



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:21 AM UTC

PDB ID : 5HD1 / pdb_00005hd1
Title : Crystal structure of antimicrobial peptide Pyrrhocoricin bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on : 2016-01-04
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

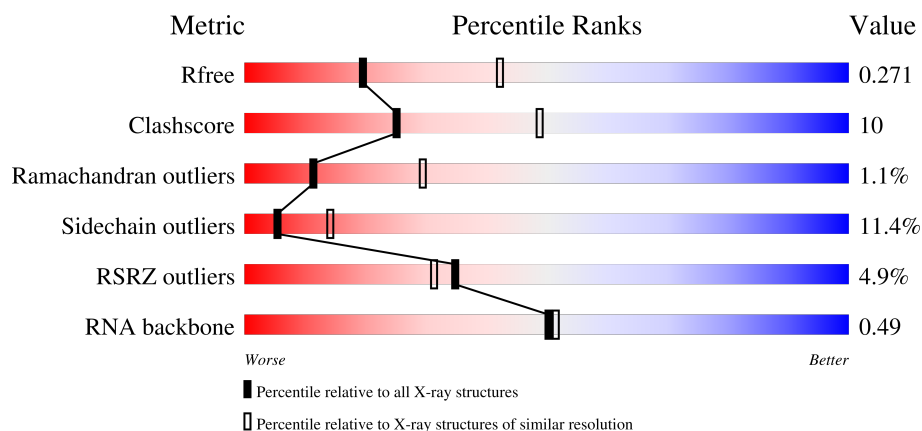
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



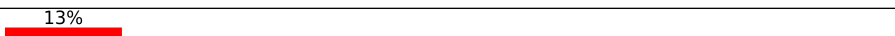
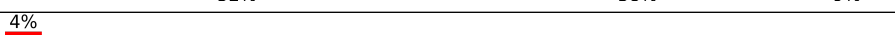
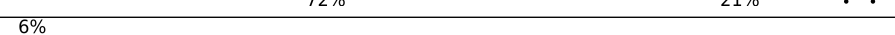
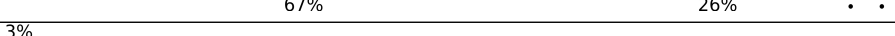
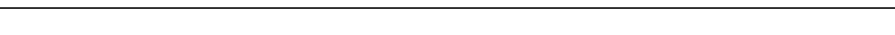
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	121	
2	2B	121	

Continued on next page...

Continued from previous page...

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

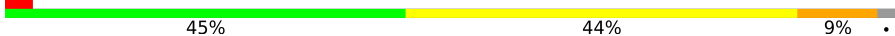
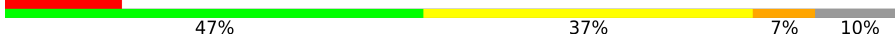
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	20	
55	2z	20	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4203	-	-	-	X
56	MG	2a	1673	-	-	-	X
58	SF4	1d	501	-	-	X	-
58	SF4	2d	501	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288775 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1074	681	202	189	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			826	513	156	154	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			715	447	140	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			671	424	133	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			811	519	148	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called P-site tRNA.

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

- Molecule 55 is a protein called Pyrrhocoricin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	16	Total	C	N	O	0	0	0
			126	82	23	21			
55	2z	16	Total	C	N	O	0	0	0
			126	82	23	21			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1233	Total	Mg	0	0
			1233	1233		
56	1B	25	Total	Mg	0	0
			25	25		
56	1D	15	Total	Mg	0	0
			15	15		
56	1E	8	Total	Mg	0	0
			8	8		
56	1F	9	Total	Mg	0	0
			9	9		
56	1G	3	Total	Mg	0	0
			3	3		
56	1H	1	Total	Mg	0	0
			1	1		
56	1N	7	Total	Mg	0	0
			7	7		
56	1O	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1P	5	Total 5	Mg 5	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	1R	8	Total 8	Mg 8	0	0
56	1T	4	Total 4	Mg 4	0	0
56	1U	6	Total 6	Mg 6	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	1	Total 1	Mg 1	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	1	Total 1	Mg 1	0	0
56	15	4	Total 4	Mg 4	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	3	Total 3	Mg 3	0	0
56	18	5	Total 5	Mg 5	0	0
56	19	3	Total 3	Mg 3	0	0
56	1a	295	Total 295	Mg 295	0	0
56	1b	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1d	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1h	2	Total 2	Mg 2	0	0
56	1k	2	Total 2	Mg 2	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1o	1	Total 1	Mg 1	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1q	2	Total 2	Mg 2	0	0
56	1r	2	Total 2	Mg 2	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1x	12	Total 12	Mg 12	0	0
56	2A	592	Total 592	Mg 592	0	0
56	2B	9	Total 9	Mg 9	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2E	6	Total 6	Mg 6	0	0
56	2F	2	Total 2	Mg 2	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	3	Total 3	Mg 3	0	0

Continued on next page...

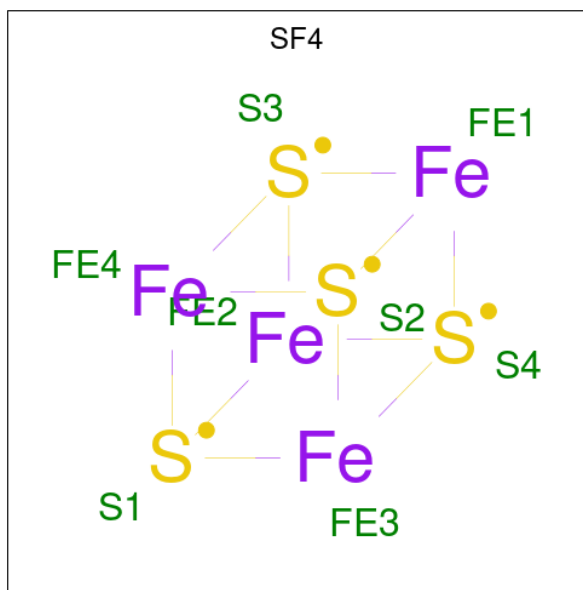
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2Q	5	Total 5	Mg 5	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	248	Total 248	Mg 248	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	2	Total 2	Mg 2	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2l	5	Total 5	Mg 5	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2u	1	Total 1	Mg 1	0	0
56	2x	4	Total 4	Mg 4	0	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2217	Total	O	0	0
			2217	2217		
59	1B	37	Total	O	0	0
			37	37		
59	1D	23	Total	O	0	0
			23	23		
59	1E	29	Total	O	0	0
			29	29		
59	1F	19	Total	O	0	0
			19	19		
59	1G	2	Total	O	0	0
			2	2		
59	1H	4	Total	O	0	0
			4	4		
59	1I	1	Total	O	0	0
			1	1		
59	1N	6	Total	O	0	0
			6	6		
59	1O	7	Total	O	0	0
			7	7		
59	1P	27	Total	O	0	0
			27	27		
59	1Q	14	Total	O	0	0
			14	14		
59	1R	11	Total	O	0	0
			11	11		
59	1S	2	Total	O	0	0
			2	2		
59	1T	13	Total	O	0	0
			13	13		
59	1U	14	Total	O	0	0
			14	14		
59	1V	7	Total	O	0	0
			7	7		
59	1W	8	Total	O	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	5	Total 5	O 5	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	7	Total 7	O 7	0	0
59	10	12	Total 12	O 12	0	0
59	11	5	Total 5	O 5	0	0
59	12	3	Total 3	O 3	0	0
59	13	4	Total 4	O 4	0	0
59	15	9	Total 9	O 9	0	0
59	16	9	Total 9	O 9	0	0
59	17	10	Total 10	O 10	0	0
59	18	12	Total 12	O 12	0	0
59	19	2	Total 2	O 2	0	0
59	1a	338	Total 338	O 338	0	0
59	1b	2	Total 2	O 2	0	0
59	1d	3	Total 3	O 3	0	0
59	1e	7	Total 7	O 7	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	3	Total 3	O 3	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1k	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1l	3	Total 3	O 3	0	0
59	1m	1	Total 1	O 1	0	0
59	1o	1	Total 1	O 1	0	0
59	1q	1	Total 1	O 1	0	0
59	1r	1	Total 1	O 1	0	0
59	1s	2	Total 2	O 2	0	0
59	1t	1	Total 1	O 1	0	0
59	1v	3	Total 3	O 3	0	0
59	1x	9	Total 9	O 9	0	0
59	2A	809	Total 809	O 809	0	0
59	2B	12	Total 12	O 12	0	0
59	2D	20	Total 20	O 20	0	0
59	2E	11	Total 11	O 11	0	0
59	2F	7	Total 7	O 7	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	3	Total 3	O 3	0	0
59	2P	3	Total 3	O 3	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
59	2T	3	Total 3	O 3	0	0
59	2U	3	Total 3	O 3	0	0

Continued on next page...

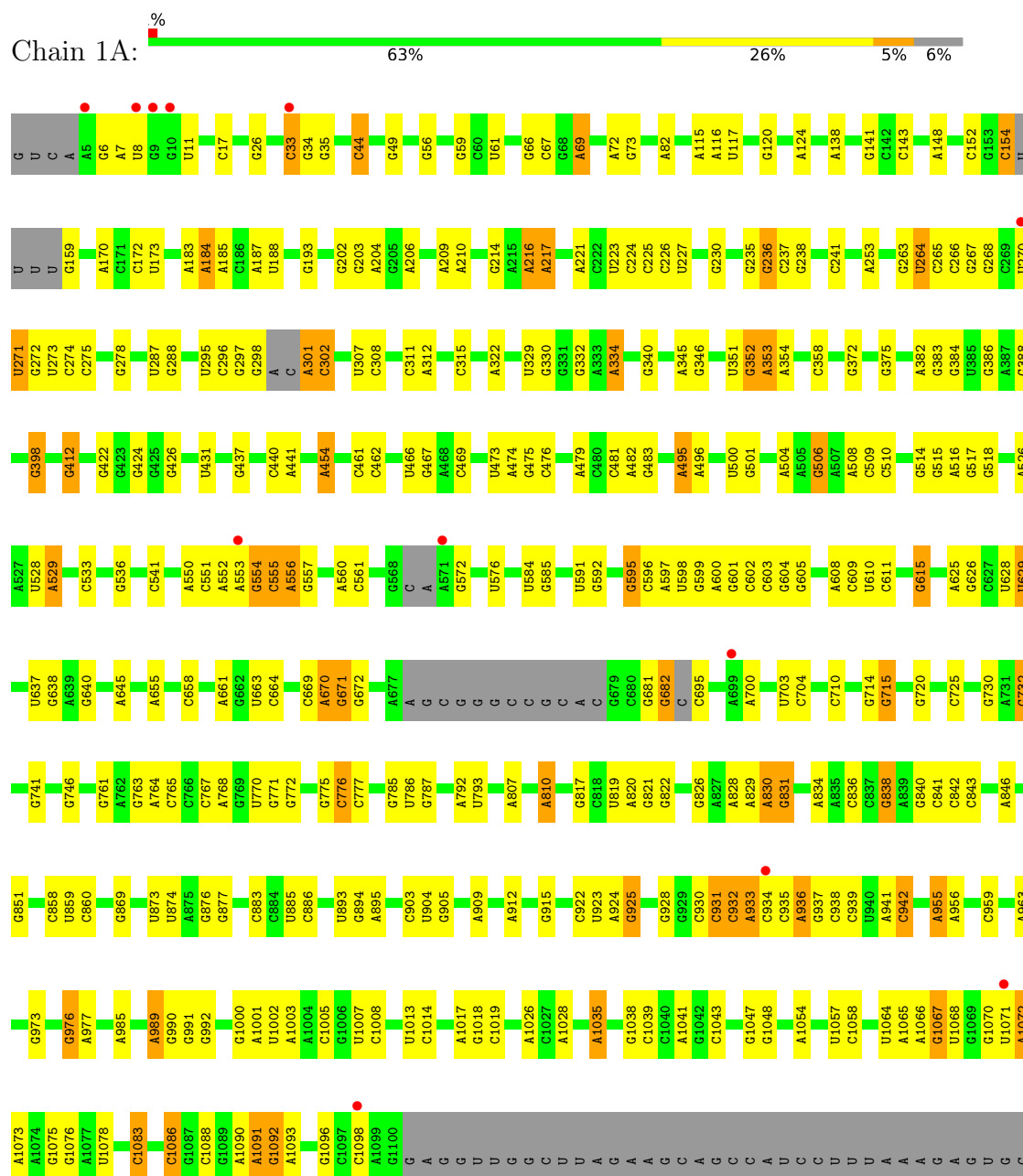
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2W	1	Total 1	O 1	0	0
59	2X	2	Total 2	O 2	0	0
59	2Y	1	Total 1	O 1	0	0
59	2Z	6	Total 6	O 6	0	0
59	20	4	Total 4	O 4	0	0
59	21	1	Total 1	O 1	0	0
59	23	1	Total 1	O 1	0	0
59	25	1	Total 1	O 1	0	0
59	27	1	Total 1	O 1	0	0
59	28	4	Total 4	O 4	0	0
59	2a	274	Total 274	O 274	0	0
59	2c	2	Total 2	O 2	0	0
59	2d	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2j	2	Total 2	O 2	0	0
59	2l	2	Total 2	O 2	0	0
59	2p	1	Total 1	O 1	0	0
59	2t	3	Total 3	O 3	0	0
59	2v	1	Total 1	O 1	0	0
59	2x	2	Total 2	O 2	0	0

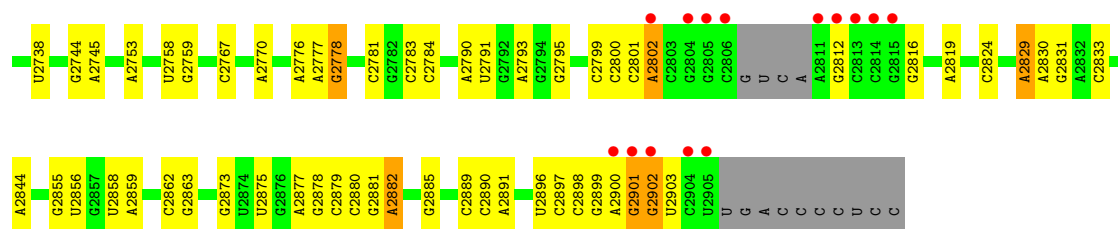
3 Residue-property plots

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.

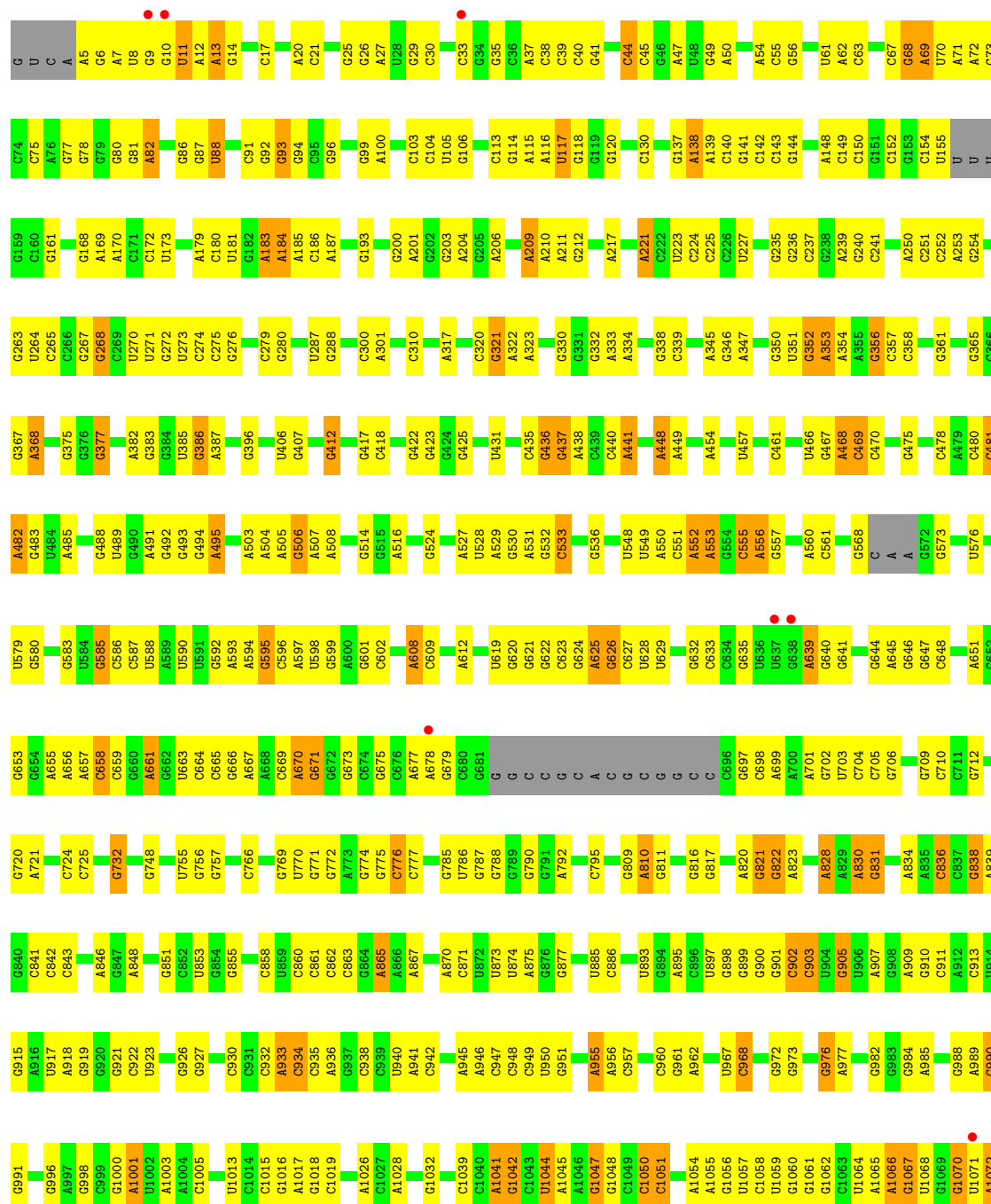
• Molecule 1: 23S Ribosomal RNA



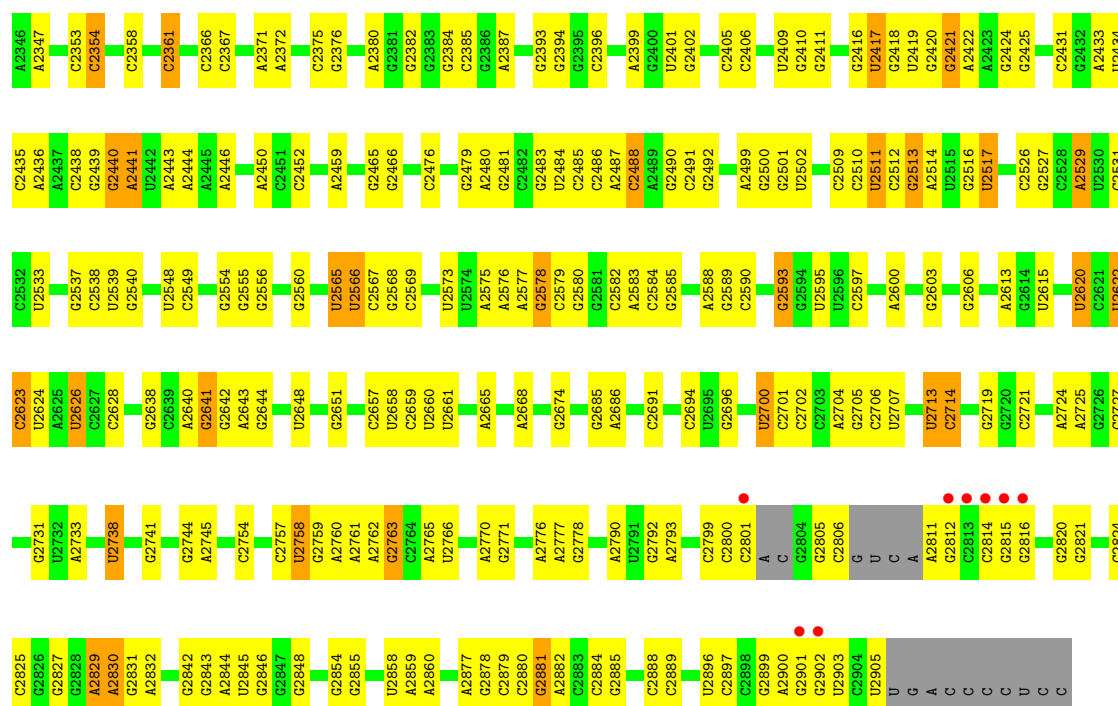
G2505	G2376	A2279	A	U2119	A1993	C1873	A1744	A1613	G1496	G1391	U1232	G
G2506	G2391	A2280	G	U2120	U2012	A1877	G1745	G1614	A1499	G1391	U1232	U
C2507	C2391	A2280	C	G2121	G2013	A1877	A1746	A1615	U1500	A1394	G1235	A
G2508	G2394	U2283	G	G2122	U2014	A1878	U1755	A1616	G1501	A1394	G1235	A
C2509	G2395	A2284	C	U2123	U2014	A1879	C1756	A1617	G1502	U1397	G1247	U
C2510	C2396	C2286	C	G2124	C2017	G1880	U1763	G1618	G1502	A1398	G1248	A
G2513	C2397	G2287	C	G	G2018	U1881	G1763	G1619	C1510	A1399	A1254	C
A2514	U2398	G2288	G	C	G2019	U1882	U1764	C1620	G1511	G1400	A1254	C
U2515	G2411	A2289	U	C	C2020	G1882	G1765	U1625	G1512	A1404	A1264	U
G2516	G2411	C2290	C	C	G2021	A1889	A1766	A1626	G1513	A1405	G1275	C
U2517	G2416	C2294	A	U	A2022	U1767	U1767	A1627	C1514	A1405	G1276	A
U2522	U2417	C2294	A	C	G2033	A1898	G1783	C1628	C1520	A1410	G1280	U
A2529	A2433	A2297	U	C	A2034	G1899	C1784	A1629	G1521	A1410	G1280	U
U2536	U2434	A2298	A	U	A2035	C1903	A1785	C1630	G1524	U1416	U1285	C
G2540	C2435	A2299	C	A	U2043	G1904	U1787	A1631	G1524	A1417	U1285	C
A2541	A2436	C2301	C	C	G2044	U1910	G1788	A1632	G1528	A1424	A1287	C
G2542	G2439	U2302	C	A	G2045	A1910	G1788	C1633	G1528	A1424	A1287	C
G2543	G2440	C2303	C	U	C2046	G1920	A1792	C1634	A1531	A1425	U1288	C
A2544	A2441	C2303	C	U	U2047	A1921	G1793	U1647	G1532	A1429	U1289	C
A2545	U2442	A2315	U	G	G2048	G1924	G1794	A1648	A1539	A1429	U1289	C
C2557	A2443	A2316	G	U	U2049	A1803	A1803	C1649	A1540	G1430	A1298	C
C2558	A2443	A2316	G	U	G2050	A1803	A1803	C1649	A1540	G1430	A1298	C
C2559	A2446	G2319	G	G	A2051	G1927	U1809	C1652	A1541	U1435	G1301	C
U2560	A2446	A2320	G	G	A2052	G1927	U1809	C1652	A1541	U1435	G1301	C
A2565	A2450	A2321	G	G	G2053	A1834	A1810	A1653	A1552	U1312	U1312	C
C2568	C2451	G2322	C	A	A2054	U1936	A1813	A1654	A1553	A1440	A1313	C
C2569	C2452	U2323	C	G	G2059	U1937	A1816	C1670	C1554	U1441	G1316	C
C2570	G2456	G2330	C	C	U2062	U1938	A1816	G1671	A1556	U1450	A1317	C
A2571	G2457	A2331	U	U	A2063	A1939	A1816	U1674	A1556	U1451	U1318	C
U2573	G2458	G2336	G	U	C2064	A1940	A1821	G1675	G1565	C1452	U1318	C
U2574	U2460	C2337	G	G	C2076	A1943	U1826	A1678	G1566	A1457	A1323	C
C2575	A2461	A2338	A	A	G2077	A1949	C1827	C1682	G1571	G1458	G1338	C
A2576	A2470	G2340	C	C	A2081	G1950	U1828	C1682	G1572	U1345	U1345	C
C2577	U2473	G2342	C	C	G2082	U1951	G1829	A1687	A1574	A1346	A1346	C
C2578	U2473	G2342	C	C	A2083	U1952	C1830	G1688	C1578	A1347	A1347	C
C2579	G2479	A2345	C	C	C2086	G1954	A1832	G1693	G	U1465	G1348	C
A2583	A2480	A2347	C	C	C2087	A1958	A1833	C1694	U	G1466	G1349	C
C2584	G2481	G2348	C	C	U2090	A1959	C1834	A1700	A	G1467	C1350	C
C2586	C2485	U2355	U	U	G2095	U1976	A1840	C1709	C	G1471	C1351	C
C2590	A2487	G2356	C	C	U2095	A1981	G1841	A1710	G1583	A1352	A1352	C
U2591	A2488	A2357	C	C	U2100	G1844	G1844	A1711	G1587	G1354	G1354	C
C2593	A2489	C2358	G	G	U2107	G1845	G1845	A1712	A1588	G1355	A1218	C
U2596	G2493	C2361	C	C	G2111	G1846	G1846	G1715	C1589	C1475	U1219	C
C2600	G2498	G2365	C	C	G2114	G1857	G1857	A1736	A1591	U1476	G1357	C
U2604	U2502	U2367	G	G	C2118	G1859	A1859	U1739	C1603	C1482	G1369	C
C2605	C2735	C2375	G	G	C2118	A1990	A1859	U1739	A1604	A1490	G1377	C
C2606	C2735	C2375	G	G	C2118	A1991	A1859	U1739	A1612	A1495	A1387	C



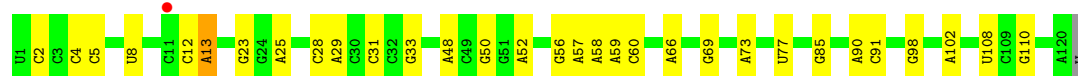
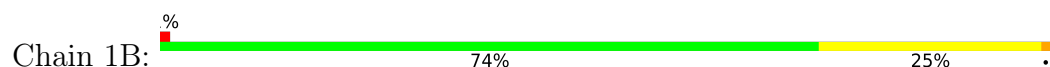
• Molecule 1: 23S Ribosomal RNA







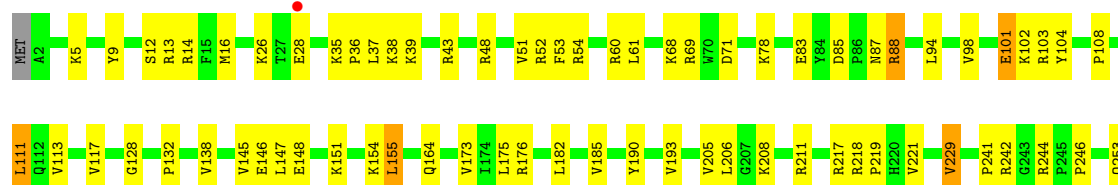
• Molecule 2: 5S Ribosomal RNA



• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

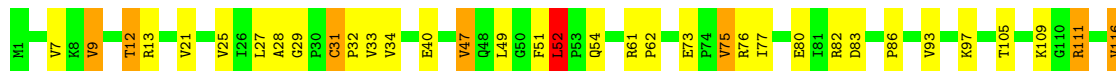




• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3



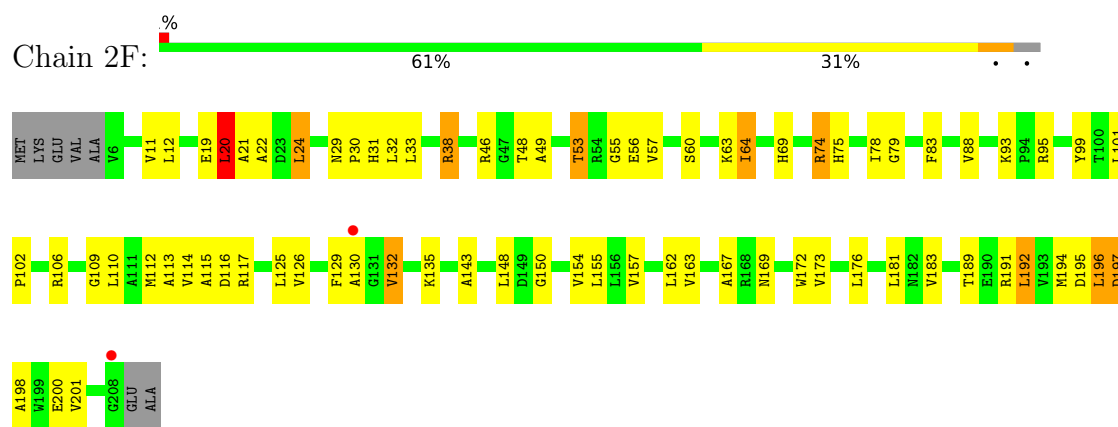
• Molecule 4: 50S ribosomal protein L3



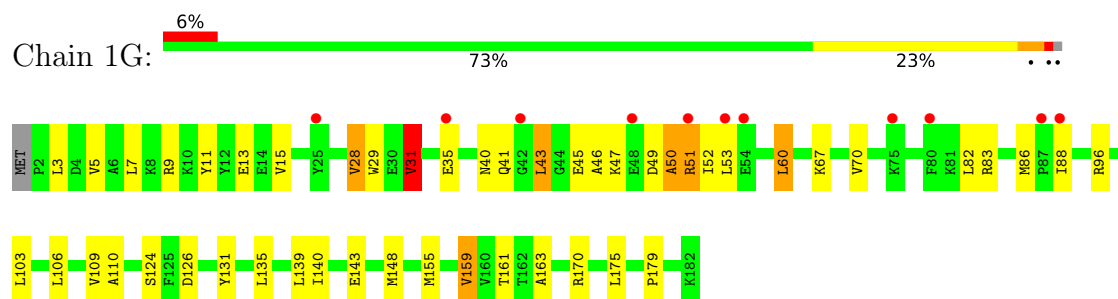
• Molecule 5: 50S ribosomal protein L4



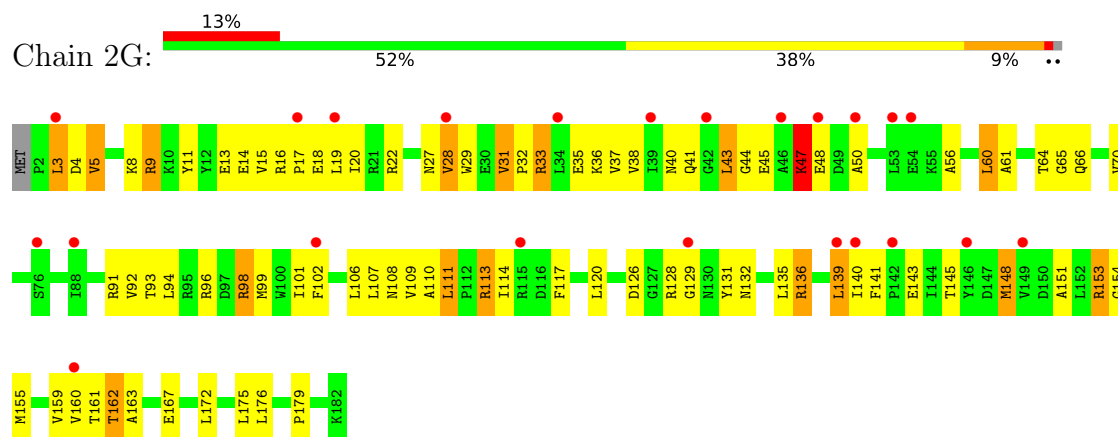
• Molecule 5: 50S ribosomal protein L4



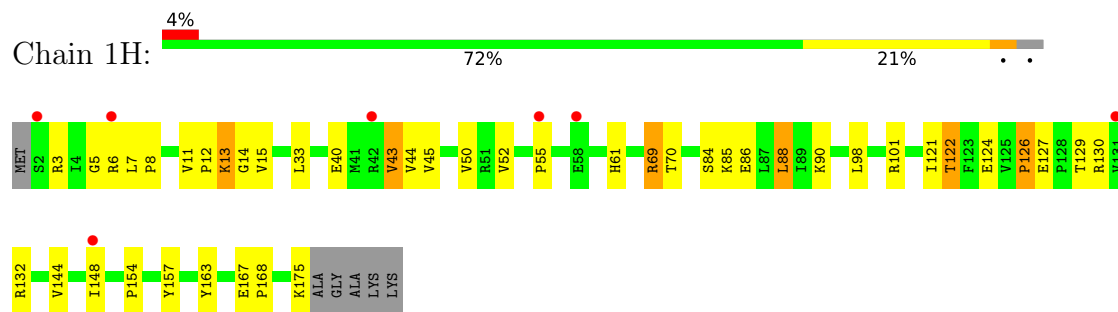
• Molecule 6: 50S ribosomal protein L5



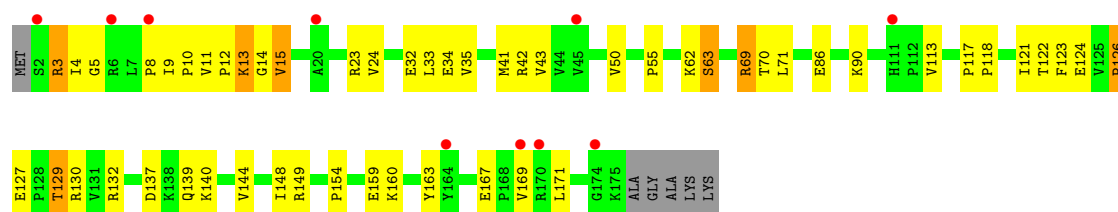
• Molecule 6: 50S ribosomal protein L5



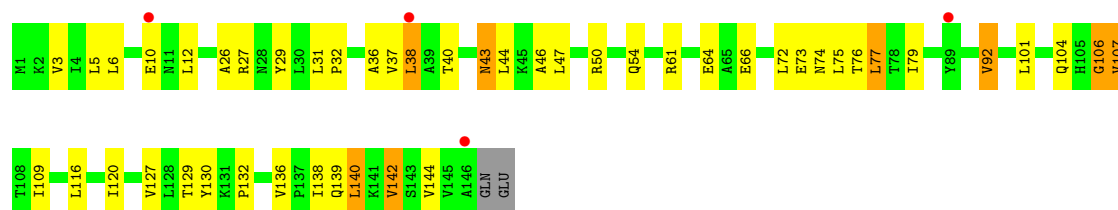
• Molecule 7: 50S ribosomal protein L6



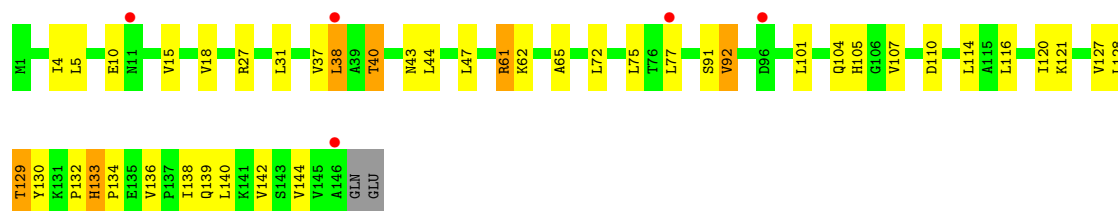
• Molecule 7: 50S ribosomal protein L6



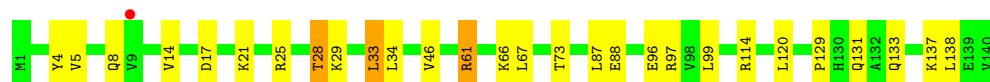
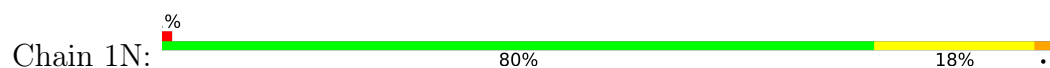
• Molecule 8: 50S ribosomal protein L9



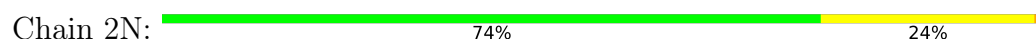
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

Chain 1O:  76% 20% .



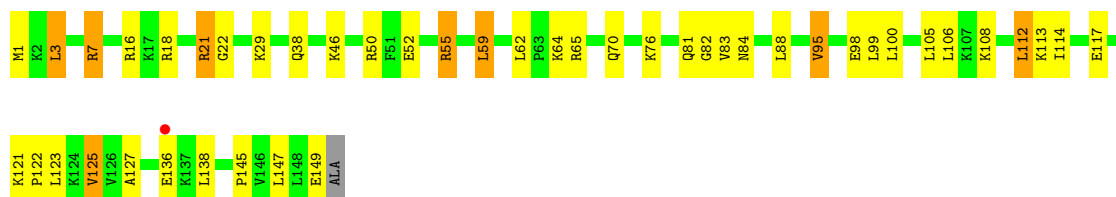
• Molecule 10: 50S ribosomal protein L14

Chain 2O:  74% 24% .



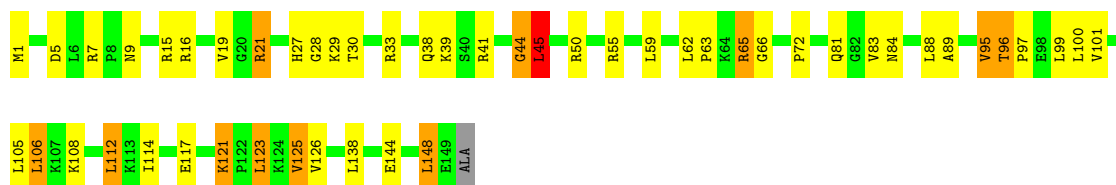
• Molecule 11: 50S ribosomal protein L15

Chain 1P:  69% 25% 5% .



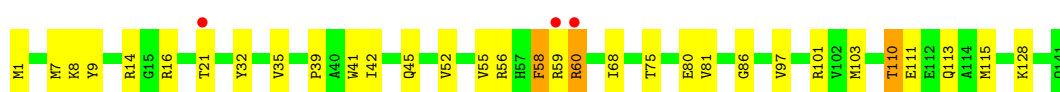
• Molecule 11: 50S ribosomal protein L15

Chain 2P:  66% 25% 7% ..



• Molecule 12: 50S ribosomal protein L16

Chain 1Q:  77% 21% .



• Molecule 12: 50S ribosomal protein L16

Chain 2Q:  71% 27% .





- Molecule 13: 50S ribosomal protein L17

Chain 1R: 74% 25% .



- Molecule 13: 50S ribosomal protein L17

Chain 2R: 68% 31% .



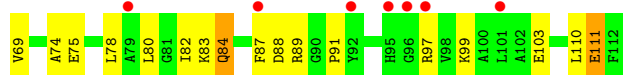
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 2% 65% 24% 9% .



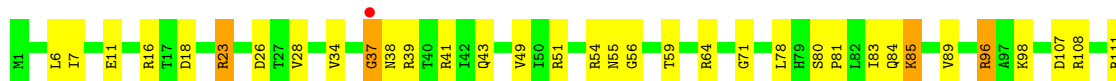
- Molecule 14: 50S ribosomal protein L18

Chain 2S: 33% 60% 31% 7% .



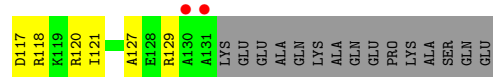
- Molecule 15: 50S ribosomal protein L19

Chain 1T: 3% 60% 27% 10% .

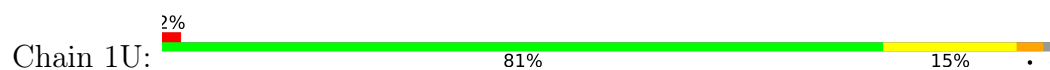




- Molecule 15: 50S ribosomal protein L19



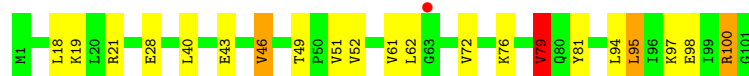
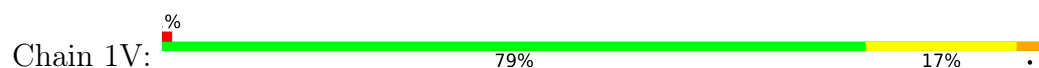
- Molecule 16: 50S ribosomal protein L20



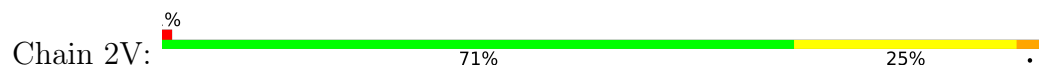
- Molecule 16: 50S ribosomal protein L20



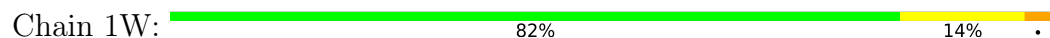
- Molecule 17: 50S ribosomal protein L21



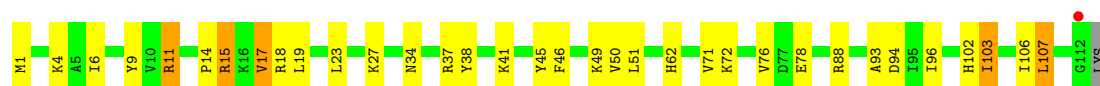
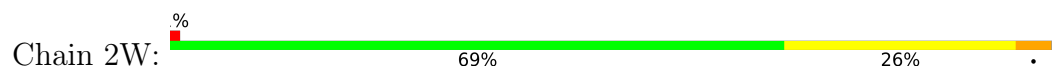
- Molecule 17: 50S ribosomal protein L21



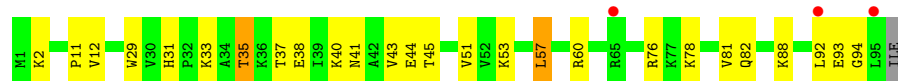
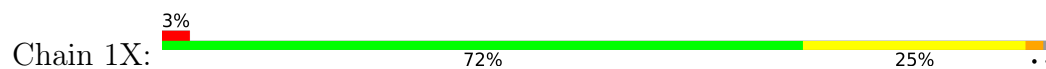
- Molecule 18: 50S ribosomal protein L22



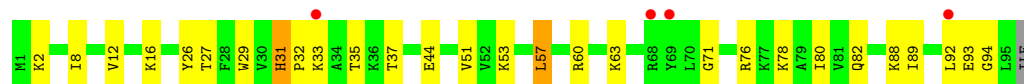
- Molecule 18: 50S ribosomal protein L22



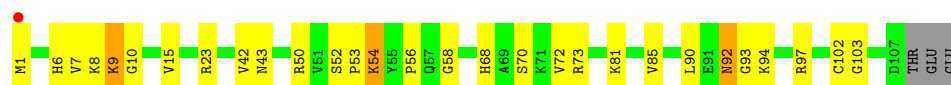
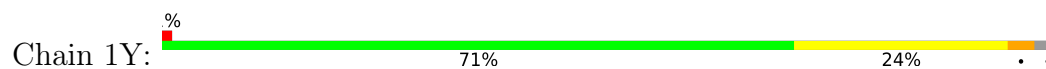
- Molecule 19: 50S ribosomal protein L23



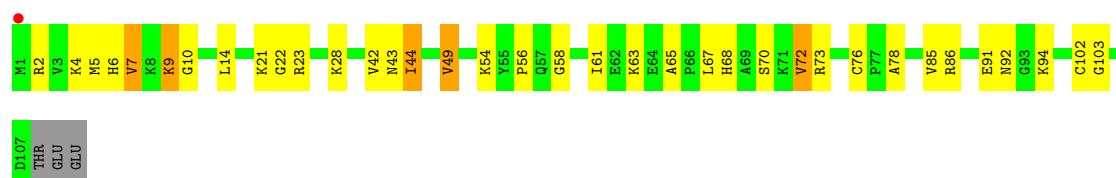
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



- [illegible]

- Chain 10: 

- Chain 20:
-
- | Amino Acid | Percentage |
|------------|------------|
| 4% | |
| 66% | |
| 20% | |
| 12% | |

- Chain 11:
-
- | Amino Acid | Percentage |
|------------|------------|
| MET | 2% |
| S2 | 81% |
| K3 | 15% |
| V4 | 2% |
| R21 | - |
| G22 | - |
| K23 | - |
| G28 | - |
| V30 | - |
| T35 | - |
| R40 | - |
| T59 | - |
| A64 | - |
| S65 | - |
| H66 | - |
| I67 | - |
| P68 | - |
| Y71 | - |
| K78 | - |
| K92 | - |
| L96 | - |
| L98 | - |

- Chain 21:
-
- | Category | Percentage |
|----------|------------|
| MET | ~1% |
| S2 | 2% |
| K3 | ~1% |
| V4 | ~1% |
| Q19 | ~1% |
| R20 | ~1% |
| R21 | ~1% |
| G22 | ~1% |
| K23 | ~1% |
| Q29 | ~1% |
| V30 | ~1% |
| T35 | ~1% |
| R40 | ~1% |
| T59 | ~1% |
| F60 | ~1% |
| R61 | ~1% |
| S65 | ~1% |
| H66 | ~1% |
| Y71 | ~1% |
| F72 | ~1% |
| L73 | ~1% |
| A77 | ~1% |
| L80 | ~1% |
| E83 | ~1% |
| G84 | ~1% |
| K92 | ~1% |
| E93 | ~1% |
| L94 | ~1% |
| L95 | ~1% |
| L96 | ~1% |
| L98 | ~1% |

- Chain 12: 

- Molecule 24: 50S ribosomal protein L29

Chain 22:  72% 22% . .



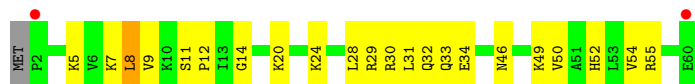
- Molecule 25: 50S ribosomal protein L30

Chain 13:  82% 13% . .



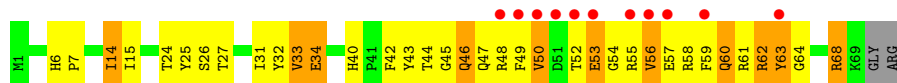
- Molecule 25: 50S ribosomal protein L30

Chain 23:  3% 62% 35% . .



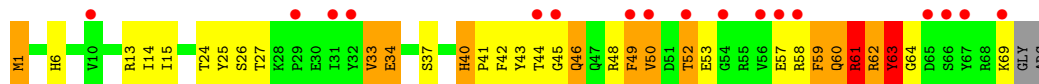
- Molecule 26: 50S ribosomal protein L31

Chain 14:  15% 46% 35% 15% .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  24% 51% 28% 15% . .



- Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 83% 12% . .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  72% 23% . .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  74% 20% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26:  65% 31% ..



- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 65% 31% ..



- Molecule 29: 50S ribosomal protein L34

Chain 27:  2% 67% 31% .



- Molecule 30: 50S ribosomal protein L35

Chain 18:  72% 26% .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  62% 32% 5% .

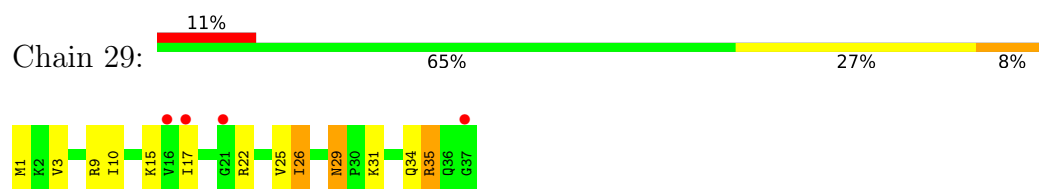


- Molecule 31: 50S ribosomal protein L36

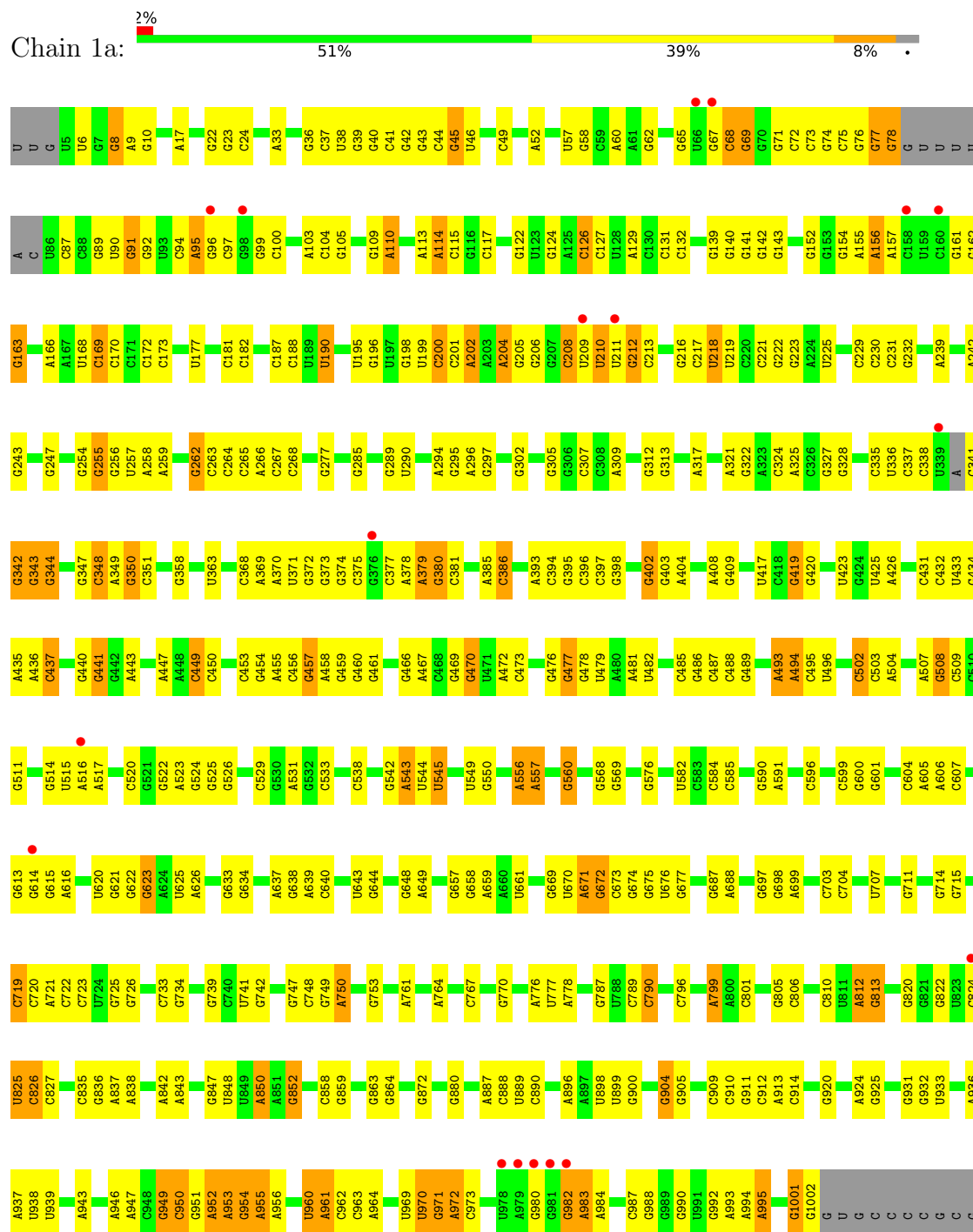
Chain 19:  3% 57% 41% .



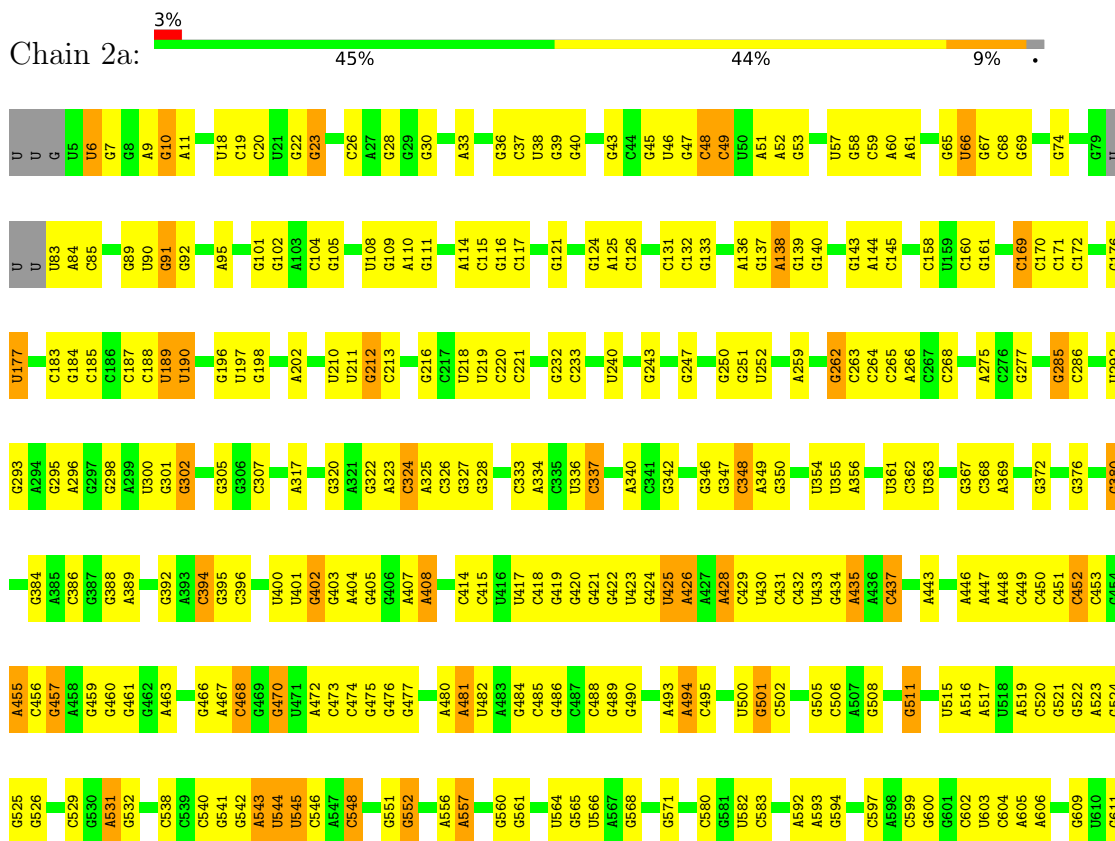
• Molecule 31: 50S ribosomal protein L36

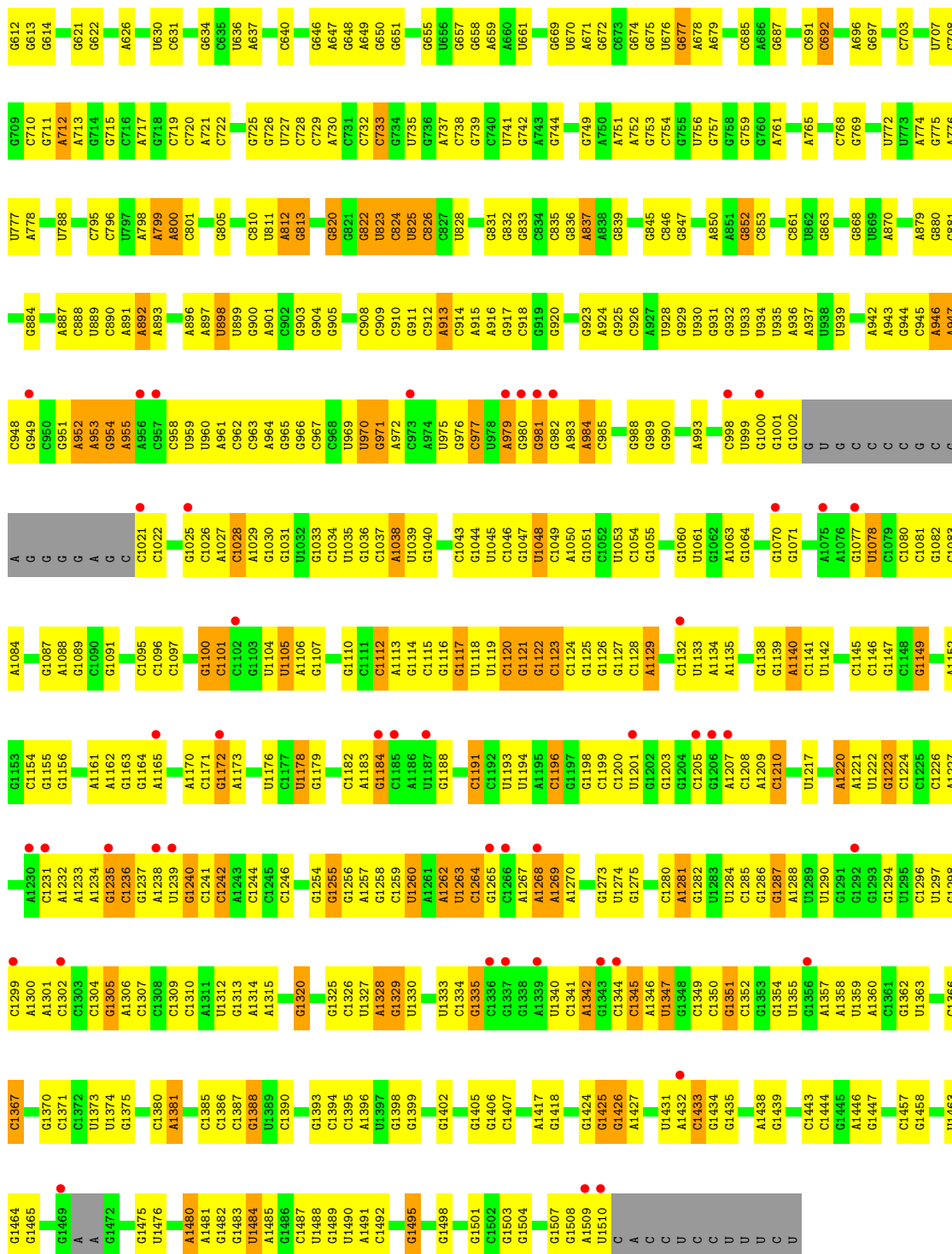


• Molecule 32: 16S Ribosomal RNA

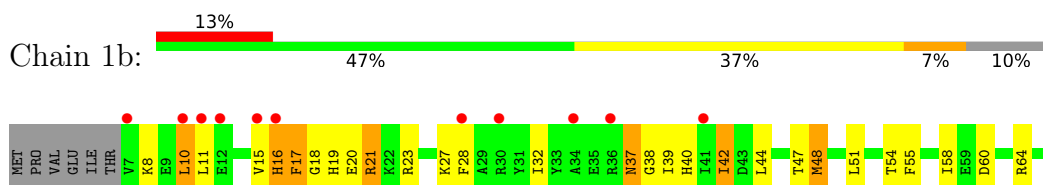


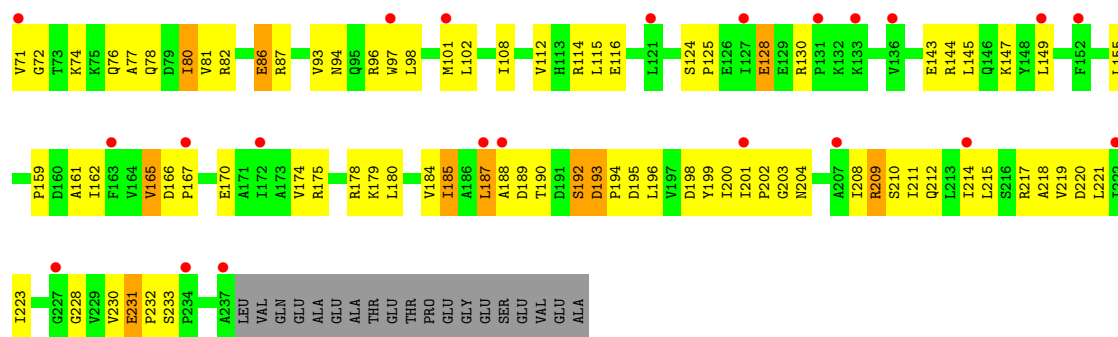
- Molecule 32: 16S Ribosomal RNA



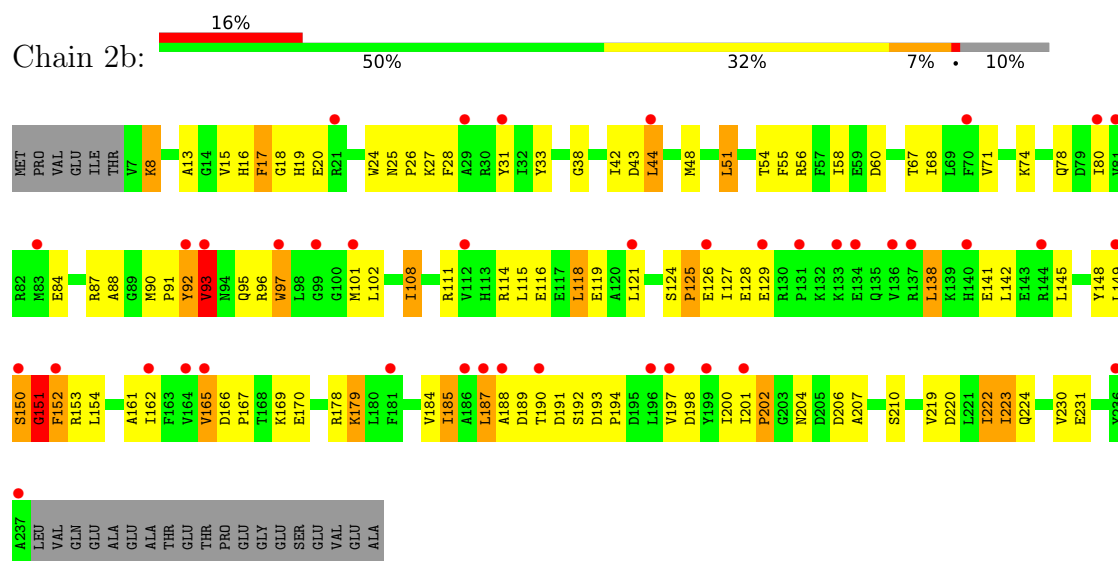


- Molecule 33: 30S ribosomal protein S2

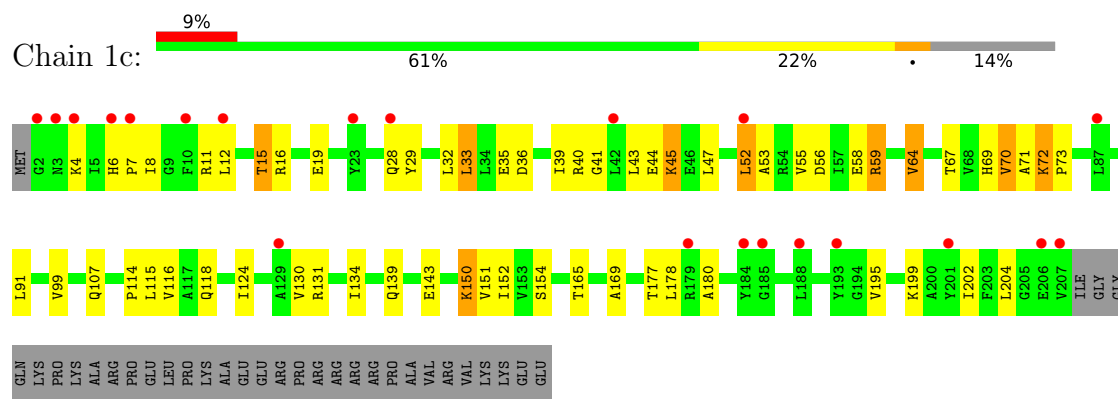




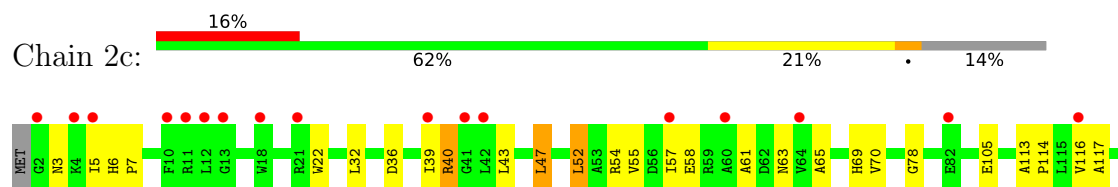
- Molecule 33: 30S ribosomal protein S2

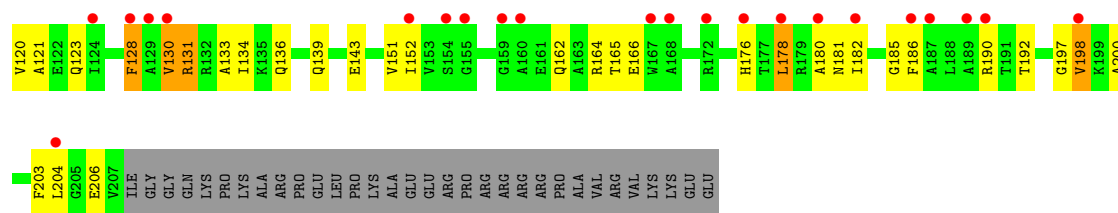


- Molecule 34: 30S ribosomal protein S3

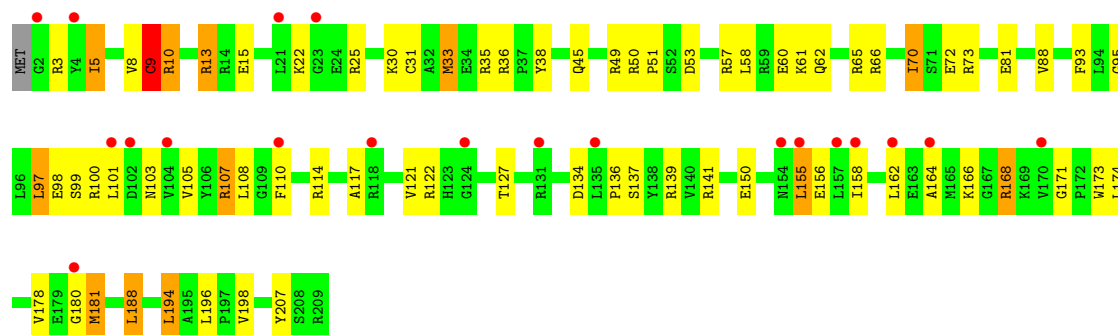


- Molecule 34: 30S ribosomal protein S3

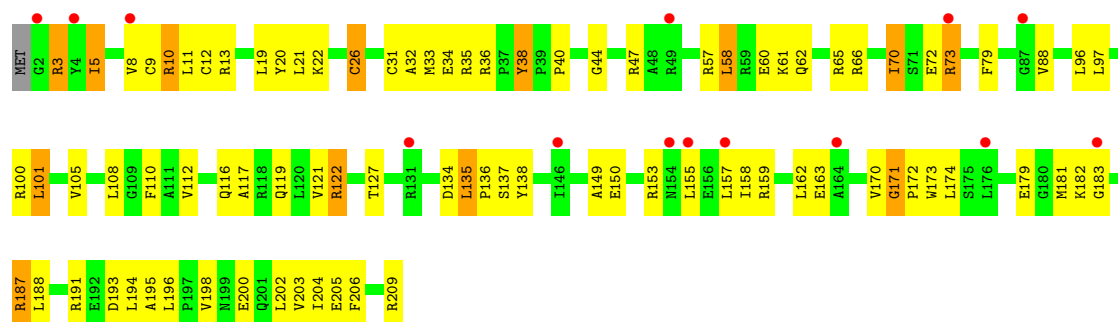




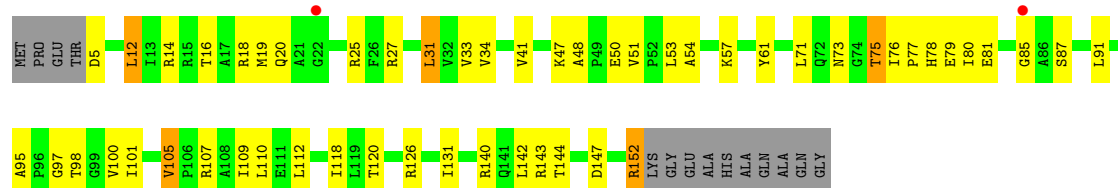
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

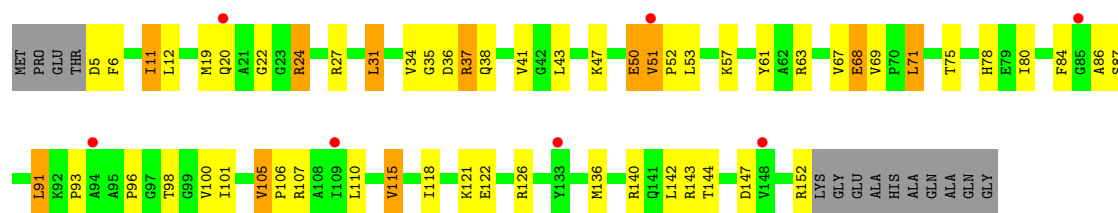


• Molecule 36: 30S ribosomal protein S5

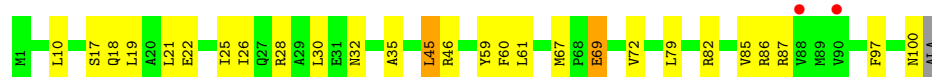
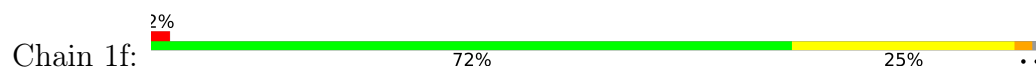


• Molecule 36: 30S ribosomal protein S5

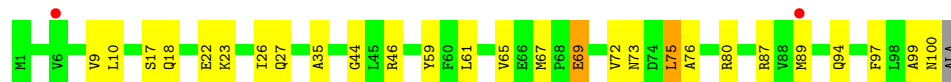
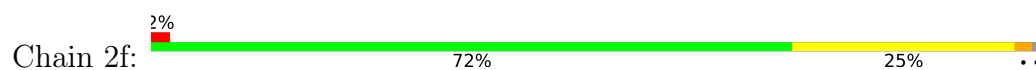




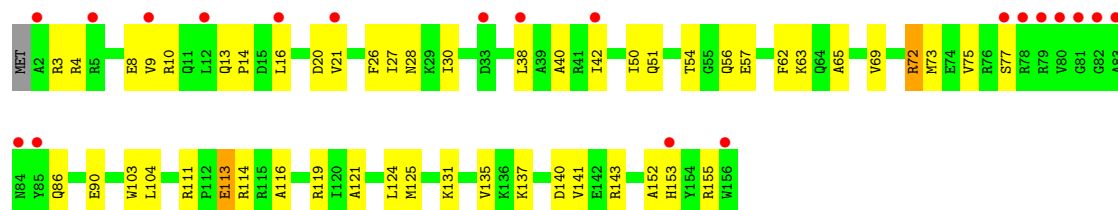
- Molecule 37: 30S ribosomal protein S6



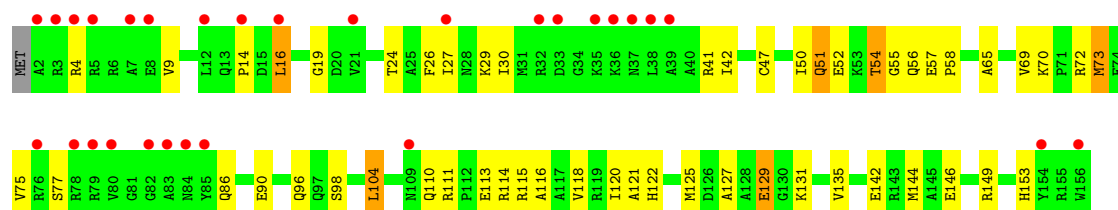
- Molecule 37: 30S ribosomal protein S6



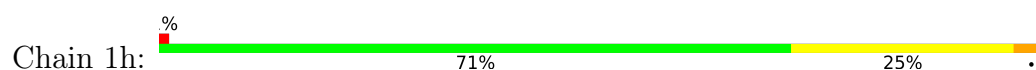
- Molecule 38: 30S ribosomal protein S7

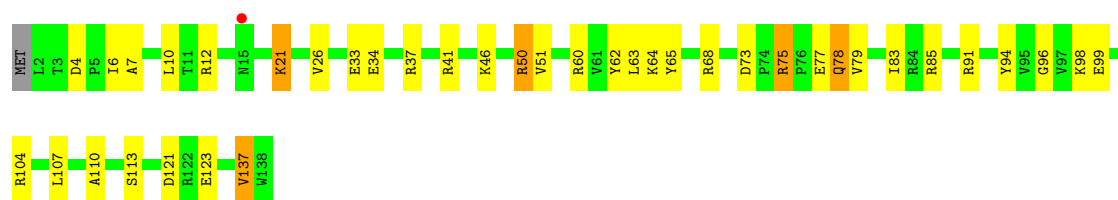


- Molecule 38: 30S ribosomal protein S7

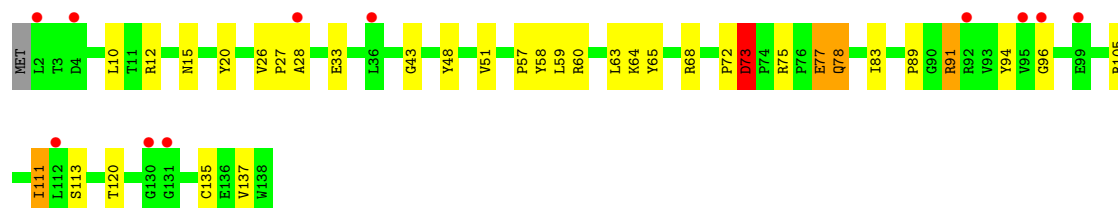
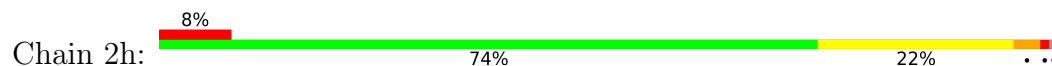


- Molecule 39: 30S ribosomal protein S8

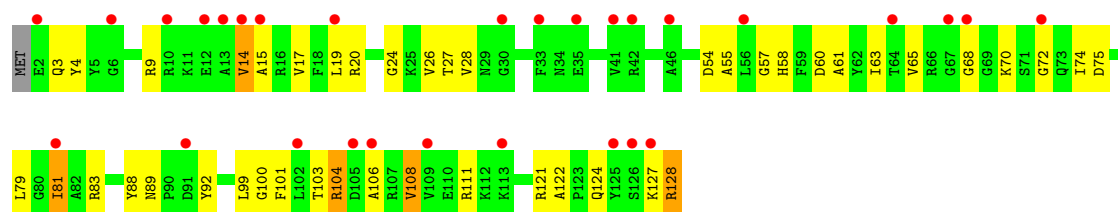




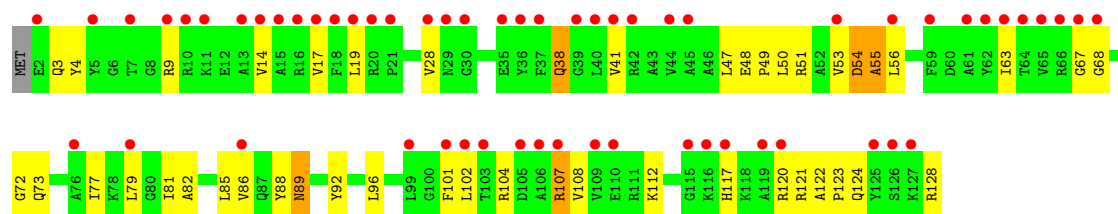
- Molecule 39: 30S ribosomal protein S8



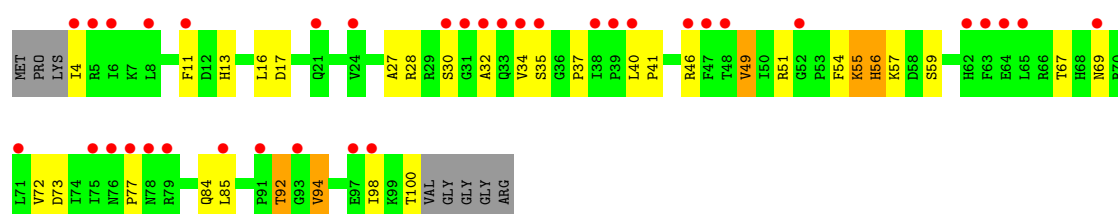
- Molecule 40: 30S ribosomal protein S9



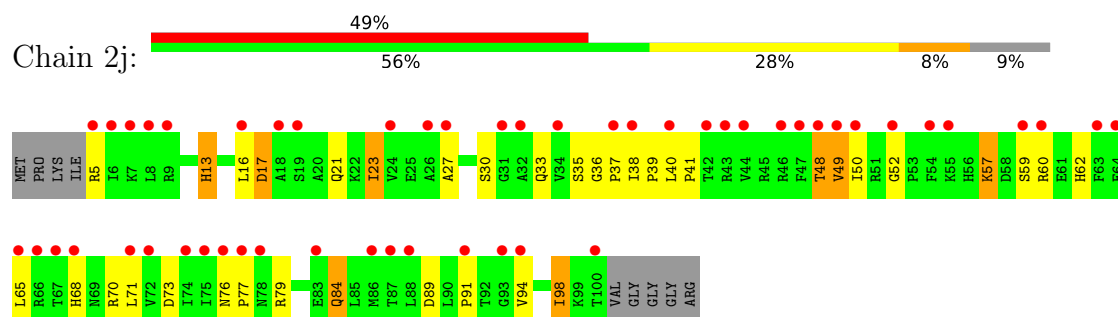
- Molecule 40: 30S ribosomal protein S9



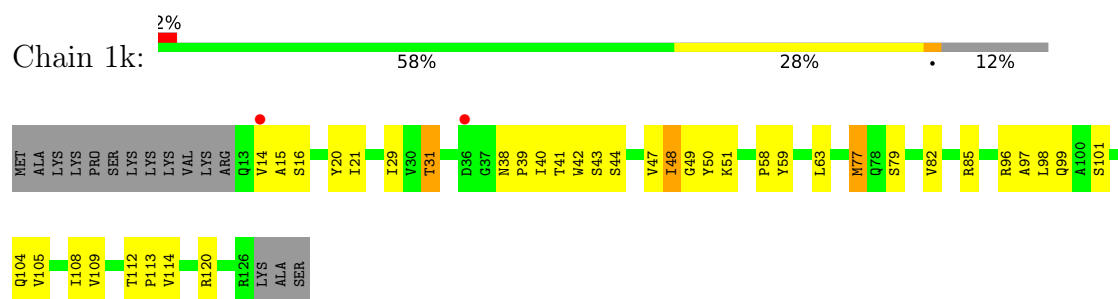
- Molecule 41: 30S ribosomal protein S10



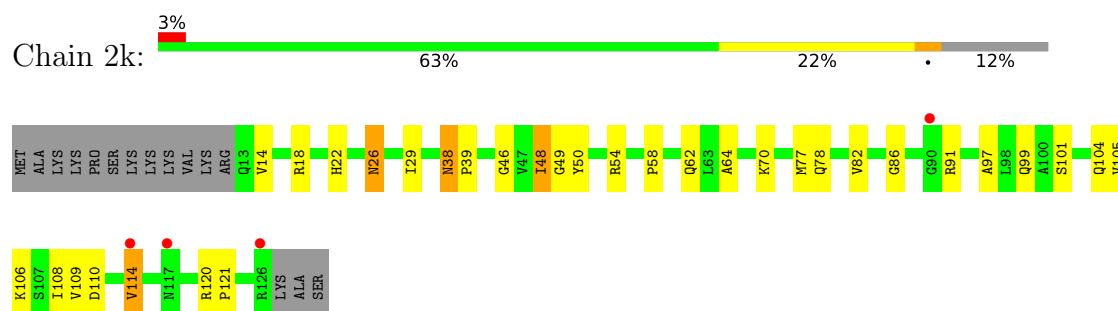
• Molecule 41: 30S ribosomal protein S10



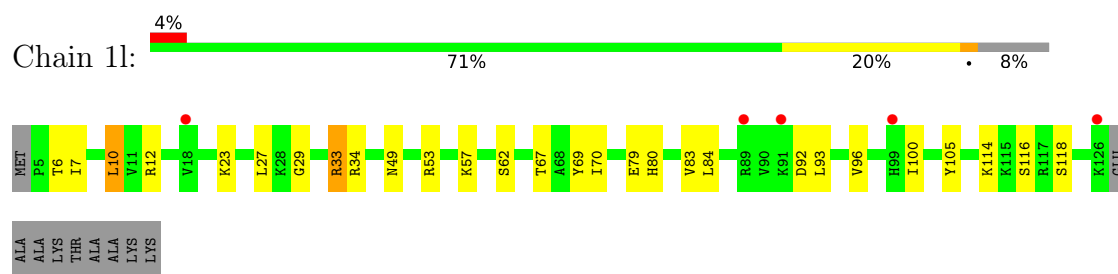
• Molecule 42: 30S ribosomal protein S11



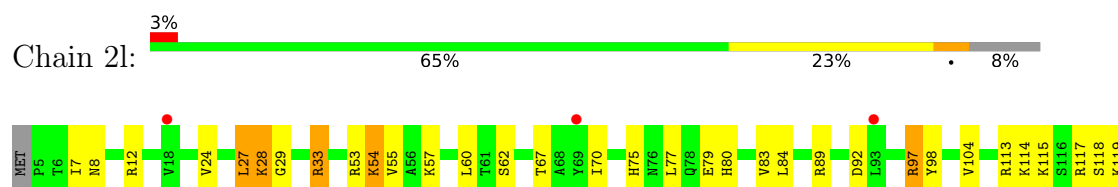
• Molecule 42: 30S ribosomal protein S11

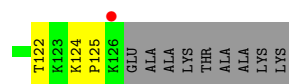


• Molecule 43: 30S ribosomal protein S12

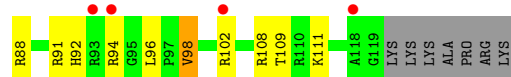
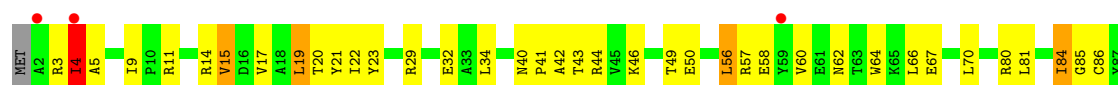


• Molecule 43: 30S ribosomal protein S12

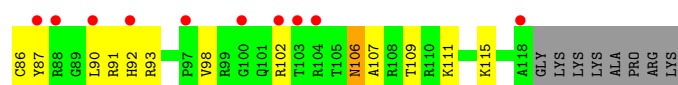
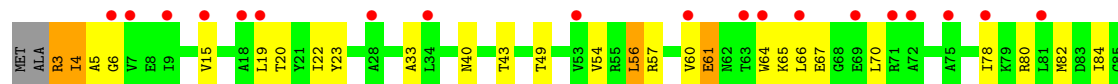




- Molecule 44: 30S ribosomal protein S13



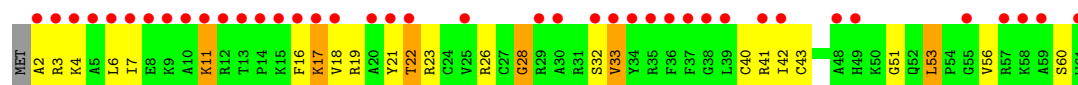
- Molecule 44: 30S ribosomal protein S13



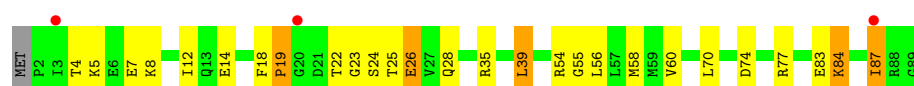
- Molecule 45: 30S ribosomal protein S14 type Z



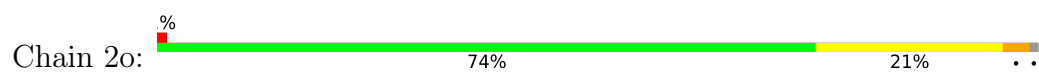
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



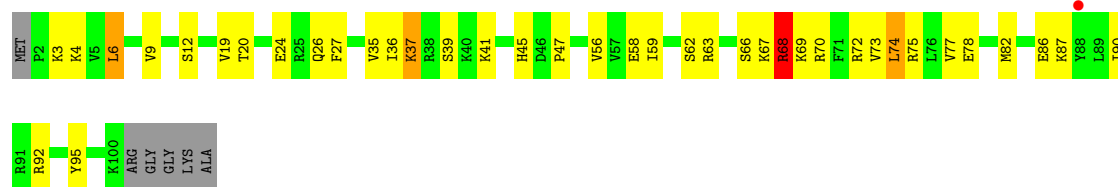
• Molecule 47: 30S ribosomal protein S16



• Molecule 47: 30S ribosomal protein S16



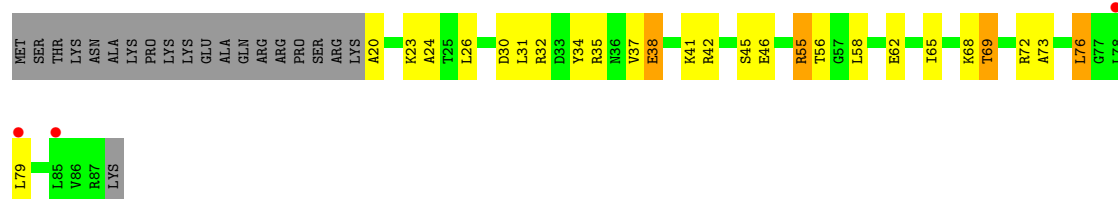
• Molecule 48: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S17



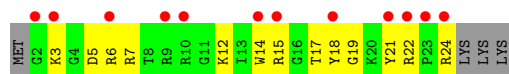
• Molecule 49: 30S ribosomal protein S18



- [illegible]



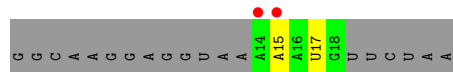
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



- Molecule 53: mRNA



- Molecule 54: P-site tRNA

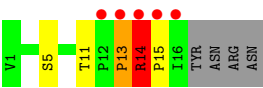


- Molecule 54: P-site tRNA

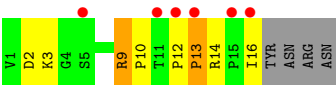


- Molecule 55: Pyrrhocoricin





● Molecule 55: Pyrrolicorin



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 450.12Å 622.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.70 49.69 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.69-2.70) 99.4 (49.69-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.220 , 0.272 0.220 , 0.271	Depositor DCC
R_{free} test set	79488 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	288775	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% 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: 5MC, 5MU, MG, PSU, ZN, SF4, 4SU

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	0.32	0/66249	0.47	1/103407 (0.0%)
1	2A	0.25	0/67298	0.44	1/105044 (0.0%)
2	1B	0.24	0/2877	0.39	0/4488
2	2B	0.27	0/2878	0.43	0/4490
3	1D	0.52	0/2186	0.89	1/2944 (0.0%)
3	2D	0.45	0/2192	0.88	3/2951 (0.1%)
4	1E	0.54	0/1592	0.92	4/2149 (0.2%)
4	2E	0.45	0/1592	0.90	2/2149 (0.1%)
5	1F	0.52	0/1619	0.91	5/2193 (0.2%)
5	2F	0.43	0/1615	0.93	3/2188 (0.1%)
6	1G	0.42	0/1450	0.89	4/1959 (0.2%)
6	2G	0.41	0/1449	0.98	5/1958 (0.3%)
7	1H	0.45	0/1356	0.89	0/1834
7	2H	0.45	0/1356	0.92	1/1834 (0.1%)
8	1I	0.42	0/1100	0.94	0/1501
8	2I	0.43	0/1076	0.95	4/1471 (0.3%)
9	1N	0.52	0/1144	0.84	0/1543
9	2N	0.41	0/1144	0.88	2/1543 (0.1%)
10	1O	0.54	0/943	0.84	0/1269
10	2O	0.44	0/943	0.88	0/1269
11	1P	0.49	0/1156	0.87	4/1537 (0.3%)
11	2P	0.42	0/1152	0.93	4/1533 (0.3%)
12	1Q	0.49	0/1143	0.82	0/1527
12	2Q	0.43	0/1143	0.89	0/1527
13	1R	0.55	0/982	0.86	0/1312
13	2R	0.42	0/982	0.79	0/1312
14	1S	0.47	0/887	0.83	0/1180
14	2S	0.41	0/880	0.89	1/1172 (0.1%)
15	1T	0.48	0/1105	0.84	0/1477
15	2T	0.39	0/1097	0.81	0/1468
16	1U	0.59	0/977	0.83	1/1301 (0.1%)
16	2U	0.44	0/977	0.81	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1V	0.51	0/782	0.82	0/1049
17	2V	0.44	0/782	0.87	0/1049
18	1W	0.59	0/897	0.86	0/1205
18	2W	0.47	0/897	0.88	1/1205 (0.1%)
19	1X	0.48	0/764	0.85	0/1025
19	2X	0.41	0/764	0.90	2/1025 (0.2%)
20	1Y	0.46	0/819	0.89	1/1095 (0.1%)
20	2Y	0.40	0/819	0.90	1/1095 (0.1%)
21	1Z	0.43	0/1502	0.88	2/2041 (0.1%)
21	2Z	0.41	0/1486	0.90	4/2022 (0.2%)
22	10	0.47	0/606	0.86	0/808
22	20	0.40	0/606	0.81	0/808
23	11	0.47	0/762	0.78	0/1014
23	21	0.43	0/762	0.79	0/1014
24	12	0.50	0/590	0.80	0/781
24	22	0.37	0/590	0.75	0/781
25	13	0.52	0/474	0.88	0/635
25	23	0.40	0/469	0.95	0/630
26	14	0.42	0/571	0.98	3/768 (0.4%)
26	24	0.47	0/545	1.08	5/737 (0.7%)
27	15	0.57	0/469	0.91	2/635 (0.3%)
27	25	0.48	0/469	0.94	0/635
28	16	0.48	0/460	0.79	0/613
28	26	0.41	0/456	0.81	0/608
29	17	0.54	0/426	0.85	2/561 (0.4%)
29	27	0.48	0/426	0.82	2/561 (0.4%)
30	18	0.53	0/525	0.85	1/691 (0.1%)
30	28	0.45	0/525	0.87	0/691
31	19	0.52	0/310	0.81	0/407
31	29	0.37	0/310	0.91	0/407
32	1a	0.22	0/35537	0.40	0/55456
32	2a	0.20	0/35680	0.38	0/55681
33	1b	0.40	0/1820	0.97	5/2468 (0.2%)
33	2b	1.62	8/1728 (0.5%)	1.16	7/2352 (0.3%)
34	1c	0.39	0/1504	0.88	2/2047 (0.1%)
34	2c	0.43	0/1435	0.88	3/1960 (0.2%)
35	1d	0.39	0/1648	0.92	4/2222 (0.2%)
35	2d	0.40	0/1659	0.92	3/2230 (0.1%)
36	1e	0.41	0/1145	0.89	5/1543 (0.3%)
36	2e	0.41	0/1111	0.93	3/1504 (0.2%)
37	1f	0.38	0/819	0.75	0/1111
37	2f	0.40	0/830	0.80	0/1125
38	1g	0.37	0/1198	0.81	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.36	0/1185	0.82	0/1602
39	1h	0.39	0/1108	0.87	2/1494 (0.1%)
39	2h	0.37	0/1094	0.90	2/1478 (0.1%)
40	1i	0.38	0/995	0.87	0/1339
40	2i	0.42	0/949	0.84	0/1284
41	1j	0.43	0/695	0.97	2/950 (0.2%)
41	2j	0.44	0/690	1.01	5/943 (0.5%)
42	1k	0.41	0/840	0.89	1/1138 (0.1%)
42	2k	0.40	0/844	0.87	2/1145 (0.2%)
43	1l	0.41	0/936	0.86	0/1263
43	2l	0.43	0/934	0.89	2/1262 (0.2%)
44	1m	0.37	0/933	0.86	1/1254 (0.1%)
44	2m	0.43	0/913	0.85	0/1230
45	1n	0.38	0/491	0.99	2/653 (0.3%)
45	2n	0.38	0/467	0.91	1/624 (0.2%)
46	1o	0.42	0/726	0.98	2/970 (0.2%)
46	2o	0.37	0/739	0.85	0/985
47	1p	0.36	0/686	0.86	0/926
47	2p	0.39	0/693	0.84	1/935 (0.1%)
48	1q	0.38	0/824	0.84	0/1105
48	2q	0.36	0/836	0.88	2/1117 (0.2%)
49	1r	0.38	0/560	0.80	0/746
49	2r	0.35	0/560	0.81	0/746
50	1s	0.38	0/657	0.93	0/890
50	2s	0.44	0/661	0.97	2/893 (0.2%)
51	1t	0.39	0/714	0.98	1/948 (0.1%)
51	2t	0.38	0/733	0.88	1/969 (0.1%)
52	1u	0.32	0/191	0.71	0/252
52	2u	0.40	0/203	0.86	0/266
53	1v	0.35	0/122	0.65	0/188
53	2v	0.29	0/122	0.46	0/188
54	1x	0.28	0/1725	0.43	0/2689
54	2x	0.28	0/1725	0.43	0/2689
55	1z	0.61	0/131	1.18	2/180 (1.1%)
55	2z	0.69	0/131	1.24	0/180
All	All	0.35	8/306330 (0.0%)	0.59	135/458260 (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
35	1d	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	29.49	2.27	1.38
33	2b	92	TYR	CD2-CE2	27.48	2.21	1.38
33	2b	151	GLY	N-CA	23.91	1.80	1.45
33	2b	92	TYR	CE1-CZ	22.53	1.92	1.38
33	2b	92	TYR	CE2-CZ	22.48	1.92	1.38

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	CA-C-N	17.98	156.66	121.41
33	2b	150	SER	C-N-CA	17.98	156.66	121.41
35	1d	10	ARG	N-CA-C	-13.64	96.51	113.97
33	2b	231	GLU	CA-C-N	12.39	133.22	119.83
33	2b	231	GLU	C-N-CA	12.39	133.22	119.83

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	1d	9	CYS	Peptide
5	2F	20	LEU	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	59154	0	29828	564	0
1	2A	60091	0	30297	814	0
2	1B	2572	0	1306	21	0
2	2B	2573	0	1306	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	54	0
3	2D	2142	0	2229	67	0
4	1E	1559	0	1618	32	0
4	2E	1559	0	1618	44	0
5	1F	1584	0	1625	31	0
5	2F	1580	0	1619	50	0
6	1G	1425	0	1443	24	0
6	2G	1424	0	1434	66	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	28	0
8	1I	1085	0	1114	27	0
8	2I	1061	0	1080	20	0
9	1N	1117	0	1184	15	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	18	0
10	2O	933	0	996	22	0
11	1P	1139	0	1223	27	0
11	2P	1135	0	1212	47	0
12	1Q	1122	0	1178	26	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	18	0
14	1S	877	0	938	27	0
14	2S	870	0	923	25	0
15	1T	1091	0	1151	34	0
15	2T	1083	0	1136	28	0
16	1U	959	0	1019	12	0
16	2U	959	0	1018	23	0
17	1V	771	0	830	9	0
17	2V	771	0	830	16	0
18	1W	886	0	940	9	0
18	2W	886	0	940	20	0
19	1X	750	0	814	18	0
19	2X	750	0	814	21	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	22	0
21	1Z	1470	0	1478	27	0
21	2Z	1454	0	1452	44	0
22	10	598	0	614	15	0
22	20	598	0	614	13	0
23	11	755	0	826	11	0
23	21	755	0	826	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	11	0
24	22	588	0	643	9	0
25	13	469	0	518	6	0
25	23	464	0	514	15	0
26	14	558	0	544	26	0
26	24	532	0	503	25	0
27	15	455	0	465	6	0
27	25	455	0	465	13	0
28	16	453	0	473	8	0
28	26	449	0	469	10	0
29	17	418	0	467	13	0
29	27	418	0	467	10	0
30	18	517	0	582	13	0
30	28	517	0	582	19	0
31	19	307	0	335	10	0
31	29	307	0	335	14	0
32	1a	31750	0	16028	478	0
32	2a	31877	0	16089	577	0
33	1b	1786	0	1744	67	0
33	2b	1697	0	1574	115	0
34	1c	1480	0	1400	42	0
34	2c	1412	0	1246	41	0
35	1d	1618	0	1579	47	0
35	2d	1630	0	1633	63	0
36	1e	1129	0	1185	33	0
36	2e	1095	0	1124	38	0
37	1f	806	0	793	19	0
37	2f	817	0	808	18	0
38	1g	1183	0	1165	23	0
38	2g	1167	0	1119	30	0
39	1h	1088	0	1126	26	0
39	2h	1074	0	1100	23	0
40	1i	976	0	973	31	0
40	2i	932	0	891	37	0
41	1j	682	0	598	23	0
41	2j	678	0	612	29	0
42	1k	826	0	829	23	0
42	2k	829	0	825	16	0
43	1l	920	0	958	16	0
43	2l	918	0	947	27	0
44	1m	923	0	962	35	0
44	2m	903	0	923	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	482	0	507	24	0
45	2n	459	0	467	30	0
46	1o	715	0	729	16	0
46	2o	728	0	760	13	0
47	1p	671	0	679	18	0
47	2p	677	0	686	17	0
48	1q	811	0	858	26	0
48	2q	823	0	891	19	0
49	1r	555	0	618	17	0
49	2r	555	0	618	22	0
50	1s	642	0	629	34	0
50	2s	646	0	644	37	0
51	1t	712	0	759	19	0
51	2t	731	0	807	18	0
52	1u	187	0	186	10	0
52	2u	199	0	208	9	0
53	1v	109	0	55	1	0
53	2v	109	0	55	1	0
54	1x	1625	0	829	14	0
54	2x	1625	0	829	17	0
55	1z	126	0	135	3	0
55	2z	126	0	135	3	0
56	10	7	0	0	0	0
56	11	3	0	0	0	0
56	12	1	0	0	0	0
56	13	1	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	3	0	0	0	0
56	18	5	0	0	0	0
56	19	3	0	0	0	0
56	1A	1233	0	0	0	0
56	1B	25	0	0	0	0
56	1D	15	0	0	0	0
56	1E	8	0	0	0	0
56	1F	9	0	0	0	0
56	1G	3	0	0	0	0
56	1H	1	0	0	0	0
56	1N	7	0	0	0	0
56	1O	3	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	8	0	0	0	0
56	1T	4	0	0	0	0
56	1U	6	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	295	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	3	0	0	0	0
56	1f	1	0	0	0	0
56	1h	2	0	0	0	0
56	1k	2	0	0	0	0
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	1	0	0	0	0
56	1p	1	0	0	0	0
56	1q	2	0	0	0	0
56	1r	2	0	0	0	0
56	1t	1	0	0	0	0
56	1x	12	0	0	0	0
56	20	1	0	0	0	0
56	23	1	0	0	0	0
56	25	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	592	0	0	0	0
56	2B	9	0	0	0	0
56	2D	6	0	0	0	0
56	2E	6	0	0	0	0
56	2F	2	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2Q	5	0	0	0	0
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	248	0	0	1	0
56	2d	1	0	0	0	0
56	2e	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2f	1	0	0	0	0
56	2l	5	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	2	0	0	0	0
56	2t	1	0	0	0	0
56	2u	1	0	0	0	0
56	2x	4	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	2	0
58	2d	8	0	0	6	0
59	10	12	0	0	0	0
59	11	5	0	0	0	0
59	12	3	0	0	0	0
59	13	4	0	0	1	0
59	15	9	0	0	0	0
59	16	9	0	0	3	0
59	17	10	0	0	1	0
59	18	12	0	0	1	0
59	19	2	0	0	0	0
59	1A	2217	0	0	121	0
59	1B	37	0	0	4	0
59	1D	23	0	0	1	0
59	1E	29	0	0	4	0
59	1F	19	0	0	1	0
59	1G	2	0	0	0	0
59	1H	4	0	0	0	0
59	1I	1	0	0	1	0
59	1N	6	0	0	2	0
59	1O	7	0	0	0	0
59	1P	27	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1Q	14	0	0	0	0
59	1R	11	0	0	0	0
59	1S	2	0	0	0	0
59	1T	13	0	0	4	0
59	1U	14	0	0	0	0
59	1V	7	0	0	0	0
59	1W	8	0	0	0	0
59	1X	5	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	7	0	0	0	0
59	1a	338	0	0	28	0
59	1b	2	0	0	0	0
59	1d	3	0	0	0	0
59	1e	7	0	0	0	0
59	1f	1	0	0	0	0
59	1h	3	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1k	1	0	0	0	0
59	1l	3	0	0	1	0
59	1m	1	0	0	0	0
59	1o	1	0	0	0	0
59	1q	1	0	0	0	0
59	1r	1	0	0	0	0
59	1s	2	0	0	2	0
59	1t	1	0	0	0	0
59	1v	3	0	0	0	0
59	1x	9	0	0	1	0
59	20	4	0	0	0	0
59	21	1	0	0	0	0
59	23	1	0	0	0	0
59	25	1	0	0	0	0
59	27	1	0	0	0	0
59	28	4	0	0	0	0
59	2A	809	0	0	86	0
59	2B	12	0	0	1	0
59	2D	20	0	0	1	0
59	2E	11	0	0	1	0
59	2F	7	0	0	0	0
59	2N	1	0	0	0	0
59	2O	3	0	0	0	0
59	2P	3	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2Q	2	0	0	0	0
59	2R	3	0	0	0	0
59	2T	3	0	0	0	0
59	2U	3	0	0	1	0
59	2W	1	0	0	0	0
59	2X	2	0	0	1	0
59	2Y	1	0	0	1	0
59	2Z	6	0	0	2	0
59	2a	274	0	0	38	0
59	2c	2	0	0	4	0
59	2d	1	0	0	0	0
59	2i	2	0	0	0	0
59	2j	2	0	0	0	0
59	2l	2	0	0	0	0
59	2p	1	0	0	0	0
59	2t	3	0	0	0	0
59	2v	1	0	0	0	0
59	2x	2	0	0	1	0
All	All	288775	0	190012	4404	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 10.

The worst 5 of 4404 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)
33:2b:92:TYR:CD1	33:2b:92:TYR:CG	1.83	1.62
33:2b:92:TYR:CG	33:2b:92:TYR:CD2	1.81	1.57
33:2b:92:TYR:CZ	33:2b:92:TYR:CE2	1.92	1.57
33:2b:92:TYR:CZ	33:2b:92:TYR:CE1	1.92	1.53
33:2b:151:GLY:N	33:2b:151:GLY:CA	1.80	1.44

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	19 (7%)	2 (1%)	18	41
4	1E	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	24	48
4	2E	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	24	48
5	1F	201/210 (96%)	192 (96%)	7 (4%)	2 (1%)	12	32
5	2F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24	48
6	1G	179/182 (98%)	164 (92%)	10 (6%)	5 (3%)	4	9
6	2G	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	5	14
7	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	21	44
7	2H	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	10	27
8	1I	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5	15
8	2I	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	9	23
9	1N	138/140 (99%)	138 (100%)	0	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18	41
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	8 (5%)	2 (1%)	9	23
11	2P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9	23
12	1Q	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	18	41
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	35
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	17
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	37
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	32
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	29
19	2X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5	14
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	17
20	2Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	32
21	1Z	184/206 (89%)	170 (92%)	14 (8%)	0	100	100
21	2Z	184/206 (89%)	168 (91%)	13 (7%)	3 (2%)	7	20
22	10	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	9	23
22	20	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	29
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	29
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%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	50 (75%)	10 (15%)	7 (10%)	0	0
26	24	67/71 (94%)	49 (73%)	12 (18%)	6 (9%)	0	0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	187 (82%)	33 (14%)	9 (4%)	2	5
33	2b	229/256 (90%)	191 (83%)	25 (11%)	13 (6%)	1	2
34	1c	204/239 (85%)	176 (86%)	27 (13%)	1 (0%)	24	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
35	1d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	12	32
35	2d	206/209 (99%)	186 (90%)	18 (9%)	2 (1%)	12	32
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	9	23
36	2e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	9	23
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	25
38	2g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9	25
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	18	41
40	1i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
40	2i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	7	20
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	2	4
41	2j	94/105 (90%)	83 (88%)	10 (11%)	1 (1%)	11	29
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	35
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	35
43	1l	120/132 (91%)	114 (95%)	5 (4%)	1 (1%)	16	37
43	2l	120/132 (91%)	115 (96%)	5 (4%)	0	100	100
44	1m	116/126 (92%)	104 (90%)	11 (10%)	1 (1%)	14	35
44	2m	114/126 (90%)	100 (88%)	12 (10%)	2 (2%)	6	18
45	1n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	19
45	2n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	27
46	2o	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	5	13
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	32
48	2q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	82/93 (88%)	69 (84%)	13 (16%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	4	11
51	1t	94/106 (89%)	82 (87%)	9 (10%)	3 (3%)	3	7
51	2t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	3	7
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	3
52	2u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	3
55	1z	14/20 (70%)	9 (64%)	3 (21%)	2 (14%)	0	0
55	2z	14/20 (70%)	7 (50%)	4 (29%)	3 (21%)	0	0
All	All	11438/12168 (94%)	10532 (92%)	776 (7%)	130 (1%)	11	29

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	126	ASP
7	1H	126	PRO
26	14	49	PHE
26	14	53	GLU

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%)	193 (90%)	22 (10%)	7	18
3	2D	216/218 (99%)	192 (89%)	24 (11%)	6	15
4	1E	164/166 (99%)	143 (87%)	21 (13%)	4	11
4	2E	164/166 (99%)	144 (88%)	20 (12%)	5	12
5	1F	160/166 (96%)	139 (87%)	21 (13%)	4	10
5	2F	159/166 (96%)	139 (87%)	20 (13%)	4	11
6	1G	143/156 (92%)	125 (87%)	18 (13%)	4	11
6	2G	142/156 (91%)	120 (84%)	22 (16%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	23
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	17
8	1I	110/124 (89%)	92 (84%)	18 (16%)	2	6
8	2I	104/124 (84%)	89 (86%)	15 (14%)	3	8
9	1N	118/119 (99%)	103 (87%)	15 (13%)	4	11
9	2N	118/119 (99%)	103 (87%)	15 (13%)	4	11
10	1O	100/100 (100%)	90 (90%)	10 (10%)	7	19
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9	23
11	1P	116/116 (100%)	101 (87%)	15 (13%)	4	10
11	2P	115/116 (99%)	101 (88%)	14 (12%)	5	12
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	32
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	23
13	1R	101/101 (100%)	84 (83%)	17 (17%)	2	6
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	9
14	1S	87/88 (99%)	73 (84%)	14 (16%)	2	6
14	2S	85/88 (97%)	67 (79%)	18 (21%)	1	3
15	1T	115/127 (91%)	103 (90%)	12 (10%)	7	17
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	20
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8	20
16	2U	93/94 (99%)	83 (89%)	10 (11%)	6	16
17	1V	80/82 (98%)	67 (84%)	13 (16%)	2	6
17	2V	80/82 (98%)	67 (84%)	13 (16%)	2	6
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7	19
18	2W	90/92 (98%)	81 (90%)	9 (10%)	7	19
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	57
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	57
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	33
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	17
21	1Z	159/179 (89%)	140 (88%)	19 (12%)	5	13
21	2Z	156/179 (87%)	137 (88%)	19 (12%)	5	12
22	10	60/67 (90%)	54 (90%)	6 (10%)	7	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	60/67 (90%)	56 (93%)	4 (7%)	15	36
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	31
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	31
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	22
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	16
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	42
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	41
26	14	60/63 (95%)	52 (87%)	8 (13%)	4	10
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	7
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	28
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	28
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	19
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	19
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	32
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	49
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	44
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	15
31	19	34/34 (100%)	31 (91%)	3 (9%)	9	23
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	23
33	1b	177/220 (80%)	149 (84%)	28 (16%)	2	7
33	2b	158/220 (72%)	138 (87%)	20 (13%)	4	11
34	1c	127/188 (68%)	116 (91%)	11 (9%)	9	24
34	2c	108/188 (57%)	95 (88%)	13 (12%)	5	12
35	1d	161/181 (89%)	138 (86%)	23 (14%)	3	8
35	2d	164/181 (91%)	141 (86%)	23 (14%)	3	9
36	1e	113/123 (92%)	99 (88%)	14 (12%)	4	11
36	2e	106/123 (86%)	89 (84%)	17 (16%)	2	6
37	1f	83/90 (92%)	78 (94%)	5 (6%)	17	41
37	2f	86/90 (96%)	79 (92%)	7 (8%)	11	27
38	1g	111/127 (87%)	97 (87%)	14 (13%)	4	11
38	2g	107/127 (84%)	93 (87%)	14 (13%)	4	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	20
39	2h	111/119 (93%)	103 (93%)	8 (7%)	13	32
40	1i	89/99 (90%)	81 (91%)	8 (9%)	9	23
40	2i	80/99 (81%)	71 (89%)	9 (11%)	5	14
41	1j	60/92 (65%)	51 (85%)	9 (15%)	3	7
41	2j	62/92 (67%)	51 (82%)	11 (18%)	2	5
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	19
42	2k	82/99 (83%)	72 (88%)	10 (12%)	5	12
43	1l	95/109 (87%)	88 (93%)	7 (7%)	13	32
43	2l	94/109 (86%)	85 (90%)	9 (10%)	8	20
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	15
44	2m	87/101 (86%)	78 (90%)	9 (10%)	7	18
45	1n	47/50 (94%)	43 (92%)	4 (8%)	10	25
45	2n	43/50 (86%)	37 (86%)	6 (14%)	3	9
46	1o	75/80 (94%)	66 (88%)	9 (12%)	5	12
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	30
47	1p	67/74 (90%)	54 (81%)	13 (19%)	1	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	6
48	1q	91/97 (94%)	83 (91%)	8 (9%)	9	23
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	54
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	9
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	9
50	1s	65/80 (81%)	58 (89%)	7 (11%)	6	16
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	9
51	1t	66/82 (80%)	55 (83%)	11 (17%)	2	6
51	2t	71/82 (87%)	64 (90%)	7 (10%)	7	19
52	1u	16/22 (73%)	15 (94%)	1 (6%)	16	39
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	15
55	1z	15/19 (79%)	13 (87%)	2 (13%)	4	10
55	2z	15/19 (79%)	12 (80%)	3 (20%)	1	4
All	All	9165/10104 (91%)	8120 (89%)	1045 (11%)	5	14

5 of 1045 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	2g	98	SER
41	2j	23	ILE
38	2g	75	VAL
52	2u	10	ARG
37	1f	69	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
24	22	38	GLN
38	2g	153	HIS
28	26	32	ASN
35	2d	74	GLN
41	2j	21	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	377 (13%)	22 (0%)
1	2A	2781/2915 (95%)	477 (17%)	23 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	119/121 (98%)	26 (21%)	2 (1%)
32	1a	1472/1521 (96%)	273 (18%)	0
32	2a	1479/1521 (97%)	278 (18%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	16 (21%)	0
54	2x	75/77 (97%)	18 (24%)	0
All	All	8865/9316 (95%)	1477 (16%)	47 (0%)

5 of 1477 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	33	C
1	1A	35	G
1	1A	44	C
1	1A	49	G

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	810	A
1	2A	1424	A
1	2A	902	C
1	2A	1102	A
1	2A	1604	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	4SU	2x	8	54	18,21,22	1.93	5 (27%)	25,30,33	1.23	3 (12%)
54	5MU	2x	54	54	19,22,23	1.41	5 (26%)	27,32,35	2.07	7 (25%)
54	PSU	1x	55	54,56	18,21,22	1.35	2 (11%)	21,30,33	2.01	3 (14%)
54	4SU	1x	8	54	18,21,22	2.14	4 (22%)	25,30,33	1.36	4 (16%)
54	PSU	2x	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	4 (19%)
54	5MC	2x	32	54	19,22,23	1.60	2 (10%)	26,32,35	1.13	3 (11%)
54	5MU	1x	54	54	19,22,23	1.54	5 (26%)	27,32,35	1.84	6 (22%)
54	5MC	1x	32	54	19,22,23	1.73	3 (15%)	26,32,35	1.22	3 (11%)

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	4SU	2x	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1x	55	54,56	-	2/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	1/7/25/26	0/2/2/2
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MU	1x	54	54	-	0/7/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/7/25/26	0/2/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	32	5MC	C5-C4	6.27	1.48	1.44
54	2x	32	5MC	C5-C4	5.63	1.48	1.44
54	1x	8	4SU	C4-N3	-4.94	1.32	1.37
54	1x	8	4SU	C4-S4	-4.59	1.60	1.68
54	2x	8	4SU	C4-N3	-4.27	1.33	1.37

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	55	PSU	N1-C2-N3	6.13	121.64	115.17
54	2x	55	PSU	N1-C2-N3	6.03	121.53	115.17
54	2x	54	5MU	N3-C2-N1	5.19	121.64	114.89
54	2x	54	5MU	C4-N3-C2	-4.96	120.83	127.34
54	1x	54	5MU	N3-C2-N1	4.93	121.30	114.89

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1x	55	PSU	O4'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	1x	55	PSU	C3'-C4'-C5'-O5'
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	1x	8	4SU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2x	8	4SU	1	0
54	1x	8	4SU	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2615 ligands modelled in this entry, 2613 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	1d	501	35	0,12,12	-	-	-		
58	SF4	2d	501	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	SF4	1d	501	35	-	-	0/6/5/5
58	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1d	501	SF4	2	0
58	2d	501	SF4	6	0

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	2746/2915 (94%)	-0.43	34 (1%) 76 75	20, 40, 84, 109	0
1	2A	2790/2915 (95%)	-0.35	29 (1%) 79 78	24, 44, 91, 107	0
2	1B	120/121 (99%)	0.19	1 (0%) 82 81	34, 63, 78, 92	0
2	2B	120/121 (99%)	0.63	4 (3%) 49 45	40, 69, 80, 94	0
3	1D	275/276 (99%)	-0.13	1 (0%) 88 87	19, 39, 57, 76	0
3	2D	275/276 (99%)	-0.11	3 (1%) 78 76	20, 41, 59, 76	0
4	1E	204/206 (99%)	-0.09	0 100 100	19, 42, 63, 80	0
4	2E	204/206 (99%)	-0.02	1 (0%) 87 86	22, 45, 65, 81	0
5	1F	203/210 (96%)	0.18	3 (1%) 72 70	19, 48, 74, 86	0
5	2F	203/210 (96%)	0.23	2 (0%) 79 78	22, 52, 76, 88	0
6	1G	181/182 (99%)	0.79	11 (6%) 27 24	53, 69, 81, 95	0
6	2G	181/182 (99%)	1.24	23 (12%) 8 7	58, 72, 83, 96	0
7	1H	174/180 (96%)	0.82	7 (4%) 42 38	45, 63, 75, 85	0
7	2H	174/180 (96%)	1.01	10 (5%) 29 26	53, 68, 78, 86	0
8	1I	146/148 (98%)	0.66	4 (2%) 56 53	48, 74, 83, 89	0
8	2I	146/148 (98%)	0.74	5 (3%) 48 44	50, 75, 83, 87	0
9	1N	140/140 (100%)	0.20	1 (0%) 84 83	28, 44, 65, 78	0
9	2N	140/140 (100%)	0.20	0 100 100	31, 49, 68, 79	0
10	1O	122/122 (100%)	-0.03	0 100 100	30, 42, 61, 66	0
10	2O	122/122 (100%)	-0.03	1 (0%) 82 81	33, 46, 62, 67	0
11	1P	149/150 (99%)	0.25	1 (0%) 84 83	21, 53, 74, 86	0
11	2P	149/150 (99%)	0.27	0 100 100	24, 56, 75, 84	0
12	1Q	141/141 (100%)	0.34	3 (2%) 63 61	33, 47, 63, 80	0
12	2Q	141/141 (100%)	0.36	3 (2%) 63 61	36, 51, 66, 79	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%)	0.05	0 100 100	27, 38, 54, 60	0
13	2R	118/118 (100%)	-0.03	0 100 100	29, 40, 56, 61	0
14	1S	110/112 (98%)	0.06	2 (1%) 67 65	33, 50, 63, 71	0
14	2S	110/112 (98%)	1.60	37 (33%) 1 1	44, 77, 85, 92	0
15	1T	131/146 (89%)	-0.11	4 (3%) 51 48	27, 40, 70, 83	0
15	2T	131/146 (89%)	0.32	3 (2%) 61 58	43, 56, 77, 87	0
16	1U	116/118 (98%)	0.12	2 (1%) 69 67	21, 35, 54, 71	0
16	2U	116/118 (98%)	0.17	0 100 100	28, 41, 59, 72	0
17	1V	101/101 (100%)	0.14	1 (0%) 79 78	25, 47, 65, 79	0
17	2V	101/101 (100%)	0.24	1 (0%) 79 78	29, 52, 70, 79	0
18	1W	112/113 (99%)	-0.19	0 100 100	25, 33, 56, 86	0
18	2W	112/113 (99%)	-0.14	1 (0%) 81 80	27, 37, 57, 88	0
19	1X	95/96 (98%)	0.26	3 (3%) 50 46	30, 45, 65, 77	0
19	2X	95/96 (98%)	0.37	4 (4%) 40 37	34, 49, 67, 78	0
20	1Y	107/110 (97%)	0.53	1 (0%) 81 80	39, 57, 74, 84	0
20	2Y	107/110 (97%)	0.65	1 (0%) 81 80	44, 60, 76, 86	0
21	1Z	186/206 (90%)	0.61	3 (1%) 70 68	48, 67, 80, 87	0
21	2Z	186/206 (90%)	0.92	7 (3%) 44 40	53, 70, 81, 89	0
22	10	75/85 (88%)	0.30	1 (1%) 75 73	28, 45, 60, 67	0
22	20	75/85 (88%)	0.44	3 (4%) 42 38	31, 50, 63, 70	0
23	11	97/98 (98%)	0.24	2 (2%) 63 61	28, 47, 73, 80	0
23	21	97/98 (98%)	0.23	2 (2%) 63 61	31, 49, 73, 79	0
24	12	70/72 (97%)	0.61	5 (7%) 22 19	43, 55, 69, 78	0
24	22	70/72 (97%)	0.50	0 100 100	46, 59, 71, 77	0
25	13	59/60 (98%)	0.26	0 100 100	29, 42, 62, 73	0
25	23	59/60 (98%)	0.29	2 (3%) 48 44	34, 47, 66, 79	0
26	14	69/71 (97%)	1.10	11 (15%) 5 4	60, 81, 93, 96	0
26	24	69/71 (97%)	1.55	17 (24%) 2 1	68, 83, 95, 101	0
27	15	59/60 (98%)	-0.31	1 (1%) 69 67	19, 36, 52, 71	0
27	25	59/60 (98%)	-0.19	0 100 100	23, 38, 56, 72	0
28	16	53/54 (98%)	-0.01	0 100 100	37, 48, 65, 69	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%)	0.19	0 100 100	38, 51, 61, 69	0
29	17	48/49 (97%)	-0.12	1 (2%) 63 61	24, 30, 63, 75	0
29	27	48/49 (97%)	-0.15	1 (2%) 63 61	26, 32, 66, 75	0
30	18	64/65 (98%)	0.11	0 100 100	30, 39, 50, 58	0
30	28	64/65 (98%)	0.33	0 100 100	33, 42, 54, 59	0
31	19	37/37 (100%)	0.58	1 (2%) 56 53	38, 48, 65, 67	0
31	29	37/37 (100%)	0.94	4 (10%) 11 9	42, 52, 66, 71	0
32	1a	1477/1521 (97%)	0.25	32 (2%) 62 59	29, 71, 95, 112	0
32	2a	1483/1521 (97%)	0.47	47 (3%) 50 46	43, 77, 98, 110	0
33	1b	231/256 (90%)	1.14	33 (14%) 6 5	65, 81, 91, 101	0
33	2b	231/256 (90%)	1.34	41 (17%) 4 3	67, 86, 94, 102	0
34	1c	206/239 (86%)	1.13	21 (10%) 12 10	66, 82, 89, 95	0
34	2c	206/239 (86%)	1.35	39 (18%) 3 3	66, 83, 90, 96	0
35	1d	208/209 (99%)	1.06	20 (9%) 13 11	56, 76, 87, 95	0
35	2d	208/209 (99%)	0.92	14 (6%) 24 21	58, 73, 84, 89	0
36	1e	148/162 (91%)	0.56	2 (1%) 73 72	43, 66, 77, 86	0
36	2e	148/162 (91%)	0.85	7 (4%) 36 33	60, 74, 84, 91	0
37	1f	100/101 (99%)	0.66	2 (2%) 65 62	57, 72, 81, 84	0
37	2f	100/101 (99%)	0.67	2 (2%) 65 62	61, 74, 82, 87	0
38	1g	155/156 (99%)	0.88	20 (12%) 7 6	60, 74, 89, 97	0
38	2g	155/156 (99%)	1.20	29 (18%) 3 3	70, 83, 91, 96	0
39	1h	137/138 (99%)	0.58	1 (0%) 84 83	49, 66, 76, 78	0
39	2h	137/138 (99%)	0.98	11 (8%) 18 15	62, 75, 82, 88	0
40	1i	127/128 (99%)	1.44	29 (22%) 2 2	60, 80, 90, 94	0
40	2i	127/128 (99%)	2.04	58 (45%) 0 0	69, 89, 96, 102	0
41	1j	97/105 (92%)	1.80	36 (37%) 1 0	61, 85, 93, 97	0
41	2j	96/105 (91%)	2.08	51 (53%) 0 0	76, 89, 97, 102	0
42	1k	114/129 (88%)	0.44	2 (1%) 67 65	40, 67, 79, 92	0
42	2k	114/129 (88%)	0.76	4 (3%) 47 43	52, 76, 85, 90	0
43	1l	122/132 (92%)	0.57	5 (4%) 41 37	42, 62, 72, 81	0
43	2l	122/132 (92%)	0.80	4 (3%) 49 45	55, 67, 77, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	1.01	7 (5%) 28 25	66, 79, 85, 91	0
44	2m	116/126 (92%)	1.58	29 (25%) 2 1	69, 81, 87, 92	0
45	1n	60/61 (98%)	1.67	15 (25%) 2 1	69, 81, 86, 92	0
45	2n	60/61 (98%)	2.55	40 (66%) 0 0	71, 82, 87, 92	0
46	1o	88/89 (98%)	0.62	3 (3%) 48 44	47, 64, 78, 85	0
46	2o	88/89 (98%)	0.67	1 (1%) 78 76	59, 71, 82, 89	0
47	1p	82/88 (93%)	1.36	12 (14%) 6 5	61, 77, 87, 92	0
47	2p	82/88 (93%)	0.99	6 (7%) 21 18	60, 70, 82, 89	0
48	1q	99/105 (94%)	0.73	1 (1%) 79 78	45, 65, 76, 78	0
48	2q	99/105 (94%)	0.75	4 (4%) 42 38	53, 71, 80, 86	0
49	1r	68/88 (77%)	0.57	3 (4%) 39 35	53, 68, 81, 87	0
49	2r	68/88 (77%)	0.79	3 (4%) 39 35	62, 74, 82, 90	0
50	1s	84/93 (90%)	1.33	12 (14%) 6 5	66, 80, 91, 94	0
50	2s	83/93 (89%)	2.01	35 (42%) 0 0	77, 90, 98, 104	0
51	1t	96/106 (90%)	1.19	18 (18%) 3 3	56, 73, 82, 88	0
51	2t	96/106 (90%)	0.97	12 (12%) 8 7	55, 72, 82, 86	0
52	1u	23/27 (85%)	1.77	12 (52%) 0 0	69, 75, 80, 81	0
52	2u	23/27 (85%)	1.98	8 (34%) 1 1	68, 78, 82, 82	0
53	1v	5/24 (20%)	1.22	2 (40%) 1 0	61, 64, 86, 94	0
53	2v	5/24 (20%)	0.94	0 100 100	65, 67, 86, 94	0
54	1x	72/77 (93%)	0.14	1 (1%) 73 72	37, 67, 85, 95	0
54	2x	72/77 (93%)	0.22	1 (1%) 73 72	39, 71, 87, 97	0
55	1z	16/20 (80%)	1.66	5 (31%) 1 1	30, 49, 74, 79	0
55	2z	16/20 (80%)	1.63	6 (37%) 1 0	32, 52, 76, 77	0
All	All	20528/21484 (95%)	0.32	1014 (4%) 35 31	19, 61, 90, 112	0

The worst 5 of 1014 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	6.6
32	1a	980	G	6.5
32	1a	981	G	5.9
38	1g	79	ARG	5.7
7	1H	2	SER	5.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	2x	55	20/21	0.82	0.12	68,72,83,84	0
54	5MC	2x	32	21/22	0.86	0.14	65,77,87,92	0
54	4SU	2x	8	20/21	0.88	0.10	69,79,87,88	0
54	5MU	2x	54	21/22	0.89	0.10	68,77,85,100	0
54	5MC	1x	32	21/22	0.92	0.12	47,63,73,74	0
54	5MU	1x	54	21/22	0.92	0.11	57,69,77,82	0
54	PSU	1x	55	20/21	0.93	0.10	63,69,80,81	0
54	4SU	1x	8	20/21	0.95	0.08	47,59,71,71	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2a	1833	1/1	0.51	0.25	94,94,94,94	0
56	MG	2a	1767	1/1	0.54	0.22	88,88,88,88	0
56	MG	1A	4047	1/1	0.54	0.23	79,79,79,79	0
56	MG	1A	3732	1/1	0.58	0.12	59,59,59,59	0
56	MG	1A	4203	1/1	0.58	0.42	71,71,71,71	0
56	MG	2a	1784	1/1	0.59	0.23	80,80,80,80	0
56	MG	1A	3352	1/1	0.59	0.33	82,82,82,82	0
56	MG	2A	3003	1/1	0.63	0.21	67,67,67,67	0
56	MG	2a	1789	1/1	0.63	0.21	69,69,69,69	0
56	MG	1a	1716	1/1	0.63	0.35	79,79,79,79	0
56	MG	2a	1837	1/1	0.63	0.23	75,75,75,75	0
56	MG	2A	3346	1/1	0.64	0.25	76,76,76,76	0
56	MG	1A	3907	1/1	0.64	0.13	53,53,53,53	0
56	MG	1a	1754	1/1	0.65	0.20	89,89,89,89	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	3517	1/1	0.65	0.18	58,58,58,58	0
56	MG	2a	1754	1/1	0.66	0.21	74,74,74,74	0
56	MG	1A	3943	1/1	0.66	0.14	74,74,74,74	0
56	MG	2Z	3001	1/1	0.66	0.16	62,62,62,62	0
56	MG	2B	3005	1/1	0.67	0.24	79,79,79,79	0
56	MG	1a	1766	1/1	0.67	0.26	73,73,73,73	0
56	MG	2a	1632	1/1	0.67	0.17	86,86,86,86	0
56	MG	2a	1655	1/1	0.67	0.18	92,92,92,92	0
56	MG	1a	1836	1/1	0.67	0.16	78,78,78,78	0
56	MG	1A	3426	1/1	0.68	0.12	65,65,65,65	0
56	MG	2a	1813	1/1	0.68	0.24	74,74,74,74	0
56	MG	1A	3913	1/1	0.68	0.23	58,58,58,58	0
56	MG	2B	3008	1/1	0.68	0.15	63,63,63,63	0
56	MG	2A	3436	1/1	0.69	0.16	55,55,55,55	0
56	MG	1a	1765	1/1	0.69	0.20	71,71,71,71	0
56	MG	1A	4035	1/1	0.69	0.20	78,78,78,78	0
56	MG	1a	1778	1/1	0.69	0.38	83,83,83,83	0
56	MG	2a	1768	1/1	0.69	0.30	86,86,86,86	0
56	MG	1a	1881	1/1	0.70	0.22	69,69,69,69	0
56	MG	2a	1608	1/1	0.70	0.27	75,75,75,75	0
56	MG	1A	4072	1/1	0.70	0.14	52,52,52,52	0
56	MG	1A	3465	1/1	0.70	0.17	71,71,71,71	0
56	MG	2A	3524	1/1	0.71	0.21	75,75,75,75	0
56	MG	1A	4104	1/1	0.71	0.20	63,63,63,63	0
56	MG	1A	3441	1/1	0.71	0.14	62,62,62,62	0
56	MG	1A	3418	1/1	0.72	0.30	52,52,52,52	0
56	MG	1A	3533	1/1	0.72	0.26	75,75,75,75	0
56	MG	2a	1668	1/1	0.72	0.25	69,69,69,69	0
56	MG	2a	1701	1/1	0.72	0.16	66,66,66,66	0
56	MG	1A	3376	1/1	0.72	0.23	69,69,69,69	0
56	MG	1A	4003	1/1	0.72	0.20	92,92,92,92	0
56	MG	2A	3515	1/1	0.73	0.20	55,55,55,55	0
56	MG	1x	112	1/1	0.73	0.21	78,78,78,78	0
56	MG	1A	4056	1/1	0.73	0.28	74,74,74,74	0
56	MG	2a	1633	1/1	0.73	0.16	70,70,70,70	0
56	MG	2A	3479	1/1	0.73	0.13	51,51,51,51	0
56	MG	1A	3127	1/1	0.74	0.19	54,54,54,54	0
56	MG	1A	3562	1/1	0.74	0.25	41,41,41,41	0
56	MG	1Q	203	1/1	0.74	0.17	64,64,64,64	0
56	MG	1a	1822	1/1	0.74	0.39	76,76,76,76	0
56	MG	1A	4064	1/1	0.74	0.24	78,78,78,78	0
56	MG	1A	3716	1/1	0.74	0.17	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	4010	1/1	0.75	0.14	76,76,76,76	0
56	MG	1A	4189	1/1	0.75	0.13	43,43,43,43	0
56	MG	2A	3233	1/1	0.75	0.20	68,68,68,68	0
56	MG	1A	3139	1/1	0.75	0.18	52,52,52,52	0
56	MG	2a	1685	1/1	0.75	0.20	83,83,83,83	0
56	MG	1a	1846	1/1	0.75	0.30	75,75,75,75	0
56	MG	1A	3918	1/1	0.75	0.15	27,27,27,27	0
56	MG	2a	1846	1/1	0.75	0.19	78,78,78,78	0
56	MG	1a	1723	1/1	0.76	0.21	69,69,69,69	0
56	MG	1a	1727	1/1	0.76	0.20	80,80,80,80	0
56	MG	1A	3876	1/1	0.76	0.17	64,64,64,64	0
56	MG	1A	3445	1/1	0.76	0.13	57,57,57,57	0
56	MG	2a	1716	1/1	0.76	0.15	70,70,70,70	0
56	MG	1a	1629	1/1	0.76	0.20	85,85,85,85	0
56	MG	1A	4191	1/1	0.76	0.14	39,39,39,39	0
56	MG	1a	1767	1/1	0.77	0.18	72,72,72,72	0
56	MG	1A	4082	1/1	0.77	0.16	85,85,85,85	0
56	MG	1A	3004	1/1	0.77	0.30	47,47,47,47	0
56	MG	1A	3658	1/1	0.77	0.19	60,60,60,60	0
56	MG	2a	1642	1/1	0.77	0.24	85,85,85,85	0
56	MG	2a	1650	1/1	0.77	0.23	82,82,82,82	0
56	MG	1A	4061	1/1	0.77	0.12	89,89,89,89	0
56	MG	1A	3842	1/1	0.77	0.22	79,79,79,79	0
56	MG	1A	3860	1/1	0.77	0.27	62,62,62,62	0
56	MG	18	104	1/1	0.77	0.19	63,63,63,63	0
56	MG	2a	1733	1/1	0.78	0.32	80,80,80,80	0
56	MG	2A	3447	1/1	0.78	0.27	61,61,61,61	0
56	MG	1A	3506	1/1	0.78	0.18	37,37,37,37	0
56	MG	1A	3536	1/1	0.78	0.11	67,67,67,67	0
56	MG	2A	3518	1/1	0.78	0.15	58,58,58,58	0
56	MG	1A	4228	1/1	0.78	0.19	58,58,58,58	0
56	MG	2a	1793	1/1	0.78	0.14	67,67,67,67	0
56	MG	2a	1796	1/1	0.78	0.23	80,80,80,80	0
56	MG	2a	1800	1/1	0.78	0.29	65,65,65,65	0
56	MG	2a	1812	1/1	0.78	0.19	75,75,75,75	0
56	MG	2A	3266	1/1	0.78	0.15	60,60,60,60	0
56	MG	2A	3279	1/1	0.78	0.15	72,72,72,72	0
56	MG	2a	1836	1/1	0.78	0.18	72,72,72,72	0
56	MG	1a	1860	1/1	0.78	0.11	68,68,68,68	0
56	MG	1a	1691	1/1	0.78	0.15	59,59,59,59	0
56	MG	2l	3003	1/1	0.78	0.26	71,71,71,71	0
56	MG	1A	3368	1/1	0.79	0.12	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3125	1/1	0.79	0.14	58,58,58,58	0
56	MG	1A	3446	1/1	0.79	0.21	45,45,45,45	0
56	MG	1A	3574	1/1	0.79	0.15	62,62,62,62	0
56	MG	1A	3912	1/1	0.79	0.19	54,54,54,54	0
56	MG	1a	1632	1/1	0.79	0.28	72,72,72,72	0
56	MG	1e	202	1/1	0.79	0.19	62,62,62,62	0
56	MG	1A	3045	1/1	0.79	0.09	60,60,60,60	0
56	MG	1A	4075	1/1	0.79	0.14	59,59,59,59	0
56	MG	1A	3365	1/1	0.79	0.27	74,74,74,74	0
56	MG	1A	3427	1/1	0.79	0.21	67,67,67,67	0
56	MG	2A	3267	1/1	0.79	0.20	62,62,62,62	0
56	MG	1A	4169	1/1	0.79	0.22	57,57,57,57	0
56	MG	1A	4173	1/1	0.79	0.17	21,21,21,21	0
56	MG	2a	1673	1/1	0.79	0.42	76,76,76,76	0
56	MG	1A	3750	1/1	0.79	0.17	43,43,43,43	0
56	MG	1A	3810	1/1	0.79	0.13	35,35,35,35	0
56	MG	1A	3537	1/1	0.80	0.20	55,55,55,55	0
56	MG	1a	1635	1/1	0.80	0.10	87,87,87,87	0
56	MG	2a	1709	1/1	0.80	0.21	78,78,78,78	0
56	MG	1q	201	1/1	0.80	0.20	65,65,65,65	0
56	MG	2A	3534	1/1	0.80	0.20	57,57,57,57	0
56	MG	2a	1734	1/1	0.80	0.20	80,80,80,80	0
56	MG	2A	3550	1/1	0.80	0.17	49,49,49,49	0
56	MG	2A	3552	1/1	0.80	0.16	59,59,59,59	0
56	MG	1A	3424	1/1	0.80	0.17	53,53,53,53	0
56	MG	2a	1769	1/1	0.80	0.19	76,76,76,76	0
56	MG	10	102	1/1	0.80	0.17	54,54,54,54	0
56	MG	1a	1721	1/1	0.80	0.17	78,78,78,78	0
56	MG	1a	1779	1/1	0.80	0.10	80,80,80,80	0
56	MG	1a	1786	1/1	0.80	0.20	64,64,64,64	0
56	MG	1A	4067	1/1	0.80	0.12	71,71,71,71	0
56	MG	2a	1805	1/1	0.80	0.21	73,73,73,73	0
56	MG	2A	3339	1/1	0.80	0.20	76,76,76,76	0
56	MG	2a	1648	1/1	0.80	0.18	79,79,79,79	0
56	MG	2a	1820	1/1	0.80	0.27	68,68,68,68	0
56	MG	2a	1823	1/1	0.80	0.22	76,76,76,76	0
56	MG	1A	3746	1/1	0.80	0.21	38,38,38,38	0
56	MG	2a	1653	1/1	0.80	0.10	85,85,85,85	0
56	MG	1a	1740	1/1	0.80	0.26	72,72,72,72	0
56	MG	1a	1847	1/1	0.80	0.20	72,72,72,72	0
56	MG	1a	1752	1/1	0.80	0.22	73,73,73,73	0
56	MG	1A	4017	1/1	0.81	0.31	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3239	1/1	0.81	0.23	64,64,64,64	0
56	MG	1A	4081	1/1	0.81	0.17	73,73,73,73	0
56	MG	1A	4028	1/1	0.81	0.12	74,74,74,74	0
56	MG	1a	1609	1/1	0.81	0.16	64,64,64,64	0
56	MG	2A	3288	1/1	0.81	0.12	46,46,46,46	0
56	MG	1a	1618	1/1	0.81	0.11	42,42,42,42	0
56	MG	1A	4086	1/1	0.81	0.24	61,61,61,61	0
56	MG	2A	3368	1/1	0.81	0.15	49,49,49,49	0
56	MG	1A	3597	1/1	0.81	0.21	49,49,49,49	0
56	MG	2a	1764	1/1	0.81	0.28	69,69,69,69	0
56	MG	1a	1812	1/1	0.81	0.17	62,62,62,62	0
56	MG	1A	4140	1/1	0.81	0.22	77,77,77,77	0
56	MG	1a	1649	1/1	0.81	0.18	83,83,83,83	0
56	MG	1a	1844	1/1	0.81	0.13	56,56,56,56	0
56	MG	2a	1786	1/1	0.81	0.23	58,58,58,58	0
56	MG	1A	3644	1/1	0.81	0.24	66,66,66,66	0
56	MG	1a	1703	1/1	0.81	0.31	61,61,61,61	0
56	MG	1A	3528	1/1	0.81	0.11	60,60,60,60	0
56	MG	1a	1870	1/1	0.81	0.12	67,67,67,67	0
56	MG	1a	1879	1/1	0.81	0.19	78,78,78,78	0
56	MG	1A	3935	1/1	0.81	0.10	29,29,29,29	0
56	MG	1A	3514	1/1	0.81	0.19	59,59,59,59	0
56	MG	1A	3461	1/1	0.81	0.22	62,62,62,62	0
56	MG	1r	3001	1/1	0.81	0.24	80,80,80,80	0
56	MG	1x	102	1/1	0.81	0.28	69,69,69,69	0
56	MG	1A	3591	1/1	0.81	0.11	55,55,55,55	0
56	MG	1B	204	1/1	0.81	0.14	49,49,49,49	0
56	MG	2a	1845	1/1	0.81	0.18	63,63,63,63	0
56	MG	2A	3043	1/1	0.81	0.18	61,61,61,61	0
56	MG	2A	3190	1/1	0.81	0.21	46,46,46,46	0
56	MG	2A	3525	1/1	0.82	0.13	49,49,49,49	0
56	MG	2A	3170	1/1	0.82	0.10	46,46,46,46	0
56	MG	1A	3594	1/1	0.82	0.11	61,61,61,61	0
56	MG	2a	1755	1/1	0.82	0.22	68,68,68,68	0
56	MG	2A	3231	1/1	0.82	0.20	81,81,81,81	0
56	MG	1a	1697	1/1	0.82	0.18	73,73,73,73	0
56	MG	1A	3466	1/1	0.82	0.23	63,63,63,63	0
56	MG	1A	4019	1/1	0.82	0.22	75,75,75,75	0
56	MG	2a	1778	1/1	0.82	0.14	61,61,61,61	0
56	MG	2a	1602	1/1	0.82	0.26	54,54,54,54	0
56	MG	1A	3634	1/1	0.82	0.09	29,29,29,29	0
56	MG	1a	1782	1/1	0.82	0.23	63,63,63,63	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	3476	1/1	0.82	0.23	61,61,61,61	0
56	MG	2a	1638	1/1	0.82	0.28	73,73,73,73	0
56	MG	1A	3438	1/1	0.82	0.14	60,60,60,60	0
56	MG	1A	3145	1/1	0.82	0.08	59,59,59,59	0
56	MG	2a	1808	1/1	0.82	0.20	65,65,65,65	0
56	MG	1A	4233	1/1	0.82	0.18	88,88,88,88	0
56	MG	2A	3405	1/1	0.82	0.17	64,64,64,64	0
56	MG	1A	3731	1/1	0.82	0.20	53,53,53,53	0
56	MG	1a	1764	1/1	0.82	0.11	73,73,73,73	0
56	MG	2A	3049	1/1	0.82	0.30	64,64,64,64	0
56	MG	2A	3480	1/1	0.82	0.17	39,39,39,39	0
56	MG	2A	3058	1/1	0.82	0.21	58,58,58,58	0
56	MG	2A	3060	1/1	0.82	0.12	46,46,46,46	0
56	MG	2A	3152	1/1	0.82	0.21	52,52,52,52	0
56	MG	2a	1731	1/1	0.82	0.20	70,70,70,70	0
56	MG	1a	1811	1/1	0.83	0.10	72,72,72,72	0
56	MG	2A	3243	1/1	0.83	0.12	59,59,59,59	0
56	MG	2A	3257	1/1	0.83	0.14	57,57,57,57	0
56	MG	1A	3050	1/1	0.83	0.10	48,48,48,48	0
56	MG	1A	3893	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3389	1/1	0.83	0.25	72,72,72,72	0
56	MG	1a	1706	1/1	0.83	0.14	51,51,51,51	0
56	MG	2a	1690	1/1	0.83	0.25	58,58,58,58	0
56	MG	2a	1697	1/1	0.83	0.13	53,53,53,53	0
56	MG	2A	3310	1/1	0.83	0.14	38,38,38,38	0
56	MG	1a	1710	1/1	0.83	0.24	58,58,58,58	0
56	MG	1A	3590	1/1	0.83	0.20	54,54,54,54	0
56	MG	2A	3367	1/1	0.83	0.19	63,63,63,63	0
56	MG	1A	3524	1/1	0.83	0.14	51,51,51,51	0
56	MG	2A	3383	1/1	0.83	0.21	44,44,44,44	0
56	MG	1A	3436	1/1	0.83	0.12	52,52,52,52	0
56	MG	1A	4071	1/1	0.83	0.17	79,79,79,79	0
56	MG	1B	210	1/1	0.83	0.15	50,50,50,50	0
56	MG	2A	3455	1/1	0.83	0.10	47,47,47,47	0
56	MG	2A	3460	1/1	0.83	0.14	74,74,74,74	0
56	MG	1a	1750	1/1	0.83	0.15	70,70,70,70	0
56	MG	1E	307	1/1	0.83	0.16	53,53,53,53	0
56	MG	2A	3498	1/1	0.83	0.14	48,48,48,48	0
56	MG	1A	3102	1/1	0.83	0.13	51,51,51,51	0
56	MG	2a	1787	1/1	0.83	0.25	65,65,65,65	0
56	MG	1a	1755	1/1	0.83	0.20	65,65,65,65	0
56	MG	1a	1756	1/1	0.83	0.17	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3609	1/1	0.83	0.14	31,31,31,31	0
56	MG	2A	3007	1/1	0.83	0.22	72,72,72,72	0
56	MG	1A	4078	1/1	0.83	0.20	62,62,62,62	0
56	MG	1A	3997	1/1	0.83	0.11	25,25,25,25	0
56	MG	2A	3571	1/1	0.83	0.28	43,43,43,43	0
56	MG	1A	3825	1/1	0.83	0.15	62,62,62,62	0
56	MG	1a	1769	1/1	0.83	0.14	66,66,66,66	0
56	MG	2A	3077	1/1	0.83	0.17	61,61,61,61	0
56	MG	2a	1827	1/1	0.83	0.38	83,83,83,83	0
56	MG	2A	3082	1/1	0.83	0.08	44,44,44,44	0
56	MG	1A	3840	1/1	0.83	0.12	69,69,69,69	0
56	MG	1A	3023	1/1	0.83	0.18	49,49,49,49	0
56	MG	1A	3425	1/1	0.83	0.22	62,62,62,62	0
56	MG	1A	3869	1/1	0.83	0.23	64,64,64,64	0
56	MG	1a	1803	1/1	0.83	0.16	60,60,60,60	0
56	MG	2q	3002	1/1	0.83	0.14	48,48,48,48	0
56	MG	2A	3399	1/1	0.84	0.19	60,60,60,60	0
56	MG	2A	3025	1/1	0.84	0.18	59,59,59,59	0
56	MG	2a	1676	1/1	0.84	0.16	64,64,64,64	0
56	MG	2a	1679	1/1	0.84	0.20	61,61,61,61	0
56	MG	2A	3435	1/1	0.84	0.10	54,54,54,54	0
56	MG	1B	201	1/1	0.84	0.18	64,64,64,64	0
56	MG	1A	3298	1/1	0.84	0.20	57,57,57,57	0
56	MG	1a	1711	1/1	0.84	0.21	75,75,75,75	0
56	MG	2a	1706	1/1	0.84	0.27	63,63,63,63	0
56	MG	1A	3432	1/1	0.84	0.14	52,52,52,52	0
56	MG	1A	3541	1/1	0.84	0.18	56,56,56,56	0
56	MG	2a	1717	1/1	0.84	0.31	71,71,71,71	0
56	MG	1Q	201	1/1	0.84	0.20	60,60,60,60	0
56	MG	2a	1732	1/1	0.84	0.20	57,57,57,57	0
56	MG	2A	3497	1/1	0.84	0.09	52,52,52,52	0
56	MG	2A	3109	1/1	0.84	0.16	55,55,55,55	0
56	MG	2a	1743	1/1	0.84	0.29	64,64,64,64	0
56	MG	2A	3130	1/1	0.84	0.11	52,52,52,52	0
56	MG	2A	3148	1/1	0.84	0.22	65,65,65,65	0
56	MG	1a	1825	1/1	0.84	0.14	59,59,59,59	0
56	MG	1A	4038	1/1	0.84	0.16	81,81,81,81	0
56	MG	1R	208	1/1	0.84	0.13	45,45,45,45	0
56	MG	2A	3535	1/1	0.84	0.20	39,39,39,39	0
56	MG	2A	3196	1/1	0.84	0.12	50,50,50,50	0
56	MG	1a	1749	1/1	0.84	0.23	78,78,78,78	0
56	MG	1A	4090	1/1	0.84	0.18	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1855	1/1	0.84	0.22	57,57,57,57	0
56	MG	1A	3434	1/1	0.84	0.12	53,53,53,53	0
56	MG	2D	306	1/1	0.84	0.14	65,65,65,65	0
56	MG	1A	3569	1/1	0.84	0.15	56,56,56,56	0
56	MG	1a	1616	1/1	0.84	0.24	74,74,74,74	0
56	MG	1A	3036	1/1	0.84	0.18	66,66,66,66	0
56	MG	2a	1619	1/1	0.84	0.11	91,91,91,91	0
56	MG	2a	1623	1/1	0.84	0.24	92,92,92,92	0
56	MG	1A	3962	1/1	0.84	0.12	55,55,55,55	0
56	MG	1A	3034	1/1	0.84	0.14	71,71,71,71	0
56	MG	1A	3529	1/1	0.84	0.11	61,61,61,61	0
56	MG	2a	1639	1/1	0.84	0.25	71,71,71,71	0
56	MG	2a	1640	1/1	0.84	0.39	72,72,72,72	0
56	MG	1A	3888	1/1	0.84	0.14	29,29,29,29	0
56	MG	1A	4213	1/1	0.84	0.11	49,49,49,49	0
56	MG	1A	3400	1/1	0.84	0.10	44,44,44,44	0
56	MG	1A	4076	1/1	0.84	0.12	71,71,71,71	0
56	MG	2A	3018	1/1	0.84	0.15	58,58,58,58	0
56	MG	2a	1656	1/1	0.84	0.08	94,94,94,94	0
56	MG	1T	201	1/1	0.85	0.20	56,56,56,56	0
56	MG	1A	3958	1/1	0.85	0.12	58,58,58,58	0
56	MG	1A	3818	1/1	0.85	0.08	32,32,32,32	0
56	MG	1A	3972	1/1	0.85	0.14	59,59,59,59	0
56	MG	2A	3441	1/1	0.85	0.15	58,58,58,58	0
56	MG	1A	3992	1/1	0.85	0.14	54,54,54,54	0
56	MG	2A	3453	1/1	0.85	0.15	49,49,49,49	0
56	MG	1A	3393	1/1	0.85	0.23	59,59,59,59	0
56	MG	1a	1777	1/1	0.85	0.31	72,72,72,72	0
56	MG	1a	1626	1/1	0.85	0.17	61,61,61,61	0
56	MG	1A	4002	1/1	0.85	0.23	82,82,82,82	0
56	MG	1A	4112	1/1	0.85	0.14	29,29,29,29	0
56	MG	2A	3089	1/1	0.85	0.14	51,51,51,51	0
56	MG	2A	3105	1/1	0.85	0.18	45,45,45,45	0
56	MG	1A	3456	1/1	0.85	0.09	41,41,41,41	0
56	MG	1a	1791	1/1	0.85	0.12	64,64,64,64	0
56	MG	1a	1639	1/1	0.85	0.20	77,77,77,77	0
56	MG	1A	3360	1/1	0.85	0.15	53,53,53,53	0
56	MG	1A	3416	1/1	0.85	0.17	60,60,60,60	0
56	MG	2a	1760	1/1	0.85	0.11	67,67,67,67	0
56	MG	2A	3173	1/1	0.85	0.18	53,53,53,53	0
56	MG	1A	3024	1/1	0.85	0.12	48,48,48,48	0
56	MG	2A	3555	1/1	0.85	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	2A	3564	1/1	0.85	0.10	35,35,35,35	0
56	MG	1A	3046	1/1	0.85	0.09	51,51,51,51	0
56	MG	2A	3579	1/1	0.85	0.17	69,69,69,69	0
56	MG	1A	3485	1/1	0.85	0.35	51,51,51,51	0
56	MG	1A	3493	1/1	0.85	0.17	58,58,58,58	0
56	MG	2a	1788	1/1	0.85	0.11	59,59,59,59	0
56	MG	1A	3899	1/1	0.85	0.12	36,36,36,36	0
56	MG	1A	4232	1/1	0.85	0.09	68,68,68,68	0
56	MG	2A	3244	1/1	0.85	0.14	49,49,49,49	0
56	MG	1A	3548	1/1	0.85	0.08	62,62,62,62	0
56	MG	1A	3500	1/1	0.85	0.15	55,55,55,55	0
56	MG	1A	3504	1/1	0.85	0.17	61,61,61,61	0
56	MG	1A	3323	1/1	0.85	0.11	58,58,58,58	0
56	MG	2A	3281	1/1	0.85	0.18	58,58,58,58	0
56	MG	1a	1747	1/1	0.85	0.25	68,68,68,68	0
56	MG	2A	3305	1/1	0.85	0.12	53,53,53,53	0
56	MG	1b	3002	1/1	0.85	0.19	88,88,88,88	0
56	MG	1B	213	1/1	0.85	0.27	59,59,59,59	0
56	MG	2A	3342	1/1	0.85	0.23	59,59,59,59	0
56	MG	1A	3780	1/1	0.85	0.11	24,24,24,24	0
56	MG	1A	3940	1/1	0.85	0.18	70,70,70,70	0
56	MG	1A	3111	1/1	0.85	0.11	59,59,59,59	0
56	MG	2e	3001	1/1	0.85	0.23	67,67,67,67	0
56	MG	1A	3944	1/1	0.85	0.19	77,77,77,77	0
56	MG	2a	1659	1/1	0.85	0.25	78,78,78,78	0
56	MG	2A	3034	1/1	0.86	0.11	58,58,58,58	0
56	MG	2a	1665	1/1	0.86	0.21	65,65,65,65	0
56	MG	1A	3675	1/1	0.86	0.15	55,55,55,55	0
56	MG	2A	3409	1/1	0.86	0.23	59,59,59,59	0
56	MG	1A	3069	1/1	0.86	0.16	50,50,50,50	0
56	MG	1a	1675	1/1	0.86	0.25	63,63,63,63	0
56	MG	2a	1680	1/1	0.86	0.23	70,70,70,70	0
56	MG	1A	3408	1/1	0.86	0.21	53,53,53,53	0
56	MG	1A	3545	1/1	0.86	0.18	56,56,56,56	0
56	MG	1a	1797	1/1	0.86	0.28	49,49,49,49	0
56	MG	1B	203	1/1	0.86	0.15	66,66,66,66	0
56	MG	1a	1810	1/1	0.86	0.16	74,74,74,74	0
56	MG	1A	3076	1/1	0.86	0.10	60,60,60,60	0
56	MG	1A	3599	1/1	0.86	0.12	60,60,60,60	0
56	MG	2A	3136	1/1	0.86	0.14	56,56,56,56	0
56	MG	1A	4110	1/1	0.86	0.34	75,75,75,75	0
56	MG	2A	3509	1/1	0.86	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3897	1/1	0.86	0.10	32,32,32,32	0
56	MG	1A	4115	1/1	0.86	0.09	36,36,36,36	0
56	MG	1A	3989	1/1	0.86	0.11	20,20,20,20	0
56	MG	1A	4161	1/1	0.86	0.14	45,45,45,45	0
56	MG	1a	1728	1/1	0.86	0.14	48,48,48,48	0
56	MG	2A	3197	1/1	0.86	0.06	49,49,49,49	0
56	MG	2A	3204	1/1	0.86	0.14	59,59,59,59	0
56	MG	2A	3209	1/1	0.86	0.09	56,56,56,56	0
56	MG	2A	3553	1/1	0.86	0.16	44,44,44,44	0
56	MG	1A	4163	1/1	0.86	0.17	61,61,61,61	0
56	MG	2A	3232	1/1	0.86	0.10	72,72,72,72	0
56	MG	1A	4164	1/1	0.86	0.26	66,66,66,66	0
56	MG	1A	4166	1/1	0.86	0.15	36,36,36,36	0
56	MG	1a	1871	1/1	0.86	0.18	55,55,55,55	0
56	MG	1a	1601	1/1	0.86	0.12	68,68,68,68	0
56	MG	1a	1751	1/1	0.86	0.13	70,70,70,70	0
56	MG	1a	1602	1/1	0.86	0.09	58,58,58,58	0
56	MG	1A	3990	1/1	0.86	0.13	53,53,53,53	0
56	MG	2A	3275	1/1	0.86	0.17	65,65,65,65	0
56	MG	1o	3001	1/1	0.86	0.13	47,47,47,47	0
56	MG	1a	1611	1/1	0.86	0.39	72,72,72,72	0
56	MG	1A	4172	1/1	0.86	0.19	22,22,22,22	0
56	MG	1A	3607	1/1	0.86	0.16	53,53,53,53	0
56	MG	1A	3558	1/1	0.86	0.12	49,49,49,49	0
56	MG	2A	3337	1/1	0.86	0.18	56,56,56,56	0
56	MG	1A	3006	1/1	0.86	0.14	64,64,64,64	0
56	MG	2A	3005	1/1	0.86	0.15	52,52,52,52	0
56	MG	2a	1646	1/1	0.86	0.19	63,63,63,63	0
56	MG	1a	1631	1/1	0.86	0.31	58,58,58,58	0
56	MG	2A	3014	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3469	1/1	0.86	0.10	57,57,57,57	0
56	MG	2a	1654	1/1	0.86	0.14	80,80,80,80	0
56	MG	1A	3309	1/1	0.86	0.38	65,65,65,65	0
56	MG	2A	3388	1/1	0.86	0.19	56,56,56,56	0
56	MG	1A	3142	1/1	0.87	0.08	61,61,61,61	0
56	MG	1A	4157	1/1	0.87	0.18	53,53,53,53	0
56	MG	1A	3515	1/1	0.87	0.17	64,64,64,64	0
56	MG	2A	3370	1/1	0.87	0.12	60,60,60,60	0
56	MG	2a	1658	1/1	0.87	0.20	79,79,79,79	0
56	MG	1A	3464	1/1	0.87	0.23	50,50,50,50	0
56	MG	2a	1660	1/1	0.87	0.10	86,86,86,86	0
56	MG	1A	3518	1/1	0.87	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	2A	3037	1/1	0.87	0.14	51,51,51,51	0
56	MG	1a	1621	1/1	0.87	0.13	64,64,64,64	0
56	MG	1A	4037	1/1	0.87	0.10	77,77,77,77	0
56	MG	2A	3414	1/1	0.87	0.20	56,56,56,56	0
56	MG	2A	3419	1/1	0.87	0.12	66,66,66,66	0
56	MG	2A	3434	1/1	0.87	0.17	58,58,58,58	0
56	MG	1A	3522	1/1	0.87	0.11	52,52,52,52	0
56	MG	1A	4039	1/1	0.87	0.12	67,67,67,67	0
56	MG	1A	3922	1/1	0.87	0.16	47,47,47,47	0
56	MG	1A	3755	1/1	0.87	0.15	52,52,52,52	0
56	MG	1A	3396	1/1	0.87	0.18	49,49,49,49	0
56	MG	2A	3096	1/1	0.87	0.15	50,50,50,50	0
56	MG	1A	4062	1/1	0.87	0.19	63,63,63,63	0
56	MG	2a	1722	1/1	0.87	0.21	71,71,71,71	0
56	MG	2a	1727	1/1	0.87	0.28	70,70,70,70	0
56	MG	2A	3107	1/1	0.87	0.12	65,65,65,65	0
56	MG	1a	1652	1/1	0.87	0.10	54,54,54,54	0
56	MG	2A	3110	1/1	0.87	0.38	64,64,64,64	0
56	MG	1a	1653	1/1	0.87	0.11	52,52,52,52	0
56	MG	1A	3353	1/1	0.87	0.11	51,51,51,51	0
56	MG	1a	1688	1/1	0.87	0.09	74,74,74,74	0
56	MG	1A	3025	1/1	0.87	0.13	52,52,52,52	0
56	MG	1a	1696	1/1	0.87	0.24	61,61,61,61	0
56	MG	1A	3955	1/1	0.87	0.18	54,54,54,54	0
56	MG	1A	3956	1/1	0.87	0.12	53,53,53,53	0
56	MG	1A	3532	1/1	0.87	0.20	55,55,55,55	0
56	MG	1A	3363	1/1	0.87	0.21	71,71,71,71	0
56	MG	2a	1773	1/1	0.87	0.20	65,65,65,65	0
56	MG	1A	3104	1/1	0.87	0.19	60,60,60,60	0
56	MG	2a	1781	1/1	0.87	0.10	56,56,56,56	0
56	MG	1a	1712	1/1	0.87	0.26	75,75,75,75	0
56	MG	2a	1785	1/1	0.87	0.20	71,71,71,71	0
56	MG	1A	3975	1/1	0.87	0.11	57,57,57,57	0
56	MG	1A	3620	1/1	0.87	0.11	37,37,37,37	0
56	MG	1A	3627	1/1	0.87	0.13	59,59,59,59	0
56	MG	1F	309	1/1	0.87	0.11	57,57,57,57	0
56	MG	1A	4089	1/1	0.87	0.13	61,61,61,61	0
56	MG	1a	1884	1/1	0.87	0.18	58,58,58,58	0
56	MG	2A	3253	1/1	0.87	0.18	58,58,58,58	0
56	MG	1a	1888	1/1	0.87	0.20	73,73,73,73	0
56	MG	1a	1731	1/1	0.87	0.26	62,62,62,62	0
56	MG	1a	1734	1/1	0.87	0.19	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	2a	1610	1/1	0.87	0.13	74,74,74,74	0
56	MG	1k	3002	1/1	0.87	0.12	68,68,68,68	0
56	MG	1A	3132	1/1	0.87	0.09	52,52,52,52	0
56	MG	1R	202	1/1	0.87	0.25	56,56,56,56	0
56	MG	1A	3314	1/1	0.87	0.12	38,38,38,38	0
56	MG	1A	3891	1/1	0.87	0.24	61,61,61,61	0
56	MG	1A	3453	1/1	0.87	0.14	51,51,51,51	0
56	MG	2a	1840	1/1	0.87	0.15	58,58,58,58	0
56	MG	2A	3320	1/1	0.87	0.11	45,45,45,45	0
56	MG	2A	3331	1/1	0.87	0.10	55,55,55,55	0
56	MG	2A	3002	1/1	0.87	0.21	58,58,58,58	0
56	MG	1A	3007	1/1	0.87	0.25	69,69,69,69	0
56	MG	2n	101	1/1	0.87	0.30	65,65,65,65	0
56	MG	1A	4117	1/1	0.87	0.18	51,51,51,51	0
56	MG	1A	3471	1/1	0.88	0.15	47,47,47,47	0
56	MG	1A	4126	1/1	0.88	0.12	56,56,56,56	0
56	MG	1A	3831	1/1	0.88	0.14	53,53,53,53	0
56	MG	1A	3059	1/1	0.88	0.08	38,38,38,38	0
56	MG	2a	1601	1/1	0.88	0.30	67,67,67,67	0
56	MG	2A	3180	1/1	0.88	0.09	43,43,43,43	0
56	MG	2a	1603	1/1	0.88	0.15	59,59,59,59	0
56	MG	1A	3065	1/1	0.88	0.09	48,48,48,48	0
56	MG	1A	4004	1/1	0.88	0.11	68,68,68,68	0
56	MG	2a	1613	1/1	0.88	0.19	65,65,65,65	0
56	MG	2a	1614	1/1	0.88	0.15	68,68,68,68	0
56	MG	1a	1636	1/1	0.88	0.13	58,58,58,58	0
56	MG	1a	1813	1/1	0.88	0.24	59,59,59,59	0
56	MG	2a	1627	1/1	0.88	0.14	63,63,63,63	0
56	MG	2A	3208	1/1	0.88	0.11	49,49,49,49	0
56	MG	1A	3852	1/1	0.88	0.12	58,58,58,58	0
56	MG	2A	3212	1/1	0.88	0.17	50,50,50,50	0
56	MG	2A	3221	1/1	0.88	0.14	48,48,48,48	0
56	MG	1a	1823	1/1	0.88	0.12	46,46,46,46	0
56	MG	1A	3163	1/1	0.88	0.17	52,52,52,52	0
56	MG	1A	3867	1/1	0.88	0.17	52,52,52,52	0
56	MG	2a	1647	1/1	0.88	0.18	82,82,82,82	0
56	MG	1A	3241	1/1	0.88	0.27	70,70,70,70	0
56	MG	1a	1665	1/1	0.88	0.20	74,74,74,74	0
56	MG	1A	3005	1/1	0.88	0.18	49,49,49,49	0
56	MG	1A	3307	1/1	0.88	0.12	37,37,37,37	0
56	MG	1A	3646	1/1	0.88	0.14	53,53,53,53	0
56	MG	1A	3549	1/1	0.88	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	4040	1/1	0.88	0.11	67,67,67,67	0
56	MG	1A	4043	1/1	0.88	0.11	62,62,62,62	0
56	MG	1A	3121	1/1	0.88	0.12	54,54,54,54	0
56	MG	2a	1664	1/1	0.88	0.18	84,84,84,84	0
56	MG	1A	3704	1/1	0.88	0.16	24,24,24,24	0
56	MG	1A	4059	1/1	0.88	0.14	60,60,60,60	0
56	MG	2a	1671	1/1	0.88	0.25	58,58,58,58	0
56	MG	1a	1895	1/1	0.88	0.12	78,78,78,78	0
56	MG	1A	3901	1/1	0.88	0.09	35,35,35,35	0
56	MG	2A	3314	1/1	0.88	0.24	63,63,63,63	0
56	MG	1A	3707	1/1	0.88	0.09	68,68,68,68	0
56	MG	1h	202	1/1	0.88	0.16	65,65,65,65	0
56	MG	1a	1717	1/1	0.88	0.38	62,62,62,62	0
56	MG	1A	3711	1/1	0.88	0.10	31,31,31,31	0
56	MG	1A	3073	1/1	0.88	0.10	69,69,69,69	0
56	MG	1a	1724	1/1	0.88	0.17	70,70,70,70	0
56	MG	1x	101	1/1	0.88	0.15	67,67,67,67	0
56	MG	1E	304	1/1	0.88	0.24	53,53,53,53	0
56	MG	1x	103	1/1	0.88	0.12	64,64,64,64	0
56	MG	1A	3564	1/1	0.88	0.16	41,41,41,41	0
56	MG	2A	3386	1/1	0.88	0.19	52,52,52,52	0
56	MG	1A	3317	1/1	0.88	0.12	73,73,73,73	0
56	MG	1A	3075	1/1	0.88	0.10	46,46,46,46	0
56	MG	2A	3401	1/1	0.88	0.14	60,60,60,60	0
56	MG	2A	3403	1/1	0.88	0.10	62,62,62,62	0
56	MG	2a	1737	1/1	0.88	0.14	64,64,64,64	0
56	MG	2a	1741	1/1	0.88	0.20	80,80,80,80	0
56	MG	1A	3575	1/1	0.88	0.16	65,65,65,65	0
56	MG	1a	1743	1/1	0.88	0.16	47,47,47,47	0
56	MG	2A	3412	1/1	0.88	0.10	44,44,44,44	0
56	MG	2A	3008	1/1	0.88	0.10	59,59,59,59	0
56	MG	2a	1762	1/1	0.88	0.13	64,64,64,64	0
56	MG	1a	1746	1/1	0.88	0.09	81,81,81,81	0
56	MG	2a	1765	1/1	0.88	0.21	65,65,65,65	0
56	MG	2A	3426	1/1	0.88	0.12	51,51,51,51	0
56	MG	1Q	204	1/1	0.88	0.19	42,42,42,42	0
56	MG	1A	3010	1/1	0.88	0.11	57,57,57,57	0
56	MG	2a	1771	1/1	0.88	0.20	50,50,50,50	0
56	MG	1A	3756	1/1	0.88	0.09	52,52,52,52	0
56	MG	1A	3759	1/1	0.88	0.13	56,56,56,56	0
56	MG	1U	201	1/1	0.88	0.11	32,32,32,32	0
56	MG	1a	1753	1/1	0.88	0.23	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3454	1/1	0.88	0.09	30,30,30,30	0
56	MG	2A	3055	1/1	0.88	0.19	60,60,60,60	0
56	MG	1U	204	1/1	0.88	0.20	55,55,55,55	0
56	MG	2A	3477	1/1	0.88	0.11	39,39,39,39	0
56	MG	1U	205	1/1	0.88	0.28	35,35,35,35	0
56	MG	2a	1790	1/1	0.88	0.17	53,53,53,53	0
56	MG	2a	1791	1/1	0.88	0.23	64,64,64,64	0
56	MG	2A	3064	1/1	0.88	0.17	34,34,34,34	0
56	MG	2A	3491	1/1	0.88	0.14	56,56,56,56	0
56	MG	2A	3076	1/1	0.88	0.13	44,44,44,44	0
56	MG	2a	1803	1/1	0.88	0.21	72,72,72,72	0
56	MG	1Z	303	1/1	0.88	0.11	64,64,64,64	0
56	MG	1A	3772	1/1	0.88	0.13	35,35,35,35	0
56	MG	1A	3138	1/1	0.88	0.09	49,49,49,49	0
56	MG	1A	3800	1/1	0.88	0.11	50,50,50,50	0
56	MG	2A	3099	1/1	0.88	0.12	54,54,54,54	0
56	MG	1A	3809	1/1	0.88	0.09	16,16,16,16	0
56	MG	1a	1608	1/1	0.88	0.16	66,66,66,66	0
56	MG	1A	3100	1/1	0.88	0.12	47,47,47,47	0
56	MG	2A	3542	1/1	0.88	0.21	33,33,33,33	0
56	MG	1A	3141	1/1	0.88	0.13	46,46,46,46	0
56	MG	2a	1839	1/1	0.88	0.13	48,48,48,48	0
56	MG	2A	3115	1/1	0.88	0.11	51,51,51,51	0
56	MG	2A	3116	1/1	0.88	0.20	48,48,48,48	0
56	MG	2A	3117	1/1	0.88	0.17	52,52,52,52	0
56	MG	2A	3563	1/1	0.88	0.14	42,42,42,42	0
56	MG	1A	4113	1/1	0.88	0.11	39,39,39,39	0
56	MG	1A	3824	1/1	0.88	0.09	56,56,56,56	0
56	MG	2A	3141	1/1	0.88	0.26	53,53,53,53	0
56	MG	2x	3003	1/1	0.88	0.19	65,65,65,65	0
56	MG	1A	3770	1/1	0.89	0.14	25,25,25,25	0
56	MG	2a	1616	1/1	0.89	0.25	60,60,60,60	0
56	MG	2a	1618	1/1	0.89	0.23	63,63,63,63	0
56	MG	1E	301	1/1	0.89	0.10	23,23,23,23	0
56	MG	1k	3001	1/1	0.89	0.21	66,66,66,66	0
56	MG	2a	1624	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3274	1/1	0.89	0.20	56,56,56,56	0
56	MG	2a	1631	1/1	0.89	0.13	49,49,49,49	0
56	MG	1A	3031	1/1	0.89	0.08	50,50,50,50	0
56	MG	2A	3276	1/1	0.89	0.26	48,48,48,48	0
56	MG	1A	4066	1/1	0.89	0.09	71,71,71,71	0
56	MG	1A	3209	1/1	0.89	0.20	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1G	203	1/1	0.89	0.20	61,61,61,61	0
56	MG	1A	3785	1/1	0.89	0.17	45,45,45,45	0
56	MG	2a	1644	1/1	0.89	0.17	60,60,60,60	0
56	MG	1a	1738	1/1	0.89	0.21	58,58,58,58	0
56	MG	1A	3487	1/1	0.89	0.15	46,46,46,46	0
56	MG	1x	111	1/1	0.89	0.18	61,61,61,61	0
56	MG	1A	4074	1/1	0.89	0.13	66,66,66,66	0
56	MG	1A	3803	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	3601	1/1	0.89	0.25	54,54,54,54	0
56	MG	1A	3489	1/1	0.89	0.15	42,42,42,42	0
56	MG	2A	3006	1/1	0.89	0.11	66,66,66,66	0
56	MG	2A	3359	1/1	0.89	0.15	39,39,39,39	0
56	MG	1A	3331	1/1	0.89	0.14	43,43,43,43	0
56	MG	1A	3351	1/1	0.89	0.19	59,59,59,59	0
56	MG	1A	3047	1/1	0.89	0.10	69,69,69,69	0
56	MG	1A	3827	1/1	0.89	0.11	70,70,70,70	0
56	MG	2A	3021	1/1	0.89	0.19	50,50,50,50	0
56	MG	1A	3978	1/1	0.89	0.31	38,38,38,38	0
56	MG	2A	3396	1/1	0.89	0.24	55,55,55,55	0
56	MG	2A	3032	1/1	0.89	0.14	45,45,45,45	0
56	MG	2A	3033	1/1	0.89	0.24	64,64,64,64	0
56	MG	18	102	1/1	0.89	0.10	40,40,40,40	0
56	MG	1A	3414	1/1	0.89	0.13	55,55,55,55	0
56	MG	1A	4106	1/1	0.89	0.17	45,45,45,45	0
56	MG	1A	3550	1/1	0.89	0.26	40,40,40,40	0
56	MG	1A	3293	1/1	0.89	0.05	42,42,42,42	0
56	MG	1A	3129	1/1	0.89	0.15	40,40,40,40	0
56	MG	2a	1707	1/1	0.89	0.16	52,52,52,52	0
56	MG	1A	4001	1/1	0.89	0.07	46,46,46,46	0
56	MG	2a	1712	1/1	0.89	0.27	62,62,62,62	0
56	MG	2A	3428	1/1	0.89	0.08	62,62,62,62	0
56	MG	1a	1771	1/1	0.89	0.10	56,56,56,56	0
56	MG	2a	1720	1/1	0.89	0.21	65,65,65,65	0
56	MG	1A	3855	1/1	0.89	0.20	62,62,62,62	0
56	MG	1A	3423	1/1	0.89	0.14	48,48,48,48	0
56	MG	1A	4134	1/1	0.89	0.09	38,38,38,38	0
56	MG	2A	3445	1/1	0.89	0.10	51,51,51,51	0
56	MG	1a	1625	1/1	0.89	0.22	74,74,74,74	0
56	MG	1a	1785	1/1	0.89	0.15	43,43,43,43	0
56	MG	2a	1736	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3697	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3102	1/1	0.89	0.12	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	3457	1/1	0.89	0.18	54,54,54,54	0
56	MG	2a	1753	1/1	0.89	0.23	76,76,76,76	0
56	MG	1a	1628	1/1	0.89	0.17	55,55,55,55	0
56	MG	2A	3462	1/1	0.89	0.11	60,60,60,60	0
56	MG	2A	3464	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3470	1/1	0.89	0.08	40,40,40,40	0
56	MG	2a	1763	1/1	0.89	0.12	69,69,69,69	0
56	MG	1A	4150	1/1	0.89	0.12	47,47,47,47	0
56	MG	1A	4007	1/1	0.89	0.09	49,49,49,49	0
56	MG	2a	1766	1/1	0.89	0.13	60,60,60,60	0
56	MG	1A	3567	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3481	1/1	0.89	0.12	48,48,48,48	0
56	MG	2A	3486	1/1	0.89	0.11	47,47,47,47	0
56	MG	2a	1770	1/1	0.89	0.20	71,71,71,71	0
56	MG	1A	4012	1/1	0.89	0.12	40,40,40,40	0
56	MG	1A	3568	1/1	0.89	0.10	52,52,52,52	0
56	MG	1A	3878	1/1	0.89	0.20	68,68,68,68	0
56	MG	1a	1818	1/1	0.89	0.22	58,58,58,58	0
56	MG	2A	3133	1/1	0.89	0.13	55,55,55,55	0
56	MG	1A	4020	1/1	0.89	0.13	69,69,69,69	0
56	MG	1A	3884	1/1	0.89	0.28	37,37,37,37	0
56	MG	1A	3304	1/1	0.89	0.16	51,51,51,51	0
56	MG	1A	3571	1/1	0.89	0.18	52,52,52,52	0
56	MG	2A	3168	1/1	0.89	0.10	48,48,48,48	0
56	MG	2A	3536	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3149	1/1	0.89	0.15	58,58,58,58	0
56	MG	1A	4197	1/1	0.89	0.16	72,72,72,72	0
56	MG	2a	1795	1/1	0.89	0.17	54,54,54,54	0
56	MG	1A	3153	1/1	0.89	0.17	49,49,49,49	0
56	MG	2A	3183	1/1	0.89	0.07	50,50,50,50	0
56	MG	1a	1851	1/1	0.89	0.23	60,60,60,60	0
56	MG	1A	3585	1/1	0.89	0.09	56,56,56,56	0
56	MG	1a	1859	1/1	0.89	0.15	67,67,67,67	0
56	MG	2a	1809	1/1	0.89	0.16	69,69,69,69	0
56	MG	2a	1810	1/1	0.89	0.22	59,59,59,59	0
56	MG	2a	1811	1/1	0.89	0.17	60,60,60,60	0
56	MG	1A	4041	1/1	0.89	0.12	65,65,65,65	0
56	MG	1a	1863	1/1	0.89	0.12	73,73,73,73	0
56	MG	2a	1815	1/1	0.89	0.21	63,63,63,63	0
56	MG	2A	3584	1/1	0.89	0.09	55,55,55,55	0
56	MG	2B	3001	1/1	0.89	0.14	62,62,62,62	0
56	MG	1a	1865	1/1	0.89	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	3372	1/1	0.89	0.17	56,56,56,56	0
56	MG	2B	3009	1/1	0.89	0.12	65,65,65,65	0
56	MG	1A	3162	1/1	0.89	0.14	50,50,50,50	0
56	MG	2G	3001	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	4050	1/1	0.89	0.11	53,53,53,53	0
56	MG	1A	3909	1/1	0.89	0.24	34,34,34,34	0
56	MG	1A	3592	1/1	0.89	0.11	54,54,54,54	0
56	MG	2d	502	1/1	0.89	0.21	48,48,48,48	0
56	MG	1a	1714	1/1	0.89	0.21	53,53,53,53	0
56	MG	2a	1606	1/1	0.89	0.27	69,69,69,69	0
56	MG	1B	209	1/1	0.89	0.28	68,68,68,68	0
56	MG	1A	3593	1/1	0.89	0.13	49,49,49,49	0
56	MG	1d	502	1/1	0.89	0.24	68,68,68,68	0
56	MG	2Q	3001	1/1	0.90	0.11	46,46,46,46	0
56	MG	1A	3673	1/1	0.90	0.14	38,38,38,38	0
56	MG	28	102	1/1	0.90	0.26	60,60,60,60	0
56	MG	1A	3502	1/1	0.90	0.15	67,67,67,67	0
56	MG	2A	3203	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3677	1/1	0.90	0.12	30,30,30,30	0
56	MG	1A	4128	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3373	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	4138	1/1	0.90	0.17	57,57,57,57	0
56	MG	1a	1627	1/1	0.90	0.08	70,70,70,70	0
56	MG	1A	4009	1/1	0.90	0.11	65,65,65,65	0
56	MG	1A	4141	1/1	0.90	0.19	68,68,68,68	0
56	MG	2a	1617	1/1	0.90	0.09	69,69,69,69	0
56	MG	1A	4145	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	4149	1/1	0.90	0.16	52,52,52,52	0
56	MG	2a	1620	1/1	0.90	0.19	51,51,51,51	0
56	MG	1A	3374	1/1	0.90	0.18	53,53,53,53	0
56	MG	1A	4153	1/1	0.90	0.20	68,68,68,68	0
56	MG	1A	3315	1/1	0.90	0.16	55,55,55,55	0
56	MG	2a	1630	1/1	0.90	0.11	60,60,60,60	0
56	MG	1a	1646	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3259	1/1	0.90	0.16	34,34,34,34	0
56	MG	1A	4159	1/1	0.90	0.19	50,50,50,50	0
56	MG	2a	1634	1/1	0.90	0.28	64,64,64,64	0
56	MG	2a	1636	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	3240	1/1	0.90	0.14	66,66,66,66	0
56	MG	1A	3318	1/1	0.90	0.17	63,63,63,63	0
56	MG	1A	3724	1/1	0.90	0.18	61,61,61,61	0
56	MG	2a	1641	1/1	0.90	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	4165	1/1	0.90	0.11	26,26,26,26	0
56	MG	1a	1680	1/1	0.90	0.15	70,70,70,70	0
56	MG	2a	1645	1/1	0.90	0.11	73,73,73,73	0
56	MG	1a	1682	1/1	0.90	0.10	57,57,57,57	0
56	MG	1A	4022	1/1	0.90	0.20	45,45,45,45	0
56	MG	2A	3304	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	4023	1/1	0.90	0.20	73,73,73,73	0
56	MG	2A	3308	1/1	0.90	0.09	56,56,56,56	0
56	MG	1a	1692	1/1	0.90	0.15	64,64,64,64	0
56	MG	2A	3312	1/1	0.90	0.13	35,35,35,35	0
56	MG	1A	4025	1/1	0.90	0.11	69,69,69,69	0
56	MG	2a	1657	1/1	0.90	0.16	58,58,58,58	0
56	MG	1A	3576	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	3581	1/1	0.90	0.09	62,62,62,62	0
56	MG	1A	3395	1/1	0.90	0.15	51,51,51,51	0
56	MG	2a	1663	1/1	0.90	0.10	74,74,74,74	0
56	MG	1A	3022	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	4198	1/1	0.90	0.07	42,42,42,42	0
56	MG	1A	4199	1/1	0.90	0.16	53,53,53,53	0
56	MG	1A	3262	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3361	1/1	0.90	0.16	53,53,53,53	0
56	MG	1x	108	1/1	0.90	0.30	56,56,56,56	0
56	MG	1A	3906	1/1	0.90	0.10	34,34,34,34	0
56	MG	1A	3402	1/1	0.90	0.11	48,48,48,48	0
56	MG	2A	3375	1/1	0.90	0.10	32,32,32,32	0
56	MG	2a	1689	1/1	0.90	0.23	60,60,60,60	0
56	MG	1a	1718	1/1	0.90	0.41	72,72,72,72	0
56	MG	2a	1695	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	3282	1/1	0.90	0.14	73,73,73,73	0
56	MG	1A	3040	1/1	0.90	0.10	46,46,46,46	0
56	MG	1A	3771	1/1	0.90	0.09	21,21,21,21	0
56	MG	1A	3012	1/1	0.90	0.14	49,49,49,49	0
56	MG	1A	3356	1/1	0.90	0.15	61,61,61,61	0
56	MG	2A	3009	1/1	0.90	0.20	35,35,35,35	0
56	MG	1B	206	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3408	1/1	0.90	0.18	57,57,57,57	0
56	MG	1a	1732	1/1	0.90	0.07	54,54,54,54	0
56	MG	2A	3020	1/1	0.90	0.08	44,44,44,44	0
56	MG	1A	3928	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3421	1/1	0.90	0.11	64,64,64,64	0
56	MG	2A	3423	1/1	0.90	0.12	60,60,60,60	0
56	MG	2A	3424	1/1	0.90	0.14	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3301	1/1	0.90	0.20	77,77,77,77	0
56	MG	1B	223	1/1	0.90	0.14	66,66,66,66	0
56	MG	2A	3429	1/1	0.90	0.13	43,43,43,43	0
56	MG	2A	3430	1/1	0.90	0.08	54,54,54,54	0
56	MG	1D	302	1/1	0.90	0.17	71,71,71,71	0
56	MG	2a	1744	1/1	0.90	0.18	69,69,69,69	0
56	MG	2a	1751	1/1	0.90	0.17	57,57,57,57	0
56	MG	1D	308	1/1	0.90	0.20	29,29,29,29	0
56	MG	1D	314	1/1	0.90	0.19	43,43,43,43	0
56	MG	2A	3044	1/1	0.90	0.15	39,39,39,39	0
56	MG	2a	1756	1/1	0.90	0.08	62,62,62,62	0
56	MG	1A	3105	1/1	0.90	0.11	43,43,43,43	0
56	MG	1A	3479	1/1	0.90	0.23	44,44,44,44	0
56	MG	1E	306	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	3946	1/1	0.90	0.17	28,28,28,28	0
56	MG	1F	307	1/1	0.90	0.36	51,51,51,51	0
56	MG	2A	3071	1/1	0.90	0.26	66,66,66,66	0
56	MG	1A	3948	1/1	0.90	0.29	39,39,39,39	0
56	MG	1A	3018	1/1	0.90	0.16	56,56,56,56	0
56	MG	2A	3079	1/1	0.90	0.27	47,47,47,47	0
56	MG	2A	3080	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3473	1/1	0.90	0.11	53,53,53,53	0
56	MG	1a	1763	1/1	0.90	0.16	88,88,88,88	0
56	MG	1A	3814	1/1	0.90	0.08	24,24,24,24	0
56	MG	2A	3095	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3817	1/1	0.90	0.08	45,45,45,45	0
56	MG	2A	3484	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	3088	1/1	0.90	0.11	57,57,57,57	0
56	MG	2A	3487	1/1	0.90	0.12	42,42,42,42	0
56	MG	2A	3490	1/1	0.90	0.16	45,45,45,45	0
56	MG	1A	3964	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3122	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3428	1/1	0.90	0.08	52,52,52,52	0
56	MG	1a	1775	1/1	0.90	0.10	55,55,55,55	0
56	MG	1A	3656	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	3985	1/1	0.90	0.24	60,60,60,60	0
56	MG	2a	1797	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3521	1/1	0.90	0.07	42,42,42,42	0
56	MG	1A	4094	1/1	0.90	0.12	34,34,34,34	0
56	MG	1a	1780	1/1	0.90	0.19	57,57,57,57	0
56	MG	2a	1806	1/1	0.90	0.13	67,67,67,67	0
56	MG	2A	3122	1/1	0.90	0.08	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3124	1/1	0.90	0.28	58,58,58,58	0
56	MG	1A	4096	1/1	0.90	0.17	22,22,22,22	0
56	MG	2A	3540	1/1	0.90	0.12	36,36,36,36	0
56	MG	1A	4102	1/1	0.90	0.10	63,63,63,63	0
56	MG	2A	3135	1/1	0.90	0.14	48,48,48,48	0
56	MG	10	103	1/1	0.90	0.13	44,44,44,44	0
56	MG	2A	3138	1/1	0.90	0.17	55,55,55,55	0
56	MG	10	106	1/1	0.90	0.18	73,73,73,73	0
56	MG	1A	3431	1/1	0.90	0.15	56,56,56,56	0
56	MG	1a	1799	1/1	0.90	0.14	60,60,60,60	0
56	MG	2a	1834	1/1	0.90	0.23	52,52,52,52	0
56	MG	2A	3162	1/1	0.90	0.23	60,60,60,60	0
56	MG	1A	3836	1/1	0.90	0.13	33,33,33,33	0
56	MG	2A	3581	1/1	0.90	0.11	46,46,46,46	0
56	MG	1A	4107	1/1	0.90	0.22	35,35,35,35	0
56	MG	1A	3659	1/1	0.90	0.16	58,58,58,58	0
56	MG	2B	3002	1/1	0.90	0.21	54,54,54,54	0
56	MG	1A	3660	1/1	0.90	0.12	46,46,46,46	0
56	MG	2A	3182	1/1	0.90	0.20	49,49,49,49	0
56	MG	1A	3849	1/1	0.90	0.11	29,29,29,29	0
56	MG	2A	3187	1/1	0.90	0.18	44,44,44,44	0
56	MG	1a	1817	1/1	0.90	0.21	59,59,59,59	0
56	MG	2u	101	1/1	0.90	0.18	60,60,60,60	0
56	MG	2O	201	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3747	1/1	0.91	0.09	22,22,22,22	0
56	MG	2A	3265	1/1	0.91	0.11	44,44,44,44	0
56	MG	1A	4052	1/1	0.91	0.10	24,24,24,24	0
56	MG	2a	1615	1/1	0.91	0.38	63,63,63,63	0
56	MG	1A	3231	1/1	0.91	0.25	53,53,53,53	0
56	MG	1a	1699	1/1	0.91	0.28	61,61,61,61	0
56	MG	1a	1700	1/1	0.91	0.21	48,48,48,48	0
56	MG	1A	3239	1/1	0.91	0.14	33,33,33,33	0
56	MG	2A	3277	1/1	0.91	0.09	38,38,38,38	0
56	MG	1A	3044	1/1	0.91	0.08	53,53,53,53	0
56	MG	1A	3332	1/1	0.91	0.08	45,45,45,45	0
56	MG	2A	3282	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3914	1/1	0.91	0.12	40,40,40,40	0
56	MG	2A	3299	1/1	0.91	0.09	25,25,25,25	0
56	MG	1A	3761	1/1	0.91	0.18	50,50,50,50	0
56	MG	1a	1713	1/1	0.91	0.28	67,67,67,67	0
56	MG	1A	3596	1/1	0.91	0.21	32,32,32,32	0
56	MG	1a	1715	1/1	0.91	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	1A	3112	1/1	0.91	0.09	63,63,63,63	0
56	MG	1A	3598	1/1	0.91	0.12	57,57,57,57	0
56	MG	1A	3403	1/1	0.91	0.14	72,72,72,72	0
56	MG	2A	3322	1/1	0.91	0.09	39,39,39,39	0
56	MG	1a	1719	1/1	0.91	0.24	58,58,58,58	0
56	MG	2a	1643	1/1	0.91	0.13	65,65,65,65	0
56	MG	2A	3334	1/1	0.91	0.14	48,48,48,48	0
56	MG	1A	3942	1/1	0.91	0.14	44,44,44,44	0
56	MG	1A	3244	1/1	0.91	0.17	45,45,45,45	0
56	MG	1A	3790	1/1	0.91	0.09	29,29,29,29	0
56	MG	2A	3004	1/1	0.91	0.07	51,51,51,51	0
56	MG	1A	3794	1/1	0.91	0.10	43,43,43,43	0
56	MG	1A	3795	1/1	0.91	0.11	58,58,58,58	0
56	MG	1F	302	1/1	0.91	0.18	39,39,39,39	0
56	MG	1A	4085	1/1	0.91	0.16	53,53,53,53	0
56	MG	1A	3114	1/1	0.91	0.20	39,39,39,39	0
56	MG	2A	3012	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3013	1/1	0.91	0.15	66,66,66,66	0
56	MG	1A	3096	1/1	0.91	0.12	50,50,50,50	0
56	MG	2A	3015	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3017	1/1	0.91	0.09	50,50,50,50	0
56	MG	1P	201	1/1	0.91	0.14	52,52,52,52	0
56	MG	1P	202	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3534	1/1	0.91	0.14	43,43,43,43	0
56	MG	2a	1670	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3023	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3359	1/1	0.91	0.17	43,43,43,43	0
56	MG	1A	3632	1/1	0.91	0.11	63,63,63,63	0
56	MG	1A	3419	1/1	0.91	0.11	75,75,75,75	0
56	MG	1R	203	1/1	0.91	0.13	59,59,59,59	0
56	MG	1A	3639	1/1	0.91	0.13	38,38,38,38	0
56	MG	1A	3977	1/1	0.91	0.09	58,58,58,58	0
56	MG	1A	3420	1/1	0.91	0.23	57,57,57,57	0
56	MG	2a	1691	1/1	0.91	0.07	45,45,45,45	0
56	MG	2A	3045	1/1	0.91	0.11	53,53,53,53	0
56	MG	2A	3427	1/1	0.91	0.08	41,41,41,41	0
56	MG	1A	4108	1/1	0.91	0.14	44,44,44,44	0
56	MG	1A	3037	1/1	0.91	0.20	43,43,43,43	0
56	MG	1a	1758	1/1	0.91	0.10	53,53,53,53	0
56	MG	2a	1708	1/1	0.91	0.40	63,63,63,63	0
56	MG	1A	3988	1/1	0.91	0.16	53,53,53,53	0
56	MG	10	101	1/1	0.91	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1713	1/1	0.91	0.23	56,56,56,56	0
56	MG	2A	3065	1/1	0.91	0.09	38,38,38,38	0
56	MG	2A	3067	1/1	0.91	0.32	54,54,54,54	0
56	MG	2A	3070	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3478	1/1	0.91	0.24	41,41,41,41	0
56	MG	1A	3124	1/1	0.91	0.10	55,55,55,55	0
56	MG	2a	1729	1/1	0.91	0.09	70,70,70,70	0
56	MG	1A	3480	1/1	0.91	0.19	35,35,35,35	0
56	MG	1A	3838	1/1	0.91	0.19	54,54,54,54	0
56	MG	18	103	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3026	1/1	0.91	0.14	56,56,56,56	0
56	MG	2a	1735	1/1	0.91	0.21	73,73,73,73	0
56	MG	2A	3461	1/1	0.91	0.18	52,52,52,52	0
56	MG	1A	3662	1/1	0.91	0.11	36,36,36,36	0
56	MG	1A	3367	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3466	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3468	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	3674	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3103	1/1	0.91	0.08	54,54,54,54	0
56	MG	2A	3474	1/1	0.91	0.07	62,62,62,62	0
56	MG	2A	3475	1/1	0.91	0.16	57,57,57,57	0
56	MG	1a	1610	1/1	0.91	0.08	57,57,57,57	0
56	MG	2a	1757	1/1	0.91	0.15	61,61,61,61	0
56	MG	1A	3856	1/1	0.91	0.18	56,56,56,56	0
56	MG	1a	1612	1/1	0.91	0.09	82,82,82,82	0
56	MG	1a	1787	1/1	0.91	0.13	51,51,51,51	0
56	MG	1a	1789	1/1	0.91	0.17	62,62,62,62	0
56	MG	2A	3485	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3858	1/1	0.91	0.13	48,48,48,48	0
56	MG	1a	1793	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3490	1/1	0.91	0.06	59,59,59,59	0
56	MG	1A	4013	1/1	0.91	0.18	56,56,56,56	0
56	MG	1A	4156	1/1	0.91	0.12	59,59,59,59	0
56	MG	1a	1806	1/1	0.91	0.09	69,69,69,69	0
56	MG	2A	3499	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3501	1/1	0.91	0.12	48,48,48,48	0
56	MG	2a	1779	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3507	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3061	1/1	0.91	0.08	58,58,58,58	0
56	MG	1A	3496	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3870	1/1	0.91	0.16	41,41,41,41	0
56	MG	2A	3520	1/1	0.91	0.10	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3871	1/1	0.91	0.17	55,55,55,55	0
56	MG	1a	1816	1/1	0.91	0.17	60,60,60,60	0
56	MG	2A	3147	1/1	0.91	0.18	47,47,47,47	0
56	MG	1A	3174	1/1	0.91	0.12	40,40,40,40	0
56	MG	1A	3063	1/1	0.91	0.16	49,49,49,49	0
56	MG	1a	1820	1/1	0.91	0.16	69,69,69,69	0
56	MG	2A	3165	1/1	0.91	0.07	33,33,33,33	0
56	MG	1A	3879	1/1	0.91	0.12	25,25,25,25	0
56	MG	2A	3547	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	4030	1/1	0.91	0.16	59,59,59,59	0
56	MG	1A	4032	1/1	0.91	0.06	77,77,77,77	0
56	MG	1a	1832	1/1	0.91	0.17	52,52,52,52	0
56	MG	2a	1807	1/1	0.91	0.15	50,50,50,50	0
56	MG	1A	4033	1/1	0.91	0.12	56,56,56,56	0
56	MG	1a	1840	1/1	0.91	0.09	51,51,51,51	0
56	MG	1a	1842	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3215	1/1	0.91	0.13	51,51,51,51	0
56	MG	1A	3886	1/1	0.91	0.15	60,60,60,60	0
56	MG	1A	3719	1/1	0.91	0.16	64,64,64,64	0
56	MG	2A	3582	1/1	0.91	0.15	38,38,38,38	0
56	MG	2a	1816	1/1	0.91	0.13	74,74,74,74	0
56	MG	1a	1848	1/1	0.91	0.09	53,53,53,53	0
56	MG	1a	1664	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3505	1/1	0.91	0.09	47,47,47,47	0
56	MG	1a	1858	1/1	0.91	0.08	78,78,78,78	0
56	MG	1a	1670	1/1	0.91	0.14	68,68,68,68	0
56	MG	2A	3214	1/1	0.91	0.06	37,37,37,37	0
56	MG	1A	3726	1/1	0.91	0.19	57,57,57,57	0
56	MG	1A	3382	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3510	1/1	0.91	0.13	42,42,42,42	0
56	MG	1a	1867	1/1	0.91	0.16	54,54,54,54	0
56	MG	2X	8001	1/1	0.91	0.15	37,37,37,37	0
56	MG	2a	1848	1/1	0.91	0.09	57,57,57,57	0
56	MG	1a	1684	1/1	0.91	0.08	52,52,52,52	0
56	MG	1a	1687	1/1	0.91	0.12	51,51,51,51	0
56	MG	1a	1872	1/1	0.91	0.15	47,47,47,47	0
56	MG	2l	3004	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3246	1/1	0.91	0.09	45,45,45,45	0
56	MG	2A	3250	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	4217	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3217	1/1	0.91	0.11	43,43,43,43	0
56	MG	1e	201	1/1	0.92	0.15	63,63,63,63	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	3713	1/1	0.92	0.06	26,26,26,26	0
56	MG	2A	3264	1/1	0.92	0.13	47,47,47,47	0
56	MG	1e	203	1/1	0.92	0.08	54,54,54,54	0
56	MG	1F	304	1/1	0.92	0.23	21,21,21,21	0
56	MG	2a	1605	1/1	0.92	0.12	74,74,74,74	0
56	MG	1A	4088	1/1	0.92	0.09	76,76,76,76	0
56	MG	2A	3269	1/1	0.92	0.14	34,34,34,34	0
56	MG	1A	3525	1/1	0.92	0.22	56,56,56,56	0
56	MG	2a	1611	1/1	0.92	0.20	48,48,48,48	0
56	MG	1G	202	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3070	1/1	0.92	0.08	48,48,48,48	0
56	MG	1N	203	1/1	0.92	0.15	44,44,44,44	0
56	MG	1r	3002	1/1	0.92	0.12	48,48,48,48	0
56	MG	1a	1725	1/1	0.92	0.19	75,75,75,75	0
56	MG	1A	4091	1/1	0.92	0.18	71,71,71,71	0
56	MG	2A	3283	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3980	1/1	0.92	0.06	42,42,42,42	0
56	MG	2A	3289	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3298	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1625	1/1	0.92	0.10	61,61,61,61	0
56	MG	1x	107	1/1	0.92	0.23	55,55,55,55	0
56	MG	2a	1629	1/1	0.92	0.19	60,60,60,60	0
56	MG	2A	3301	1/1	0.92	0.20	40,40,40,40	0
56	MG	1A	3981	1/1	0.92	0.09	59,59,59,59	0
56	MG	1x	109	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3013	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	4103	1/1	0.92	0.11	35,35,35,35	0
56	MG	2a	1635	1/1	0.92	0.21	66,66,66,66	0
56	MG	2A	3311	1/1	0.92	0.11	57,57,57,57	0
56	MG	1a	1736	1/1	0.92	0.36	76,76,76,76	0
56	MG	1a	1737	1/1	0.92	0.09	67,67,67,67	0
56	MG	2A	3315	1/1	0.92	0.11	41,41,41,41	0
56	MG	2A	3317	1/1	0.92	0.14	35,35,35,35	0
56	MG	1A	3859	1/1	0.92	0.06	44,44,44,44	0
56	MG	1A	3175	1/1	0.92	0.06	40,40,40,40	0
56	MG	1A	3863	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3866	1/1	0.92	0.06	41,41,41,41	0
56	MG	1T	203	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3595	1/1	0.92	0.07	65,65,65,65	0
56	MG	1A	3186	1/1	0.92	0.23	39,39,39,39	0
56	MG	1A	3131	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3348	1/1	0.92	0.06	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1Z	302	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3106	1/1	0.92	0.13	47,47,47,47	0
56	MG	1A	3375	1/1	0.92	0.22	57,57,57,57	0
56	MG	1A	3877	1/1	0.92	0.08	56,56,56,56	0
56	MG	1A	3600	1/1	0.92	0.21	54,54,54,54	0
56	MG	1A	3039	1/1	0.92	0.10	48,48,48,48	0
56	MG	1a	1761	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3024	1/1	0.92	0.12	51,51,51,51	0
56	MG	12	3001	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3390	1/1	0.92	0.21	56,56,56,56	0
56	MG	2a	1666	1/1	0.92	0.21	62,62,62,62	0
56	MG	2a	1667	1/1	0.92	0.20	60,60,60,60	0
56	MG	2A	3394	1/1	0.92	0.25	61,61,61,61	0
56	MG	2A	3027	1/1	0.92	0.15	47,47,47,47	0
56	MG	2A	3397	1/1	0.92	0.20	45,45,45,45	0
56	MG	16	101	1/1	0.92	0.17	47,47,47,47	0
56	MG	2a	1675	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3880	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3377	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3404	1/1	0.92	0.12	58,58,58,58	0
56	MG	2A	3035	1/1	0.92	0.13	57,57,57,57	0
56	MG	2A	3036	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3546	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3040	1/1	0.92	0.25	52,52,52,52	0
56	MG	2a	1694	1/1	0.92	0.25	60,60,60,60	0
56	MG	1A	3618	1/1	0.92	0.17	40,40,40,40	0
56	MG	2A	3416	1/1	0.92	0.09	58,58,58,58	0
56	MG	1a	1770	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3890	1/1	0.92	0.07	45,45,45,45	0
56	MG	1a	1604	1/1	0.92	0.13	79,79,79,79	0
56	MG	1a	1776	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3056	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3016	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	4152	1/1	0.92	0.19	54,54,54,54	0
56	MG	1A	3388	1/1	0.92	0.25	65,65,65,65	0
56	MG	1A	3894	1/1	0.92	0.09	27,27,27,27	0
56	MG	2a	1718	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3140	1/1	0.92	0.06	43,43,43,43	0
56	MG	1A	4029	1/1	0.92	0.22	64,64,64,64	0
56	MG	1A	3898	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3442	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3553	1/1	0.92	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	3113	1/1	0.92	0.13	49,49,49,49	0
56	MG	1A	3042	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3645	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	1795	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	3440	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3801	1/1	0.92	0.08	40,40,40,40	0
56	MG	1A	3566	1/1	0.92	0.13	44,44,44,44	0
56	MG	2A	3097	1/1	0.92	0.08	42,42,42,42	0
56	MG	1A	3805	1/1	0.92	0.09	54,54,54,54	0
56	MG	2a	1745	1/1	0.92	0.25	52,52,52,52	0
56	MG	2a	1748	1/1	0.92	0.20	51,51,51,51	0
56	MG	1a	1634	1/1	0.92	0.25	61,61,61,61	0
56	MG	1A	3333	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	4044	1/1	0.92	0.14	72,72,72,72	0
56	MG	1a	1637	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3920	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3398	1/1	0.92	0.20	46,46,46,46	0
56	MG	2a	1758	1/1	0.92	0.10	89,89,89,89	0
56	MG	1A	3032	1/1	0.92	0.12	50,50,50,50	0
56	MG	2a	1761	1/1	0.92	0.10	69,69,69,69	0
56	MG	1A	4204	1/1	0.92	0.18	56,56,56,56	0
56	MG	1A	4054	1/1	0.92	0.11	56,56,56,56	0
56	MG	1a	1657	1/1	0.92	0.13	54,54,54,54	0
56	MG	1A	3250	1/1	0.92	0.21	45,45,45,45	0
56	MG	1a	1829	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	4223	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	4227	1/1	0.92	0.08	34,34,34,34	0
56	MG	1a	1838	1/1	0.92	0.08	41,41,41,41	0
56	MG	1a	1839	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3142	1/1	0.92	0.23	56,56,56,56	0
56	MG	2a	1772	1/1	0.92	0.14	57,57,57,57	0
56	MG	1a	1672	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	4057	1/1	0.92	0.18	71,71,71,71	0
56	MG	2A	3151	1/1	0.92	0.20	38,38,38,38	0
56	MG	2A	3506	1/1	0.92	0.08	52,52,52,52	0
56	MG	1a	1843	1/1	0.92	0.13	63,63,63,63	0
56	MG	2A	3508	1/1	0.92	0.11	41,41,41,41	0
56	MG	1a	1679	1/1	0.92	0.23	52,52,52,52	0
56	MG	2A	3511	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3939	1/1	0.92	0.10	34,34,34,34	0
56	MG	1A	3572	1/1	0.92	0.39	35,35,35,35	0
56	MG	2A	3519	1/1	0.92	0.09	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	1683	1/1	0.92	0.16	52,52,52,52	0
56	MG	2a	1792	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3017	1/1	0.92	0.16	50,50,50,50	0
56	MG	1a	1852	1/1	0.92	0.15	62,62,62,62	0
56	MG	1A	4063	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3531	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	3068	1/1	0.92	0.21	54,54,54,54	0
56	MG	2a	1801	1/1	0.92	0.20	64,64,64,64	0
56	MG	1a	1690	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	3291	1/1	0.92	0.21	57,57,57,57	0
56	MG	2A	3537	1/1	0.92	0.14	49,49,49,49	0
56	MG	1a	1861	1/1	0.92	0.15	50,50,50,50	0
56	MG	1a	1862	1/1	0.92	0.20	50,50,50,50	0
56	MG	2A	3546	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3682	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3548	1/1	0.92	0.18	53,53,53,53	0
56	MG	1a	1864	1/1	0.92	0.15	74,74,74,74	0
56	MG	1A	3692	1/1	0.92	0.21	37,37,37,37	0
56	MG	1A	3519	1/1	0.92	0.26	51,51,51,51	0
56	MG	2A	3210	1/1	0.92	0.13	50,50,50,50	0
56	MG	2a	1819	1/1	0.92	0.27	56,56,56,56	0
56	MG	2A	3558	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3161	1/1	0.92	0.17	47,47,47,47	0
56	MG	1B	224	1/1	0.92	0.17	59,59,59,59	0
56	MG	2a	1832	1/1	0.92	0.08	59,59,59,59	0
56	MG	2A	3568	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3957	1/1	0.92	0.16	46,46,46,46	0
56	MG	1D	305	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3589	1/1	0.92	0.31	56,56,56,56	0
56	MG	1a	1883	1/1	0.92	0.12	62,62,62,62	0
56	MG	2A	3235	1/1	0.92	0.12	44,44,44,44	0
56	MG	2A	3237	1/1	0.92	0.22	67,67,67,67	0
56	MG	1A	3844	1/1	0.92	0.09	33,33,33,33	0
56	MG	1A	4080	1/1	0.92	0.10	56,56,56,56	0
56	MG	2B	3006	1/1	0.92	0.26	57,57,57,57	0
56	MG	1A	3845	1/1	0.92	0.06	22,22,22,22	0
56	MG	2e	3002	1/1	0.92	0.14	68,68,68,68	0
56	MG	2l	3002	1/1	0.92	0.09	74,74,74,74	0
56	MG	2A	3245	1/1	0.92	0.08	58,58,58,58	0
56	MG	1b	3001	1/1	0.92	0.13	78,78,78,78	0
56	MG	2A	3247	1/1	0.92	0.12	34,34,34,34	0
56	MG	2p	101	1/1	0.92	0.14	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	3971	1/1	0.92	0.08	47,47,47,47	0
56	MG	1A	3003	1/1	0.92	0.25	60,60,60,60	0
56	MG	2x	3002	1/1	0.92	0.20	57,57,57,57	0
56	MG	2A	3256	1/1	0.92	0.14	53,53,53,53	0
56	MG	2F	301	1/1	0.93	0.09	38,38,38,38	0
56	MG	1B	212	1/1	0.93	0.22	53,53,53,53	0
56	MG	1a	1704	1/1	0.93	0.32	55,55,55,55	0
56	MG	1A	3588	1/1	0.93	0.06	51,51,51,51	0
56	MG	1a	1707	1/1	0.93	0.23	45,45,45,45	0
56	MG	1a	1708	1/1	0.93	0.22	61,61,61,61	0
56	MG	25	502	1/1	0.93	0.21	54,54,54,54	0
56	MG	1a	1709	1/1	0.93	0.15	75,75,75,75	0
56	MG	1B	219	1/1	0.93	0.07	60,60,60,60	0
56	MG	1B	220	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	3495	1/1	0.93	0.07	41,41,41,41	0
56	MG	1A	3176	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3763	1/1	0.93	0.21	53,53,53,53	0
56	MG	1A	3765	1/1	0.93	0.08	19,19,19,19	0
56	MG	1A	3499	1/1	0.93	0.10	58,58,58,58	0
56	MG	2A	3285	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3286	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3287	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3300	1/1	0.93	0.12	44,44,44,44	0
56	MG	1D	315	1/1	0.93	0.07	39,39,39,39	0
56	MG	2A	3295	1/1	0.93	0.07	47,47,47,47	0
56	MG	1x	105	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3097	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	4069	1/1	0.93	0.06	37,37,37,37	0
56	MG	1E	305	1/1	0.93	0.28	35,35,35,35	0
56	MG	1x	110	1/1	0.93	0.16	68,68,68,68	0
56	MG	1A	3773	1/1	0.93	0.09	31,31,31,31	0
56	MG	1A	3110	1/1	0.93	0.07	43,43,43,43	0
56	MG	1a	1726	1/1	0.93	0.07	56,56,56,56	0
56	MG	1F	301	1/1	0.93	0.15	56,56,56,56	0
56	MG	2A	3313	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3929	1/1	0.93	0.18	55,55,55,55	0
56	MG	1A	3933	1/1	0.93	0.07	29,29,29,29	0
56	MG	1A	3782	1/1	0.93	0.12	28,28,28,28	0
56	MG	1F	308	1/1	0.93	0.12	61,61,61,61	0
56	MG	1A	3371	1/1	0.93	0.08	41,41,41,41	0
56	MG	2A	3326	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3328	1/1	0.93	0.07	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	3305	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	3941	1/1	0.93	0.16	32,32,32,32	0
56	MG	1N	201	1/1	0.93	0.12	54,54,54,54	0
56	MG	1a	1742	1/1	0.93	0.17	52,52,52,52	0
56	MG	1N	202	1/1	0.93	0.21	54,54,54,54	0
56	MG	2A	3345	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3027	1/1	0.93	0.17	36,36,36,36	0
56	MG	1A	4084	1/1	0.93	0.15	73,73,73,73	0
56	MG	2A	3350	1/1	0.93	0.09	54,54,54,54	0
56	MG	2a	1649	1/1	0.93	0.18	77,77,77,77	0
56	MG	2A	3353	1/1	0.93	0.11	29,29,29,29	0
56	MG	2a	1652	1/1	0.93	0.08	86,86,86,86	0
56	MG	2A	3358	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3430	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3308	1/1	0.93	0.12	43,43,43,43	0
56	MG	1Q	202	1/1	0.93	0.17	35,35,35,35	0
56	MG	1A	3126	1/1	0.93	0.14	31,31,31,31	0
56	MG	2A	3369	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3312	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3951	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3376	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3028	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3143	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3387	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	4093	1/1	0.93	0.13	29,29,29,29	0
56	MG	2A	3389	1/1	0.93	0.10	46,46,46,46	0
56	MG	1a	1757	1/1	0.93	0.15	70,70,70,70	0
56	MG	1A	3084	1/1	0.93	0.30	53,53,53,53	0
56	MG	1a	1760	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3383	1/1	0.93	0.14	42,42,42,42	0
56	MG	1A	3813	1/1	0.93	0.06	39,39,39,39	0
56	MG	2A	3041	1/1	0.93	0.27	49,49,49,49	0
56	MG	2A	3402	1/1	0.93	0.09	47,47,47,47	0
56	MG	2a	1683	1/1	0.93	0.16	67,67,67,67	0
56	MG	1U	203	1/1	0.93	0.18	42,42,42,42	0
56	MG	2a	1687	1/1	0.93	0.23	54,54,54,54	0
56	MG	1A	3385	1/1	0.93	0.22	43,43,43,43	0
56	MG	1A	3963	1/1	0.93	0.11	45,45,45,45	0
56	MG	1W	3005	1/1	0.93	0.13	24,24,24,24	0
56	MG	2a	1693	1/1	0.93	0.19	50,50,50,50	0
56	MG	1A	3815	1/1	0.93	0.07	32,32,32,32	0
56	MG	1A	3816	1/1	0.93	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3413	1/1	0.93	0.20	54,54,54,54	0
56	MG	2a	1698	1/1	0.93	0.08	62,62,62,62	0
56	MG	2A	3057	1/1	0.93	0.07	34,34,34,34	0
56	MG	2a	1705	1/1	0.93	0.13	60,60,60,60	0
56	MG	1A	3625	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3059	1/1	0.93	0.19	59,59,59,59	0
56	MG	1A	3527	1/1	0.93	0.10	48,48,48,48	0
56	MG	1A	3443	1/1	0.93	0.08	59,59,59,59	0
56	MG	1A	3387	1/1	0.93	0.09	54,54,54,54	0
56	MG	2A	3066	1/1	0.93	0.29	60,60,60,60	0
56	MG	2a	1714	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	4114	1/1	0.93	0.08	47,47,47,47	0
56	MG	15	105	1/1	0.93	0.12	35,35,35,35	0
56	MG	1A	3530	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1781	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3128	1/1	0.93	0.27	46,46,46,46	0
56	MG	2a	1723	1/1	0.93	0.15	61,61,61,61	0
56	MG	2a	1724	1/1	0.93	0.31	58,58,58,58	0
56	MG	2a	1725	1/1	0.93	0.18	63,63,63,63	0
56	MG	1A	4120	1/1	0.93	0.19	50,50,50,50	0
56	MG	2A	3439	1/1	0.93	0.07	48,48,48,48	0
56	MG	1A	4125	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3832	1/1	0.93	0.15	47,47,47,47	0
56	MG	2A	3444	1/1	0.93	0.06	30,30,30,30	0
56	MG	1A	3449	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3090	1/1	0.93	0.05	38,38,38,38	0
56	MG	1a	1790	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	4132	1/1	0.93	0.18	52,52,52,52	0
56	MG	2a	1738	1/1	0.93	0.24	36,36,36,36	0
56	MG	1a	1792	1/1	0.93	0.08	34,34,34,34	0
56	MG	1A	4133	1/1	0.93	0.20	47,47,47,47	0
56	MG	1A	3052	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3648	1/1	0.93	0.11	46,46,46,46	0
56	MG	2a	1746	1/1	0.93	0.14	43,43,43,43	0
56	MG	2a	1747	1/1	0.93	0.26	67,67,67,67	0
56	MG	1a	1798	1/1	0.93	0.10	59,59,59,59	0
56	MG	2a	1749	1/1	0.93	0.23	68,68,68,68	0
56	MG	1A	3649	1/1	0.93	0.08	26,26,26,26	0
56	MG	1A	3392	1/1	0.93	0.17	46,46,46,46	0
56	MG	1A	3998	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	1617	1/1	0.93	0.17	61,61,61,61	0
56	MG	1A	4146	1/1	0.93	0.14	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3458	1/1	0.93	0.16	28,28,28,28	0
56	MG	1a	1623	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3127	1/1	0.93	0.18	49,49,49,49	0
56	MG	1a	1624	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3160	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	4151	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3463	1/1	0.93	0.23	39,39,39,39	0
56	MG	1a	1821	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	3329	1/1	0.93	0.05	62,62,62,62	0
56	MG	1A	4006	1/1	0.93	0.10	36,36,36,36	0
56	MG	2A	3489	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3669	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3670	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3330	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3130	1/1	0.93	0.22	49,49,49,49	0
56	MG	1A	3862	1/1	0.93	0.07	34,34,34,34	0
56	MG	1A	3468	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3552	1/1	0.93	0.07	42,42,42,42	0
56	MG	2a	1780	1/1	0.93	0.17	56,56,56,56	0
56	MG	1a	1643	1/1	0.93	0.09	64,64,64,64	0
56	MG	1A	3260	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3686	1/1	0.93	0.15	27,27,27,27	0
56	MG	1A	3470	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3513	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3514	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3696	1/1	0.93	0.15	45,45,45,45	0
56	MG	1a	1656	1/1	0.93	0.17	53,53,53,53	0
56	MG	1a	1849	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3193	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3194	1/1	0.93	0.08	50,50,50,50	0
56	MG	2a	1794	1/1	0.93	0.19	46,46,46,46	0
56	MG	1a	1850	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3091	1/1	0.93	0.15	50,50,50,50	0
56	MG	2A	3527	1/1	0.93	0.15	44,44,44,44	0
56	MG	2a	1799	1/1	0.93	0.22	65,65,65,65	0
56	MG	2A	3199	1/1	0.93	0.08	34,34,34,34	0
56	MG	1a	1659	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3472	1/1	0.93	0.09	47,47,47,47	0
56	MG	2a	1804	1/1	0.93	0.24	63,63,63,63	0
56	MG	1a	1856	1/1	0.93	0.20	64,64,64,64	0
56	MG	1A	3339	1/1	0.93	0.47	48,48,48,48	0
56	MG	1A	3405	1/1	0.93	0.22	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	3272	1/1	0.93	0.12	46,46,46,46	0
56	MG	2A	3545	1/1	0.93	0.07	54,54,54,54	0
56	MG	2A	3213	1/1	0.93	0.08	40,40,40,40	0
56	MG	1A	3883	1/1	0.93	0.16	49,49,49,49	0
56	MG	1A	3116	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3228	1/1	0.93	0.05	63,63,63,63	0
56	MG	1A	3481	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	3720	1/1	0.93	0.07	47,47,47,47	0
56	MG	2a	1817	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3484	1/1	0.93	0.16	34,34,34,34	0
56	MG	2A	3556	1/1	0.93	0.10	33,33,33,33	0
56	MG	1a	1866	1/1	0.93	0.20	72,72,72,72	0
56	MG	2a	1825	1/1	0.93	0.15	63,63,63,63	0
56	MG	2A	3562	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3133	1/1	0.93	0.05	55,55,55,55	0
56	MG	1A	3892	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3567	1/1	0.93	0.14	49,49,49,49	0
56	MG	2A	3241	1/1	0.93	0.07	41,41,41,41	0
56	MG	1A	3417	1/1	0.93	0.11	30,30,30,30	0
56	MG	2A	3577	1/1	0.93	0.07	40,40,40,40	0
56	MG	1a	1689	1/1	0.93	0.14	62,62,62,62	0
56	MG	1a	1877	1/1	0.93	0.17	59,59,59,59	0
56	MG	1A	3056	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	4048	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3248	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3295	1/1	0.93	0.20	45,45,45,45	0
56	MG	2A	3251	1/1	0.93	0.11	22,22,22,22	0
56	MG	2l	3001	1/1	0.93	0.12	66,66,66,66	0
56	MG	1A	3582	1/1	0.93	0.08	46,46,46,46	0
56	MG	1B	208	1/1	0.93	0.08	38,38,38,38	0
56	MG	1A	3584	1/1	0.93	0.07	50,50,50,50	0
56	MG	2l	3005	1/1	0.93	0.08	48,48,48,48	0
56	MG	2D	301	1/1	0.93	0.14	51,51,51,51	0
56	MG	2D	302	1/1	0.93	0.08	52,52,52,52	0
56	MG	2D	304	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3296	1/1	0.93	0.24	56,56,56,56	0
56	MG	2E	301	1/1	0.93	0.10	23,23,23,23	0
56	MG	2E	304	1/1	0.93	0.09	40,40,40,40	0
56	MG	1A	3613	1/1	0.94	0.21	51,51,51,51	0
56	MG	1A	3616	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3617	1/1	0.94	0.09	11,11,11,11	0
56	MG	1A	3357	1/1	0.94	0.14	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3541	1/1	0.94	0.19	51,51,51,51	0
56	MG	1A	3819	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3123	1/1	0.94	0.15	58,58,58,58	0
56	MG	1A	3822	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	4016	1/1	0.94	0.11	65,65,65,65	0
56	MG	2A	3129	1/1	0.94	0.20	56,56,56,56	0
56	MG	1B	221	1/1	0.94	0.09	44,44,44,44	0
56	MG	1B	222	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3134	1/1	0.94	0.19	49,49,49,49	0
56	MG	2A	3554	1/1	0.94	0.06	35,35,35,35	0
56	MG	1A	3513	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	4018	1/1	0.94	0.23	27,27,27,27	0
56	MG	1B	225	1/1	0.94	0.07	33,33,33,33	0
56	MG	2A	3560	1/1	0.94	0.17	41,41,41,41	0
56	MG	1D	301	1/1	0.94	0.21	37,37,37,37	0
56	MG	1a	1759	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3624	1/1	0.94	0.17	43,43,43,43	0
56	MG	1A	3277	1/1	0.94	0.14	39,39,39,39	0
56	MG	2A	3150	1/1	0.94	0.09	46,46,46,46	0
56	MG	1a	1762	1/1	0.94	0.17	67,67,67,67	0
56	MG	1A	3030	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3578	1/1	0.94	0.23	45,45,45,45	0
56	MG	1D	309	1/1	0.94	0.16	56,56,56,56	0
56	MG	2A	3164	1/1	0.94	0.08	43,43,43,43	0
56	MG	1D	313	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3583	1/1	0.94	0.24	39,39,39,39	0
56	MG	2A	3166	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3631	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3095	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3292	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3177	1/1	0.94	0.15	42,42,42,42	0
56	MG	2B	3007	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3839	1/1	0.94	0.11	56,56,56,56	0
56	MG	1A	3637	1/1	0.94	0.11	48,48,48,48	0
56	MG	1a	1774	1/1	0.94	0.08	63,63,63,63	0
56	MG	2A	3185	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3060	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3843	1/1	0.94	0.10	46,46,46,46	0
56	MG	1E	308	1/1	0.94	0.09	29,29,29,29	0
56	MG	2E	302	1/1	0.94	0.13	27,27,27,27	0
56	MG	1A	3642	1/1	0.94	0.11	26,26,26,26	0
56	MG	2E	305	1/1	0.94	0.12	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3294	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3847	1/1	0.94	0.09	33,33,33,33	0
56	MG	1F	305	1/1	0.94	0.17	69,69,69,69	0
56	MG	2O	202	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3071	1/1	0.94	0.14	60,60,60,60	0
56	MG	2Q	3002	1/1	0.94	0.14	53,53,53,53	0
56	MG	1a	1783	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3207	1/1	0.94	0.26	60,60,60,60	0
56	MG	23	101	1/1	0.94	0.11	56,56,56,56	0
56	MG	1A	3192	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3854	1/1	0.94	0.09	36,36,36,36	0
56	MG	1A	3647	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3195	1/1	0.94	0.11	37,37,37,37	0
56	MG	1H	8001	1/1	0.94	0.12	72,72,72,72	0
56	MG	1A	3442	1/1	0.94	0.07	50,50,50,50	0
56	MG	2A	3216	1/1	0.94	0.13	33,33,33,33	0
56	MG	1A	3299	1/1	0.94	0.09	34,34,34,34	0
56	MG	1A	3444	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3196	1/1	0.94	0.09	48,48,48,48	0
56	MG	2a	1612	1/1	0.94	0.25	59,59,59,59	0
56	MG	1A	3197	1/1	0.94	0.18	50,50,50,50	0
56	MG	1A	4055	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3200	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3668	1/1	0.94	0.10	38,38,38,38	0
56	MG	2A	3238	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3208	1/1	0.94	0.12	17,17,17,17	0
56	MG	2A	3240	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	4060	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3455	1/1	0.94	0.15	58,58,58,58	0
56	MG	1R	204	1/1	0.94	0.13	56,56,56,56	0
56	MG	1R	205	1/1	0.94	0.10	49,49,49,49	0
56	MG	2a	1626	1/1	0.94	0.23	74,74,74,74	0
56	MG	1a	1815	1/1	0.94	0.10	43,43,43,43	0
56	MG	1R	207	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3540	1/1	0.94	0.25	45,45,45,45	0
56	MG	1A	3873	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3306	1/1	0.94	0.25	41,41,41,41	0
56	MG	1T	204	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3255	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3384	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3051	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4068	1/1	0.94	0.08	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	2A	3261	1/1	0.94	0.10	41,41,41,41	0
56	MG	2A	3262	1/1	0.94	0.09	36,36,36,36	0
56	MG	1a	1828	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3678	1/1	0.94	0.06	27,27,27,27	0
56	MG	1V	201	1/1	0.94	0.11	44,44,44,44	0
56	MG	1a	1835	1/1	0.94	0.07	36,36,36,36	0
56	MG	2A	3268	1/1	0.94	0.05	33,33,33,33	0
56	MG	1W	3001	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3271	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3272	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3273	1/1	0.94	0.12	56,56,56,56	0
56	MG	1W	3004	1/1	0.94	0.14	31,31,31,31	0
56	MG	1A	3462	1/1	0.94	0.19	64,64,64,64	0
56	MG	1A	3043	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3216	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3064	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3390	1/1	0.94	0.06	46,46,46,46	0
56	MG	1A	4077	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	3700	1/1	0.94	0.14	28,28,28,28	0
56	MG	11	101	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3555	1/1	0.94	0.08	51,51,51,51	0
56	MG	2a	1661	1/1	0.94	0.11	64,64,64,64	0
56	MG	13	101	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3556	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3709	1/1	0.94	0.12	29,29,29,29	0
56	MG	1A	3467	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3896	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3712	1/1	0.94	0.11	28,28,28,28	0
56	MG	18	105	1/1	0.94	0.11	37,37,37,37	0
56	MG	19	103	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3218	1/1	0.94	0.17	35,35,35,35	0
56	MG	1A	3715	1/1	0.94	0.12	22,22,22,22	0
56	MG	1A	3223	1/1	0.94	0.15	40,40,40,40	0
56	MG	1A	3905	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3718	1/1	0.94	0.15	39,39,39,39	0
56	MG	1A	3394	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3908	1/1	0.94	0.25	37,37,37,37	0
56	MG	1A	4098	1/1	0.94	0.08	24,24,24,24	0
56	MG	1a	1613	1/1	0.94	0.30	61,61,61,61	0
56	MG	2A	3319	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	4101	1/1	0.94	0.11	39,39,39,39	0
56	MG	1A	3077	1/1	0.94	0.06	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3323	1/1	0.94	0.13	35,35,35,35	0
56	MG	2A	3324	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3146	1/1	0.94	0.06	46,46,46,46	0
56	MG	1a	1880	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3474	1/1	0.94	0.17	61,61,61,61	0
56	MG	2a	1702	1/1	0.94	0.18	51,51,51,51	0
56	MG	1a	1882	1/1	0.94	0.12	59,59,59,59	0
56	MG	1a	1622	1/1	0.94	0.14	43,43,43,43	0
56	MG	1A	3727	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3917	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3344	1/1	0.94	0.17	47,47,47,47	0
56	MG	1a	1893	1/1	0.94	0.08	59,59,59,59	0
56	MG	1a	1894	1/1	0.94	0.17	65,65,65,65	0
56	MG	1A	3729	1/1	0.94	0.20	44,44,44,44	0
56	MG	1A	3570	1/1	0.94	0.17	49,49,49,49	0
56	MG	2A	3351	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3352	1/1	0.94	0.07	31,31,31,31	0
56	MG	1A	3147	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3354	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3356	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3357	1/1	0.94	0.08	29,29,29,29	0
56	MG	1A	3743	1/1	0.94	0.08	45,45,45,45	0
56	MG	2a	1726	1/1	0.94	0.15	61,61,61,61	0
56	MG	1A	3326	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3932	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3079	1/1	0.94	0.06	63,63,63,63	0
56	MG	1f	3001	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	4119	1/1	0.94	0.11	35,35,35,35	0
56	MG	1A	3934	1/1	0.94	0.06	27,27,27,27	0
56	MG	1A	4121	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3748	1/1	0.94	0.08	30,30,30,30	0
56	MG	1A	3083	1/1	0.94	0.11	44,44,44,44	0
56	MG	1q	202	1/1	0.94	0.19	55,55,55,55	0
56	MG	1A	4127	1/1	0.94	0.14	29,29,29,29	0
56	MG	2a	1742	1/1	0.94	0.09	56,56,56,56	0
56	MG	1a	1645	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3751	1/1	0.94	0.23	43,43,43,43	0
56	MG	1A	3246	1/1	0.94	0.04	13,13,13,13	0
56	MG	1A	3406	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3109	1/1	0.94	0.21	62,62,62,62	0
56	MG	1x	106	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3760	1/1	0.94	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	2a	1750	1/1	0.94	0.19	54,54,54,54	0
56	MG	1A	3411	1/1	0.94	0.17	43,43,43,43	0
56	MG	1a	1658	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3488	1/1	0.94	0.07	44,44,44,44	0
56	MG	1a	1663	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	4142	1/1	0.94	0.10	39,39,39,39	0
56	MG	2A	3406	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	4144	1/1	0.94	0.20	67,67,67,67	0
56	MG	1a	1666	1/1	0.94	0.05	51,51,51,51	0
56	MG	1a	1667	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3252	1/1	0.94	0.08	48,48,48,48	0
56	MG	1a	1671	1/1	0.94	0.21	55,55,55,55	0
56	MG	1A	3953	1/1	0.94	0.14	65,65,65,65	0
56	MG	2A	3418	1/1	0.94	0.18	58,58,58,58	0
56	MG	1a	1674	1/1	0.94	0.24	63,63,63,63	0
56	MG	1A	4147	1/1	0.94	0.10	40,40,40,40	0
56	MG	1a	1677	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3766	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3769	1/1	0.94	0.12	45,45,45,45	0
56	MG	1a	1681	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3334	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3491	1/1	0.94	0.06	63,63,63,63	0
56	MG	1A	3960	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	4154	1/1	0.94	0.13	33,33,33,33	0
56	MG	1A	3337	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3437	1/1	0.94	0.05	41,41,41,41	0
56	MG	1A	3254	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	3340	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3965	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3443	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3966	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3970	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3497	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3451	1/1	0.94	0.06	41,41,41,41	0
56	MG	1A	3783	1/1	0.94	0.25	58,58,58,58	0
56	MG	1A	3498	1/1	0.94	0.06	46,46,46,46	0
56	MG	1A	3789	1/1	0.94	0.08	30,30,30,30	0
56	MG	1A	3347	1/1	0.94	0.18	61,61,61,61	0
56	MG	2A	3039	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	4174	1/1	0.94	0.17	62,62,62,62	0
56	MG	2a	1798	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	4176	1/1	0.94	0.18	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3042	1/1	0.94	0.15	50,50,50,50	0
56	MG	1A	4178	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	4185	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	3792	1/1	0.94	0.08	21,21,21,21	0
56	MG	2A	3471	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3348	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	4193	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3983	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3476	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3984	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	3501	1/1	0.94	0.16	36,36,36,36	0
56	MG	1A	4202	1/1	0.94	0.29	67,67,67,67	0
56	MG	1A	3053	1/1	0.94	0.18	54,54,54,54	0
56	MG	2a	1814	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3482	1/1	0.94	0.07	34,34,34,34	0
56	MG	1A	3087	1/1	0.94	0.12	51,51,51,51	0
56	MG	1A	4211	1/1	0.94	0.16	31,31,31,31	0
56	MG	2a	1818	1/1	0.94	0.16	63,63,63,63	0
56	MG	1a	1720	1/1	0.94	0.13	58,58,58,58	0
56	MG	1A	4212	1/1	0.94	0.09	40,40,40,40	0
56	MG	2a	1821	1/1	0.94	0.17	66,66,66,66	0
56	MG	2A	3488	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3069	1/1	0.94	0.26	58,58,58,58	0
56	MG	1A	3268	1/1	0.94	0.07	34,34,34,34	0
56	MG	2a	1829	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	4216	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3991	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3602	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3994	1/1	0.94	0.06	62,62,62,62	0
56	MG	1A	3806	1/1	0.94	0.14	66,66,66,66	0
56	MG	2a	1838	1/1	0.94	0.14	54,54,54,54	0
56	MG	1a	1729	1/1	0.94	0.25	49,49,49,49	0
56	MG	1a	1730	1/1	0.94	0.09	56,56,56,56	0
56	MG	2a	1842	1/1	0.94	0.29	54,54,54,54	0
56	MG	2a	1844	1/1	0.94	0.17	64,64,64,64	0
56	MG	1A	3808	1/1	0.94	0.11	14,14,14,14	0
56	MG	2A	3092	1/1	0.94	0.19	34,34,34,34	0
56	MG	2A	3510	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	4000	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3605	1/1	0.94	0.10	40,40,40,40	0
56	MG	1B	202	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3098	1/1	0.94	0.11	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3516	1/1	0.94	0.06	32,32,32,32	0
56	MG	1A	3020	1/1	0.94	0.14	38,38,38,38	0
56	MG	2A	3101	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3508	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3104	1/1	0.94	0.06	49,49,49,49	0
56	MG	1a	1739	1/1	0.94	0.10	64,64,64,64	0
56	MG	2A	3106	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3610	1/1	0.94	0.11	36,36,36,36	0
56	MG	2x	3001	1/1	0.94	0.07	68,68,68,68	0
56	MG	2A	3108	1/1	0.94	0.15	30,30,30,30	0
56	MG	1B	207	1/1	0.94	0.15	52,52,52,52	0
57	ZN	2n	102	1/1	0.94	0.08	100,100,100,100	0
56	MG	1A	4177	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3566	1/1	0.95	0.05	32,32,32,32	0
56	MG	1A	3123	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3857	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3569	1/1	0.95	0.11	32,32,32,32	0
56	MG	1A	3319	1/1	0.95	0.12	58,58,58,58	0
56	MG	2A	3572	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3575	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	4190	1/1	0.95	0.22	51,51,51,51	0
56	MG	2A	3224	1/1	0.95	0.05	38,38,38,38	0
56	MG	2A	3225	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3580	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3227	1/1	0.95	0.06	51,51,51,51	0
56	MG	1a	1641	1/1	0.95	0.22	58,58,58,58	0
56	MG	2A	3230	1/1	0.95	0.07	57,57,57,57	0
56	MG	1a	1857	1/1	0.95	0.08	70,70,70,70	0
56	MG	2A	3585	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3698	1/1	0.95	0.20	51,51,51,51	0
56	MG	1a	1644	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3320	1/1	0.95	0.07	57,57,57,57	0
56	MG	1A	4195	1/1	0.95	0.07	32,32,32,32	0
56	MG	1a	1648	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3861	1/1	0.95	0.14	43,43,43,43	0
56	MG	1a	1651	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3701	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	4021	1/1	0.95	0.11	33,33,33,33	0
56	MG	2D	303	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	4200	1/1	0.95	0.14	47,47,47,47	0
56	MG	1a	1868	1/1	0.95	0.18	63,63,63,63	0
56	MG	1A	3702	1/1	0.95	0.08	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3864	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	4024	1/1	0.95	0.07	46,46,46,46	0
56	MG	1a	1875	1/1	0.95	0.07	57,57,57,57	0
56	MG	1A	3865	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	4027	1/1	0.95	0.13	72,72,72,72	0
56	MG	1A	3703	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	4215	1/1	0.95	0.07	44,44,44,44	0
56	MG	1A	3152	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3706	1/1	0.95	0.06	25,25,25,25	0
56	MG	2Q	3003	1/1	0.95	0.16	50,50,50,50	0
56	MG	2Q	3004	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	4218	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	4031	1/1	0.95	0.11	39,39,39,39	0
56	MG	20	101	1/1	0.95	0.11	56,56,56,56	0
56	MG	1a	1890	1/1	0.95	0.12	49,49,49,49	0
56	MG	1a	1891	1/1	0.95	0.19	68,68,68,68	0
56	MG	1a	1673	1/1	0.95	0.18	54,54,54,54	0
56	MG	1A	4226	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3324	1/1	0.95	0.15	38,38,38,38	0
56	MG	1a	1676	1/1	0.95	0.16	69,69,69,69	0
56	MG	1A	3099	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4034	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3482	1/1	0.95	0.16	49,49,49,49	0
56	MG	1A	3327	1/1	0.95	0.17	29,29,29,29	0
56	MG	1A	3328	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3714	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3577	1/1	0.95	0.12	56,56,56,56	0
56	MG	1a	1685	1/1	0.95	0.13	61,61,61,61	0
56	MG	2A	3280	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3580	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	4042	1/1	0.95	0.07	50,50,50,50	0
56	MG	1p	101	1/1	0.95	0.20	63,63,63,63	0
56	MG	2A	3284	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3882	1/1	0.95	0.15	29,29,29,29	0
56	MG	1A	3062	1/1	0.95	0.21	49,49,49,49	0
56	MG	1A	3248	1/1	0.95	0.07	31,31,31,31	0
56	MG	1A	3412	1/1	0.95	0.19	37,37,37,37	0
56	MG	1t	3001	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	4049	1/1	0.95	0.08	37,37,37,37	0
56	MG	2a	1628	1/1	0.95	0.13	66,66,66,66	0
56	MG	2A	3296	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3721	1/1	0.95	0.08	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	3249	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3586	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3302	1/1	0.95	0.07	30,30,30,30	0
56	MG	1a	1702	1/1	0.95	0.22	41,41,41,41	0
56	MG	1A	3101	1/1	0.95	0.12	54,54,54,54	0
56	MG	2A	3307	1/1	0.95	0.06	35,35,35,35	0
56	MG	2a	1637	1/1	0.95	0.09	60,60,60,60	0
56	MG	1A	3009	1/1	0.95	0.20	31,31,31,31	0
56	MG	1A	3078	1/1	0.95	0.06	54,54,54,54	0
56	MG	1A	3256	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3258	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3259	1/1	0.95	0.15	46,46,46,46	0
56	MG	1D	303	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3021	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3316	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3261	1/1	0.95	0.13	22,22,22,22	0
56	MG	1A	3903	1/1	0.95	0.07	41,41,41,41	0
56	MG	1D	311	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3321	1/1	0.95	0.16	43,43,43,43	0
56	MG	1A	3749	1/1	0.95	0.07	15,15,15,15	0
56	MG	1A	3080	1/1	0.95	0.13	51,51,51,51	0
56	MG	1A	3035	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3503	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	4070	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3269	1/1	0.95	0.09	20,20,20,20	0
56	MG	1A	3271	1/1	0.95	0.17	38,38,38,38	0
56	MG	2A	3016	1/1	0.95	0.05	56,56,56,56	0
56	MG	2A	3338	1/1	0.95	0.08	61,61,61,61	0
56	MG	1A	4073	1/1	0.95	0.11	58,58,58,58	0
56	MG	2A	3341	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3429	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3343	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3019	1/1	0.95	0.05	59,59,59,59	0
56	MG	1A	3180	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3915	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3347	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3762	1/1	0.95	0.08	10,10,10,10	0
56	MG	1A	3604	1/1	0.95	0.09	66,66,66,66	0
56	MG	2a	1672	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	4079	1/1	0.95	0.14	28,28,28,28	0
56	MG	2A	3026	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3764	1/1	0.95	0.18	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1677	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3509	1/1	0.95	0.07	50,50,50,50	0
56	MG	2A	3031	1/1	0.95	0.17	46,46,46,46	0
56	MG	1G	201	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3923	1/1	0.95	0.07	53,53,53,53	0
56	MG	1a	1735	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3181	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3365	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3107	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3931	1/1	0.95	0.07	36,36,36,36	0
56	MG	1A	3433	1/1	0.95	0.10	66,66,66,66	0
56	MG	1A	3611	1/1	0.95	0.15	40,40,40,40	0
56	MG	2a	1696	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3371	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3372	1/1	0.95	0.06	34,34,34,34	0
56	MG	2a	1699	1/1	0.95	0.17	46,46,46,46	0
56	MG	1N	206	1/1	0.95	0.06	29,29,29,29	0
56	MG	1O	3002	1/1	0.95	0.13	51,51,51,51	0
56	MG	1a	1745	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3384	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3385	1/1	0.95	0.16	36,36,36,36	0
56	MG	1O	3003	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3362	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3047	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3284	1/1	0.95	0.06	37,37,37,37	0
56	MG	2A	3050	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3052	1/1	0.95	0.12	31,31,31,31	0
56	MG	2A	3054	1/1	0.95	0.13	41,41,41,41	0
56	MG	1A	3936	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3286	1/1	0.95	0.12	40,40,40,40	0
56	MG	2a	1721	1/1	0.95	0.16	52,52,52,52	0
56	MG	2A	3400	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	4095	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3001	1/1	0.95	0.18	37,37,37,37	0
56	MG	1R	201	1/1	0.95	0.09	26,26,26,26	0
56	MG	1A	3520	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3061	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3063	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3784	1/1	0.95	0.11	65,65,65,65	0
56	MG	1A	3622	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	3521	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3134	1/1	0.95	0.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3626	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3369	1/1	0.95	0.20	32,32,32,32	0
56	MG	1A	3630	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3073	1/1	0.95	0.15	48,48,48,48	0
56	MG	2A	3420	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3422	1/1	0.95	0.20	51,51,51,51	0
56	MG	2A	3075	1/1	0.95	0.11	24,24,24,24	0
56	MG	1A	4109	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3796	1/1	0.95	0.04	46,46,46,46	0
56	MG	2A	3078	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3370	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3137	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3086	1/1	0.95	0.22	43,43,43,43	0
56	MG	2A	3084	1/1	0.95	0.19	49,49,49,49	0
56	MG	2A	3085	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3057	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3961	1/1	0.95	0.11	34,34,34,34	0
56	MG	1A	3206	1/1	0.95	0.19	46,46,46,46	0
56	MG	1a	1772	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3531	1/1	0.95	0.33	51,51,51,51	0
56	MG	1X	3001	1/1	0.95	0.07	44,44,44,44	0
56	MG	2a	1759	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	3058	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	4124	1/1	0.95	0.17	33,33,33,33	0
56	MG	2A	3100	1/1	0.95	0.08	38,38,38,38	0
56	MG	2A	3448	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3449	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3454	1/1	0.95	0.09	56,56,56,56	0
56	MG	1A	3090	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	3028	1/1	0.95	0.18	39,39,39,39	0
56	MG	10	104	1/1	0.95	0.09	61,61,61,61	0
56	MG	2A	3456	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	3380	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3459	1/1	0.95	0.17	43,43,43,43	0
56	MG	1a	1784	1/1	0.95	0.16	64,64,64,64	0
56	MG	11	102	1/1	0.95	0.07	34,34,34,34	0
56	MG	2a	1777	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3973	1/1	0.95	0.09	55,55,55,55	0
56	MG	2A	3465	1/1	0.95	0.05	39,39,39,39	0
56	MG	2A	3111	1/1	0.95	0.13	48,48,48,48	0
56	MG	2A	3467	1/1	0.95	0.12	60,60,60,60	0
56	MG	2a	1783	1/1	0.95	0.13	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	2A	3114	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3460	1/1	0.95	0.15	58,58,58,58	0
56	MG	15	104	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	4137	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3543	1/1	0.95	0.24	46,46,46,46	0
56	MG	17	101	1/1	0.95	0.30	35,35,35,35	0
56	MG	17	103	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3125	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3478	1/1	0.95	0.14	49,49,49,49	0
56	MG	18	101	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3128	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3115	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3979	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3483	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3820	1/1	0.95	0.09	17,17,17,17	0
56	MG	1a	1802	1/1	0.95	0.07	59,59,59,59	0
56	MG	1A	4143	1/1	0.95	0.11	34,34,34,34	0
56	MG	1a	1805	1/1	0.95	0.14	66,66,66,66	0
56	MG	2A	3137	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3144	1/1	0.95	0.07	49,49,49,49	0
56	MG	1a	1807	1/1	0.95	0.14	60,60,60,60	0
56	MG	1A	3661	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3146	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3014	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3666	1/1	0.95	0.07	30,30,30,30	0
56	MG	1a	1605	1/1	0.95	0.09	66,66,66,66	0
56	MG	1a	1606	1/1	0.95	0.08	65,65,65,65	0
56	MG	1a	1607	1/1	0.95	0.09	73,73,73,73	0
56	MG	2A	3156	1/1	0.95	0.16	49,49,49,49	0
56	MG	2A	3160	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3161	1/1	0.95	0.20	48,48,48,48	0
56	MG	1A	3074	1/1	0.95	0.16	41,41,41,41	0
56	MG	1A	3386	1/1	0.95	0.27	43,43,43,43	0
56	MG	1A	3834	1/1	0.95	0.11	36,36,36,36	0
56	MG	1A	3224	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3228	1/1	0.95	0.12	25,25,25,25	0
56	MG	2A	3169	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3993	1/1	0.95	0.12	32,32,32,32	0
56	MG	2a	1824	1/1	0.95	0.06	41,41,41,41	0
56	MG	2A	3172	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3229	1/1	0.95	0.10	23,23,23,23	0
56	MG	2a	1828	1/1	0.95	0.11	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3523	1/1	0.95	0.09	27,27,27,27	0
56	MG	1a	1826	1/1	0.95	0.06	53,53,53,53	0
56	MG	2A	3179	1/1	0.95	0.15	31,31,31,31	0
56	MG	1a	1827	1/1	0.95	0.11	44,44,44,44	0
56	MG	2a	1835	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3181	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3533	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3019	1/1	0.95	0.30	49,49,49,49	0
56	MG	1A	3676	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3999	1/1	0.95	0.09	55,55,55,55	0
56	MG	2A	3186	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3539	1/1	0.95	0.08	43,43,43,43	0
56	MG	1a	1834	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3557	1/1	0.95	0.09	53,53,53,53	0
56	MG	2a	1847	1/1	0.95	0.22	46,46,46,46	0
56	MG	2A	3192	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3234	1/1	0.95	0.31	31,31,31,31	0
56	MG	1A	3679	1/1	0.95	0.06	24,24,24,24	0
56	MG	1A	3236	1/1	0.95	0.10	63,63,63,63	0
56	MG	1A	3148	1/1	0.95	0.18	40,40,40,40	0
56	MG	1a	1841	1/1	0.95	0.16	49,49,49,49	0
56	MG	2A	3551	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3200	1/1	0.95	0.30	40,40,40,40	0
56	MG	1A	3850	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3691	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3206	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3473	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3557	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	4175	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3694	1/1	0.95	0.10	29,29,29,29	0
56	MG	1a	1633	1/1	0.95	0.06	64,64,64,64	0
56	MG	2x	3004	1/1	0.95	0.19	62,62,62,62	0
57	ZN	24	501	1/1	0.95	0.07	122,122,122,122	0
56	MG	2A	3211	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3996	1/1	0.96	0.05	43,43,43,43	0
56	MG	10	105	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3603	1/1	0.96	0.08	60,60,60,60	0
56	MG	10	107	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3409	1/1	0.96	0.20	33,33,33,33	0
56	MG	1A	3410	1/1	0.96	0.15	22,22,22,22	0
56	MG	2O	203	1/1	0.96	0.08	47,47,47,47	0
56	MG	11	103	1/1	0.96	0.04	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3606	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3167	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3608	1/1	0.96	0.08	62,62,62,62	0
56	MG	2Q	3005	1/1	0.96	0.05	43,43,43,43	0
56	MG	2A	3325	1/1	0.96	0.12	28,28,28,28	0
56	MG	2Y	502	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3717	1/1	0.96	0.13	59,59,59,59	0
56	MG	2A	3327	1/1	0.96	0.23	50,50,50,50	0
56	MG	1A	3169	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3329	1/1	0.96	0.10	55,55,55,55	0
56	MG	28	101	1/1	0.96	0.17	40,40,40,40	0
56	MG	16	103	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	4005	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3413	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3170	1/1	0.96	0.07	31,31,31,31	0
56	MG	2a	1604	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	4008	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3340	1/1	0.96	0.09	57,57,57,57	0
56	MG	2a	1607	1/1	0.96	0.22	45,45,45,45	0
56	MG	1A	3361	1/1	0.96	0.11	35,35,35,35	0
56	MG	2a	1609	1/1	0.96	0.12	55,55,55,55	0
56	MG	1A	3722	1/1	0.96	0.15	38,38,38,38	0
56	MG	1A	4160	1/1	0.96	0.16	45,45,45,45	0
56	MG	19	101	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	4011	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3723	1/1	0.96	0.05	11,11,11,11	0
56	MG	1A	3257	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	4014	1/1	0.96	0.05	39,39,39,39	0
56	MG	2A	3349	1/1	0.96	0.10	64,64,64,64	0
56	MG	1A	4015	1/1	0.96	0.09	15,15,15,15	0
56	MG	1A	4167	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3210	1/1	0.96	0.16	48,48,48,48	0
56	MG	2a	1622	1/1	0.96	0.13	70,70,70,70	0
56	MG	1A	3538	1/1	0.96	0.07	57,57,57,57	0
56	MG	1a	1800	1/1	0.96	0.09	37,37,37,37	0
56	MG	2A	3355	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3728	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3874	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3619	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3475	1/1	0.96	0.14	50,50,50,50	0
56	MG	2A	3360	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3621	1/1	0.96	0.14	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3363	1/1	0.96	0.08	30,30,30,30	0
56	MG	2A	3364	1/1	0.96	0.07	44,44,44,44	0
56	MG	1A	3734	1/1	0.96	0.04	42,42,42,42	0
56	MG	1A	4183	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3735	1/1	0.96	0.10	57,57,57,57	0
56	MG	1A	3742	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	4026	1/1	0.96	0.11	44,44,44,44	0
56	MG	1A	3033	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	4192	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3374	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3092	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	4194	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3377	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3382	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3094	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3422	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3041	1/1	0.96	0.22	44,44,44,44	0
56	MG	2A	3113	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3629	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3264	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	4201	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3483	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3391	1/1	0.96	0.13	55,55,55,55	0
56	MG	2A	3393	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3119	1/1	0.96	0.12	53,53,53,53	0
56	MG	2A	3120	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3121	1/1	0.96	0.18	49,49,49,49	0
56	MG	2A	3398	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3219	1/1	0.96	0.08	24,24,24,24	0
56	MG	1A	4036	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3895	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3758	1/1	0.96	0.04	46,46,46,46	0
56	MG	2A	3126	1/1	0.96	0.29	47,47,47,47	0
56	MG	1a	1640	1/1	0.96	0.14	62,62,62,62	0
56	MG	1a	1837	1/1	0.96	0.05	43,43,43,43	0
56	MG	2a	1669	1/1	0.96	0.07	69,69,69,69	0
56	MG	1A	3633	1/1	0.96	0.10	29,29,29,29	0
56	MG	1A	3048	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3131	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3410	1/1	0.96	0.05	36,36,36,36	0
56	MG	2A	3132	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3635	1/1	0.96	0.07	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3900	1/1	0.96	0.05	45,45,45,45	0
56	MG	2a	1678	1/1	0.96	0.28	60,60,60,60	0
56	MG	2A	3415	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3636	1/1	0.96	0.13	29,29,29,29	0
56	MG	2a	1681	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3417	1/1	0.96	0.11	51,51,51,51	0
56	MG	2a	1684	1/1	0.96	0.09	44,44,44,44	0
56	MG	1a	1647	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3554	1/1	0.96	0.11	61,61,61,61	0
56	MG	2a	1688	1/1	0.96	0.16	49,49,49,49	0
56	MG	1a	1845	1/1	0.96	0.14	48,48,48,48	0
56	MG	2A	3421	1/1	0.96	0.04	40,40,40,40	0
56	MG	1A	4224	1/1	0.96	0.25	23,23,23,23	0
56	MG	2a	1692	1/1	0.96	0.16	59,59,59,59	0
56	MG	1A	4045	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3145	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	4046	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3486	1/1	0.96	0.09	32,32,32,32	0
56	MG	1a	1654	1/1	0.96	0.20	51,51,51,51	0
56	MG	1a	1655	1/1	0.96	0.22	47,47,47,47	0
56	MG	1A	4230	1/1	0.96	0.19	47,47,47,47	0
56	MG	1a	1853	1/1	0.96	0.19	53,53,53,53	0
56	MG	2A	3154	1/1	0.96	0.06	41,41,41,41	0
56	MG	2a	1704	1/1	0.96	0.08	67,67,67,67	0
56	MG	1A	3640	1/1	0.96	0.19	53,53,53,53	0
56	MG	2A	3158	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3641	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3767	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3183	1/1	0.96	0.12	35,35,35,35	0
56	MG	2a	1710	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3910	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3322	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3227	1/1	0.96	0.20	27,27,27,27	0
56	MG	2A	3167	1/1	0.96	0.05	31,31,31,31	0
56	MG	1A	3560	1/1	0.96	0.06	44,44,44,44	0
56	MG	1a	1668	1/1	0.96	0.14	44,44,44,44	0
56	MG	2a	1719	1/1	0.96	0.23	43,43,43,43	0
56	MG	1a	1669	1/1	0.96	0.11	54,54,54,54	0
56	MG	2A	3171	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	4058	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3184	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3916	1/1	0.96	0.12	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	211	1/1	0.96	0.05	34,34,34,34	0
56	MG	2A	3459	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3775	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	3777	1/1	0.96	0.12	31,31,31,31	0
56	MG	2a	1730	1/1	0.96	0.09	66,66,66,66	0
56	MG	1A	3278	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3492	1/1	0.96	0.19	52,52,52,52	0
56	MG	1a	1678	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	1878	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	4065	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3188	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3189	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3650	1/1	0.96	0.12	50,50,50,50	0
56	MG	2a	1739	1/1	0.96	0.22	39,39,39,39	0
56	MG	2a	1740	1/1	0.96	0.13	31,31,31,31	0
56	MG	2A	3191	1/1	0.96	0.19	48,48,48,48	0
56	MG	1A	3924	1/1	0.96	0.05	19,19,19,19	0
56	MG	1A	3652	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3653	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	3930	1/1	0.96	0.12	47,47,47,47	0
56	MG	1a	1885	1/1	0.96	0.06	66,66,66,66	0
56	MG	1a	1887	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3788	1/1	0.96	0.07	34,34,34,34	0
56	MG	1a	1889	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3378	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3379	1/1	0.96	0.14	26,26,26,26	0
56	MG	1D	306	1/1	0.96	0.08	13,13,13,13	0
56	MG	1A	3280	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3381	1/1	0.96	0.06	44,44,44,44	0
56	MG	1D	310	1/1	0.96	0.07	46,46,46,46	0
56	MG	1a	1693	1/1	0.96	0.20	49,49,49,49	0
56	MG	1A	3049	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3938	1/1	0.96	0.07	16,16,16,16	0
56	MG	1a	1698	1/1	0.96	0.07	57,57,57,57	0
56	MG	2A	3492	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3493	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3496	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3188	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3663	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3664	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3500	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3665	1/1	0.96	0.09	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3503	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3504	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3226	1/1	0.96	0.20	64,64,64,64	0
56	MG	1A	3573	1/1	0.96	0.07	44,44,44,44	0
56	MG	1l	201	1/1	0.96	0.06	50,50,50,50	0
56	MG	2a	1776	1/1	0.96	0.18	55,55,55,55	0
56	MG	2A	3229	1/1	0.96	0.07	38,38,38,38	0
56	MG	1n	502	1/1	0.96	0.13	59,59,59,59	0
56	MG	1A	3667	1/1	0.96	0.06	23,23,23,23	0
56	MG	1A	3945	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3232	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	4087	1/1	0.96	0.09	66,66,66,66	0
56	MG	1A	3290	1/1	0.96	0.07	15,15,15,15	0
56	MG	1A	3949	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3190	1/1	0.96	0.18	25,25,25,25	0
56	MG	1A	3811	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	4092	1/1	0.96	0.08	69,69,69,69	0
56	MG	1A	3671	1/1	0.96	0.11	30,30,30,30	0
56	MG	1A	3672	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3191	1/1	0.96	0.11	35,35,35,35	0
56	MG	2A	3526	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3119	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3959	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	4099	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3336	1/1	0.96	0.08	56,56,56,56	0
56	MG	1a	1722	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3447	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3193	1/1	0.96	0.15	23,23,23,23	0
56	MG	1A	3450	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	4105	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3821	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3260	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3544	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3451	1/1	0.96	0.09	38,38,38,38	0
56	MG	1P	204	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3681	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3587	1/1	0.96	0.07	59,59,59,59	0
56	MG	2A	3010	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3684	1/1	0.96	0.06	29,29,29,29	0
56	MG	1A	3338	1/1	0.96	0.05	32,32,32,32	0
56	MG	1A	3194	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3833	1/1	0.96	0.08	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3976	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3098	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	4118	1/1	0.96	0.06	37,37,37,37	0
56	MG	1R	206	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3516	1/1	0.96	0.12	59,59,59,59	0
56	MG	1A	3837	1/1	0.96	0.07	50,50,50,50	0
56	MG	1a	1744	1/1	0.96	0.12	44,44,44,44	0
56	MG	2a	1822	1/1	0.96	0.10	71,71,71,71	0
56	MG	1A	3346	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3565	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	4122	1/1	0.96	0.17	26,26,26,26	0
56	MG	1A	3297	1/1	0.96	0.11	37,37,37,37	0
56	MG	1a	1748	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3011	1/1	0.96	0.06	49,49,49,49	0
56	MG	2a	1830	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3570	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3030	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3350	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3082	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3576	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3986	1/1	0.96	0.10	70,70,70,70	0
56	MG	1A	4130	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3290	1/1	0.96	0.05	26,26,26,26	0
56	MG	2A	3291	1/1	0.96	0.08	30,30,30,30	0
56	MG	2A	3294	1/1	0.96	0.13	34,34,34,34	0
56	MG	2a	1843	1/1	0.96	0.10	43,43,43,43	0
56	MG	1V	202	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	4131	1/1	0.96	0.15	32,32,32,32	0
56	MG	2A	3297	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3199	1/1	0.96	0.10	35,35,35,35	0
56	MG	2A	3587	1/1	0.96	0.19	44,44,44,44	0
56	MG	2A	3588	1/1	0.96	0.23	42,42,42,42	0
56	MG	2A	3589	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3590	1/1	0.96	0.15	55,55,55,55	0
56	MG	2A	3592	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3038	1/1	0.96	0.17	45,45,45,45	0
56	MG	2A	3300	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3523	1/1	0.96	0.08	50,50,50,50	0
56	MG	1W	3006	1/1	0.96	0.04	35,35,35,35	0
56	MG	2A	3303	1/1	0.96	0.20	56,56,56,56	0
56	MG	1A	3165	1/1	0.96	0.12	42,42,42,42	0
56	MG	2q	3001	1/1	0.96	0.29	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	1Z	301	1/1	0.96	0.08	63,63,63,63	0
56	MG	2A	3306	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	4135	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3705	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3354	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3046	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3526	1/1	0.96	0.12	70,70,70,70	0
56	MG	1A	3303	1/1	0.96	0.07	44,44,44,44	0
56	MG	1A	3868	1/1	0.97	0.12	59,59,59,59	0
56	MG	1A	3657	1/1	0.97	0.16	39,39,39,39	0
56	MG	2A	3362	1/1	0.97	0.07	42,42,42,42	0
56	MG	1E	302	1/1	0.97	0.07	50,50,50,50	0
56	MG	1E	303	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3578	1/1	0.97	0.18	53,53,53,53	0
56	MG	1a	1854	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3995	1/1	0.97	0.22	32,32,32,32	0
56	MG	1A	3008	1/1	0.97	0.11	57,57,57,57	0
56	MG	1A	3872	1/1	0.97	0.07	16,16,16,16	0
56	MG	1A	3281	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3118	1/1	0.97	0.13	44,44,44,44	0
56	MG	2A	3373	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3448	1/1	0.97	0.08	35,35,35,35	0
56	MG	1F	303	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3233	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3285	1/1	0.97	0.23	30,30,30,30	0
56	MG	2A	3378	1/1	0.97	0.12	55,55,55,55	0
56	MG	2A	3379	1/1	0.97	0.09	31,31,31,31	0
56	MG	2A	3381	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3335	1/1	0.97	0.16	36,36,36,36	0
56	MG	2A	3139	1/1	0.97	0.17	37,37,37,37	0
56	MG	2A	3140	1/1	0.97	0.18	41,41,41,41	0
56	MG	1A	3391	1/1	0.97	0.05	29,29,29,29	0
56	MG	1a	1686	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3143	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3144	1/1	0.97	0.20	45,45,45,45	0
56	MG	1A	3881	1/1	0.97	0.05	16,16,16,16	0
56	MG	1A	3002	1/1	0.97	0.05	54,54,54,54	0
56	MG	1a	1869	1/1	0.97	0.11	62,62,62,62	0
56	MG	1A	3287	1/1	0.97	0.13	40,40,40,40	0
56	MG	2A	3149	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3395	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3172	1/1	0.97	0.14	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	3457	1/1	0.97	0.04	22,22,22,22	0
56	MG	1a	1873	1/1	0.97	0.10	42,42,42,42	0
56	MG	1a	1874	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3887	1/1	0.97	0.05	40,40,40,40	0
56	MG	2A	3157	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3237	1/1	0.97	0.12	24,24,24,24	0
56	MG	2A	3159	1/1	0.97	0.11	37,37,37,37	0
56	MG	1a	1694	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	1695	1/1	0.97	0.05	56,56,56,56	0
56	MG	1A	3238	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3163	1/1	0.97	0.12	36,36,36,36	0
56	MG	1N	204	1/1	0.97	0.07	44,44,44,44	0
56	MG	1N	205	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3411	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	4136	1/1	0.97	0.08	38,38,38,38	0
56	MG	1N	207	1/1	0.97	0.04	41,41,41,41	0
56	MG	1a	1701	1/1	0.97	0.20	47,47,47,47	0
56	MG	1a	1886	1/1	0.97	0.09	40,40,40,40	0
56	MG	1O	3001	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3397	1/1	0.97	0.07	57,57,57,57	0
56	MG	2a	1651	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3341	1/1	0.97	0.07	25,25,25,25	0
56	MG	1a	1705	1/1	0.97	0.05	46,46,46,46	0
56	MG	2A	3174	1/1	0.97	0.15	38,38,38,38	0
56	MG	2A	3175	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3176	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3343	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3778	1/1	0.97	0.07	30,30,30,30	0
56	MG	2A	3425	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3779	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	3401	1/1	0.97	0.09	30,30,30,30	0
56	MG	2a	1662	1/1	0.97	0.06	71,71,71,71	0
56	MG	1A	3781	1/1	0.97	0.11	25,25,25,25	0
56	MG	1A	3173	1/1	0.97	0.13	40,40,40,40	0
56	MG	2A	3184	1/1	0.97	0.12	29,29,29,29	0
56	MG	2A	3431	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3432	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3433	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3151	1/1	0.97	0.08	31,31,31,31	0
56	MG	1Q	205	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3120	1/1	0.97	0.16	37,37,37,37	0
56	MG	1A	4148	1/1	0.97	0.11	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	3349	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3440	1/1	0.97	0.11	37,37,37,37	0
56	MG	1h	201	1/1	0.97	0.12	60,60,60,60	0
56	MG	1A	3902	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3786	1/1	0.97	0.11	18,18,18,18	0
56	MG	1A	3904	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3407	1/1	0.97	0.16	48,48,48,48	0
56	MG	2A	3446	1/1	0.97	0.12	53,53,53,53	0
56	MG	2a	1682	1/1	0.97	0.13	54,54,54,54	0
56	MG	2A	3195	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3202	1/1	0.97	0.08	26,26,26,26	0
56	MG	1A	3203	1/1	0.97	0.14	30,30,30,30	0
56	MG	2a	1686	1/1	0.97	0.07	44,44,44,44	0
56	MG	2A	3198	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3452	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3687	1/1	0.97	0.10	21,21,21,21	0
56	MG	1A	3793	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3688	1/1	0.97	0.13	19,19,19,19	0
56	MG	1A	3911	1/1	0.97	0.12	25,25,25,25	0
56	MG	1A	4162	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3458	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3689	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	3054	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3535	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3178	1/1	0.97	0.23	39,39,39,39	0
56	MG	2A	3463	1/1	0.97	0.13	40,40,40,40	0
56	MG	1x	104	1/1	0.97	0.11	42,42,42,42	0
56	MG	1W	3002	1/1	0.97	0.18	41,41,41,41	0
56	MG	1a	1733	1/1	0.97	0.11	49,49,49,49	0
56	MG	1W	3003	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3215	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3469	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3695	1/1	0.97	0.11	40,40,40,40	0
56	MG	2A	3220	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	4168	1/1	0.97	0.13	26,26,26,26	0
56	MG	2A	3223	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	3804	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	4170	1/1	0.97	0.10	10,10,10,10	0
56	MG	1Y	502	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3001	1/1	0.97	0.04	38,38,38,38	0
56	MG	1A	4171	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3179	1/1	0.97	0.16	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3919	1/1	0.97	0.06	16,16,16,16	0
56	MG	1A	3355	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	3921	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	3539	1/1	0.97	0.05	41,41,41,41	0
56	MG	2A	3234	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3612	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3155	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	4179	1/1	0.97	0.15	34,34,34,34	0
56	MG	2a	1728	1/1	0.97	0.14	52,52,52,52	0
56	MG	2A	3011	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	4180	1/1	0.97	0.24	33,33,33,33	0
56	MG	1A	4182	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3242	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3925	1/1	0.97	0.05	39,39,39,39	0
56	MG	2A	3494	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3495	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3926	1/1	0.97	0.05	15,15,15,15	0
56	MG	1A	4186	1/1	0.97	0.14	17,17,17,17	0
56	MG	1A	3927	1/1	0.97	0.05	30,30,30,30	0
56	MG	15	102	1/1	0.97	0.19	45,45,45,45	0
56	MG	1A	3415	1/1	0.97	0.11	46,46,46,46	0
56	MG	2A	3249	1/1	0.97	0.08	29,29,29,29	0
56	MG	2A	3502	1/1	0.97	0.05	30,30,30,30	0
56	MG	1A	4051	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3812	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3505	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	4053	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3254	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3302	1/1	0.97	0.04	15,15,15,15	0
56	MG	1A	3212	1/1	0.97	0.16	63,63,63,63	0
56	MG	1A	4196	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3255	1/1	0.97	0.05	68,68,68,68	0
56	MG	1A	3157	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3029	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3158	1/1	0.97	0.07	18,18,18,18	0
56	MG	2A	3263	1/1	0.97	0.08	30,30,30,30	0
56	MG	1A	3067	1/1	0.97	0.14	37,37,37,37	0
56	MG	1a	1768	1/1	0.97	0.11	32,32,32,32	0
56	MG	1A	3551	1/1	0.97	0.13	53,53,53,53	0
56	MG	1A	3185	1/1	0.97	0.05	24,24,24,24	0
56	MG	2A	3522	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3366	1/1	0.97	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	3081	1/1	0.97	0.10	47,47,47,47	0
56	MG	1a	1773	1/1	0.97	0.06	25,25,25,25	0
56	MG	1a	1603	1/1	0.97	0.05	59,59,59,59	0
56	MG	1A	4205	1/1	0.97	0.05	36,36,36,36	0
56	MG	2A	3529	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3530	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	4206	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3532	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	4209	1/1	0.97	0.23	27,27,27,27	0
56	MG	1A	4210	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3310	1/1	0.97	0.12	37,37,37,37	0
56	MG	2a	1774	1/1	0.97	0.27	57,57,57,57	0
56	MG	2a	1775	1/1	0.97	0.07	62,62,62,62	0
56	MG	2A	3278	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3221	1/1	0.97	0.08	36,36,36,36	0
56	MG	2A	3538	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3826	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3313	1/1	0.97	0.07	56,56,56,56	0
56	MG	1A	3828	1/1	0.97	0.10	44,44,44,44	0
56	MG	2A	3048	1/1	0.97	0.12	43,43,43,43	0
56	MG	2A	3543	1/1	0.97	0.19	47,47,47,47	0
56	MG	1A	3830	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3222	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3051	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	4220	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	4221	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3549	1/1	0.97	0.20	47,47,47,47	0
56	MG	1a	1788	1/1	0.97	0.10	46,46,46,46	0
56	MG	1a	1620	1/1	0.97	0.15	38,38,38,38	0
56	MG	1A	3559	1/1	0.97	0.13	41,41,41,41	0
56	MG	2A	3292	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3293	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3187	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	4225	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	3952	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3561	1/1	0.97	0.08	51,51,51,51	0
56	MG	2A	3559	1/1	0.97	0.25	42,42,42,42	0
56	MG	2A	3062	1/1	0.97	0.10	35,35,35,35	0
56	MG	1a	1796	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3835	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3266	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3563	1/1	0.97	0.16	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3267	1/1	0.97	0.04	23,23,23,23	0
56	MG	2A	3068	1/1	0.97	0.14	46,46,46,46	0
56	MG	1a	1630	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	3725	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	3565	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3841	1/1	0.97	0.17	46,46,46,46	0
56	MG	2A	3074	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3494	1/1	0.97	0.19	59,59,59,59	0
56	MG	1B	205	1/1	0.97	0.20	57,57,57,57	0
56	MG	1A	3038	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3225	1/1	0.97	0.22	35,35,35,35	0
56	MG	1A	3321	1/1	0.97	0.09	47,47,47,47	0
56	MG	1a	1814	1/1	0.97	0.12	56,56,56,56	0
56	MG	2A	3081	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3318	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3846	1/1	0.97	0.05	23,23,23,23	0
56	MG	2A	3083	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	3967	1/1	0.97	0.04	20,20,20,20	0
56	MG	2A	3586	1/1	0.97	0.08	33,33,33,33	0
56	MG	2a	1826	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3226	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3087	1/1	0.97	0.14	41,41,41,41	0
56	MG	2A	3088	1/1	0.97	0.04	27,27,27,27	0
56	MG	1A	3733	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3437	1/1	0.97	0.09	33,33,33,33	0
56	MG	2A	3091	1/1	0.97	0.04	39,39,39,39	0
56	MG	1B	217	1/1	0.97	0.06	36,36,36,36	0
56	MG	2B	3003	1/1	0.97	0.19	51,51,51,51	0
56	MG	2A	3094	1/1	0.97	0.18	49,49,49,49	0
56	MG	1A	3851	1/1	0.97	0.11	33,33,33,33	0
56	MG	2A	3332	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3029	1/1	0.97	0.25	55,55,55,55	0
56	MG	1a	1824	1/1	0.97	0.14	59,59,59,59	0
56	MG	2a	1841	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	3736	1/1	0.97	0.04	42,42,42,42	0
56	MG	1a	1650	1/1	0.97	0.25	52,52,52,52	0
56	MG	1A	3740	1/1	0.97	0.13	32,32,32,32	0
56	MG	1A	3741	1/1	0.97	0.06	44,44,44,44	0
56	MG	2D	305	1/1	0.97	0.14	29,29,29,29	0
56	MG	1A	4097	1/1	0.97	0.17	27,27,27,27	0
56	MG	1a	1830	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3275	1/1	0.97	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2E	303	1/1	0.97	0.16	44,44,44,44	0
56	MG	1A	3276	1/1	0.97	0.36	34,34,34,34	0
56	MG	2f	3001	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3744	1/1	0.97	0.07	49,49,49,49	0
56	MG	2E	306	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3651	1/1	0.97	0.14	52,52,52,52	0
56	MG	2F	302	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3164	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3136	1/1	0.97	0.15	37,37,37,37	0
56	MG	1a	1660	1/1	0.97	0.22	47,47,47,47	0
56	MG	1a	1661	1/1	0.97	0.08	34,34,34,34	0
56	MG	1a	1662	1/1	0.97	0.10	42,42,42,42	0
56	MG	2t	3001	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3654	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	3987	1/1	0.97	0.06	12,12,12,12	0
56	MG	1A	3655	1/1	0.97	0.05	30,30,30,30	0
56	MG	1A	3279	1/1	0.97	0.11	41,41,41,41	0
56	MG	1D	312	1/1	0.97	0.14	41,41,41,41	0
57	ZN	1n	501	1/1	0.97	0.06	93,93,93,93	0
56	MG	1A	3752	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3754	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3178	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	4187	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	4188	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3166	1/1	0.98	0.04	21,21,21,21	0
56	MG	2A	3053	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3182	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3547	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3220	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3937	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3404	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3791	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3198	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3251	1/1	0.98	0.07	36,36,36,36	0
56	MG	1a	1638	1/1	0.98	0.07	18,18,18,18	0
56	MG	1A	3452	1/1	0.98	0.07	48,48,48,48	0
56	MG	2A	3472	1/1	0.98	0.04	52,52,52,52	0
56	MG	2N	8001	1/1	0.98	0.04	55,55,55,55	0
56	MG	1A	3364	1/1	0.98	0.11	43,43,43,43	0
56	MG	2A	3336	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3066	1/1	0.98	0.11	41,41,41,41	0
56	MG	1a	1642	1/1	0.98	0.06	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	3797	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3288	1/1	0.98	0.09	13,13,13,13	0
56	MG	1A	4111	1/1	0.98	0.16	32,32,32,32	0
56	MG	1P	203	1/1	0.98	0.12	26,26,26,26	0
56	MG	1a	1876	1/1	0.98	0.07	37,37,37,37	0
56	MG	2A	3202	1/1	0.98	0.05	40,40,40,40	0
56	MG	2A	3072	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3947	1/1	0.98	0.09	13,13,13,13	0
56	MG	1P	205	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3289	1/1	0.98	0.11	24,24,24,24	0
56	MG	1A	3168	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	4207	1/1	0.98	0.19	30,30,30,30	0
56	MG	2a	1752	1/1	0.98	0.14	51,51,51,51	0
56	MG	1A	3950	1/1	0.98	0.03	16,16,16,16	0
56	MG	1A	3875	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3201	1/1	0.98	0.14	17,17,17,17	0
56	MG	1A	3730	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3954	1/1	0.98	0.08	53,53,53,53	0
56	MG	1A	4214	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3135	1/1	0.98	0.06	49,49,49,49	0
56	MG	2A	3219	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3807	1/1	0.98	0.03	18,18,18,18	0
56	MG	2A	3086	1/1	0.98	0.11	48,48,48,48	0
56	MG	1A	3015	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3615	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	4219	1/1	0.98	0.14	25,25,25,25	0
56	MG	1T	202	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3204	1/1	0.98	0.18	27,27,27,27	0
56	MG	2A	3366	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3205	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	4222	1/1	0.98	0.08	68,68,68,68	0
56	MG	1A	3511	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	4129	1/1	0.98	0.06	56,56,56,56	0
56	MG	1A	3885	1/1	0.98	0.12	46,46,46,46	0
56	MG	1A	3739	1/1	0.98	0.10	22,22,22,22	0
56	MG	1A	3512	1/1	0.98	0.05	41,41,41,41	0
56	MG	2A	3512	1/1	0.98	0.08	36,36,36,36	0
56	MG	1A	3093	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	4229	1/1	0.98	0.26	33,33,33,33	0
56	MG	1A	3889	1/1	0.98	0.03	29,29,29,29	0
56	MG	2A	3103	1/1	0.98	0.10	39,39,39,39	0
56	MG	2A	3517	1/1	0.98	0.03	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	1782	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	4231	1/1	0.98	0.13	17,17,17,17	0
56	MG	1A	3230	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3968	1/1	0.98	0.03	34,34,34,34	0
56	MG	1A	3969	1/1	0.98	0.05	58,58,58,58	0
56	MG	1A	3207	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	3263	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3680	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3159	1/1	0.98	0.09	26,26,26,26	0
56	MG	1a	1794	1/1	0.98	0.10	24,24,24,24	0
56	MG	1A	3974	1/1	0.98	0.08	54,54,54,54	0
56	MG	2A	3528	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3265	1/1	0.98	0.07	12,12,12,12	0
56	MG	1A	3072	1/1	0.98	0.11	32,32,32,32	0
56	MG	2A	3252	1/1	0.98	0.07	56,56,56,56	0
56	MG	2A	3392	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3628	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3118	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3089	1/1	0.98	0.08	53,53,53,53	0
56	MG	1A	3235	1/1	0.98	0.25	36,36,36,36	0
56	MG	2a	1802	1/1	0.98	0.10	53,53,53,53	0
56	MG	1a	1801	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3753	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	3342	1/1	0.98	0.07	30,30,30,30	0
56	MG	1a	1804	1/1	0.98	0.10	42,42,42,42	0
56	MG	1B	215	1/1	0.98	0.07	31,31,31,31	0
56	MG	1B	216	1/1	0.98	0.08	54,54,54,54	0
56	MG	1A	3982	1/1	0.98	0.06	42,42,42,42	0
56	MG	1a	1808	1/1	0.98	0.12	33,33,33,33	0
56	MG	1a	1809	1/1	0.98	0.09	41,41,41,41	0
56	MG	1B	218	1/1	0.98	0.07	27,27,27,27	0
56	MG	2A	3407	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3829	1/1	0.98	0.07	54,54,54,54	0
56	MG	15	103	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	3690	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3211	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	4155	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3757	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3344	1/1	0.98	0.10	41,41,41,41	0
56	MG	1A	4158	1/1	0.98	0.16	23,23,23,23	0
56	MG	1a	1819	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3693	1/1	0.98	0.08	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3345	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	3270	1/1	0.98	0.06	26,26,26,26	0
56	MG	1D	304	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3561	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	3477	1/1	0.98	0.06	26,26,26,26	0
56	MG	1A	3108	1/1	0.98	0.17	46,46,46,46	0
56	MG	1D	307	1/1	0.98	0.04	27,27,27,27	0
56	MG	2a	1831	1/1	0.98	0.11	60,60,60,60	0
56	MG	19	104	1/1	0.98	0.12	59,59,59,59	0
56	MG	1A	3213	1/1	0.98	0.16	23,23,23,23	0
56	MG	1A	3699	1/1	0.98	0.09	20,20,20,20	0
56	MG	1A	3274	1/1	0.98	0.04	29,29,29,29	0
56	MG	1a	1831	1/1	0.98	0.12	51,51,51,51	0
56	MG	1A	3214	1/1	0.98	0.07	38,38,38,38	0
56	MG	2A	3153	1/1	0.98	0.12	29,29,29,29	0
56	MG	1a	1833	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3573	1/1	0.98	0.09	42,42,42,42	0
56	MG	2A	3574	1/1	0.98	0.10	30,30,30,30	0
56	MG	2A	3155	1/1	0.98	0.11	37,37,37,37	0
56	MG	1A	3768	1/1	0.98	0.06	17,17,17,17	0
56	MG	1A	3435	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3311	1/1	0.98	0.09	35,35,35,35	0
56	MG	1A	3150	1/1	0.98	0.07	22,22,22,22	0
56	MG	1A	3085	1/1	0.98	0.13	43,43,43,43	0
56	MG	1A	3848	1/1	0.98	0.04	23,23,23,23	0
56	MG	1A	3439	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3242	1/1	0.98	0.15	22,22,22,22	0
56	MG	1A	3708	1/1	0.98	0.12	30,30,30,30	0
56	MG	1a	1614	1/1	0.98	0.05	59,59,59,59	0
56	MG	2a	1700	1/1	0.98	0.08	55,55,55,55	0
56	MG	1a	1615	1/1	0.98	0.04	52,52,52,52	0
56	MG	1A	3243	1/1	0.98	0.06	24,24,24,24	0
56	MG	1A	3853	1/1	0.98	0.08	35,35,35,35	0
56	MG	1A	3710	1/1	0.98	0.11	37,37,37,37	0
56	MG	1a	1619	1/1	0.98	0.06	31,31,31,31	0
56	MG	2A	3591	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3316	1/1	0.98	0.10	41,41,41,41	0
56	MG	2A	3450	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	4181	1/1	0.98	0.06	27,27,27,27	0
56	MG	2a	1711	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3117	1/1	0.98	0.18	43,43,43,43	0
56	MG	2B	3004	1/1	0.98	0.08	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3399	1/1	0.98	0.08	5,5,5,5	0
56	MG	2a	1715	1/1	0.98	0.13	65,65,65,65	0
57	ZN	14	501	1/1	0.98	0.04	104,104,104,104	0
56	MG	1A	4184	1/1	0.98	0.10	58,58,58,58	0
57	ZN	2Y	501	1/1	0.98	0.03	83,83,83,83	0
56	MG	1A	3542	1/1	0.98	0.06	37,37,37,37	0
57	ZN	29	501	1/1	0.98	0.04	61,61,61,61	0
56	MG	1A	3358	1/1	0.98	0.05	46,46,46,46	0
58	SF4	1d	501	8/8	0.98	0.05	62,69,78,87	0
58	SF4	2d	501	8/8	0.98	0.04	62,78,83,91	0
56	MG	2A	3205	1/1	0.99	0.03	23,23,23,23	0
56	MG	1A	3737	1/1	0.99	0.07	18,18,18,18	0
56	MG	2A	3258	1/1	0.99	0.09	34,34,34,34	0
56	MG	1B	214	1/1	0.99	0.03	37,37,37,37	0
56	MG	1A	3787	1/1	0.99	0.07	33,33,33,33	0
56	MG	1A	3738	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3273	1/1	0.99	0.03	18,18,18,18	0
56	MG	1F	306	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3283	1/1	0.99	0.12	25,25,25,25	0
56	MG	17	102	1/1	0.99	0.03	42,42,42,42	0
56	MG	1A	3638	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	4083	1/1	0.99	0.04	45,45,45,45	0
56	MG	1U	202	1/1	0.99	0.07	25,25,25,25	0
56	MG	2a	1703	1/1	0.99	0.03	60,60,60,60	0
56	MG	2A	3438	1/1	0.99	0.03	26,26,26,26	0
56	MG	2A	3380	1/1	0.99	0.04	47,47,47,47	0
56	MG	2A	3217	1/1	0.99	0.18	36,36,36,36	0
56	MG	2A	3270	1/1	0.99	0.03	23,23,23,23	0
56	MG	2A	3218	1/1	0.99	0.07	36,36,36,36	0
56	MG	1A	3154	1/1	0.99	0.08	21,21,21,21	0
56	MG	1A	4116	1/1	0.99	0.07	17,17,17,17	0
56	MG	1A	3325	1/1	0.99	0.07	37,37,37,37	0
56	MG	2A	3222	1/1	0.99	0.08	29,29,29,29	0
56	MG	2A	3330	1/1	0.99	0.07	41,41,41,41	0
56	MG	1U	206	1/1	0.99	0.12	32,32,32,32	0
56	MG	1A	3623	1/1	0.99	0.07	21,21,21,21	0
56	MG	2A	3333	1/1	0.99	0.04	55,55,55,55	0
56	MG	1A	3055	1/1	0.99	0.05	54,54,54,54	0
56	MG	2A	3335	1/1	0.99	0.05	39,39,39,39	0
56	MG	1A	3643	1/1	0.99	0.12	12,12,12,12	0
56	MG	1A	3189	1/1	0.99	0.06	26,26,26,26	0
56	MG	1A	3798	1/1	0.99	0.08	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	4123	1/1	0.99	0.17	31,31,31,31	0
56	MG	1A	3799	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3683	1/1	0.99	0.06	44,44,44,44	0
56	MG	1A	3579	1/1	0.99	0.15	38,38,38,38	0
56	MG	2A	3093	1/1	0.99	0.07	51,51,51,51	0
56	MG	1a	1892	1/1	0.99	0.15	54,54,54,54	0
56	MG	1A	3802	1/1	0.99	0.06	20,20,20,20	0
56	MG	2A	3236	1/1	0.99	0.05	45,45,45,45	0
56	MG	1A	3774	1/1	0.99	0.03	23,23,23,23	0
56	MG	1A	3685	1/1	0.99	0.08	17,17,17,17	0
56	MG	1A	3776	1/1	0.99	0.07	25,25,25,25	0
56	MG	1A	3245	1/1	0.99	0.14	30,30,30,30	0
56	MG	1A	3253	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	4100	1/1	0.99	0.14	22,22,22,22	0
56	MG	2a	1674	1/1	0.99	0.13	46,46,46,46	0
56	MG	1A	3177	1/1	0.99	0.10	14,14,14,14	0
56	MG	1A	3583	1/1	0.99	0.05	46,46,46,46	0
56	MG	1A	3614	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	3507	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3544	1/1	0.99	0.04	10,10,10,10	0
56	MG	1A	4139	1/1	0.99	0.17	38,38,38,38	0
56	MG	1a	1741	1/1	0.99	0.20	47,47,47,47	0
57	ZN	1Y	501	1/1	0.99	0.03	66,66,66,66	0
56	MG	2a	1621	1/1	0.99	0.03	47,47,47,47	0
57	ZN	15	101	1/1	0.99	0.09	60,60,60,60	0
57	ZN	16	102	1/1	0.99	0.02	32,32,32,32	0
56	MG	2A	3022	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	4208	1/1	0.99	0.07	29,29,29,29	0
56	MG	2A	3201	1/1	0.99	0.04	25,25,25,25	0
57	ZN	26	501	1/1	0.99	0.03	55,55,55,55	0
56	MG	1A	3247	1/1	0.99	0.07	27,27,27,27	0
56	MG	2A	3112	1/1	0.99	0.13	34,34,34,34	0
56	MG	1A	3171	1/1	0.99	0.07	30,30,30,30	0
56	MG	2A	3309	1/1	0.99	0.12	35,35,35,35	0
57	ZN	19	102	1/1	1.00	0.01	36,36,36,36	0
56	MG	1A	3745	1/1	1.00	0.03	43,43,43,43	0
56	MG	1A	3156	1/1	1.00	0.06	29,29,29,29	0
56	MG	1A	3823	1/1	1.00	0.03	11,11,11,11	0
57	ZN	25	501	1/1	1.00	0.06	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.