,61,61,61	0
56	MG	2A	3529	1/1	0.89	0.14	42,42,42,42	0
56	MG	2A	3534	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3807	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3811	1/1	0.89	0.10	26,26,26,26	0
56	MG	1A	3959	1/1	0.89	0.16	66,66,66,66	0
56	MG	2A	3264	1/1	0.89	0.28	71,71,71,71	0
56	MG	2a	1655	1/1	0.89	0.25	67,67,67,67	0
56	MG	2a	1657	1/1	0.89	0.17	64,64,64,64	0
56	MG	2a	1659	1/1	0.89	0.17	69,69,69,69	0
56	MG	1A	3539	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3817	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3582	1/1	0.89	0.16	65,65,65,65	0
56	MG	2a	1681	1/1	0.89	0.21	50,50,50,50	0
56	MG	1a	1665	1/1	0.89	0.17	64,64,64,64	0
56	MG	2A	3586	1/1	0.89	0.19	66,66,66,66	0
56	MG	1a	1667	1/1	0.89	0.27	58,58,58,58	0
56	MG	2a	1693	1/1	0.89	0.20	59,59,59,59	0
56	MG	1B	223	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3702	1/1	0.89	0.19	55,55,55,55	0
56	MG	2A	3605	1/1	0.89	0.12	42,42,42,42	0
56	MG	2A	3019	1/1	0.89	0.37	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3608	1/1	0.89	0.13	74,74,74,74	0
56	MG	2a	1710	1/1	0.89	0.20	76,76,76,76	0
56	MG	1a	1671	1/1	0.89	0.11	56,56,56,56	0
56	MG	2A	3283	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	3542	1/1	0.89	0.14	63,63,63,63	0
56	MG	2a	1721	1/1	0.89	0.23	55,55,55,55	0
56	MG	1A	3825	1/1	0.89	0.14	47,47,47,47	0
56	MG	1B	231	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	3498	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3707	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	4001	1/1	0.89	0.11	45,45,45,45	0
56	MG	1a	1693	1/1	0.89	0.25	52,52,52,52	0
56	MG	2a	1754	1/1	0.89	0.17	70,70,70,70	0
56	MG	2a	1761	1/1	0.89	0.13	54,54,54,54	0
56	MG	2A	3663	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1697	1/1	0.89	0.27	64,64,64,64	0
56	MG	1A	3171	1/1	0.89	0.10	44,44,44,44	0
56	MG	1a	1700	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3716	1/1	0.89	0.12	53,53,53,53	0
56	MG	2A	3681	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3041	1/1	0.89	0.23	56,56,56,56	0
56	MG	2A	3318	1/1	0.89	0.29	66,66,66,66	0
56	MG	1A	3573	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3634	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3695	1/1	0.89	0.17	40,40,40,40	0
56	MG	2A	3322	1/1	0.89	0.11	49,49,49,49	0
56	MG	2A	3323	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3092	1/1	0.89	0.12	64,64,64,64	0
56	MG	2a	1798	1/1	0.89	0.16	68,68,68,68	0
56	MG	2a	1801	1/1	0.89	0.11	68,68,68,68	0
56	MG	2A	3700	1/1	0.89	0.24	60,60,60,60	0
56	MG	2A	3095	1/1	0.89	0.20	60,60,60,60	0
56	MG	1G	202	1/1	0.89	0.18	59,59,59,59	0
56	MG	1G	203	1/1	0.89	0.09	69,69,69,69	0
56	MG	1A	3062	1/1	0.89	0.17	67,67,67,67	0
56	MG	2A	3101	1/1	0.89	0.27	70,70,70,70	0
56	MG	1A	3053	1/1	0.89	0.15	48,48,48,48	0
56	MG	2a	1817	1/1	0.89	0.18	50,50,50,50	0
56	MG	1A	4039	1/1	0.89	0.15	61,61,61,61	0
56	MG	2A	3729	1/1	0.89	0.20	54,54,54,54	0
56	MG	2A	3343	1/1	0.89	0.15	67,67,67,67	0
56	MG	2A	3344	1/1	0.89	0.09	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3758	1/1	0.89	0.11	45,45,45,45	0
56	MG	2A	3749	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3331	1/1	0.89	0.16	54,54,54,54	0
56	MG	1A	3906	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3758	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	4068	1/1	0.89	0.09	49,49,49,49	0
56	MG	1A	3913	1/1	0.89	0.10	64,64,64,64	0
56	MG	2A	3147	1/1	0.89	0.25	49,49,49,49	0
56	MG	2A	3769	1/1	0.89	0.12	70,70,70,70	0
56	MG	1a	1759	1/1	0.89	0.22	66,66,66,66	0
56	MG	2A	3779	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3370	1/1	0.89	0.16	67,67,67,67	0
56	MG	1a	1761	1/1	0.89	0.12	50,50,50,50	0
56	MG	2A	3787	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3915	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3172	1/1	0.89	0.22	51,51,51,51	0
56	MG	1A	3938	1/1	0.90	0.12	63,63,63,63	0
56	MG	1A	3341	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3838	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	3429	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3635	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3799	1/1	0.90	0.15	58,58,58,58	0
56	MG	1x	107	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3644	1/1	0.90	0.16	46,46,46,46	0
56	MG	2A	3248	1/1	0.90	0.13	57,57,57,57	0
56	MG	2B	213	1/1	0.90	0.16	66,66,66,66	0
56	MG	1A	3536	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3656	1/1	0.90	0.09	40,40,40,40	0
56	MG	1A	3431	1/1	0.90	0.09	44,44,44,44	0
56	MG	1A	3342	1/1	0.90	0.14	33,33,33,33	0
56	MG	2E	307	1/1	0.90	0.17	53,53,53,53	0
56	MG	1B	224	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3437	1/1	0.90	0.14	51,51,51,51	0
56	MG	2Q	203	1/1	0.90	0.09	64,64,64,64	0
56	MG	2R	201	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3009	1/1	0.90	0.20	46,46,46,46	0
56	MG	1A	3976	1/1	0.90	0.10	26,26,26,26	0
56	MG	1A	3442	1/1	0.90	0.18	36,36,36,36	0
56	MG	2A	3015	1/1	0.90	0.37	69,69,69,69	0
56	MG	25	102	1/1	0.90	0.15	50,50,50,50	0
56	MG	25	104	1/1	0.90	0.23	53,53,53,53	0
56	MG	1A	3354	1/1	0.90	0.16	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1602	1/1	0.90	0.18	73,73,73,73	0
56	MG	1A	3987	1/1	0.90	0.26	40,40,40,40	0
56	MG	1a	1678	1/1	0.90	0.16	60,60,60,60	0
56	MG	2A	3528	1/1	0.90	0.16	59,59,59,59	0
56	MG	1A	3299	1/1	0.90	0.18	55,55,55,55	0
56	MG	2A	3032	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3037	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3699	1/1	0.90	0.14	44,44,44,44	0
56	MG	1a	1684	1/1	0.90	0.39	63,63,63,63	0
56	MG	1A	3831	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	3246	1/1	0.90	0.22	67,67,67,67	0
56	MG	2A	3566	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3294	1/1	0.90	0.24	59,59,59,59	0
56	MG	1A	4005	1/1	0.90	0.11	73,73,73,73	0
56	MG	2A	3584	1/1	0.90	0.15	50,50,50,50	0
56	MG	2a	1630	1/1	0.90	0.25	54,54,54,54	0
56	MG	1A	3583	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	4007	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3070	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3584	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3309	1/1	0.90	0.10	59,59,59,59	0
56	MG	1a	1706	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3313	1/1	0.90	0.14	61,61,61,61	0
56	MG	2A	3314	1/1	0.90	0.13	63,63,63,63	0
56	MG	2a	1647	1/1	0.90	0.27	64,64,64,64	0
56	MG	1A	3850	1/1	0.90	0.19	66,66,66,66	0
56	MG	1A	3858	1/1	0.90	0.09	35,35,35,35	0
56	MG	1A	3866	1/1	0.90	0.13	44,44,44,44	0
56	MG	2A	3632	1/1	0.90	0.11	73,73,73,73	0
56	MG	2A	3635	1/1	0.90	0.23	70,70,70,70	0
56	MG	2a	1658	1/1	0.90	0.22	44,44,44,44	0
56	MG	1N	205	1/1	0.90	0.24	62,62,62,62	0
56	MG	2a	1663	1/1	0.90	0.21	54,54,54,54	0
56	MG	2a	1669	1/1	0.90	0.18	61,61,61,61	0
56	MG	1a	1715	1/1	0.90	0.20	62,62,62,62	0
56	MG	2A	3645	1/1	0.90	0.16	57,57,57,57	0
56	MG	2A	3647	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3872	1/1	0.90	0.10	35,35,35,35	0
56	MG	1O	205	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	4035	1/1	0.90	0.10	65,65,65,65	0
56	MG	2a	1691	1/1	0.90	0.49	65,65,65,65	0
56	MG	1S	201	1/1	0.90	0.34	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3362	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3328	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3364	1/1	0.90	0.09	45,45,45,45	0
56	MG	1W	203	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3673	1/1	0.90	0.18	58,58,58,58	0
56	MG	2a	1705	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3115	1/1	0.90	0.14	73,73,73,73	0
56	MG	2a	1708	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3179	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3682	1/1	0.90	0.16	66,66,66,66	0
56	MG	2a	1715	1/1	0.90	0.27	59,59,59,59	0
56	MG	1X	106	1/1	0.90	0.07	32,32,32,32	0
56	MG	2A	3342	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	4046	1/1	0.90	0.12	55,55,55,55	0
56	MG	2a	1726	1/1	0.90	0.22	77,77,77,77	0
56	MG	2a	1727	1/1	0.90	0.20	55,55,55,55	0
56	MG	2A	3137	1/1	0.90	0.22	65,65,65,65	0
56	MG	2A	3351	1/1	0.90	0.20	73,73,73,73	0
56	MG	2a	1734	1/1	0.90	0.35	65,65,65,65	0
56	MG	1a	1755	1/1	0.90	0.12	64,64,64,64	0
56	MG	1Z	301	1/1	0.90	0.16	59,59,59,59	0
56	MG	2a	1743	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3588	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3357	1/1	0.90	0.23	64,64,64,64	0
56	MG	2a	1751	1/1	0.90	0.10	41,41,41,41	0
56	MG	1A	4060	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3709	1/1	0.90	0.09	56,56,56,56	0
56	MG	2a	1762	1/1	0.90	0.11	70,70,70,70	0
56	MG	2A	3711	1/1	0.90	0.19	58,58,58,58	0
56	MG	2a	1764	1/1	0.90	0.14	64,64,64,64	0
56	MG	1A	4064	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3364	1/1	0.90	0.28	71,71,71,71	0
56	MG	2A	3717	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3170	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3379	1/1	0.90	0.18	76,76,76,76	0
56	MG	15	105	1/1	0.90	0.23	55,55,55,55	0
56	MG	15	110	1/1	0.90	0.08	55,55,55,55	0
56	MG	1a	1775	1/1	0.90	0.24	50,50,50,50	0
56	MG	1A	3325	1/1	0.90	0.16	51,51,51,51	0
56	MG	2a	1788	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3594	1/1	0.90	0.22	51,51,51,51	0
56	MG	2a	1791	1/1	0.90	0.12	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1782	1/1	0.90	0.12	57,57,57,57	0
56	MG	2A	3746	1/1	0.90	0.20	59,59,59,59	0
56	MG	1A	3069	1/1	0.90	0.10	49,49,49,49	0
56	MG	2A	3393	1/1	0.90	0.15	73,73,73,73	0
56	MG	2A	3397	1/1	0.90	0.13	63,63,63,63	0
56	MG	2A	3202	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3600	1/1	0.90	0.09	29,29,29,29	0
56	MG	2A	3404	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1793	1/1	0.90	0.12	77,77,77,77	0
56	MG	1A	3917	1/1	0.90	0.15	52,52,52,52	0
56	MG	2A	3770	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3777	1/1	0.90	0.12	68,68,68,68	0
56	MG	1A	3242	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	4078	1/1	0.90	0.17	51,51,51,51	0
56	MG	2a	1822	1/1	0.90	0.29	68,68,68,68	0
56	MG	2A	3416	1/1	0.90	0.36	54,54,54,54	0
56	MG	2A	3211	1/1	0.90	0.24	67,67,67,67	0
56	MG	2A	3212	1/1	0.90	0.20	64,64,64,64	0
56	MG	2g	201	1/1	0.90	0.23	72,72,72,72	0
56	MG	2A	3788	1/1	0.90	0.10	69,69,69,69	0
56	MG	1A	3417	1/1	0.90	0.20	56,56,56,56	0
56	MG	2q	203	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	4084	1/1	0.90	0.16	46,46,46,46	0
56	MG	1f	202	1/1	0.90	0.17	63,63,63,63	0
56	MG	1a	1627	1/1	0.90	0.20	46,46,46,46	0
56	MG	2w	102	1/1	0.90	0.16	82,82,82,82	0
56	MG	2A	3437	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3440	1/1	0.90	0.27	56,56,56,56	0
56	MG	2w	105	1/1	0.90	0.11	76,76,76,76	0
56	MG	2A	3808	1/1	0.90	0.08	48,48,48,48	0
56	MG	1a	1632	1/1	0.90	0.18	60,60,60,60	0
56	MG	1a	1635	1/1	0.90	0.24	75,75,75,75	0
56	MG	2A	3446	1/1	0.90	0.27	61,61,61,61	0
56	MG	1A	3207	1/1	0.90	0.09	56,56,56,56	0
56	MG	1a	1638	1/1	0.90	0.34	66,66,66,66	0
56	MG	2A	3824	1/1	0.90	0.08	50,50,50,50	0
56	MG	2A	3454	1/1	0.90	0.20	42,42,42,42	0
56	MG	2y	106	1/1	0.90	0.26	64,64,64,64	0
56	MG	2A	3834	1/1	0.90	0.09	55,55,55,55	0
59	ZN	14	102	1/1	0.90	0.17	134,134,134,134	0
56	MG	1A	4036	1/1	0.91	0.10	75,75,75,75	0
56	MG	1A	4037	1/1	0.91	0.09	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3841	1/1	0.91	0.19	61,61,61,61	0
56	MG	2A	3219	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3220	1/1	0.91	0.25	64,64,64,64	0
56	MG	10	102	1/1	0.91	0.11	58,58,58,58	0
56	MG	2B	204	1/1	0.91	0.16	66,66,66,66	0
56	MG	10	107	1/1	0.91	0.16	59,59,59,59	0
56	MG	1a	1796	1/1	0.91	0.10	66,66,66,66	0
56	MG	2A	3228	1/1	0.91	0.23	60,60,60,60	0
56	MG	1A	3015	1/1	0.91	0.11	38,38,38,38	0
56	MG	2B	214	1/1	0.91	0.08	74,74,74,74	0
56	MG	2A	3472	1/1	0.91	0.12	46,46,46,46	0
56	MG	2B	217	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	4041	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	4042	1/1	0.91	0.14	38,38,38,38	0
56	MG	1A	3462	1/1	0.91	0.12	56,56,56,56	0
56	MG	2E	306	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3466	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	3212	1/1	0.91	0.07	37,37,37,37	0
56	MG	2F	301	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	4057	1/1	0.91	0.10	50,50,50,50	0
56	MG	2N	201	1/1	0.91	0.15	75,75,75,75	0
56	MG	2O	201	1/1	0.91	0.18	65,65,65,65	0
56	MG	1A	3877	1/1	0.91	0.09	42,42,42,42	0
56	MG	1A	3883	1/1	0.91	0.08	25,25,25,25	0
56	MG	2U	201	1/1	0.91	0.08	60,60,60,60	0
56	MG	1A	4061	1/1	0.91	0.13	50,50,50,50	0
56	MG	1A	3885	1/1	0.91	0.19	70,70,70,70	0
56	MG	2Z	301	1/1	0.91	0.10	77,77,77,77	0
56	MG	1w	102	1/1	0.91	0.24	68,68,68,68	0
56	MG	20	103	1/1	0.91	0.19	56,56,56,56	0
56	MG	1A	4066	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3102	1/1	0.91	0.12	65,65,65,65	0
56	MG	2A	3513	1/1	0.91	0.12	49,49,49,49	0
56	MG	27	102	1/1	0.91	0.18	58,58,58,58	0
56	MG	28	102	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3515	1/1	0.91	0.10	37,37,37,37	0
56	MG	1w	106	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3519	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3374	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3104	1/1	0.91	0.21	42,42,42,42	0
56	MG	2a	1606	1/1	0.91	0.18	56,56,56,56	0
56	MG	2A	3526	1/1	0.91	0.13	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	101	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3324	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3730	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	4073	1/1	0.91	0.09	52,52,52,52	0
56	MG	2A	3543	1/1	0.91	0.14	38,38,38,38	0
56	MG	1a	1639	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3277	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3279	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	1624	1/1	0.91	0.12	63,63,63,63	0
56	MG	2A	3554	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3595	1/1	0.91	0.07	28,28,28,28	0
56	MG	1A	3115	1/1	0.91	0.22	40,40,40,40	0
56	MG	2a	1632	1/1	0.91	0.33	60,60,60,60	0
56	MG	2A	3001	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3508	1/1	0.91	0.21	37,37,37,37	0
56	MG	1a	1643	1/1	0.91	0.22	56,56,56,56	0
56	MG	1a	1646	1/1	0.91	0.15	54,54,54,54	0
56	MG	1a	1648	1/1	0.91	0.37	61,61,61,61	0
56	MG	2a	1640	1/1	0.91	0.15	60,60,60,60	0
56	MG	2A	3590	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3592	1/1	0.91	0.17	63,63,63,63	0
56	MG	1A	3749	1/1	0.91	0.08	20,20,20,20	0
56	MG	1A	4082	1/1	0.91	0.10	36,36,36,36	0
56	MG	1A	3750	1/1	0.91	0.13	44,44,44,44	0
56	MG	2a	1649	1/1	0.91	0.24	71,71,71,71	0
56	MG	2A	3298	1/1	0.91	0.16	58,58,58,58	0
56	MG	2a	1652	1/1	0.91	0.27	57,57,57,57	0
56	MG	1A	3752	1/1	0.91	0.10	22,22,22,22	0
56	MG	2A	3607	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3601	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3307	1/1	0.91	0.23	70,70,70,70	0
56	MG	1A	3939	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3621	1/1	0.91	0.14	38,38,38,38	0
56	MG	2a	1668	1/1	0.91	0.24	54,54,54,54	0
56	MG	2A	3629	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3131	1/1	0.91	0.17	43,43,43,43	0
56	MG	1a	1666	1/1	0.91	0.18	64,64,64,64	0
56	MG	2a	1674	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3327	1/1	0.91	0.19	62,62,62,62	0
56	MG	2A	3637	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3945	1/1	0.91	0.10	41,41,41,41	0
56	MG	2a	1689	1/1	0.91	0.21	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3142	1/1	0.91	0.11	50,50,50,50	0
56	MG	2A	3641	1/1	0.91	0.23	65,65,65,65	0
56	MG	2A	3642	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3643	1/1	0.91	0.16	63,63,63,63	0
56	MG	1A	3630	1/1	0.91	0.09	48,48,48,48	0
56	MG	2a	1697	1/1	0.91	0.34	67,67,67,67	0
56	MG	2a	1699	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	3953	1/1	0.91	0.06	44,44,44,44	0
56	MG	1A	3332	1/1	0.91	0.15	52,52,52,52	0
56	MG	1a	1675	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3061	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3660	1/1	0.91	0.17	68,68,68,68	0
56	MG	2A	3063	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3067	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3664	1/1	0.91	0.19	66,66,66,66	0
56	MG	1A	3632	1/1	0.91	0.10	22,22,22,22	0
56	MG	1A	3531	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3074	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3670	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3960	1/1	0.91	0.13	66,66,66,66	0
56	MG	2A	3674	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3962	1/1	0.91	0.10	73,73,73,73	0
56	MG	2a	1731	1/1	0.91	0.33	67,67,67,67	0
56	MG	2A	3337	1/1	0.91	0.22	61,61,61,61	0
56	MG	1A	3254	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3339	1/1	0.91	0.20	71,71,71,71	0
56	MG	2a	1739	1/1	0.91	0.22	71,71,71,71	0
56	MG	1a	1690	1/1	0.91	0.25	46,46,46,46	0
56	MG	2a	1742	1/1	0.91	0.07	74,74,74,74	0
56	MG	1A	3641	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3968	1/1	0.91	0.12	71,71,71,71	0
56	MG	2A	3691	1/1	0.91	0.23	65,65,65,65	0
56	MG	1A	3340	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3648	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3537	1/1	0.91	0.23	60,60,60,60	0
56	MG	1a	1705	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3981	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1708	1/1	0.91	0.14	70,70,70,70	0
56	MG	2a	1767	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3198	1/1	0.91	0.08	43,43,43,43	0
56	MG	2a	1773	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3824	1/1	0.91	0.10	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3658	1/1	0.91	0.09	25,25,25,25	0
56	MG	1F	313	1/1	0.91	0.15	35,35,35,35	0
56	MG	1A	3151	1/1	0.91	0.13	41,41,41,41	0
56	MG	2a	1779	1/1	0.91	0.11	82,82,82,82	0
56	MG	2A	3366	1/1	0.91	0.10	70,70,70,70	0
56	MG	2A	3367	1/1	0.91	0.12	56,56,56,56	0
56	MG	1a	1719	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3369	1/1	0.91	0.13	69,69,69,69	0
56	MG	2A	3132	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3993	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1721	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3740	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3741	1/1	0.91	0.17	59,59,59,59	0
56	MG	1G	204	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3376	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3386	1/1	0.91	0.22	62,62,62,62	0
56	MG	1A	3264	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3829	1/1	0.91	0.15	59,59,59,59	0
56	MG	1A	3443	1/1	0.91	0.11	50,50,50,50	0
56	MG	2a	1808	1/1	0.91	0.24	56,56,56,56	0
56	MG	2a	1810	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3392	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3270	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3395	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3396	1/1	0.91	0.18	74,74,74,74	0
56	MG	1A	3836	1/1	0.91	0.11	64,64,64,64	0
56	MG	2A	3774	1/1	0.91	0.09	62,62,62,62	0
56	MG	2A	3398	1/1	0.91	0.12	61,61,61,61	0
56	MG	1Q	205	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3178	1/1	0.91	0.13	50,50,50,50	0
56	MG	2A	3780	1/1	0.91	0.11	70,70,70,70	0
56	MG	1A	3450	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3783	1/1	0.91	0.10	55,55,55,55	0
56	MG	1R	201	1/1	0.91	0.10	45,45,45,45	0
56	MG	2I	205	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3408	1/1	0.91	0.27	47,47,47,47	0
56	MG	2A	3409	1/1	0.91	0.24	47,47,47,47	0
56	MG	1a	1752	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3794	1/1	0.91	0.20	60,60,60,60	0
56	MG	1A	3839	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3412	1/1	0.91	0.25	45,45,45,45	0
56	MG	1A	4012	1/1	0.91	0.12	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3288	1/1	0.91	0.17	48,48,48,48	0
56	MG	1T	201	1/1	0.91	0.10	73,73,73,73	0
56	MG	1V	201	1/1	0.91	0.17	37,37,37,37	0
56	MG	1V	206	1/1	0.91	0.09	56,56,56,56	0
56	MG	1A	3580	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3432	1/1	0.91	0.28	62,62,62,62	0
56	MG	1A	3855	1/1	0.91	0.15	68,68,68,68	0
56	MG	1A	4024	1/1	0.91	0.08	31,31,31,31	0
56	MG	2y	104	1/1	0.91	0.13	81,81,81,81	0
56	MG	1a	1778	1/1	0.91	0.11	46,46,46,46	0
56	MG	1a	1779	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	4030	1/1	0.91	0.14	34,34,34,34	0
56	MG	1A	3456	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3497	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	3432	1/1	0.92	0.17	51,51,51,51	0
56	MG	2D	308	1/1	0.92	0.09	60,60,60,60	0
56	MG	1x	112	1/1	0.92	0.20	59,59,59,59	0
56	MG	2A	3265	1/1	0.92	0.25	59,59,59,59	0
56	MG	1A	4011	1/1	0.92	0.17	61,61,61,61	0
56	MG	2E	308	1/1	0.92	0.11	42,42,42,42	0
56	MG	1E	306	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3741	1/1	0.92	0.10	59,59,59,59	0
56	MG	2F	303	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3880	1/1	0.92	0.11	22,22,22,22	0
56	MG	1F	303	1/1	0.92	0.15	55,55,55,55	0
56	MG	1F	304	1/1	0.92	0.29	71,71,71,71	0
56	MG	2Q	201	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	4016	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	4019	1/1	0.92	0.14	54,54,54,54	0
56	MG	2R	202	1/1	0.92	0.19	49,49,49,49	0
56	MG	1a	1680	1/1	0.92	0.18	67,67,67,67	0
56	MG	1F	314	1/1	0.92	0.10	65,65,65,65	0
56	MG	2W	201	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3014	1/1	0.92	0.20	66,66,66,66	0
56	MG	1a	1682	1/1	0.92	0.19	63,63,63,63	0
56	MG	1A	3335	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3368	1/1	0.92	0.14	47,47,47,47	0
56	MG	2I	101	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3107	1/1	0.92	0.25	50,50,50,50	0
56	MG	1A	4026	1/1	0.92	0.08	55,55,55,55	0
56	MG	2A	3558	1/1	0.92	0.15	62,62,62,62	0
56	MG	25	106	1/1	0.92	0.27	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3890	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3372	1/1	0.92	0.10	46,46,46,46	0
56	MG	1a	1694	1/1	0.92	0.27	53,53,53,53	0
56	MG	2A	3578	1/1	0.92	0.11	75,75,75,75	0
56	MG	2A	3579	1/1	0.92	0.18	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.26	54,54,54,54	0
56	MG	2A	3301	1/1	0.92	0.12	48,48,48,48	0
56	MG	1N	206	1/1	0.92	0.07	53,53,53,53	0
56	MG	2A	3046	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3757	1/1	0.92	0.11	24,24,24,24	0
56	MG	2A	3591	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3028	1/1	0.92	0.12	63,63,63,63	0
56	MG	1a	1702	1/1	0.92	0.21	51,51,51,51	0
56	MG	2A	3598	1/1	0.92	0.14	63,63,63,63	0
56	MG	1a	1703	1/1	0.92	0.06	43,43,43,43	0
56	MG	1P	205	1/1	0.92	0.16	42,42,42,42	0
56	MG	2A	3064	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3065	1/1	0.92	0.17	67,67,67,67	0
56	MG	2a	1626	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3317	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3376	1/1	0.92	0.24	39,39,39,39	0
56	MG	1A	3766	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3640	1/1	0.92	0.06	25,25,25,25	0
56	MG	1A	3453	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3627	1/1	0.92	0.15	60,60,60,60	0
56	MG	2A	3628	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3543	1/1	0.92	0.07	63,63,63,63	0
56	MG	2a	1637	1/1	0.92	0.22	55,55,55,55	0
56	MG	1a	1713	1/1	0.92	0.24	49,49,49,49	0
56	MG	1A	3290	1/1	0.92	0.18	71,71,71,71	0
56	MG	1A	3791	1/1	0.92	0.09	56,56,56,56	0
56	MG	1a	1718	1/1	0.92	0.11	58,58,58,58	0
56	MG	2a	1645	1/1	0.92	0.24	62,62,62,62	0
56	MG	1A	3793	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3297	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3655	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3395	1/1	0.92	0.32	40,40,40,40	0
56	MG	1a	1727	1/1	0.92	0.19	58,58,58,58	0
56	MG	1A	3944	1/1	0.92	0.13	69,69,69,69	0
56	MG	2A	3107	1/1	0.92	0.19	70,70,70,70	0
56	MG	1a	1731	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3558	1/1	0.92	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3654	1/1	0.92	0.10	59,59,59,59	0
56	MG	1A	3946	1/1	0.92	0.11	45,45,45,45	0
56	MG	2a	1660	1/1	0.92	0.07	59,59,59,59	0
56	MG	2A	3346	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3350	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3947	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3118	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3662	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3816	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3123	1/1	0.92	0.26	57,57,57,57	0
56	MG	2a	1679	1/1	0.92	0.11	64,64,64,64	0
56	MG	2A	3360	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3671	1/1	0.92	0.17	50,50,50,50	0
56	MG	10	103	1/1	0.92	0.11	40,40,40,40	0
56	MG	2A	3125	1/1	0.92	0.36	67,67,67,67	0
56	MG	2A	3675	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3130	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3131	1/1	0.92	0.27	82,82,82,82	0
56	MG	1a	1748	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3683	1/1	0.92	0.10	56,56,56,56	0
56	MG	2a	1698	1/1	0.92	0.16	60,60,60,60	0
56	MG	10	104	1/1	0.92	0.16	58,58,58,58	0
56	MG	10	106	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3145	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3146	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3461	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3399	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3155	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3156	1/1	0.92	0.21	59,59,59,59	0
56	MG	2A	3379	1/1	0.92	0.15	71,71,71,71	0
56	MG	2A	3384	1/1	0.92	0.18	66,66,66,66	0
56	MG	2A	3161	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3706	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3821	1/1	0.92	0.25	60,60,60,60	0
56	MG	2a	1722	1/1	0.92	0.21	55,55,55,55	0
56	MG	1a	1762	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	4077	1/1	0.92	0.07	53,53,53,53	0
56	MG	2a	1728	1/1	0.92	0.29	50,50,50,50	0
56	MG	1a	1766	1/1	0.92	0.14	58,58,58,58	0
56	MG	2A	3175	1/1	0.92	0.12	48,48,48,48	0
56	MG	2a	1732	1/1	0.92	0.18	62,62,62,62	0
56	MG	1A	3406	1/1	0.92	0.23	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3177	1/1	0.92	0.40	56,56,56,56	0
56	MG	1a	1769	1/1	0.92	0.10	68,68,68,68	0
56	MG	16	101	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3472	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3733	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3348	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3185	1/1	0.92	0.23	62,62,62,62	0
56	MG	2A	3405	1/1	0.92	0.24	63,63,63,63	0
56	MG	2a	1750	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	1773	1/1	0.92	0.12	58,58,58,58	0
56	MG	2A	3743	1/1	0.92	0.16	43,43,43,43	0
56	MG	2a	1758	1/1	0.92	0.18	69,69,69,69	0
56	MG	1A	3684	1/1	0.92	0.09	26,26,26,26	0
56	MG	2A	3190	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3747	1/1	0.92	0.08	71,71,71,71	0
56	MG	1a	1776	1/1	0.92	0.17	57,57,57,57	0
56	MG	1A	4086	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3485	1/1	0.92	0.09	49,49,49,49	0
56	MG	2a	1771	1/1	0.92	0.19	69,69,69,69	0
56	MG	2a	1772	1/1	0.92	0.11	68,68,68,68	0
56	MG	2A	3413	1/1	0.92	0.17	36,36,36,36	0
56	MG	2A	3763	1/1	0.92	0.16	64,64,64,64	0
56	MG	2A	3205	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	4088	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3419	1/1	0.92	0.25	62,62,62,62	0
56	MG	1a	1610	1/1	0.92	0.19	65,65,65,65	0
56	MG	2A	3423	1/1	0.92	0.28	63,63,63,63	0
56	MG	2A	3772	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3773	1/1	0.92	0.08	55,55,55,55	0
56	MG	1A	4089	1/1	0.92	0.13	53,53,53,53	0
56	MG	1a	1614	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3427	1/1	0.92	0.29	60,60,60,60	0
56	MG	2A	3429	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3412	1/1	0.92	0.17	69,69,69,69	0
56	MG	2A	3431	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3782	1/1	0.92	0.16	65,65,65,65	0
56	MG	2a	1797	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3349	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	1799	1/1	0.92	0.16	73,73,73,73	0
56	MG	1A	3972	1/1	0.92	0.15	54,54,54,54	0
56	MG	1a	1629	1/1	0.92	0.27	63,63,63,63	0
56	MG	2a	1803	1/1	0.92	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3252	1/1	0.92	0.17	57,57,57,57	0
56	MG	2a	1806	1/1	0.92	0.18	80,80,80,80	0
56	MG	1A	3328	1/1	0.92	0.16	49,49,49,49	0
56	MG	1a	1802	1/1	0.92	0.07	60,60,60,60	0
56	MG	2A	3443	1/1	0.92	0.30	54,54,54,54	0
56	MG	1a	1636	1/1	0.92	0.11	51,51,51,51	0
56	MG	1B	210	1/1	0.92	0.17	41,41,41,41	0
56	MG	1e	202	1/1	0.92	0.09	64,64,64,64	0
56	MG	1A	3501	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3426	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3456	1/1	0.92	0.27	67,67,67,67	0
56	MG	2A	3229	1/1	0.92	0.30	55,55,55,55	0
56	MG	1A	3844	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3461	1/1	0.92	0.20	72,72,72,72	0
56	MG	2A	3463	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3823	1/1	0.92	0.07	47,47,47,47	0
56	MG	2A	3466	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3205	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3309	1/1	0.92	0.32	57,57,57,57	0
56	MG	2q	201	1/1	0.92	0.27	69,69,69,69	0
56	MG	1A	3598	1/1	0.92	0.10	30,30,30,30	0
56	MG	2t	201	1/1	0.92	0.21	60,60,60,60	0
56	MG	1A	3997	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3517	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3840	1/1	0.92	0.12	70,70,70,70	0
56	MG	2A	3241	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3363	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3845	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3867	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3869	1/1	0.92	0.15	61,61,61,61	0
56	MG	2x	101	1/1	0.92	0.18	60,60,60,60	0
56	MG	2B	203	1/1	0.92	0.25	63,63,63,63	0
56	MG	1A	3520	1/1	0.92	0.10	53,53,53,53	0
56	MG	1B	234	1/1	0.92	0.09	70,70,70,70	0
56	MG	2B	208	1/1	0.92	0.20	56,56,56,56	0
56	MG	2A	3487	1/1	0.92	0.13	61,61,61,61	0
56	MG	1D	310	1/1	0.92	0.18	47,47,47,47	0
56	MG	2B	212	1/1	0.92	0.18	76,76,76,76	0
56	MG	1A	3734	1/1	0.92	0.06	41,41,41,41	0
56	MG	2A	3492	1/1	0.92	0.13	56,56,56,56	0
56	MG	1x	109	1/1	0.92	0.20	65,65,65,65	0
58	WC9	1A	4098	34/34	0.92	0.12	27,38,47,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3496	1/1	0.92	0.08	52,52,52,52	0
59	ZN	24	501	1/1	0.92	0.19	142,142,142,142	0
56	MG	2A	3500	1/1	0.93	0.11	35,35,35,35	0
56	MG	1A	3926	1/1	0.93	0.13	63,63,63,63	0
56	MG	1A	3036	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3387	1/1	0.93	0.16	26,26,26,26	0
56	MG	1a	1647	1/1	0.93	0.12	52,52,52,52	0
56	MG	2A	3259	1/1	0.93	0.15	55,55,55,55	0
56	MG	2F	305	1/1	0.93	0.08	42,42,42,42	0
56	MG	2G	201	1/1	0.93	0.17	67,67,67,67	0
56	MG	1x	103	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3262	1/1	0.93	0.14	56,56,56,56	0
56	MG	2P	202	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3934	1/1	0.93	0.08	65,65,65,65	0
56	MG	2Q	202	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3747	1/1	0.93	0.17	49,49,49,49	0
56	MG	1a	1651	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3112	1/1	0.93	0.14	35,35,35,35	0
56	MG	2T	202	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3481	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3270	1/1	0.93	0.15	59,59,59,59	0
56	MG	1a	1659	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3016	1/1	0.93	0.30	57,57,57,57	0
56	MG	1B	214	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3597	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3488	1/1	0.93	0.08	62,62,62,62	0
56	MG	1A	3400	1/1	0.93	0.13	55,55,55,55	0
56	MG	23	102	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3763	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3402	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3562	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3284	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3285	1/1	0.93	0.22	64,64,64,64	0
56	MG	28	101	1/1	0.93	0.25	58,58,58,58	0
56	MG	2A	3573	1/1	0.93	0.12	61,61,61,61	0
56	MG	1a	1669	1/1	0.93	0.15	65,65,65,65	0
56	MG	2A	3287	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3288	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3949	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3607	1/1	0.93	0.07	24,24,24,24	0
56	MG	1A	3776	1/1	0.93	0.06	30,30,30,30	0
56	MG	2A	3589	1/1	0.93	0.13	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3293	1/1	0.93	0.24	55,55,55,55	0
56	MG	1B	227	1/1	0.93	0.09	41,41,41,41	0
56	MG	2a	1612	1/1	0.93	0.34	69,69,69,69	0
56	MG	1a	1674	1/1	0.93	0.21	62,62,62,62	0
56	MG	1A	3955	1/1	0.93	0.12	43,43,43,43	0
56	MG	2a	1616	1/1	0.93	0.14	67,67,67,67	0
56	MG	1A	3088	1/1	0.93	0.17	50,50,50,50	0
56	MG	2A	3599	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3408	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3034	1/1	0.93	0.14	60,60,60,60	0
56	MG	2a	1623	1/1	0.93	0.18	64,64,64,64	0
56	MG	2A	3603	1/1	0.93	0.16	46,46,46,46	0
56	MG	2a	1625	1/1	0.93	0.19	58,58,58,58	0
56	MG	1A	3783	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3306	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3409	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	3503	1/1	0.93	0.11	55,55,55,55	0
56	MG	2a	1631	1/1	0.93	0.27	54,54,54,54	0
56	MG	1A	3963	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3614	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1685	1/1	0.93	0.21	62,62,62,62	0
56	MG	1a	1686	1/1	0.93	0.29	66,66,66,66	0
56	MG	1A	3964	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3505	1/1	0.93	0.11	63,63,63,63	0
56	MG	1E	302	1/1	0.93	0.17	50,50,50,50	0
56	MG	1A	3794	1/1	0.93	0.06	22,22,22,22	0
56	MG	1A	3141	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3344	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3066	1/1	0.93	0.09	49,49,49,49	0
56	MG	1E	314	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3804	1/1	0.93	0.17	57,57,57,57	0
56	MG	1a	1699	1/1	0.93	0.41	60,60,60,60	0
56	MG	2A	3072	1/1	0.93	0.18	49,49,49,49	0
56	MG	2A	3326	1/1	0.93	0.36	51,51,51,51	0
56	MG	2A	3644	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3974	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3805	1/1	0.93	0.17	60,60,60,60	0
56	MG	2A	3329	1/1	0.93	0.23	72,72,72,72	0
56	MG	1A	3511	1/1	0.93	0.37	46,46,46,46	0
56	MG	2A	3333	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3079	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3081	1/1	0.93	0.14	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1704	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3980	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3809	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3025	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3415	1/1	0.93	0.25	56,56,56,56	0
56	MG	2a	1675	1/1	0.93	0.20	56,56,56,56	0
56	MG	1A	3814	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	3001	1/1	0.93	0.11	37,37,37,37	0
56	MG	2A	3345	1/1	0.93	0.13	60,60,60,60	0
56	MG	2a	1683	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3099	1/1	0.93	0.15	57,57,57,57	0
56	MG	2a	1687	1/1	0.93	0.17	43,43,43,43	0
56	MG	1A	3647	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3351	1/1	0.93	0.14	58,58,58,58	0
56	MG	2A	3106	1/1	0.93	0.19	68,68,68,68	0
56	MG	1A	3820	1/1	0.93	0.18	43,43,43,43	0
56	MG	1A	4003	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3424	1/1	0.93	0.11	41,41,41,41	0
56	MG	1Q	203	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3652	1/1	0.93	0.07	29,29,29,29	0
56	MG	2A	3687	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3527	1/1	0.93	0.25	47,47,47,47	0
56	MG	2A	3119	1/1	0.93	0.24	62,62,62,62	0
56	MG	1a	1725	1/1	0.93	0.18	53,53,53,53	0
56	MG	2a	1704	1/1	0.93	0.09	59,59,59,59	0
56	MG	1a	1726	1/1	0.93	0.15	45,45,45,45	0
56	MG	1A	3217	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3826	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3157	1/1	0.93	0.19	58,58,58,58	0
56	MG	2a	1711	1/1	0.93	0.31	59,59,59,59	0
56	MG	1A	3101	1/1	0.93	0.14	68,68,68,68	0
56	MG	2a	1714	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3243	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3055	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3135	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3035	1/1	0.93	0.35	31,31,31,31	0
56	MG	1A	3541	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3380	1/1	0.93	0.10	56,56,56,56	0
56	MG	2A	3715	1/1	0.93	0.25	52,52,52,52	0
56	MG	2A	3144	1/1	0.93	0.28	49,49,49,49	0
56	MG	1A	3365	1/1	0.93	0.16	46,46,46,46	0
56	MG	1A	3249	1/1	0.93	0.13	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3843	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3390	1/1	0.93	0.11	69,69,69,69	0
56	MG	1a	1750	1/1	0.93	0.22	51,51,51,51	0
56	MG	2a	1735	1/1	0.93	0.27	59,59,59,59	0
56	MG	2A	3731	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3151	1/1	0.93	0.22	58,58,58,58	0
56	MG	1A	3180	1/1	0.93	0.19	50,50,50,50	0
56	MG	2A	3394	1/1	0.93	0.06	62,62,62,62	0
56	MG	1a	1753	1/1	0.93	0.08	73,73,73,73	0
56	MG	2a	1745	1/1	0.93	0.12	64,64,64,64	0
56	MG	2a	1747	1/1	0.93	0.13	70,70,70,70	0
56	MG	1A	3691	1/1	0.93	0.06	50,50,50,50	0
56	MG	2A	3162	1/1	0.93	0.24	55,55,55,55	0
56	MG	1A	3693	1/1	0.93	0.06	26,26,26,26	0
56	MG	2A	3399	1/1	0.93	0.08	65,65,65,65	0
56	MG	2a	1753	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3853	1/1	0.93	0.12	45,45,45,45	0
56	MG	2a	1757	1/1	0.93	0.19	68,68,68,68	0
56	MG	2A	3166	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3751	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3168	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3854	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3697	1/1	0.93	0.10	28,28,28,28	0
56	MG	1A	3444	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3860	1/1	0.93	0.15	33,33,33,33	0
56	MG	2a	1770	1/1	0.93	0.24	63,63,63,63	0
56	MG	2A	3766	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3552	1/1	0.93	0.33	42,42,42,42	0
56	MG	1A	3251	1/1	0.93	0.16	47,47,47,47	0
56	MG	1A	3703	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	4052	1/1	0.93	0.08	23,23,23,23	0
56	MG	2A	3183	1/1	0.93	0.17	65,65,65,65	0
56	MG	1A	3448	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3418	1/1	0.93	0.17	39,39,39,39	0
56	MG	17	106	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3421	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3186	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3571	1/1	0.93	0.19	31,31,31,31	0
56	MG	1a	1777	1/1	0.93	0.09	68,68,68,68	0
56	MG	1A	3105	1/1	0.93	0.10	32,32,32,32	0
56	MG	2A	3193	1/1	0.93	0.29	65,65,65,65	0
56	MG	2A	3196	1/1	0.93	0.20	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3786	1/1	0.93	0.12	66,66,66,66	0
56	MG	2A	3198	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3709	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3183	1/1	0.93	0.19	72,72,72,72	0
56	MG	1A	3881	1/1	0.93	0.09	30,30,30,30	0
56	MG	2A	3434	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3377	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1607	1/1	0.93	0.17	60,60,60,60	0
56	MG	2A	3438	1/1	0.93	0.22	56,56,56,56	0
56	MG	2a	1805	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3439	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3884	1/1	0.93	0.08	23,23,23,23	0
56	MG	1A	3717	1/1	0.93	0.11	49,49,49,49	0
56	MG	2a	1809	1/1	0.93	0.14	64,64,64,64	0
56	MG	2A	3814	1/1	0.93	0.14	58,58,58,58	0
56	MG	2a	1812	1/1	0.93	0.12	60,60,60,60	0
56	MG	1a	1795	1/1	0.93	0.17	54,54,54,54	0
56	MG	1a	1613	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3720	1/1	0.93	0.07	37,37,37,37	0
56	MG	1a	1616	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3257	1/1	0.93	0.10	44,44,44,44	0
56	MG	2a	1820	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3457	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3829	1/1	0.93	0.15	63,63,63,63	0
56	MG	1a	1804	1/1	0.93	0.16	59,59,59,59	0
56	MG	1a	1805	1/1	0.93	0.20	51,51,51,51	0
56	MG	2e	201	1/1	0.93	0.07	70,70,70,70	0
56	MG	1a	1806	1/1	0.93	0.19	65,65,65,65	0
56	MG	1a	1624	1/1	0.93	0.22	49,49,49,49	0
56	MG	2A	3837	1/1	0.93	0.14	65,65,65,65	0
56	MG	2l	201	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3224	1/1	0.93	0.15	55,55,55,55	0
56	MG	2l	203	1/1	0.93	0.11	64,64,64,64	0
56	MG	1a	1626	1/1	0.93	0.16	52,52,52,52	0
56	MG	2m	201	1/1	0.93	0.24	68,68,68,68	0
56	MG	2A	3226	1/1	0.93	0.10	65,65,65,65	0
56	MG	1b	301	1/1	0.93	0.14	66,66,66,66	0
56	MG	2A	3843	1/1	0.93	0.07	62,62,62,62	0
56	MG	1d	301	1/1	0.93	0.43	68,68,68,68	0
56	MG	2A	3471	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3728	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3729	1/1	0.93	0.09	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3382	1/1	0.93	0.11	43,43,43,43	0
56	MG	2B	205	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3475	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3908	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3383	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3236	1/1	0.93	0.08	46,46,46,46	0
56	MG	2x	103	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3482	1/1	0.93	0.25	50,50,50,50	0
56	MG	1p	101	1/1	0.93	0.23	49,49,49,49	0
56	MG	1A	3384	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3240	1/1	0.93	0.16	56,56,56,56	0
56	MG	2B	216	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3916	1/1	0.93	0.08	45,45,45,45	0
56	MG	1A	4085	1/1	0.93	0.13	42,42,42,42	0
56	MG	2D	301	1/1	0.93	0.14	49,49,49,49	0
56	MG	1w	103	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3247	1/1	0.93	0.09	62,62,62,62	0
58	WC9	2A	3846	34/34	0.93	0.12	43,52,58,60	0
56	MG	1A	3736	1/1	0.93	0.20	52,52,52,52	0
56	MG	1A	3463	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3565	1/1	0.94	0.21	50,50,50,50	0
56	MG	1x	102	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3488	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3361	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3902	1/1	0.94	0.14	34,34,34,34	0
56	MG	1x	105	1/1	0.94	0.20	66,66,66,66	0
56	MG	2D	306	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3084	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3577	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3446	1/1	0.94	0.28	63,63,63,63	0
56	MG	2A	3498	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3909	1/1	0.94	0.06	34,34,34,34	0
56	MG	1A	3735	1/1	0.94	0.05	16,16,16,16	0
56	MG	1A	3293	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3504	1/1	0.94	0.24	46,46,46,46	0
56	MG	2F	302	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3581	1/1	0.94	0.09	45,45,45,45	0
56	MG	1a	1655	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3740	1/1	0.94	0.06	32,32,32,32	0
56	MG	2A	3516	1/1	0.94	0.07	37,37,37,37	0
56	MG	1a	1657	1/1	0.94	0.13	64,64,64,64	0
56	MG	2A	3274	1/1	0.94	0.12	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3919	1/1	0.94	0.08	46,46,46,46	0
56	MG	1B	201	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3525	1/1	0.94	0.19	53,53,53,53	0
56	MG	1A	3296	1/1	0.94	0.12	62,62,62,62	0
56	MG	1B	206	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3281	1/1	0.94	0.26	67,67,67,67	0
56	MG	1A	3449	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1664	1/1	0.94	0.12	60,60,60,60	0
56	MG	2U	202	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3221	1/1	0.94	0.06	49,49,49,49	0
56	MG	1B	211	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3546	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3748	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3027	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3028	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3555	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3366	1/1	0.94	0.12	63,63,63,63	0
56	MG	2A	3290	1/1	0.94	0.13	68,68,68,68	0
56	MG	1A	3367	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3564	1/1	0.94	0.08	36,36,36,36	0
56	MG	25	105	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3033	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3060	1/1	0.94	0.18	57,57,57,57	0
56	MG	27	103	1/1	0.94	0.32	52,52,52,52	0
56	MG	2A	3570	1/1	0.94	0.18	51,51,51,51	0
56	MG	2A	3571	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3941	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3038	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3753	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3756	1/1	0.94	0.09	20,20,20,20	0
56	MG	2A	3583	1/1	0.94	0.16	61,61,61,61	0
56	MG	1A	3589	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3233	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3303	1/1	0.94	0.08	48,48,48,48	0
56	MG	2a	1610	1/1	0.94	0.27	64,64,64,64	0
56	MG	2A	3587	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3304	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3305	1/1	0.94	0.13	58,58,58,58	0
56	MG	2a	1614	1/1	0.94	0.21	54,54,54,54	0
56	MG	1A	3305	1/1	0.94	0.32	60,60,60,60	0
56	MG	2A	3055	1/1	0.94	0.19	65,65,65,65	0
56	MG	1B	230	1/1	0.94	0.08	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3764	1/1	0.94	0.12	26,26,26,26	0
56	MG	2A	3310	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3311	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3601	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3375	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3950	1/1	0.94	0.06	24,24,24,24	0
56	MG	2A	3604	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3768	1/1	0.94	0.07	35,35,35,35	0
56	MG	1B	235	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3952	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3068	1/1	0.94	0.14	63,63,63,63	0
56	MG	2A	3609	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3167	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3612	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3774	1/1	0.94	0.06	69,69,69,69	0
56	MG	1A	3775	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3617	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3619	1/1	0.94	0.10	61,61,61,61	0
56	MG	2a	1639	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3073	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3626	1/1	0.94	0.12	58,58,58,58	0
56	MG	2a	1642	1/1	0.94	0.20	54,54,54,54	0
56	MG	1A	3464	1/1	0.94	0.15	65,65,65,65	0
56	MG	1E	303	1/1	0.94	0.23	45,45,45,45	0
56	MG	1a	1696	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3170	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3631	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3468	1/1	0.94	0.08	64,64,64,64	0
56	MG	2A	3634	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1651	1/1	0.94	0.13	63,63,63,63	0
56	MG	2A	3082	1/1	0.94	0.10	50,50,50,50	0
56	MG	1E	310	1/1	0.94	0.07	17,17,17,17	0
56	MG	1A	3961	1/1	0.94	0.09	60,60,60,60	0
56	MG	2a	1656	1/1	0.94	0.15	76,76,76,76	0
56	MG	2A	3639	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3332	1/1	0.94	0.19	63,63,63,63	0
56	MG	1a	1701	1/1	0.94	0.22	61,61,61,61	0
56	MG	2A	3334	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1662	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3335	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3314	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3784	1/1	0.94	0.09	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3315	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3609	1/1	0.94	0.10	10,10,10,10	0
56	MG	1F	312	1/1	0.94	0.13	57,57,57,57	0
56	MG	1a	1707	1/1	0.94	0.18	60,60,60,60	0
56	MG	2A	3657	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3658	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3479	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3104	1/1	0.94	0.12	48,48,48,48	0
56	MG	2a	1685	1/1	0.94	0.30	54,54,54,54	0
56	MG	1A	3480	1/1	0.94	0.09	41,41,41,41	0
56	MG	1F	315	1/1	0.94	0.09	41,41,41,41	0
56	MG	2a	1688	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3109	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3348	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3970	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3622	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3318	1/1	0.94	0.19	51,51,51,51	0
56	MG	2A	3353	1/1	0.94	0.22	56,56,56,56	0
56	MG	2a	1696	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3672	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3803	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3628	1/1	0.94	0.08	23,23,23,23	0
56	MG	1A	3629	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3676	1/1	0.94	0.08	74,74,74,74	0
56	MG	2A	3358	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3359	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3806	1/1	0.94	0.10	30,30,30,30	0
56	MG	2a	1706	1/1	0.94	0.24	57,57,57,57	0
56	MG	1A	3482	1/1	0.94	0.11	56,56,56,56	0
56	MG	1O	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1724	1/1	0.94	0.23	57,57,57,57	0
56	MG	1O	204	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3244	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3486	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3017	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3133	1/1	0.94	0.22	61,61,61,61	0
56	MG	2a	1719	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3134	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3490	1/1	0.94	0.13	33,33,33,33	0
56	MG	2A	3136	1/1	0.94	0.07	62,62,62,62	0
56	MG	2a	1724	1/1	0.94	0.23	53,53,53,53	0
56	MG	1a	1736	1/1	0.94	0.14	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3375	1/1	0.94	0.18	52,52,52,52	0
56	MG	2A	3703	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3704	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3138	1/1	0.94	0.11	55,55,55,55	0
56	MG	2A	3378	1/1	0.94	0.29	55,55,55,55	0
56	MG	1A	3638	1/1	0.94	0.08	38,38,38,38	0
56	MG	1A	3068	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3388	1/1	0.94	0.16	27,27,27,27	0
56	MG	2a	1737	1/1	0.94	0.22	59,59,59,59	0
56	MG	2A	3385	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3389	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3499	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3393	1/1	0.94	0.29	61,61,61,61	0
56	MG	1U	209	1/1	0.94	0.14	54,54,54,54	0
56	MG	2a	1744	1/1	0.94	0.11	71,71,71,71	0
56	MG	2A	3725	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3726	1/1	0.94	0.11	74,74,74,74	0
56	MG	2A	3152	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3116	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3122	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3732	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3158	1/1	0.94	0.20	39,39,39,39	0
56	MG	2A	3734	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3736	1/1	0.94	0.15	53,53,53,53	0
56	MG	1a	1751	1/1	0.94	0.17	53,53,53,53	0
56	MG	2a	1760	1/1	0.94	0.24	59,59,59,59	0
56	MG	1A	3329	1/1	0.94	0.09	38,38,38,38	0
56	MG	1W	206	1/1	0.94	0.13	27,27,27,27	0
56	MG	1a	1754	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3742	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3129	1/1	0.94	0.10	66,66,66,66	0
56	MG	1a	1758	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3401	1/1	0.94	0.06	59,59,59,59	0
56	MG	1X	104	1/1	0.94	0.25	43,43,43,43	0
56	MG	1a	1760	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3405	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3752	1/1	0.94	0.16	68,68,68,68	0
56	MG	1Y	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3754	1/1	0.94	0.11	81,81,81,81	0
56	MG	2A	3755	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3661	1/1	0.94	0.09	29,29,29,29	0
56	MG	1Y	205	1/1	0.94	0.15	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1782	1/1	0.94	0.17	61,61,61,61	0
56	MG	2a	1783	1/1	0.94	0.07	62,62,62,62	0
56	MG	2A	3759	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3180	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3007	1/1	0.94	0.08	39,39,39,39	0
56	MG	2A	3765	1/1	0.94	0.07	48,48,48,48	0
56	MG	1A	3673	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	1790	1/1	0.94	0.22	60,60,60,60	0
56	MG	1A	3333	1/1	0.94	0.21	52,52,52,52	0
56	MG	1A	3334	1/1	0.94	0.23	56,56,56,56	0
56	MG	2A	3415	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3194	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3338	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	4025	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3420	1/1	0.94	0.14	50,50,50,50	0
56	MG	2A	3775	1/1	0.94	0.13	64,64,64,64	0
56	MG	1A	3051	1/1	0.94	0.09	24,24,24,24	0
56	MG	11	103	1/1	0.94	0.17	62,62,62,62	0
56	MG	11	105	1/1	0.94	0.10	62,62,62,62	0
56	MG	12	101	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	4029	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	3845	1/1	0.94	0.12	24,24,24,24	0
56	MG	1A	3846	1/1	0.94	0.09	30,30,30,30	0
56	MG	1a	1784	1/1	0.94	0.11	49,49,49,49	0
56	MG	15	109	1/1	0.94	0.10	39,39,39,39	0
56	MG	2a	1811	1/1	0.94	0.19	60,60,60,60	0
56	MG	1A	3103	1/1	0.94	0.06	25,25,25,25	0
56	MG	1A	3849	1/1	0.94	0.21	36,36,36,36	0
56	MG	2A	3789	1/1	0.94	0.08	44,44,44,44	0
56	MG	17	105	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3261	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3795	1/1	0.94	0.12	59,59,59,59	0
56	MG	2a	1819	1/1	0.94	0.22	66,66,66,66	0
56	MG	1A	3851	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3419	1/1	0.94	0.13	50,50,50,50	0
56	MG	1a	1799	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3146	1/1	0.94	0.09	34,34,34,34	0
56	MG	2A	3441	1/1	0.94	0.27	53,53,53,53	0
56	MG	2d	301	1/1	0.94	0.30	59,59,59,59	0
56	MG	2A	3216	1/1	0.94	0.16	52,52,52,52	0
56	MG	2A	3809	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3694	1/1	0.94	0.06	11,11,11,11	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3263	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3445	1/1	0.94	0.25	49,49,49,49	0
56	MG	2A	3817	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4051	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3345	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3449	1/1	0.94	0.34	53,53,53,53	0
56	MG	1A	3538	1/1	0.94	0.13	47,47,47,47	0
56	MG	2A	3451	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3452	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3701	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3455	1/1	0.94	0.10	69,69,69,69	0
56	MG	1a	1809	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3147	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3540	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3268	1/1	0.94	0.21	56,56,56,56	0
56	MG	1f	201	1/1	0.94	0.11	59,59,59,59	0
56	MG	1a	1618	1/1	0.94	0.06	55,55,55,55	0
56	MG	1A	3081	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	4067	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3844	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3353	1/1	0.94	0.06	50,50,50,50	0
56	MG	1a	1625	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3287	1/1	0.94	0.05	45,45,45,45	0
56	MG	1A	3156	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3438	1/1	0.94	0.22	45,45,45,45	0
56	MG	1a	1631	1/1	0.94	0.27	57,57,57,57	0
56	MG	1A	3554	1/1	0.94	0.20	49,49,49,49	0
56	MG	2B	207	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3439	1/1	0.94	0.31	44,44,44,44	0
56	MG	1A	3213	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3562	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3894	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3484	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3355	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	3706	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3879	1/1	0.95	0.05	43,43,43,43	0
56	MG	2A	3007	1/1	0.95	0.32	58,58,58,58	0
56	MG	1a	1644	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3357	1/1	0.95	0.09	60,60,60,60	0
56	MG	2F	306	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3560	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3708	1/1	0.95	0.12	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3548	1/1	0.95	0.11	57,57,57,57	0
56	MG	2P	201	1/1	0.95	0.10	63,63,63,63	0
56	MG	1A	4083	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3565	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3017	1/1	0.95	0.23	50,50,50,50	0
56	MG	2A	3018	1/1	0.95	0.24	49,49,49,49	0
56	MG	2A	3569	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3127	1/1	0.95	0.15	56,56,56,56	0
56	MG	1a	1654	1/1	0.95	0.06	48,48,48,48	0
56	MG	2T	203	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3553	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3886	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3271	1/1	0.95	0.08	38,38,38,38	0
56	MG	2V	202	1/1	0.95	0.05	56,56,56,56	0
56	MG	1A	3718	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3300	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3719	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3302	1/1	0.95	0.28	45,45,45,45	0
56	MG	1A	3895	1/1	0.95	0.21	24,24,24,24	0
56	MG	20	104	1/1	0.95	0.11	61,61,61,61	0
56	MG	1A	3896	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3588	1/1	0.95	0.27	67,67,67,67	0
56	MG	2A	3036	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1662	1/1	0.95	0.13	65,65,65,65	0
56	MG	25	103	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3555	1/1	0.95	0.28	47,47,47,47	0
56	MG	1A	3898	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3723	1/1	0.95	0.09	64,64,64,64	0
56	MG	26	101	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3595	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3596	1/1	0.95	0.09	50,50,50,50	0
56	MG	1B	204	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3901	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3047	1/1	0.95	0.14	39,39,39,39	0
56	MG	2a	1601	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3281	1/1	0.95	0.13	29,29,29,29	0
56	MG	2A	3052	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3203	1/1	0.95	0.10	22,22,22,22	0
56	MG	1A	3727	1/1	0.95	0.06	36,36,36,36	0
56	MG	1B	212	1/1	0.95	0.17	56,56,56,56	0
56	MG	1B	213	1/1	0.95	0.13	56,56,56,56	0
56	MG	2a	1608	1/1	0.95	0.26	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3907	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3559	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3560	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3610	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3047	1/1	0.95	0.04	27,27,27,27	0
56	MG	1A	3206	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3613	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3569	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3451	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3918	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3013	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	3454	1/1	0.95	0.18	43,43,43,43	0
56	MG	2A	3623	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3330	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3136	1/1	0.95	0.27	39,39,39,39	0
56	MG	1a	1687	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3077	1/1	0.95	0.15	59,59,59,59	0
56	MG	1a	1688	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3929	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3080	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3294	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3743	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3636	1/1	0.95	0.17	39,39,39,39	0
56	MG	1a	1692	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3295	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3085	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3086	1/1	0.95	0.30	45,45,45,45	0
56	MG	1A	3935	1/1	0.95	0.06	66,66,66,66	0
56	MG	1A	3936	1/1	0.95	0.08	48,48,48,48	0
56	MG	2A	3093	1/1	0.95	0.14	53,53,53,53	0
56	MG	1D	306	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3347	1/1	0.95	0.31	77,77,77,77	0
56	MG	2A	3646	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3096	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3027	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3649	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3089	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3652	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3653	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3940	1/1	0.95	0.08	54,54,54,54	0
56	MG	2A	3656	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3373	1/1	0.95	0.15	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3214	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3216	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3105	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3302	1/1	0.95	0.09	29,29,29,29	0
56	MG	2A	3662	1/1	0.95	0.07	47,47,47,47	0
56	MG	1E	308	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3754	1/1	0.95	0.08	28,28,28,28	0
56	MG	2a	1666	1/1	0.95	0.24	61,61,61,61	0
56	MG	1A	3467	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3143	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3668	1/1	0.95	0.19	49,49,49,49	0
56	MG	2a	1671	1/1	0.95	0.22	55,55,55,55	0
56	MG	1A	3591	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3114	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3471	1/1	0.95	0.10	52,52,52,52	0
56	MG	2a	1676	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3219	1/1	0.95	0.14	47,47,47,47	0
56	MG	2a	1678	1/1	0.95	0.10	55,55,55,55	0
56	MG	1F	307	1/1	0.95	0.11	45,45,45,45	0
56	MG	1F	308	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3308	1/1	0.95	0.05	43,43,43,43	0
56	MG	1A	3477	1/1	0.95	0.17	59,59,59,59	0
56	MG	2A	3678	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3090	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3954	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3127	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3312	1/1	0.95	0.16	44,44,44,44	0
56	MG	1A	3771	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3223	1/1	0.95	0.09	44,44,44,44	0
56	MG	1a	1723	1/1	0.95	0.24	47,47,47,47	0
56	MG	2a	1694	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3383	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3224	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3602	1/1	0.95	0.07	28,28,28,28	0
56	MG	1A	3604	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3605	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3782	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3225	1/1	0.95	0.12	56,56,56,56	0
56	MG	1a	1734	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3004	1/1	0.95	0.05	27,27,27,27	0
56	MG	1O	203	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3487	1/1	0.95	0.08	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3967	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3789	1/1	0.95	0.07	37,37,37,37	0
56	MG	2a	1709	1/1	0.95	0.12	69,69,69,69	0
56	MG	1a	1743	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3320	1/1	0.95	0.18	36,36,36,36	0
56	MG	1A	3619	1/1	0.95	0.07	27,27,27,27	0
56	MG	2A	3157	1/1	0.95	0.20	64,64,64,64	0
56	MG	1A	3621	1/1	0.95	0.04	33,33,33,33	0
56	MG	2A	3402	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3795	1/1	0.95	0.04	19,19,19,19	0
56	MG	2A	3720	1/1	0.95	0.05	71,71,71,71	0
56	MG	1A	3798	1/1	0.95	0.28	27,27,27,27	0
56	MG	1A	3232	1/1	0.95	0.25	42,42,42,42	0
56	MG	1A	3397	1/1	0.95	0.21	41,41,41,41	0
56	MG	2a	1725	1/1	0.95	0.17	62,62,62,62	0
56	MG	2A	3727	1/1	0.95	0.08	69,69,69,69	0
56	MG	1A	3493	1/1	0.95	0.23	40,40,40,40	0
56	MG	2A	3167	1/1	0.95	0.09	41,41,41,41	0
56	MG	1T	202	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3169	1/1	0.95	0.11	59,59,59,59	0
56	MG	1U	202	1/1	0.95	0.16	35,35,35,35	0
56	MG	1U	204	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3173	1/1	0.95	0.20	65,65,65,65	0
56	MG	2A	3174	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3984	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3031	1/1	0.95	0.20	26,26,26,26	0
56	MG	1V	205	1/1	0.95	0.11	31,31,31,31	0
56	MG	1A	3496	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3497	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3236	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3401	1/1	0.95	0.10	49,49,49,49	0
56	MG	1X	102	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3096	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3998	1/1	0.95	0.07	25,25,25,25	0
56	MG	1A	3100	1/1	0.95	0.07	62,62,62,62	0
56	MG	1A	3160	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3407	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3642	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3059	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3194	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3164	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3761	1/1	0.95	0.09	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3509	1/1	0.95	0.34	44,44,44,44	0
56	MG	1A	3002	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3512	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3654	1/1	0.95	0.07	21,21,21,21	0
56	MG	2a	1765	1/1	0.95	0.07	52,52,52,52	0
56	MG	1a	1783	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3513	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3207	1/1	0.95	0.16	52,52,52,52	0
56	MG	1a	1786	1/1	0.95	0.17	67,67,67,67	0
56	MG	1A	3514	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3061	1/1	0.95	0.10	27,27,27,27	0
56	MG	2A	3447	1/1	0.95	0.21	55,55,55,55	0
56	MG	1a	1790	1/1	0.95	0.05	54,54,54,54	0
56	MG	1a	1791	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3413	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3214	1/1	0.95	0.11	53,53,53,53	0
56	MG	2a	1780	1/1	0.95	0.18	66,66,66,66	0
56	MG	13	103	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3453	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3011	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3666	1/1	0.95	0.04	22,22,22,22	0
56	MG	15	103	1/1	0.95	0.17	38,38,38,38	0
56	MG	2A	3785	1/1	0.95	0.06	51,51,51,51	0
56	MG	1A	3671	1/1	0.95	0.12	38,38,38,38	0
56	MG	15	106	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3221	1/1	0.95	0.09	69,69,69,69	0
56	MG	2A	3462	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3790	1/1	0.95	0.09	44,44,44,44	0
56	MG	2a	1793	1/1	0.95	0.07	59,59,59,59	0
56	MG	15	108	1/1	0.95	0.07	47,47,47,47	0
56	MG	2a	1795	1/1	0.95	0.20	76,76,76,76	0
56	MG	2A	3793	1/1	0.95	0.08	34,34,34,34	0
56	MG	2A	3465	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3067	1/1	0.95	0.08	30,30,30,30	0
56	MG	1A	4027	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3838	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3524	1/1	0.95	0.24	32,32,32,32	0
56	MG	1A	4031	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	4033	1/1	0.95	0.08	41,41,41,41	0
56	MG	1a	1810	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3840	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3810	1/1	0.95	0.07	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3841	1/1	0.95	0.08	20,20,20,20	0
56	MG	2A	3813	1/1	0.95	0.13	80,80,80,80	0
56	MG	2A	3476	1/1	0.95	0.08	39,39,39,39	0
56	MG	1e	201	1/1	0.95	0.30	59,59,59,59	0
56	MG	2A	3478	1/1	0.95	0.22	63,63,63,63	0
56	MG	2A	3818	1/1	0.95	0.05	31,31,31,31	0
56	MG	2A	3235	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1601	1/1	0.95	0.20	52,52,52,52	0
56	MG	1a	1602	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	3525	1/1	0.95	0.09	36,36,36,36	0
56	MG	2a	1818	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3037	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3826	1/1	0.95	0.16	59,59,59,59	0
56	MG	1m	3001	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3832	1/1	0.95	0.13	58,58,58,58	0
56	MG	2a	1823	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	4040	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3681	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3255	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	3847	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3528	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3251	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	3181	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	4048	1/1	0.95	0.10	45,45,45,45	0
56	MG	1a	1617	1/1	0.95	0.05	54,54,54,54	0
56	MG	2A	3499	1/1	0.95	0.22	71,71,71,71	0
56	MG	2l	204	1/1	0.95	0.07	68,68,68,68	0
56	MG	1A	3686	1/1	0.95	0.11	27,27,27,27	0
56	MG	2A	3257	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1621	1/1	0.95	0.26	61,61,61,61	0
56	MG	1A	3111	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3506	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3018	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3533	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3514	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3072	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3857	1/1	0.95	0.10	40,40,40,40	0
56	MG	2B	209	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	4063	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3347	1/1	0.95	0.19	38,38,38,38	0
56	MG	2A	3522	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3269	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($\text{\AA}^2$)	Q<0.9
56	MG	1A	3859	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3042	1/1	0.95	0.06	32,32,32,32	0
56	MG	1x	110	1/1	0.95	0.31	67,67,67,67	0
56	MG	1A	3862	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3078	1/1	0.95	0.25	54,54,54,54	0
56	MG	2A	3530	1/1	0.95	0.14	42,42,42,42	0
56	MG	2D	303	1/1	0.95	0.28	55,55,55,55	0
56	MG	2A	3531	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3533	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3350	1/1	0.95	0.16	30,30,30,30	0
57	K	2A	3459	1/1	0.95	0.10	73,73,73,73	0
56	MG	1A	3265	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3267	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3197	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3545	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3491	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3020	1/1	0.96	0.20	44,44,44,44	0
56	MG	2F	307	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3910	1/1	0.96	0.06	65,65,65,65	0
56	MG	2A	3572	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3024	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3575	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3577	1/1	0.96	0.08	70,70,70,70	0
56	MG	1B	203	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3026	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3404	1/1	0.96	0.12	51,51,51,51	0
56	MG	2Q	204	1/1	0.96	0.10	57,57,57,57	0
56	MG	1a	1650	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3914	1/1	0.96	0.06	54,54,54,54	0
56	MG	2R	203	1/1	0.96	0.16	56,56,56,56	0
56	MG	1a	1652	1/1	0.96	0.08	50,50,50,50	0
56	MG	1a	1653	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3603	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3063	1/1	0.96	0.29	63,63,63,63	0
56	MG	1A	3337	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3755	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3040	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3066	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3052	1/1	0.96	0.15	29,29,29,29	0
56	MG	2A	3594	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3269	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3759	1/1	0.96	0.07	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	219	1/1	0.96	0.24	53,53,53,53	0
56	MG	23	101	1/1	0.96	0.06	50,50,50,50	0
56	MG	2A	3048	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3049	1/1	0.96	0.11	32,32,32,32	0
56	MG	1B	220	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3760	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3614	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3054	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3762	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3056	1/1	0.96	0.27	56,56,56,56	0
56	MG	1A	3616	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3059	1/1	0.96	0.10	56,56,56,56	0
56	MG	2A	3060	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3617	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3158	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3411	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3159	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3343	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3272	1/1	0.96	0.19	57,57,57,57	0
56	MG	2A	3616	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3627	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3618	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3275	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3276	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3622	1/1	0.96	0.14	51,51,51,51	0
56	MG	1a	1679	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3780	1/1	0.96	0.08	21,21,21,21	0
56	MG	1B	236	1/1	0.96	0.06	39,39,39,39	0
56	MG	1D	302	1/1	0.96	0.09	26,26,26,26	0
56	MG	1D	304	1/1	0.96	0.16	36,36,36,36	0
56	MG	1A	3418	1/1	0.96	0.06	40,40,40,40	0
56	MG	1D	309	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3093	1/1	0.96	0.10	27,27,27,27	0
56	MG	2a	1619	1/1	0.96	0.07	74,74,74,74	0
56	MG	2A	3633	1/1	0.96	0.08	52,52,52,52	0
56	MG	2a	1621	1/1	0.96	0.17	82,82,82,82	0
56	MG	1A	3285	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3422	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3423	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3636	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	3790	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3118	1/1	0.96	0.16	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1628	1/1	0.96	0.31	61,61,61,61	0
56	MG	1A	3639	1/1	0.96	0.05	28,28,28,28	0
56	MG	2A	3349	1/1	0.96	0.06	67,67,67,67	0
56	MG	2A	3090	1/1	0.96	0.32	58,58,58,58	0
56	MG	1A	3425	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3121	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3797	1/1	0.96	0.05	23,23,23,23	0
56	MG	1E	313	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3427	1/1	0.96	0.16	50,50,50,50	0
56	MG	2A	3356	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3522	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3645	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3651	1/1	0.96	0.08	34,34,34,34	0
56	MG	1F	305	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3801	1/1	0.96	0.04	38,38,38,38	0
56	MG	1A	3523	1/1	0.96	0.14	43,43,43,43	0
56	MG	2a	1644	1/1	0.96	0.08	76,76,76,76	0
56	MG	2A	3655	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3165	1/1	0.96	0.17	35,35,35,35	0
56	MG	1F	311	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3094	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3650	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3291	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3969	1/1	0.96	0.10	63,63,63,63	0
56	MG	1G	201	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3653	1/1	0.96	0.07	22,22,22,22	0
56	MG	2a	1654	1/1	0.96	0.08	60,60,60,60	0
56	MG	1A	3810	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3117	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3356	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3433	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3975	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3377	1/1	0.96	0.20	41,41,41,41	0
56	MG	2a	1661	1/1	0.96	0.16	61,61,61,61	0
56	MG	1N	204	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3228	1/1	0.96	0.14	37,37,37,37	0
56	MG	2a	1665	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3530	1/1	0.96	0.15	39,39,39,39	0
56	MG	2A	3381	1/1	0.96	0.17	58,58,58,58	0
56	MG	1A	3979	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3436	1/1	0.96	0.23	46,46,46,46	0
56	MG	2A	3128	1/1	0.96	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3679	1/1	0.96	0.06	65,65,65,65	0
56	MG	2a	1673	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3818	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3387	1/1	0.96	0.12	64,64,64,64	0
56	MG	1A	3982	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3124	1/1	0.96	0.23	41,41,41,41	0
56	MG	1A	3664	1/1	0.96	0.06	23,23,23,23	0
56	MG	1Q	201	1/1	0.96	0.12	33,33,33,33	0
56	MG	2a	1680	1/1	0.96	0.26	65,65,65,65	0
56	MG	1a	1730	1/1	0.96	0.10	51,51,51,51	0
56	MG	2a	1682	1/1	0.96	0.25	54,54,54,54	0
56	MG	2A	3688	1/1	0.96	0.07	30,30,30,30	0
56	MG	2a	1684	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3231	1/1	0.96	0.10	57,57,57,57	0
56	MG	1Q	204	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3125	1/1	0.96	0.21	33,33,33,33	0
56	MG	2A	3693	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3140	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3696	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3141	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3672	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3143	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3178	1/1	0.96	0.11	36,36,36,36	0
56	MG	1R	205	1/1	0.96	0.16	33,33,33,33	0
56	MG	1A	3298	1/1	0.96	0.13	39,39,39,39	0
56	MG	1a	1742	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3148	1/1	0.96	0.21	35,35,35,35	0
56	MG	1A	3235	1/1	0.96	0.09	31,31,31,31	0
56	MG	2A	3406	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3126	1/1	0.96	0.23	34,34,34,34	0
56	MG	1A	3679	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3153	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3154	1/1	0.96	0.26	48,48,48,48	0
56	MG	1a	1746	1/1	0.96	0.05	59,59,59,59	0
56	MG	1a	1747	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3830	1/1	0.96	0.05	33,33,33,33	0
56	MG	2A	3722	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3237	1/1	0.96	0.17	34,34,34,34	0
56	MG	1U	203	1/1	0.96	0.09	38,38,38,38	0
56	MG	2a	1712	1/1	0.96	0.28	59,59,59,59	0
56	MG	1A	3833	1/1	0.96	0.06	58,58,58,58	0
56	MG	1U	207	1/1	0.96	0.10	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3241	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3026	1/1	0.96	0.13	41,41,41,41	0
56	MG	2a	1718	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3730	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3369	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3685	1/1	0.96	0.06	63,63,63,63	0
56	MG	1W	202	1/1	0.96	0.16	41,41,41,41	0
56	MG	1A	3005	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	4014	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3737	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3687	1/1	0.96	0.07	38,38,38,38	0
56	MG	1X	101	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3688	1/1	0.96	0.09	41,41,41,41	0
56	MG	1a	1767	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3019	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	4020	1/1	0.96	0.09	51,51,51,51	0
56	MG	1X	107	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3745	1/1	0.96	0.14	66,66,66,66	0
56	MG	1Y	201	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3310	1/1	0.96	0.24	63,63,63,63	0
56	MG	2A	3748	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3692	1/1	0.96	0.09	29,29,29,29	0
56	MG	2a	1741	1/1	0.96	0.06	72,72,72,72	0
56	MG	2A	3750	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3132	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3184	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3695	1/1	0.96	0.10	54,54,54,54	0
56	MG	2a	1746	1/1	0.96	0.12	58,58,58,58	0
56	MG	1Z	303	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3248	1/1	0.96	0.26	50,50,50,50	0
56	MG	10	101	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3698	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3134	1/1	0.96	0.09	42,42,42,42	0
56	MG	2a	1752	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3195	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3762	1/1	0.96	0.08	54,54,54,54	0
56	MG	2a	1755	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3852	1/1	0.96	0.07	50,50,50,50	0
56	MG	10	105	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	4032	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3201	1/1	0.96	0.21	70,70,70,70	0
56	MG	1A	3460	1/1	0.96	0.26	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	10	108	1/1	0.96	0.07	44,44,44,44	0
56	MG	11	102	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3378	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3316	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3381	1/1	0.96	0.15	29,29,29,29	0
56	MG	13	102	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3563	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3776	1/1	0.96	0.18	62,62,62,62	0
56	MG	1A	3193	1/1	0.96	0.26	30,30,30,30	0
56	MG	2a	1774	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3465	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3570	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3863	1/1	0.96	0.15	31,31,31,31	0
56	MG	1a	1803	1/1	0.96	0.06	58,58,58,58	0
56	MG	2A	3468	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3864	1/1	0.96	0.21	38,38,38,38	0
56	MG	15	107	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3135	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3321	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3712	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3870	1/1	0.96	0.06	40,40,40,40	0
56	MG	17	102	1/1	0.96	0.16	34,34,34,34	0
56	MG	2a	1787	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3223	1/1	0.96	0.35	42,42,42,42	0
56	MG	1A	4053	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	4054	1/1	0.96	0.06	42,42,42,42	0
56	MG	18	101	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	4056	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3797	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3575	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	4058	1/1	0.96	0.07	52,52,52,52	0
56	MG	1k	201	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3576	1/1	0.96	0.17	53,53,53,53	0
56	MG	1l	202	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3874	1/1	0.96	0.07	29,29,29,29	0
56	MG	2a	1800	1/1	0.96	0.17	57,57,57,57	0
56	MG	1A	3875	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3323	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3578	1/1	0.96	0.08	48,48,48,48	0
56	MG	1a	1606	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3469	1/1	0.96	0.14	51,51,51,51	0
56	MG	1a	1608	1/1	0.96	0.06	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3057	1/1	0.96	0.17	45,45,45,45	0
56	MG	1a	1611	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3244	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3029	1/1	0.96	0.32	29,29,29,29	0
56	MG	1A	3882	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3473	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3475	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3825	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3507	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3508	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3830	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	3043	1/1	0.96	0.21	27,27,27,27	0
56	MG	2A	3512	1/1	0.96	0.09	71,71,71,71	0
56	MG	1A	3392	1/1	0.96	0.07	50,50,50,50	0
56	MG	1a	1619	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3478	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3256	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3201	1/1	0.96	0.09	32,32,32,32	0
56	MG	1x	106	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3520	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3892	1/1	0.96	0.18	48,48,48,48	0
56	MG	1x	108	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3893	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3394	1/1	0.96	0.12	66,66,66,66	0
56	MG	1A	3258	1/1	0.96	0.04	39,39,39,39	0
56	MG	1A	3024	1/1	0.96	0.08	29,29,29,29	0
56	MG	1a	1628	1/1	0.96	0.08	51,51,51,51	0
56	MG	1x	114	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	3483	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3271	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3737	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3535	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3536	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3537	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3538	1/1	0.96	0.09	40,40,40,40	0
56	MG	2v	103	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3593	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3542	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3002	1/1	0.96	0.15	43,43,43,43	0
56	MG	1a	1634	1/1	0.96	0.26	58,58,58,58	0
56	MG	2A	3004	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3278	1/1	0.96	0.07	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2B	218	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3087	1/1	0.96	0.31	38,38,38,38	0
56	MG	1A	3006	1/1	0.96	0.21	54,54,54,54	0
56	MG	2A	3552	1/1	0.96	0.07	37,37,37,37	0
56	MG	2x	105	1/1	0.96	0.07	61,61,61,61	0
56	MG	2D	304	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3149	1/1	0.96	0.18	39,39,39,39	0
56	MG	2A	3008	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3557	1/1	0.96	0.10	57,57,57,57	0
56	MG	2y	103	1/1	0.96	0.05	66,66,66,66	0
56	MG	1A	3150	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3559	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3010	1/1	0.96	0.28	57,57,57,57	0
56	MG	1A	4091	1/1	0.96	0.20	65,65,65,65	0
56	MG	1A	3489	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	4094	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	4095	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3403	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	4097	1/1	0.96	0.16	42,42,42,42	0
56	MG	2A	3087	1/1	0.97	0.06	48,48,48,48	0
56	MG	2W	203	1/1	0.97	0.11	58,58,58,58	0
56	MG	2X	101	1/1	0.97	0.06	59,59,59,59	0
56	MG	1P	202	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3322	1/1	0.97	0.13	35,35,35,35	0
56	MG	2A	3091	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3396	1/1	0.97	0.04	28,28,28,28	0
56	MG	1a	1710	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	4010	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3020	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3398	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	4013	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3044	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3625	1/1	0.97	0.05	43,43,43,43	0
56	MG	1a	1716	1/1	0.97	0.13	44,44,44,44	0
56	MG	1R	202	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3102	1/1	0.97	0.10	39,39,39,39	0
56	MG	27	101	1/1	0.97	0.04	44,44,44,44	0
56	MG	2A	3103	1/1	0.97	0.11	44,44,44,44	0
56	MG	1R	203	1/1	0.97	0.14	28,28,28,28	0
56	MG	1R	204	1/1	0.97	0.25	37,37,37,37	0
56	MG	1A	3711	1/1	0.97	0.15	48,48,48,48	0
56	MG	1R	206	1/1	0.97	0.17	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3253	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3714	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3196	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	4021	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3113	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3148	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3362	1/1	0.97	0.05	59,59,59,59	0
56	MG	1a	1728	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3116	1/1	0.97	0.17	53,53,53,53	0
56	MG	1U	201	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3856	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3256	1/1	0.97	0.13	39,39,39,39	0
56	MG	1a	1732	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3121	1/1	0.97	0.15	40,40,40,40	0
56	MG	1a	1733	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3030	1/1	0.97	0.08	29,29,29,29	0
56	MG	1U	205	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3373	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3330	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3126	1/1	0.97	0.07	46,46,46,46	0
56	MG	1U	208	1/1	0.97	0.22	30,30,30,30	0
56	MG	1A	3199	1/1	0.97	0.20	25,25,25,25	0
56	MG	1A	4028	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3861	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3722	1/1	0.97	0.08	27,27,27,27	0
56	MG	1W	201	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3382	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3200	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3260	1/1	0.97	0.08	50,50,50,50	0
56	MG	1W	205	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3865	1/1	0.97	0.22	31,31,31,31	0
56	MG	1A	4034	1/1	0.97	0.08	23,23,23,23	0
56	MG	2A	3139	1/1	0.97	0.12	49,49,49,49	0
56	MG	2A	3667	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3119	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3120	1/1	0.97	0.30	42,42,42,42	0
56	MG	1X	103	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3868	1/1	0.97	0.20	41,41,41,41	0
56	MG	1X	105	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	4038	1/1	0.97	0.17	63,63,63,63	0
56	MG	1a	1757	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3495	1/1	0.97	0.10	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3599	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3336	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3731	1/1	0.97	0.04	54,54,54,54	0
56	MG	1Y	204	1/1	0.97	0.21	52,52,52,52	0
56	MG	1a	1763	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3154	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3155	1/1	0.97	0.27	36,36,36,36	0
56	MG	1A	3073	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3049	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3416	1/1	0.97	0.06	50,50,50,50	0
56	MG	2A	3159	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3160	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3606	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3209	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3692	1/1	0.97	0.05	53,53,53,53	0
56	MG	1A	3608	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	3504	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3165	1/1	0.97	0.06	58,58,58,58	0
56	MG	1a	1774	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3210	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3746	1/1	0.97	0.10	48,48,48,48	0
56	MG	2a	1664	1/1	0.97	0.15	44,44,44,44	0
56	MG	1A	3076	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3507	1/1	0.97	0.26	32,32,32,32	0
56	MG	2a	1667	1/1	0.97	0.05	43,43,43,43	0
56	MG	2A	3702	1/1	0.97	0.04	49,49,49,49	0
56	MG	2A	3171	1/1	0.97	0.08	59,59,59,59	0
56	MG	11	101	1/1	0.97	0.29	43,43,43,43	0
56	MG	1A	3888	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3708	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3889	1/1	0.97	0.09	25,25,25,25	0
56	MG	2A	3424	1/1	0.97	0.23	51,51,51,51	0
56	MG	1A	3050	1/1	0.97	0.06	22,22,22,22	0
56	MG	11	106	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3714	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3079	1/1	0.97	0.19	45,45,45,45	0
56	MG	2A	3428	1/1	0.97	0.29	62,62,62,62	0
56	MG	12	102	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3179	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3346	1/1	0.97	0.16	32,32,32,32	0
56	MG	2A	3721	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3620	1/1	0.97	0.05	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3723	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3274	1/1	0.97	0.06	39,39,39,39	0
56	MG	15	101	1/1	0.97	0.16	35,35,35,35	0
56	MG	2A	3435	1/1	0.97	0.20	49,49,49,49	0
56	MG	1A	3161	1/1	0.97	0.36	34,34,34,34	0
56	MG	1A	3624	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3039	1/1	0.97	0.31	43,43,43,43	0
56	MG	1A	3218	1/1	0.97	0.16	40,40,40,40	0
56	MG	1A	3900	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3283	1/1	0.97	0.39	32,32,32,32	0
56	MG	2A	3191	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3192	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3352	1/1	0.97	0.13	49,49,49,49	0
56	MG	1a	1801	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3519	1/1	0.97	0.04	49,49,49,49	0
56	MG	2a	1700	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3284	1/1	0.97	0.08	48,48,48,48	0
56	MG	17	101	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3199	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3521	1/1	0.97	0.08	52,52,52,52	0
56	MG	17	103	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3633	1/1	0.97	0.04	15,15,15,15	0
56	MG	1A	3128	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3767	1/1	0.97	0.07	47,47,47,47	0
56	MG	18	102	1/1	0.97	0.09	47,47,47,47	0
56	MG	18	103	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3912	1/1	0.97	0.06	47,47,47,47	0
56	MG	18	105	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3286	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3434	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3637	1/1	0.97	0.05	30,30,30,30	0
56	MG	2a	1716	1/1	0.97	0.11	64,64,64,64	0
56	MG	2A	3464	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3772	1/1	0.97	0.11	65,65,65,65	0
56	MG	1A	3773	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3757	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3220	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	4093	1/1	0.97	0.06	43,43,43,43	0
56	MG	2a	1723	1/1	0.97	0.26	52,52,52,52	0
56	MG	2A	3760	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3083	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3166	1/1	0.97	0.08	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3922	1/1	0.97	0.05	65,65,65,65	0
56	MG	1a	1609	1/1	0.97	0.15	48,48,48,48	0
56	MG	2a	1729	1/1	0.97	0.17	66,66,66,66	0
56	MG	1A	3777	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3927	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3778	1/1	0.97	0.04	29,29,29,29	0
56	MG	1A	3359	1/1	0.97	0.19	59,59,59,59	0
56	MG	1A	3130	1/1	0.97	0.10	38,38,38,38	0
56	MG	1a	1615	1/1	0.97	0.08	53,53,53,53	0
56	MG	2a	1736	1/1	0.97	0.23	57,57,57,57	0
56	MG	2A	3479	1/1	0.97	0.08	47,47,47,47	0
56	MG	1B	205	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3933	1/1	0.97	0.11	59,59,59,59	0
56	MG	1A	3643	1/1	0.97	0.06	28,28,28,28	0
56	MG	1B	208	1/1	0.97	0.11	54,54,54,54	0
56	MG	1a	1620	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3232	1/1	0.97	0.50	47,47,47,47	0
56	MG	2A	3486	1/1	0.97	0.15	43,43,43,43	0
56	MG	1B	209	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3441	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3168	1/1	0.97	0.14	59,59,59,59	0
56	MG	1A	3937	1/1	0.97	0.04	43,43,43,43	0
56	MG	2A	3237	1/1	0.97	0.16	47,47,47,47	0
56	MG	2A	3493	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3646	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3787	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3292	1/1	0.97	0.13	25,25,25,25	0
56	MG	1B	216	1/1	0.97	0.06	58,58,58,58	0
56	MG	1B	217	1/1	0.97	0.09	45,45,45,45	0
56	MG	2a	1756	1/1	0.97	0.09	39,39,39,39	0
56	MG	1A	3226	1/1	0.97	0.07	28,28,28,28	0
56	MG	2A	3501	1/1	0.97	0.09	34,34,34,34	0
56	MG	2a	1759	1/1	0.97	0.10	66,66,66,66	0
56	MG	1A	3534	1/1	0.97	0.04	22,22,22,22	0
56	MG	2A	3245	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3796	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3246	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3799	1/1	0.97	0.16	36,36,36,36	0
56	MG	1a	1633	1/1	0.97	0.12	35,35,35,35	0
56	MG	2a	1766	1/1	0.97	0.17	55,55,55,55	0
56	MG	2A	3803	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3535	1/1	0.97	0.15	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3249	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3792	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3445	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3227	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3169	1/1	0.97	0.04	39,39,39,39	0
56	MG	1A	3229	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3040	1/1	0.97	0.21	28,28,28,28	0
56	MG	1A	3085	1/1	0.97	0.09	34,34,34,34	0
56	MG	2A	3518	1/1	0.97	0.09	54,54,54,54	0
56	MG	1B	228	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3659	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3172	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3011	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3820	1/1	0.97	0.06	54,54,54,54	0
56	MG	1a	1645	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3370	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3177	1/1	0.97	0.09	18,18,18,18	0
56	MG	1A	3301	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3016	1/1	0.97	0.20	50,50,50,50	0
56	MG	1A	3667	1/1	0.97	0.08	22,22,22,22	0
56	MG	1A	3669	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3532	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3831	1/1	0.97	0.13	57,57,57,57	0
56	MG	1A	3958	1/1	0.97	0.10	55,55,55,55	0
56	MG	1D	301	1/1	0.97	0.08	32,32,32,32	0
56	MG	2A	3021	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3808	1/1	0.97	0.15	24,24,24,24	0
56	MG	1D	303	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3276	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	3546	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3547	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3234	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3812	1/1	0.97	0.08	34,34,34,34	0
56	MG	1D	311	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3549	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	3550	1/1	0.97	0.05	29,29,29,29	0
56	MG	1A	3815	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3550	1/1	0.97	0.07	30,30,30,30	0
56	MG	1E	301	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3551	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3133	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3556	1/1	0.97	0.06	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3039	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3458	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3041	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3064	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3306	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3044	1/1	0.97	0.21	50,50,50,50	0
56	MG	1A	3108	1/1	0.97	0.28	27,27,27,27	0
56	MG	1A	3822	1/1	0.97	0.05	43,43,43,43	0
56	MG	1A	3240	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3109	1/1	0.97	0.05	36,36,36,36	0
56	MG	1E	315	1/1	0.97	0.04	36,36,36,36	0
56	MG	1F	301	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3977	1/1	0.97	0.07	30,30,30,30	0
56	MG	1a	1677	1/1	0.97	0.06	38,38,38,38	0
56	MG	2D	302	1/1	0.97	0.21	51,51,51,51	0
56	MG	2d	302	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3311	1/1	0.97	0.05	51,51,51,51	0
56	MG	2f	201	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3574	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3561	1/1	0.97	0.06	17,17,17,17	0
56	MG	2A	3576	1/1	0.97	0.08	74,74,74,74	0
56	MG	1F	306	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3057	1/1	0.97	0.09	55,55,55,55	0
56	MG	2E	303	1/1	0.97	0.15	49,49,49,49	0
56	MG	2E	304	1/1	0.97	0.18	49,49,49,49	0
56	MG	2E	305	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3138	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3690	1/1	0.97	0.09	28,28,28,28	0
56	MG	2q	202	1/1	0.97	0.05	77,77,77,77	0
56	MG	1A	3010	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3009	1/1	0.97	0.08	24,24,24,24	0
56	MG	2A	3062	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3567	1/1	0.97	0.08	25,25,25,25	0
56	MG	1A	3185	1/1	0.97	0.03	32,32,32,32	0
56	MG	1A	3990	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3386	1/1	0.97	0.21	26,26,26,26	0
56	MG	1A	3696	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3470	1/1	0.97	0.13	42,42,42,42	0
56	MG	2F	308	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3994	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3995	1/1	0.97	0.07	28,28,28,28	0
56	MG	2A	3071	1/1	0.97	0.17	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3321	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3996	1/1	0.97	0.04	25,25,25,25	0
56	MG	1A	3114	1/1	0.97	0.09	36,36,36,36	0
56	MG	1N	201	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3075	1/1	0.97	0.12	54,54,54,54	0
56	MG	1N	202	1/1	0.97	0.07	38,38,38,38	0
56	MG	1N	203	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3317	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	4000	1/1	0.97	0.06	38,38,38,38	0
56	MG	2T	201	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3188	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3474	1/1	0.97	0.07	42,42,42,42	0
57	K	1A	3557	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3842	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3319	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3192	1/1	0.97	0.28	39,39,39,39	0
56	MG	1A	3145	1/1	0.97	0.09	30,30,30,30	0
56	MG	1P	201	1/1	0.97	0.17	31,31,31,31	0
56	MG	2D	305	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3502	1/1	0.98	0.12	32,32,32,32	0
56	MG	17	104	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	4062	1/1	0.98	0.06	31,31,31,31	0
56	MG	2E	301	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3258	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3391	1/1	0.98	0.08	60,60,60,60	0
56	MG	2A	3260	1/1	0.98	0.05	65,65,65,65	0
56	MG	2A	3549	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3082	1/1	0.98	0.10	35,35,35,35	0
56	MG	2A	3551	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	4065	1/1	0.98	0.14	43,43,43,43	0
56	MG	2A	3263	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3239	1/1	0.98	0.21	29,29,29,29	0
56	MG	2A	3716	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	3046	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3710	1/1	0.98	0.15	45,45,45,45	0
56	MG	1a	1717	1/1	0.98	0.11	35,35,35,35	0
56	MG	1A	3568	1/1	0.98	0.32	33,33,33,33	0
56	MG	1A	3056	1/1	0.98	0.03	24,24,24,24	0
56	MG	1A	3033	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3452	1/1	0.98	0.15	38,38,38,38	0
56	MG	1H	201	1/1	0.98	0.15	60,60,60,60	0
56	MG	1A	3878	1/1	0.98	0.09	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4074	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3796	1/1	0.98	0.04	50,50,50,50	0
56	MG	2A	3568	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3572	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3510	1/1	0.98	0.19	40,40,40,40	0
56	MG	1A	3574	1/1	0.98	0.03	41,41,41,41	0
56	MG	2A	3417	1/1	0.98	0.23	50,50,50,50	0
56	MG	1A	4079	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3162	1/1	0.98	0.21	51,51,51,51	0
56	MG	2R	204	1/1	0.98	0.12	48,48,48,48	0
56	MG	2A	3735	1/1	0.98	0.17	64,64,64,64	0
56	MG	1A	4081	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3106	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3802	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3721	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1735	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3580	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3202	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3086	1/1	0.98	0.18	31,31,31,31	0
56	MG	2A	3150	1/1	0.98	0.14	39,39,39,39	0
56	MG	1P	203	1/1	0.98	0.21	24,24,24,24	0
56	MG	1A	3515	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3247	1/1	0.98	0.15	37,37,37,37	0
56	MG	20	102	1/1	0.98	0.09	52,52,52,52	0
56	MG	1a	1741	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3891	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3986	1/1	0.98	0.05	11,11,11,11	0
56	MG	2A	3295	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3726	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3204	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3058	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3651	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3071	1/1	0.98	0.04	11,11,11,11	0
56	MG	1A	3110	1/1	0.98	0.18	29,29,29,29	0
56	MG	2A	3029	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3034	1/1	0.98	0.21	29,29,29,29	0
56	MG	1A	3733	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3137	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3303	1/1	0.98	0.16	24,24,24,24	0
56	MG	2A	3035	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3999	1/1	0.98	0.04	39,39,39,39	0
56	MG	2a	1768	1/1	0.98	0.09	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3657	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3022	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	4002	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3211	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3739	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3660	1/1	0.98	0.05	22,22,22,22	0
56	MG	2A	3771	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3139	1/1	0.98	0.12	36,36,36,36	0
56	MG	1U	206	1/1	0.98	0.25	35,35,35,35	0
56	MG	1A	3742	1/1	0.98	0.05	41,41,41,41	0
56	MG	1a	1765	1/1	0.98	0.07	53,53,53,53	0
56	MG	1A	3911	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3460	1/1	0.98	0.14	25,25,25,25	0
56	MG	1A	3307	1/1	0.98	0.08	39,39,39,39	0
56	MG	1A	3744	1/1	0.98	0.03	20,20,20,20	0
56	MG	2A	3620	1/1	0.98	0.05	37,37,37,37	0
56	MG	1V	202	1/1	0.98	0.19	31,31,31,31	0
56	MG	2A	3051	1/1	0.98	0.17	49,49,49,49	0
56	MG	1V	203	1/1	0.98	0.08	28,28,28,28	0
56	MG	2A	3624	1/1	0.98	0.04	49,49,49,49	0
56	MG	1V	204	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3113	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3173	1/1	0.98	0.31	33,33,33,33	0
56	MG	1A	3215	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3668	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3174	1/1	0.98	0.14	25,25,25,25	0
56	MG	1W	204	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3792	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3832	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	4017	1/1	0.98	0.03	24,24,24,24	0
56	MG	1A	4018	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3197	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3175	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3834	1/1	0.98	0.04	59,59,59,59	0
56	MG	2A	3800	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3925	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3802	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3751	1/1	0.98	0.06	40,40,40,40	0
56	MG	1a	1785	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3203	1/1	0.98	0.04	52,52,52,52	0
56	MG	1A	3008	1/1	0.98	0.08	25,25,25,25	0
56	MG	1a	1787	1/1	0.98	0.08	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3928	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3092	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3930	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3021	1/1	0.98	0.06	30,30,30,30	0
56	MG	2A	3812	1/1	0.98	0.05	34,34,34,34	0
56	MG	1a	1792	1/1	0.98	0.05	60,60,60,60	0
56	MG	2A	3490	1/1	0.98	0.08	61,61,61,61	0
56	MG	1A	3421	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3816	1/1	0.98	0.08	64,64,64,64	0
56	MG	1a	1794	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	3117	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3266	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3077	1/1	0.98	0.03	27,27,27,27	0
56	MG	1A	3038	1/1	0.98	0.10	24,24,24,24	0
56	MG	1A	3045	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3097	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3098	1/1	0.98	0.10	19,19,19,19	0
56	MG	1a	1676	1/1	0.98	0.14	52,52,52,52	0
56	MG	1D	305	1/1	0.98	0.07	18,18,18,18	0
56	MG	2A	3827	1/1	0.98	0.12	55,55,55,55	0
56	MG	2A	3828	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3186	1/1	0.98	0.14	38,38,38,38	0
56	MG	1D	307	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3088	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3611	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3612	1/1	0.98	0.06	53,53,53,53	0
56	MG	2A	3509	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3273	1/1	0.98	0.07	29,29,29,29	0
56	MG	2A	3511	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3152	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3769	1/1	0.98	0.06	25,25,25,25	0
56	MG	2A	3839	1/1	0.98	0.15	42,42,42,42	0
56	MG	2A	3094	1/1	0.98	0.06	49,49,49,49	0
56	MG	1A	3153	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3189	1/1	0.98	0.07	37,37,37,37	0
56	MG	11	104	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	4044	1/1	0.98	0.03	22,22,22,22	0
56	MG	1A	3277	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3677	1/1	0.98	0.04	33,33,33,33	0
56	MG	1E	304	1/1	0.98	0.11	27,27,27,27	0
56	MG	1E	305	1/1	0.98	0.17	33,33,33,33	0
56	MG	13	101	1/1	0.98	0.04	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3278	1/1	0.98	0.14	24,24,24,24	0
56	MG	1A	4047	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3279	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3527	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	4049	1/1	0.98	0.05	10,10,10,10	0
56	MG	1E	311	1/1	0.98	0.12	22,22,22,22	0
56	MG	2A	3108	1/1	0.98	0.12	58,58,58,58	0
56	MG	1A	3280	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3190	1/1	0.98	0.21	42,42,42,42	0
56	MG	1A	3623	1/1	0.98	0.05	18,18,18,18	0
56	MG	1A	3440	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	4055	1/1	0.98	0.05	28,28,28,28	0
56	MG	2A	3694	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3282	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3123	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3099	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3540	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3080	1/1	0.98	0.04	23,23,23,23	0
59	ZN	2Y	501	1/1	0.98	0.04	95,95,95,95	0
56	MG	1A	3065	1/1	0.98	0.08	37,37,37,37	0
56	MG	2A	3553	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	3074	1/1	0.99	0.04	16,16,16,16	0
56	MG	1A	3191	1/1	0.99	0.08	42,42,42,42	0
56	MG	1A	3484	1/1	0.99	0.18	38,38,38,38	0
56	MG	1F	309	1/1	0.99	0.12	31,31,31,31	0
56	MG	1A	3923	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	3924	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3670	1/1	0.99	0.04	27,27,27,27	0
56	MG	1A	3014	1/1	0.99	0.04	28,28,28,28	0
56	MG	1A	3140	1/1	0.99	0.04	16,16,16,16	0
56	MG	2A	3686	1/1	0.99	0.03	64,64,64,64	0
56	MG	2A	3563	1/1	0.99	0.08	39,39,39,39	0
56	MG	1A	3012	1/1	0.99	0.04	30,30,30,30	0
56	MG	2A	3505	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3003	1/1	0.99	0.06	23,23,23,23	0
56	MG	2A	3023	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	3675	1/1	0.99	0.08	20,20,20,20	0
56	MG	2A	3129	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	4050	1/1	0.99	0.08	24,24,24,24	0
56	MG	1A	3626	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	3765	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3677	1/1	0.99	0.03	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	15	104	1/1	0.99	0.28	29,29,29,29	0
56	MG	2A	3188	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3582	1/1	0.99	0.13	33,33,33,33	0
56	MG	2A	3031	1/1	0.99	0.11	34,34,34,34	0
56	MG	1a	1630	1/1	0.99	0.20	45,45,45,45	0
56	MG	1A	3070	1/1	0.99	0.10	17,17,17,17	0
56	MG	1A	3973	1/1	0.99	0.09	19,19,19,19	0
56	MG	2A	3705	1/1	0.99	0.10	33,33,33,33	0
56	MG	2A	3521	1/1	0.99	0.08	41,41,41,41	0
56	MG	2A	3707	1/1	0.99	0.07	39,39,39,39	0
56	MG	1D	308	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3680	1/1	0.99	0.06	27,27,27,27	0
56	MG	2A	3710	1/1	0.99	0.05	37,37,37,37	0
56	MG	1A	3144	1/1	0.99	0.13	24,24,24,24	0
56	MG	1A	3564	1/1	0.99	0.18	39,39,39,39	0
56	MG	1A	3390	1/1	0.99	0.13	30,30,30,30	0
56	MG	1A	3566	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	3903	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3904	1/1	0.99	0.04	35,35,35,35	0
56	MG	2X	102	1/1	0.99	0.08	51,51,51,51	0
56	MG	1A	3222	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3871	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3983	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3023	1/1	0.99	0.03	12,12,12,12	0
56	MG	1P	204	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3176	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3597	1/1	0.99	0.14	66,66,66,66	0
56	MG	1E	307	1/1	0.99	0.06	25,25,25,25	0
56	MG	1A	3238	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3032	1/1	0.99	0.12	27,27,27,27	0
56	MG	2A	3539	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3988	1/1	0.99	0.08	23,23,23,23	0
56	MG	1A	3989	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3615	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3380	1/1	0.99	0.22	29,29,29,29	0
56	MG	1A	3663	1/1	0.99	0.02	34,34,34,34	0
56	MG	2A	3798	1/1	0.99	0.03	45,45,45,45	0
56	MG	1A	3048	1/1	0.99	0.09	37,37,37,37	0
56	MG	1A	3665	1/1	0.99	0.06	22,22,22,22	0
56	MG	1F	302	1/1	0.99	0.15	26,26,26,26	0
56	MG	1a	1756	1/1	0.99	0.06	55,55,55,55	0
56	MG	1A	3430	1/1	0.99	0.07	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	ZN	1Y	206	1/1	0.99	0.03	75,75,75,75	0
56	MG	1A	3785	1/1	0.99	0.03	17,17,17,17	0
59	ZN	1n	103	1/1	0.99	0.03	66,66,66,66	0
56	MG	1A	3786	1/1	0.99	0.04	17,17,17,17	0
56	MG	2A	3494	1/1	0.99	0.07	48,48,48,48	0
59	ZN	29	501	1/1	0.99	0.03	72,72,72,72	0
59	ZN	2n	501	1/1	0.99	0.03	84,84,84,84	0
60	SF4	1d	302	8/8	0.99	0.04	60,64,69,72	0
60	SF4	2d	303	8/8	0.99	0.04	52,65,72,78	0
59	ZN	19	102	1/1	1.00	0.03	42,42,42,42	0
56	MG	1A	3920	1/1	1.00	0.02	13,13,13,13	0
56	MG	1A	3610	1/1	1.00	0.05	32,32,32,32	0
56	MG	1A	3713	1/1	1.00	0.05	17,17,17,17	0
59	ZN	25	107	1/1	1.00	0.05	55,55,55,55	0
59	ZN	26	102	1/1	1.00	0.03	61,61,61,61	0
56	MG	1Q	202	1/1	1.00	0.02	31,31,31,31	0
56	MG	2A	3581	1/1	1.00	0.02	39,39,39,39	0
59	ZN	15	111	1/1	1.00	0.07	47,47,47,47	0
59	ZN	16	102	1/1	1.00	0.02	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.