



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:56 PM UTC

PDB ID : 5DOY / pdb_00005doy
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with antibiotic Hygromycin A, mRNA and three tRNAs in the A, P and E sites at 2.6Å resolution
Authors : Polikanov, Y.S.; Starosta, A.L.; Juette, M.F.; Altman, R.B.; Terry, D.S.; Lu, W.; Burnett, B.J.; Dinos, G.; Reynolds, K.; Blanchard, S.C.; Steitz, T.A.; Wilson, D.N.
Deposited on : 2015-09-11
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

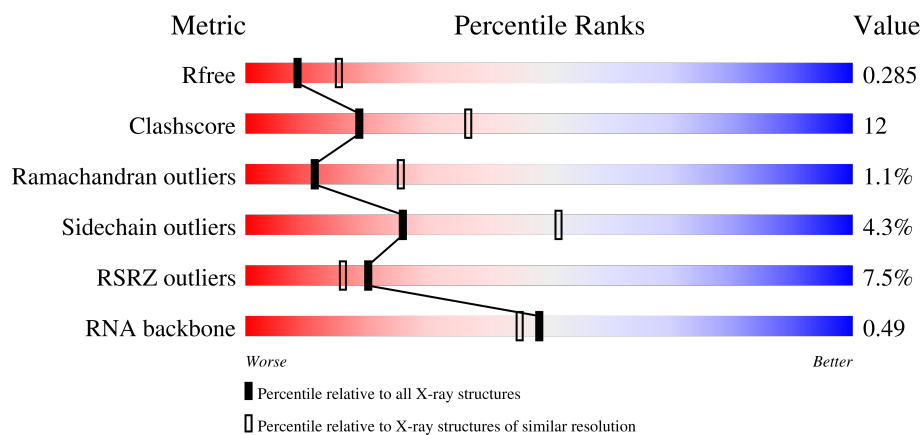
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

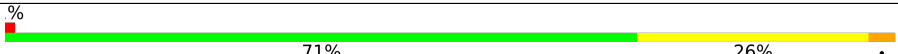
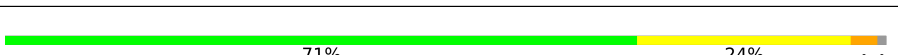
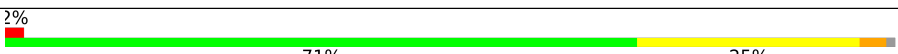
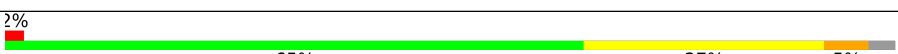
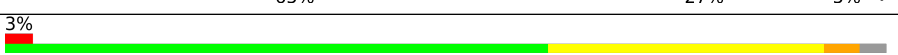
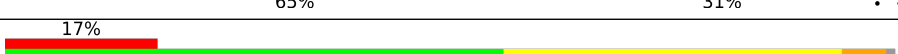
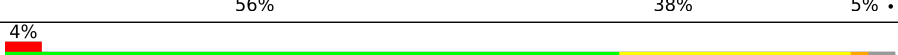
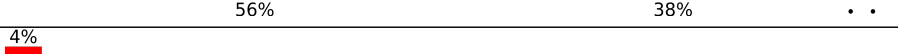
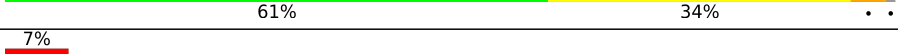
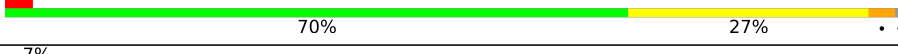
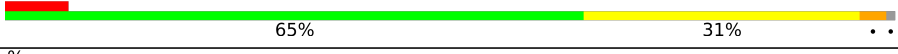
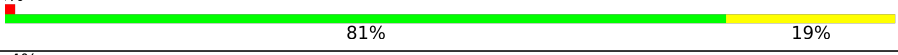
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	SF4	1d	501	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 298925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

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

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1429	916	256	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

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

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

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

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

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

Continued on next page...

Continued from previous page...

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

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

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

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

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

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

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

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

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

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

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

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

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

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

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

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

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

Continued on next page...

Continued from previous page...

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

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

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

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

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

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

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

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

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

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

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

- Molecule 33 is a protein called 30S Ribosomal Protein S2.

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

- Molecule 34 is a protein called 30S Ribosomal Protein S3.

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

- Molecule 35 is a protein called 30S Ribosomal Protein S4.

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

- Molecule 36 is a protein called 30S Ribosomal Protein S5.

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

- Molecule 37 is a protein called 30S Ribosomal Protein S6.

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

- Molecule 38 is a protein called 30S Ribosomal Protein S7.

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

- Molecule 39 is a protein called 30S Ribosomal Protein S8.

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

- Molecule 40 is a protein called 30S Ribosomal Protein S9.

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

- Molecule 41 is a protein called 30S Ribosomal Protein S10.

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

- Molecule 42 is a protein called 30S Ribosomal Protein S11.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 30S Ribosomal Protein S12.

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

- Molecule 44 is a protein called 30S Ribosomal Protein S13.

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

- Molecule 45 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 46 is a protein called 30S Ribosomal Protein S15.

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

- Molecule 47 is a protein called 30S Ribosomal Protein S16.

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

- Molecule 48 is a protein called 30S Ribosomal Protein S17.

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

- Molecule 49 is a protein called 30S Ribosomal Protein S18.

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

- Molecule 50 is a protein called 30S Ribosomal Protein S19.

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

- Molecule 51 is a protein called 30S Ribosomal Protein S20.

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

- Molecule 52 is a protein called 30S Ribosomal Protein THX.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	14	Total	C	N	O	P	0	0	0
			281	125	51	91	14			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	75	Total 1574	C 704	N 283	O 512	P 73	S 2	0	0	1
54	1y	74	Total 1581	C 707	N 285	O 515	P 73	S 1	0	0	0
54	2w	74	Total 1547	C 688	N 278	O 507	P 73	S 1	0	0	1
54	2y	73	Total 1561	C 698	N 283	O 507	P 72	S 1	0	0	0

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	963	Total	Mg	0	0
			963	963		
56	1B	29	Total	Mg	0	0
			29	29		
56	1D	5	Total	Mg	0	0
			5	5		
56	1E	6	Total	Mg	0	0
			6	6		
56	1F	7	Total	Mg	0	0
			7	7		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	7	Total	Mg	0	0
			7	7		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	239	Total 239	Mg 239	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	6	Total 6	Mg 6	0	0
56	1x	10	Total 10	Mg 10	0	0
56	1y	2	Total 2	Mg 2	0	0
56	2A	673	Total 673	Mg 673	0	0
56	2B	18	Total 18	Mg 18	0	0
56	2D	4	Total 4	Mg 4	0	0
56	2E	5	Total 5	Mg 5	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2O	2	Total 2	Mg 2	0	0
56	2P	1	Total 1	Mg 1	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2T	1	Total 1	Mg 1	0	0
56	2U	4	Total 4	Mg 4	0	0
56	2V	1	Total 1	Mg 1	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	3	Total 3	Mg 3	0	0
56	23	1	Total 1	Mg 1	0	0
56	26	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2a	196	Total 196	Mg 196	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	1	Total 1	Mg 1	0	0

Continued on next page...

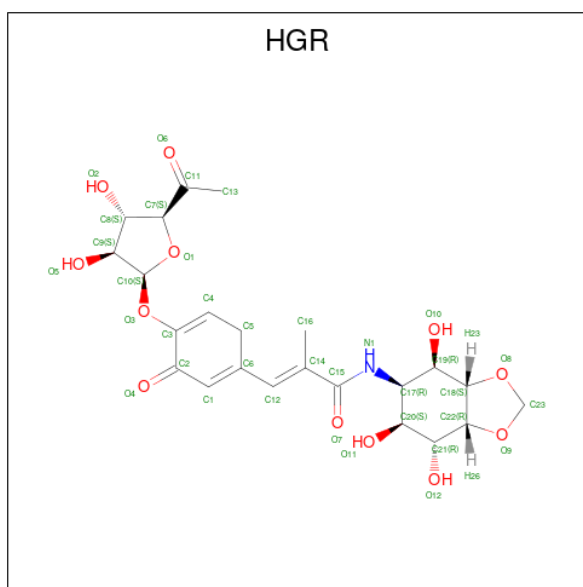
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2w	3	Total	Mg	0	0
			3	3		
56	2x	2	Total	Mg	0	0
			2	2		

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

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

- Molecule 58 is Hygromycin A (CCD ID: HGR) (formula: C₂₃H₂₉NO₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			36	23	1	12		
58	2A	1	Total	C	N	O	0	0
			36	23	1	12		

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

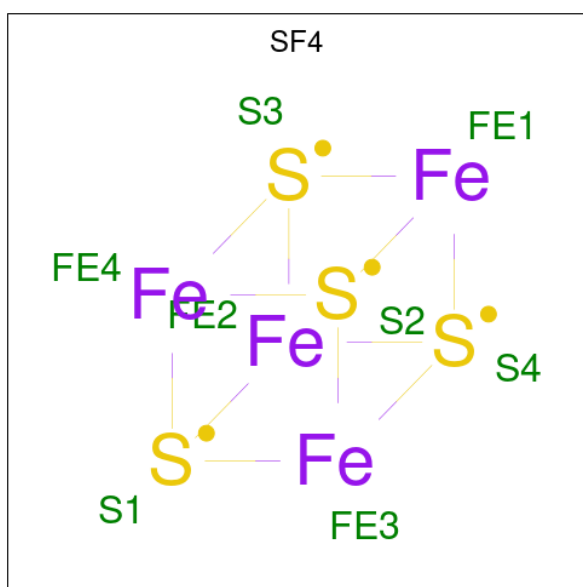
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

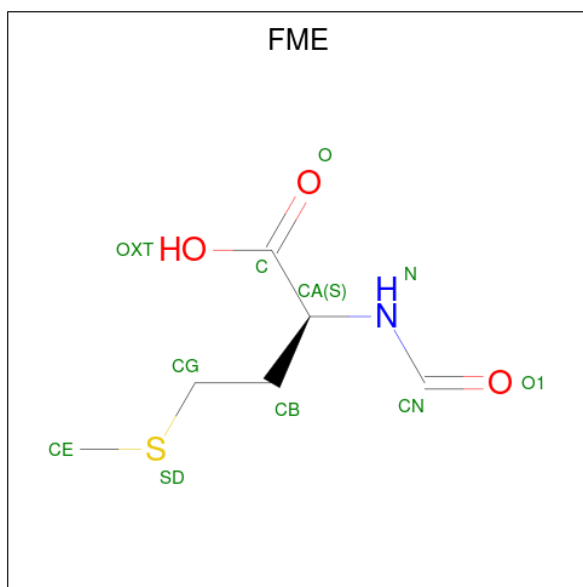
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

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



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

- Molecule 61 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	1x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		
61	2x	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1577	Total	O	0	0
			1577	1577		
62	1B	43	Total	O	0	0
			43	43		
62	1D	23	Total	O	0	0
			23	23		
62	1E	25	Total	O	0	0
			25	25		
62	1F	17	Total	O	0	0
			17	17		
62	1G	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1H	1	Total 1	O 1	0	0
62	1N	3	Total 3	O 3	0	0
62	1O	4	Total 4	O 4	0	0
62	1P	20	Total 20	O 20	0	0
62	1Q	4	Total 4	O 4	0	0
62	1R	5	Total 5	O 5	0	0
62	1S	3	Total 3	O 3	0	0
62	1T	4	Total 4	O 4	0	0
62	1U	9	Total 9	O 9	0	0
62	1V	5	Total 5	O 5	0	0
62	1W	8	Total 8	O 8	0	0
62	1X	7	Total 7	O 7	0	0
62	1Y	2	Total 2	O 2	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	9	Total 9	O 9	0	0
62	11	3	Total 3	O 3	0	0
62	12	4	Total 4	O 4	0	0
62	13	3	Total 3	O 3	0	0
62	14	1	Total 1	O 1	0	0
62	15	4	Total 4	O 4	0	0
62	16	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	17	5	Total 5	O 5	0	0
62	18	10	Total 10	O 10	0	0
62	19	1	Total 1	O 1	0	0
62	1a	287	Total 287	O 287	0	0
62	1e	1	Total 1	O 1	0	0
62	1h	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	4	Total 4	O 4	0	0
62	1m	1	Total 1	O 1	0	0
62	1n	1	Total 1	O 1	0	0
62	1o	1	Total 1	O 1	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	1	Total 1	O 1	0	0
62	1s	1	Total 1	O 1	0	0
62	1v	3	Total 3	O 3	0	0
62	1w	8	Total 8	O 8	0	0
62	1x	6	Total 6	O 6	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1063	Total 1063	O 1063	0	0
62	2B	10	Total 10	O 10	0	0
62	2D	20	Total 20	O 20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2E	9	Total 9	O 9	0	0
62	2F	7	Total 7	O 7	0	0
62	2I	1	Total 1	O 1	0	0
62	2N	2	Total 2	O 2	0	0
62	2O	1	Total 1	O 1	0	0
62	2P	14	Total 14	O 14	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	2	Total 2	O 2	0	0
62	2U	1	Total 1	O 1	0	0
62	2V	2	Total 2	O 2	0	0
62	2W	2	Total 2	O 2	0	0
62	2X	3	Total 3	O 3	0	0
62	2Y	1	Total 1	O 1	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	4	Total 4	O 4	0	0
62	21	3	Total 3	O 3	0	0
62	23	1	Total 1	O 1	0	0
62	25	2	Total 2	O 2	0	0
62	26	2	Total 2	O 2	0	0
62	28	5	Total 5	O 5	0	0

Continued on next page...

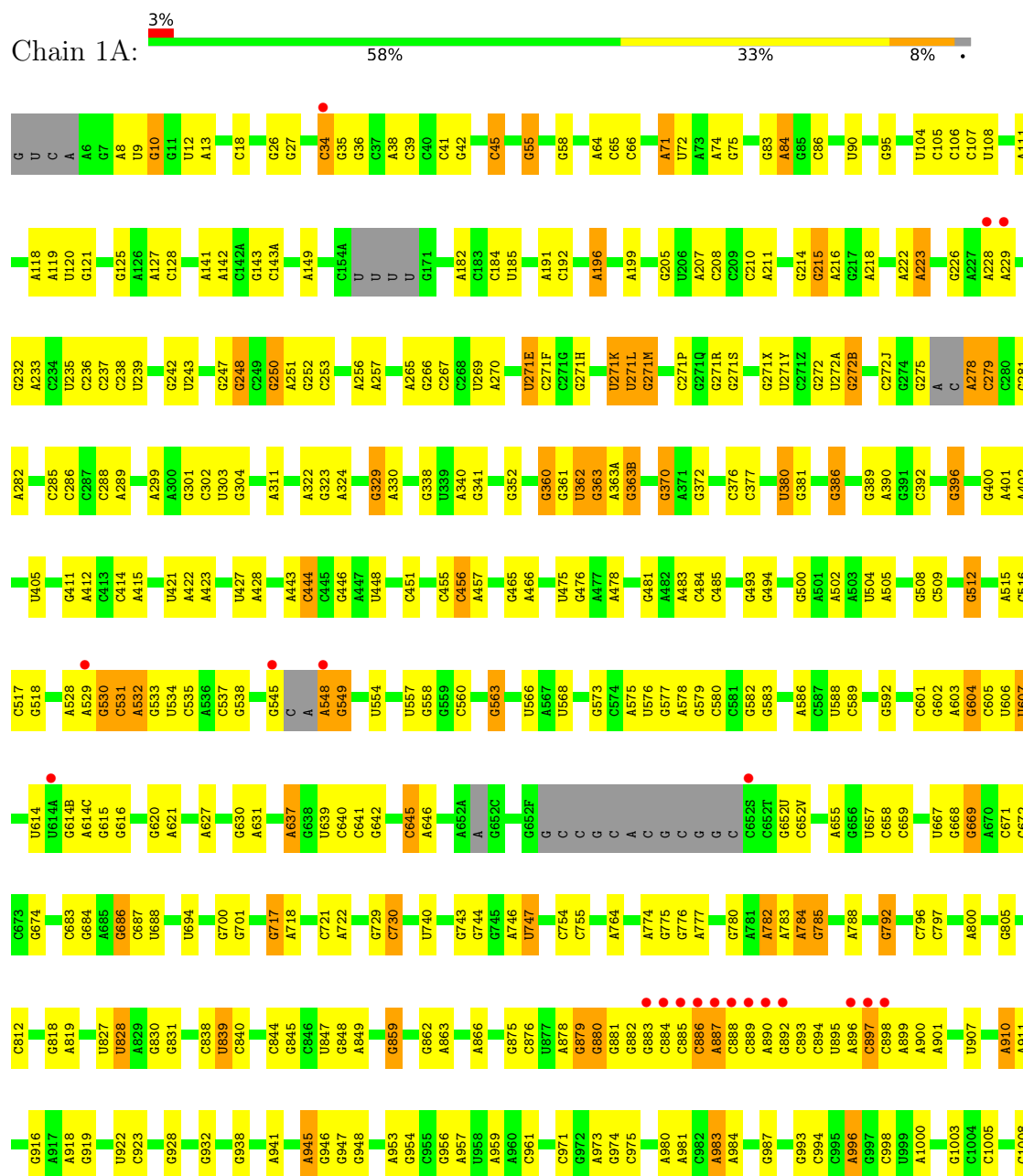
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	29	1	Total 1	O 1	0	0
62	2a	213	Total 213	O 213	0	0
62	2d	3	Total 3	O 3	0	0
62	2g	2	Total 2	O 2	0	0
62	2i	2	Total 2	O 2	0	0
62	2j	5	Total 5	O 5	0	0
62	2l	3	Total 3	O 3	0	0
62	2n	1	Total 1	O 1	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	3	Total 3	O 3	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	1	Total 1	O 1	0	0
62	2w	2	Total 2	O 2	0	0
62	2x	6	Total 6	O 6	0	0

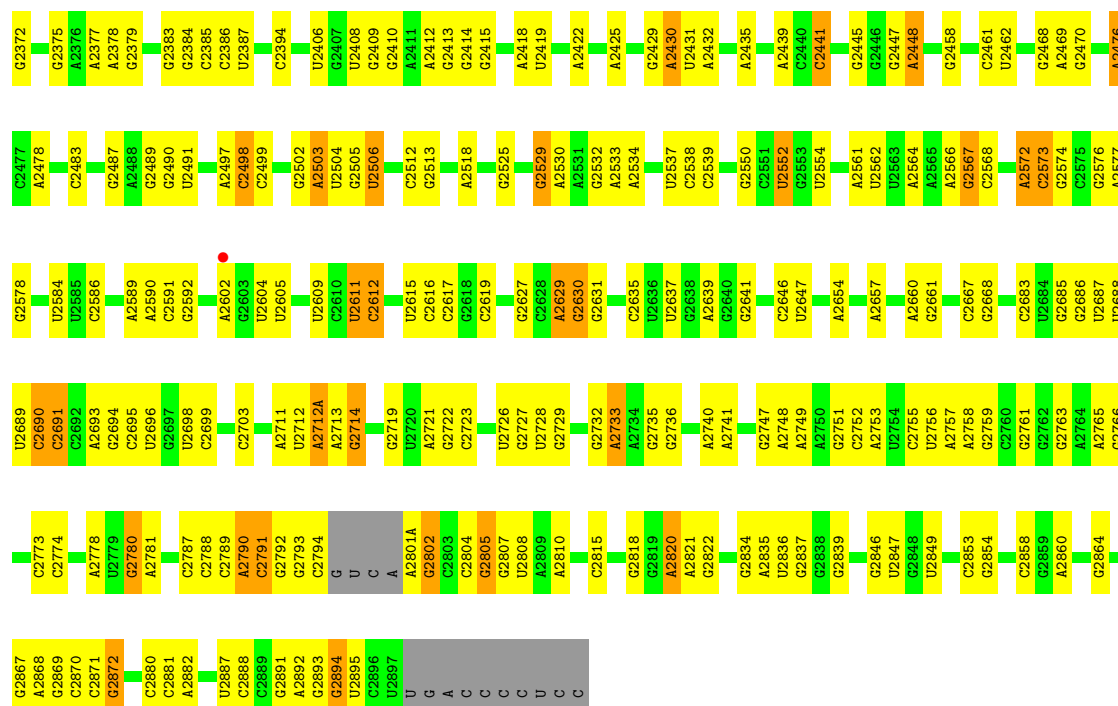
3 Residue-property plots

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.

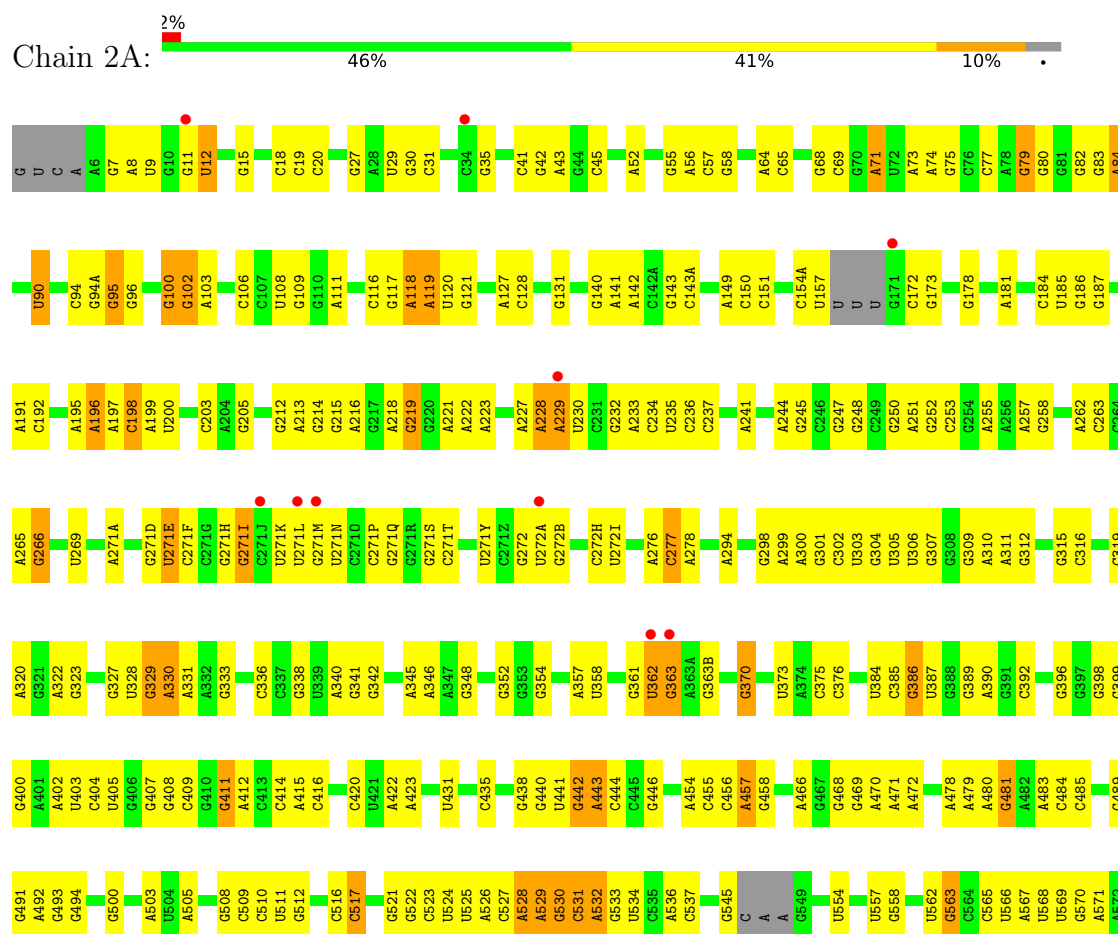
• Molecule 1: 23S Ribosomal RNA



A2287	C2175	G2002	G1906	G1793	C1683	A1554	G1442	G1338	A1253	C1153	C1079	A1009
A2288	A2176	G2012	G1907	U1794	C1684	A1557	A1445	U1341	A1254	G1154	C1080	A1010
A2289	C2177	A2013	C1908	U1796	U1688	A1558	A1446	A1342	U1255	A1155	U1081	G1011
G2290	A2118	A2014	U1911	C1797	U1693	A1566	G1448	U1352	C1257	A1156	U1082	U1012
C2291	A2119	G2018	A1912	U1798	U1696	A1569	A1449	A1353	C1258	C1161	A1084	U1014
C2292	G2181	G2018	A1913	C1799	G1696	A1589	G1450	A1354	G1259	G1164	A1085	G1022
U2296	G2182	U2022	A1914	C1800	G1697	A1589	A1452	A1355	C1260	U1165	A1086	U1023
C2297	C2183	G2023	U1915	A1801	A1698	U1578	A1453	G1356	C1261	C1166	G1087	G1024
A2298	G2124	A2023	A1916	A1802	G1699	A1579	G1455	U1357	U1262	U1169	A1088	G1025
C2299	G2125	U2028	A1918	A1803	G1700	A1580	G1461	A1358	U1263	G1170	U1090	U1026
U2306	A2126	G2032	A1919	A1810	A1701	G1581	G1462	A1359	A1264	G1169	U1091	A1027
U2189	G2127	A2031	U1920	G1811	G1702	C1584	G1466	A1360	A1265	C1171	G1092	A1028
G2190	C2128	A2032	U1921	A1815	G1703	A1586	C1467	U1267	A1268	G1173	G1093	A1032
G2191	U2130	A2033	U1927	A1816	U1709	A1587	C1468	A1268	U1274	U1174	U1094	A1033
G2192	U2131	G2033	A1928	G1817	C1710	C1588	C1471	A1269	A1275	U1175	A1095	U1034
C2196	U2132	A2042	G1929	U1823	U1713	C1589	U1471	A1365	G1270	G1176	A1096	G1035
U2197	A2134	C2043	U1930	G1824	G1714	U1602	G1478	G1371	A1272	C1178	U1097	U1036
A2198	A2135	G2049	U1936	G1825	G1717	U1609	G1478	U1372	A1273	C1179	G1099	G1039
G2206	C2136	G2050	A1937	A1825	G1718	A1610	G1482	A1379	A1274	G1183	U1101	C1041
G2207	C2137	A2051	A1938	G1826	G1718	A1610	G1484	G1380	A1275	U1184	C1102	G1042
G2220	C2138	G2052	U1939	C1827	A1722	G1630	G1493	A1384	G1276	G1185	A1103	G1043
G2221	C2140	G2053	U1942	A1829	U1739	A1608	C1494	A1385	A1277	G1186	G1104	G1044
G2222	G2141	A2054	U1946	C1830	C1745A	A1609	A1494	G1386	A1287	U1187	U1105	A1045
G2223	C2142	G2055	U1947	U1833	G1746	A1610	A1495	C1387	U1292	G1188	G1106	A1046
G2224	C2143	G2056	U1948	U1837	G1750	G1630	A1508	U1394	C1293	G1197	U1108	G1047
A2225	U2144	G2056	U1949	C1837	G1756	G1636	C1509	A1395	U1297	U1198	C1109	A1048
U2233	C2145	A2059	A1952	U1843	U1759	A1637	A1509A	U1396	C1297	C1201	G1111	G1051
G2234	G2146	A2060	A1953	C1843	G1764	A1637	A1509B	U1400	U1300	A1204	G1112	C1052
A2327	C2147	G2061	U1954	G1846	A1763	U1638	U1512	G1401	A1301	G1113	U1113	C1053
G2238	G2148	G2069	U1955	A1847	U1763	U1639	C1513	G1402	A1302	G1114	G1114	A1054
G2239	U2150	U2074	C1958	A1848	G1764	A1641	U1514	C1403	G1303	A1210	G1115	G1055
U2243	G2151	U2075	U1962	G1849	C1765	G1645	U1518	C1404	U1306	U1211	C1116	G1056
U2244	G2152	U2086	U1963	G1850	G1765	C1646	G1519	U1405	C1306	C1218	G1122	A1057
A2335	G2153	G2087	U1967	U1851	U1766	C1647	G1526	U1406	U1313	G1219	G1125	G1058
G2340	G2154	G2087	U1968	C1852	C1767	G1648	G1527	U1407	U1314	A1220	G1126	G1059
G2341	G2155	G2083	A1969	A1854	U1768	C1648	U1528	G1421	C1320	G1230	U1128	U
A2267	A2157	U2098	U1970	G1861	G1769	G1653	A1528A	G1416	C1315	G1235	A1128	G1062
A2268	G2159	U2096	A1971	C1866	A1773	A1654	A1528A	C1417	U1316	U1238	A1129	G1063
A2269	C2160	C2097	A1972	C1866	U1778	A1654	C1531	G1418	A1317	G1239	U1130	G1064
G2270	C2161	U2098	U1972	C1866	U1778	U1659	C1532	A1419	C1318	U1240	C1135	U1065
G2351	G2162	U2099	G1985	A1877	U1779	U1659	G1532	U1420	G1319	A1430	C1136	U1066
U2272	C2163	G2100	A1986	G1878	A1780	A1664	G1532	G1421	C1320	A1241	G1137	A1067
A2273	C2164	G2101	U1986	G1878	C1781	A1664	G1532	G1421	C1320	A1241	G1137	A1068
A2274	G2165	U2102	U1989	C1881	C1782	A1669	G1532	G1421	C1320	A1241	G1137	A1068
G2277	U2167	C2105	G1989	C1881	C1782	A1669	G1532	G1421	C1320	A1241	G1137	A1068
A2278	C2168	G2106	G1992	C1882	A1783	C1670	G1537	G1428	U1328	G1238	U1141	A1070
G2279	A2169	C2107	U1993	C1882	A1784	C1670	G1537	G1429	U1329	G1239	U1141	G1071
A2361	A2170	C2108	U1996	A1889	A1785	U1540	U1540	C1430	C1330	U1240	A1143	A1073
G2364	A2171	U2109	C1996	A1890	A1786	G1674	U1541	C1431	A1331	A1241	A1144	G1074
C2284	U2172	G2110	G1997	G1899	C1790	C1675	A1542	C1432	G1332	G1244	G1149	G1075
C2285	A2173	U2113	A2001	A1900	A1791	G1678	C1547	U1433	C1333	G1244	C1150	G1076
A2286	C2174	U2113	A2001	A1900	A1791	G1678	C1547	G1441	G1337	G1252	G1150	A1077



• Molecule 1: 23S Ribosomal RNA

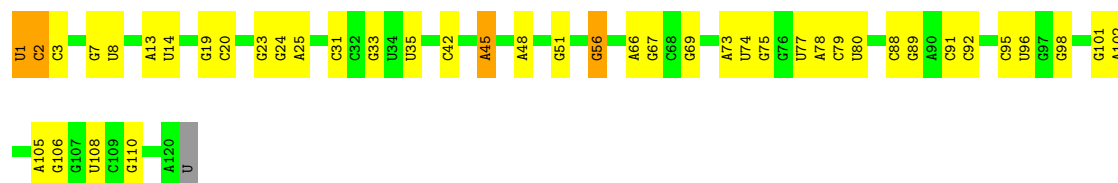




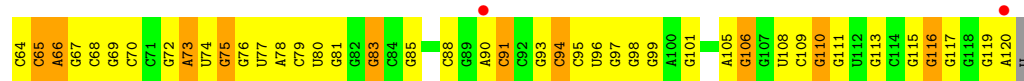
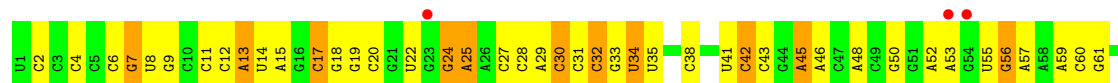
C2767	U2696	U2615	U2357	A2450	U2357	A2287	A2198	A2133	A2062	G1973	G1883	C1782	A1655
C2768		C2616	C2358	G2454	C2359	U2291	A2199	A2134	C2063	A1978	A1889	A1783	C1656
C2769	C2699	C2617	C2538	G2454	C2360	C2292	C2200	A2135	C2064		A1890	A1784	C1657
C2770	C2700	A2621	A2361	U2462	A2361	C2293	G2206	C2138	C2066	C1987	C1894	A1786	C1662
C2771	C2701	U2462	C2364	U2462	C2365	C2294	G2207	C2139	G2069	C1988	C1895	C1663	C1663
C2772	C2702	U2462	C2365	C2465	C2366	C2295	G2208	C2140	G2070			A1654	A1654
C2773	C2703	C2465	C2366	C2465	C2367	C2296	A2203	C2141	A2071	U1991	G1899	C1790	A1665
A2778	C2704	C2628	A2369	A2469	A2369	C2297	U2218	C2142	C2072	G1992	A1900	A1791	G1666
U2779	C2706	C2627	A2370	A2469	A2370	A2298	U2218	C2143	C2073	U1993			
C2785	A2711	G2628	G2371	C2474	G2371		G2224	C2144	U2074	G1996	G1906	U1794	C1670
U2788	U2712	A2629	C2474	C2474	A2225		A2225	U2144	U2074	G1997		U1796	U1671
C2788	A2712A	G2630	C2475	C2475	A2226		A2226	C2145	U2075	G1998	U1911	G1674	G1674
C2789	A2713	G2631	A2476	A2476	A2227		A2227	G2146	C2078	C1999	U1912	C1675	C1675
A	G2714	A2632	A2477	A2477	C2228		C2228	G2147	U2079	G2000	A1913	U1798	
C	G2715	G2633	A2478	A2478	C2229		C2229	G2148	G2080	A2001	C1914	U1799	
								G2149	C2081	G2002	U1915	U1688	U1688
C2792	G2719	U2637	C2483	C2483	U2232		U2232	U2150	C2081		A1916	A1802	A1689
G2793		G2638	G2484	G2484	U2233		U2233	G2151	G2087	C2006	U1917	A1803	G1686
C2794		A2639	C2485	C2485	G2234		G2234	G2152			A1918	A1804	G1687
G	G2722	G2640	G2486	G2486	G2235		G2235	G2153	G2090	G2010	A1919	U1805	G1697
U	C2723		G2487	G2487	G2236		G2236	G2154		G2011	A1920	U1806	A1698
C	U2726	G2645	G2488	A2488	C2313		C2313	G2155	G2093	G2012	G1921	A1810	G1699
A	G2727	C2646	A2489	A2489	G2315		G2315	G2156	G2094	A2013	G1922	A1700	A1700
A2801A	U2728	U2647	C2385	C2385	G2316		G2316	G2157	G2095	A2014	U1923	A1701	A1701
G2802	G2729	C2648	C2386	C2386	C2317		U2244	G2158	C2096		C1924	A1812	G1702
C2803	C2730	U2649	A2387	U2387	G2318		U2245	G2159	U2097	A2019		G1813	G1703
C2804	G2731	U2650	A2388	A2388	G2319		G2246	G2160	C2097	C2021	A1928	A1814	C1711
G2805	G2732		A2393	A2393	A2320		A2247	G2161	U2098	A2020	A1937	A1815	C1712
G2807	A2733	G2655	C2394	C2394	G2321		C2248	G2162	U2099	G2022	A1938	A1816	U1713
U2808			G2397	G2397	A2322		U2249	G2163		G2023	U1939	A1817	G1714
A2809	G2736	A2660	C2499	C2499	G2323		G2250	G2164	G2104	A2030		G1824	U1720
G2810	G2737	G2661	G2502	G2502	C2324		G2251	G2165	C2105	G2038	A1936	G1827	G1721
G2812		A2662	U2400	U2400	G2325		G2252	G2166	C2106	A2031	A1937	A1828	A1722
	A2740	G2663	A2503	A2503	C2326		G2253	G2167	C2107	G2032	A1938	A1829	A1739
C2815	C2741	A2664	U2504	U2504	A2327		G2254	G2168	C2108	A2033	U1939	G1830	G1740
C2816	C2742	G2665	G2505	G2505	C2328		G2255	G2169	U2109			U1833	G1746
G2817	C2743	C2666	U2506	U2506	G2329			G2170	G2110		C1942	G1835	G1756
G2818	G2744		C2507	C2507	U2330		C2261	G2171	G2111	G2037	C1946	G1836	U1757
C2819	C2745	G2669	G2508	G2508	G2331		U2262	G2172	G2112	G2038	U1947	G1837	G1758
A2820	U2746		G2509	G2509	U2332		C2263	G2173	A2114	C2040	U1951	G1838	U1762
G2821	G2747	G2673	C2510	C2510	A2333		C2264	G2174	G2115	A2042	A1952	G1839	G1763
G2822	A2748	G2674	U2511	U2511	G2334		A2267	G2175	G2116	C2045		A1847	G1764
A2823	A2750	A2675	G2512	G2512	A2335		A2268	G2176	G2117	G2046	U1955	A1848	
	G2751		G2513	G2513	A2336			G2177	A2117	U2041			G1772
G2833	C2752	A2679	U2514	U2514	G2337		U2272	G2178	U2118		C1962	A1853	G1773
A2834	A2753	U2682	A2430	A2430			A2273	G2179	G2125	G2049	U1963	C2050	C1774
G2835	U2754	C2683	U2431	U2431	G2344		A2274	G2180	G2126	A2051		G1857	U1775
U2836	C2755	U2684	A2432	A2432	G2345		A2275	G2181	G2127		C1967	G1858	G1776
G2837	U2756	G2685	A2433	A2433	C2346		C2276	G2182	G2128		U1968	U1777	U1777
G2838	A2757		A2434	A2434	C2347		U2277	G2183	G2129		A1969	U1778	U1778
G2839	U2758	A2435	G2348	G2348	U2348		A2278	G2184	C2129		A1970	G1877	U1779
G2846	G2759	G2526	A2439	A2439	C2350		C2279	G2185	G2130		A1971	G1878	U1780
U2847	C2760	G2527	G2351	G2351	G2351		G2282	G2186	G2131			U1781	
G2848	G2761	U2689	A2352	A2352	C2352		C2283	G2187	G2132				
G2849		C2690	G2353	G2353	G2353		C2284	G2188	U2130				
U2849	A2764	A2693	C2354	C2354	G2354		C2285	G2189	G2131				
G2852	G2766	G2694	A2448	A2448	C2355		A2286	G2190	U2132				
		C2695	U2449	U2449	G2356			G2191					



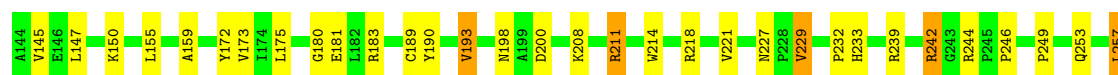
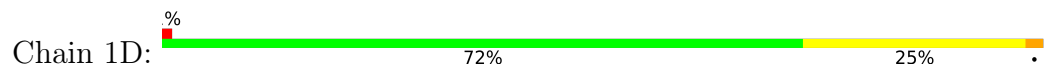
• Molecule 2: 5S Ribosomal RNA



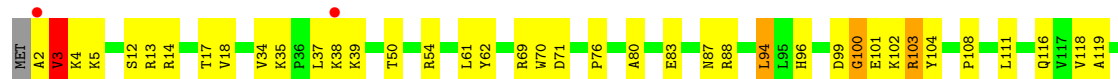
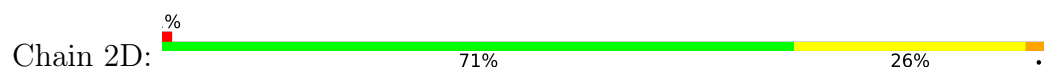
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S Ribosomal Protein L2



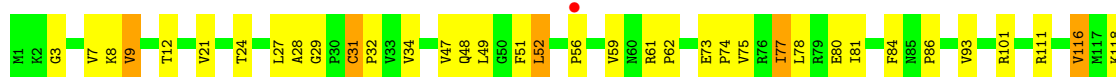
• Molecule 3: 50S Ribosomal Protein L2





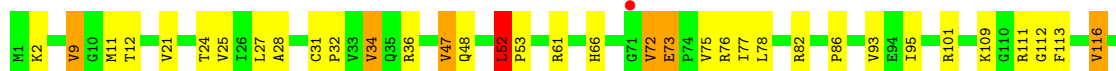
• Molecule 4: 50S Ribosomal Protein L3

Chain 1E: 71% 24% ..



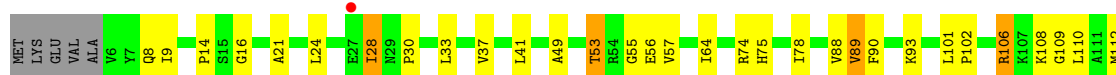
• Molecule 4: 50S Ribosomal Protein L3

Chain 2E: 71% 25% ..



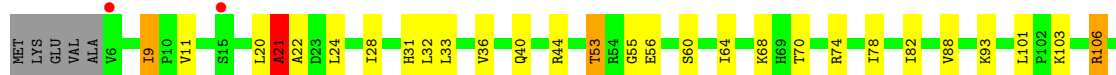
• Molecule 5: 50S Ribosomal Protein L4

Chain 1F: 65% 27% 5% .



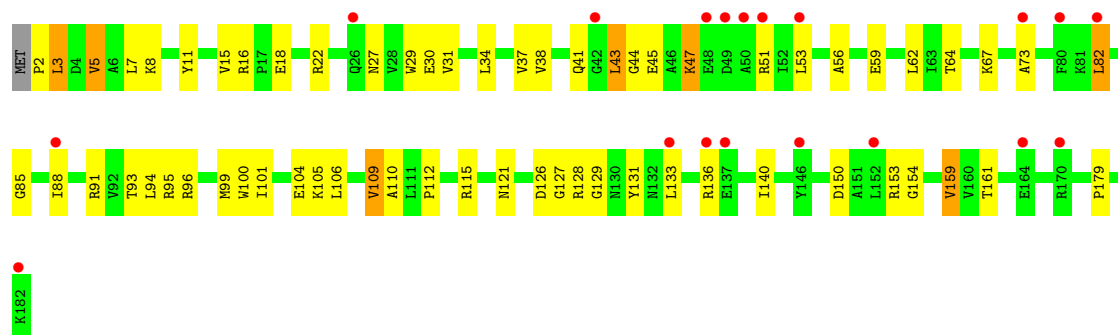
• Molecule 5: 50S Ribosomal Protein L4

Chain 2F: 61% 31% .

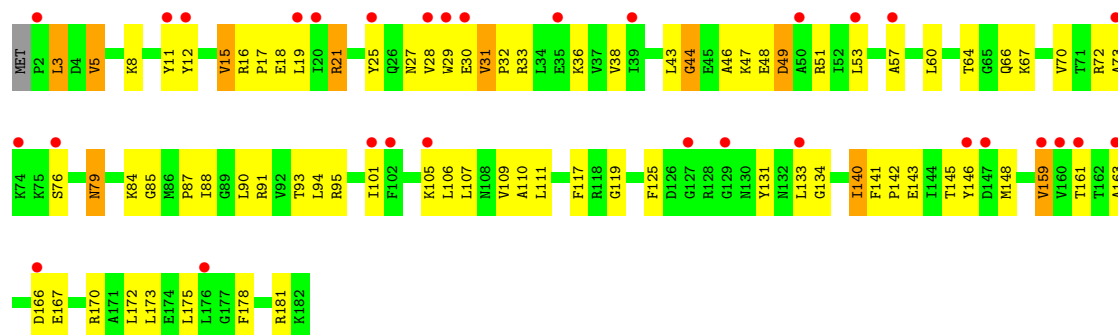




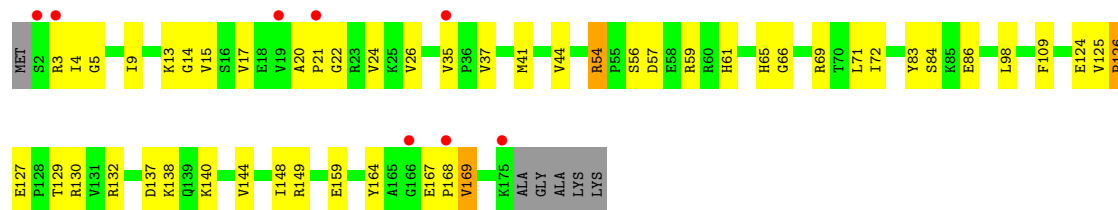
• Molecule 6: 50S Ribosomal Protein L5



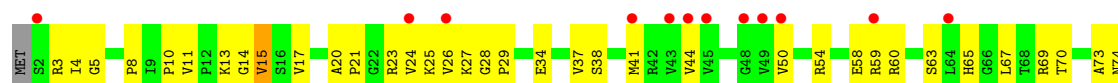
• Molecule 6: 50S Ribosomal Protein L5

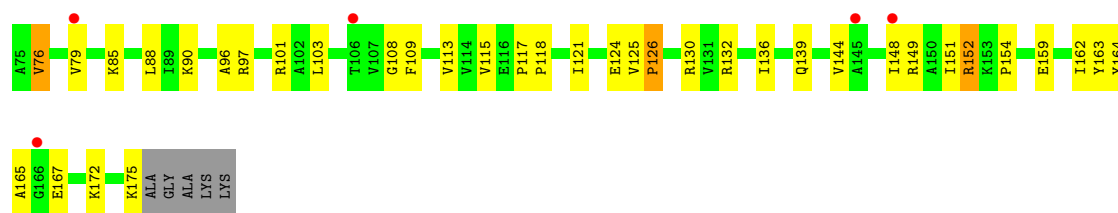


• Molecule 7: 50S Ribosomal Protein L6

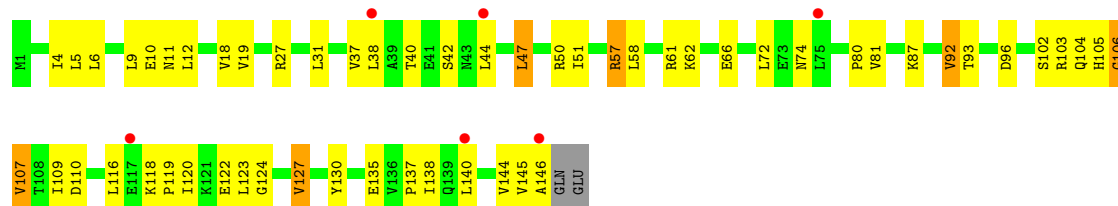


• Molecule 7: 50S Ribosomal Protein L6

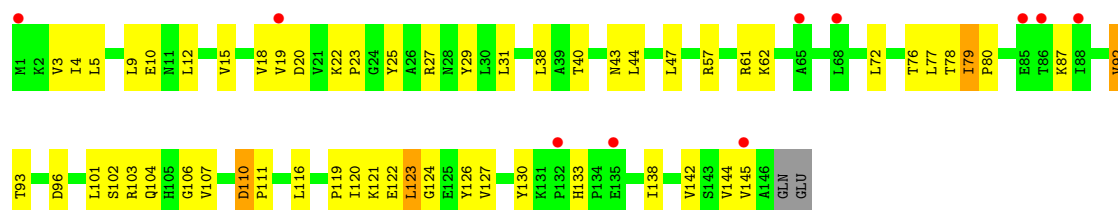




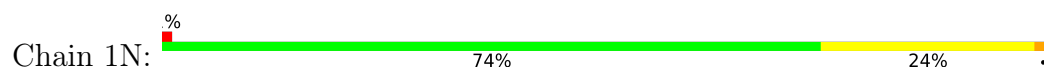
• Molecule 8: 50S Ribosomal Protein L9



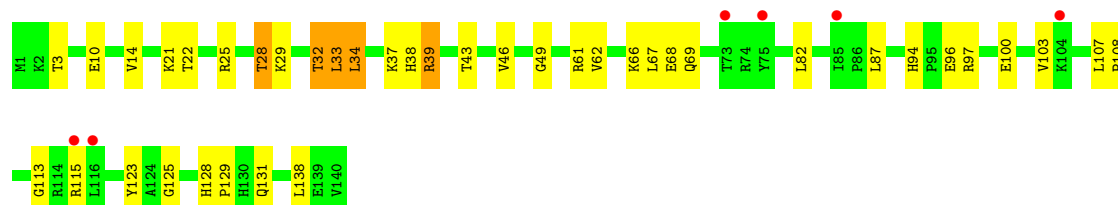
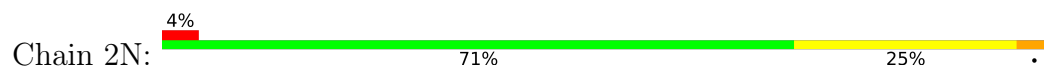
• Molecule 8: 50S Ribosomal Protein L9



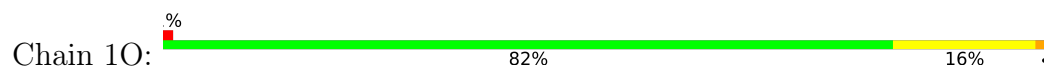
• Molecule 9: 50S Ribosomal Protein L13



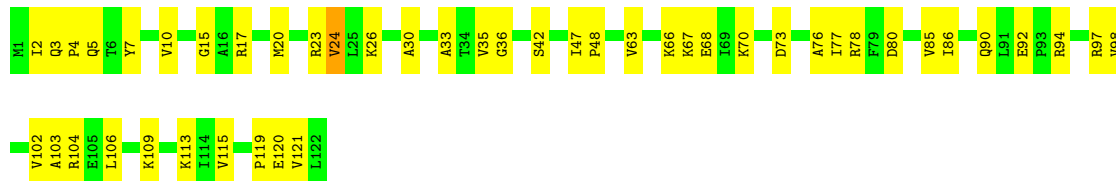
• Molecule 9: 50S Ribosomal Protein L13



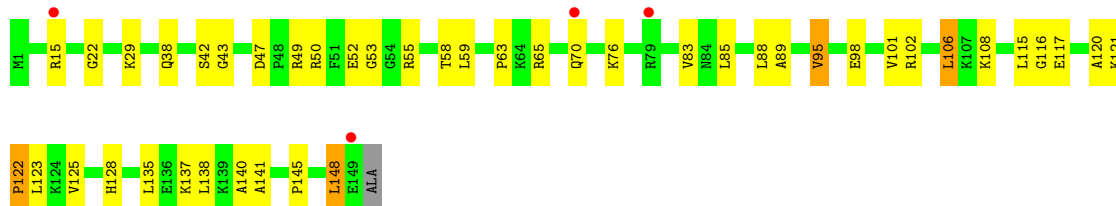
- Molecule 10: 50S Ribosomal Protein L14



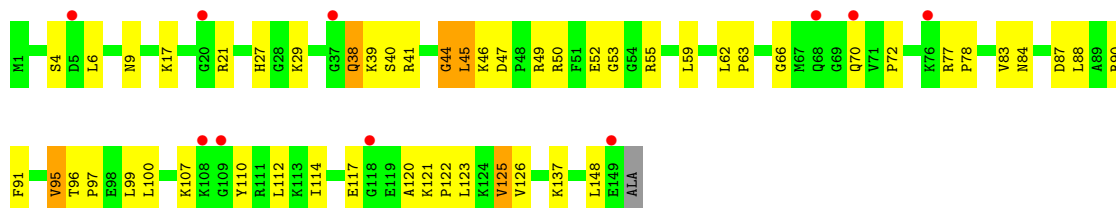
- Molecule 10: 50S Ribosomal Protein L14



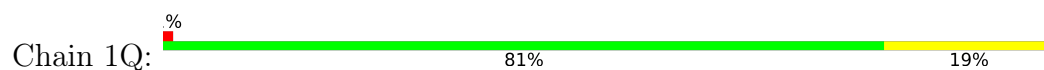
- Molecule 11: 50S Ribosomal Protein L15



- Molecule 11: 50S Ribosomal Protein L15

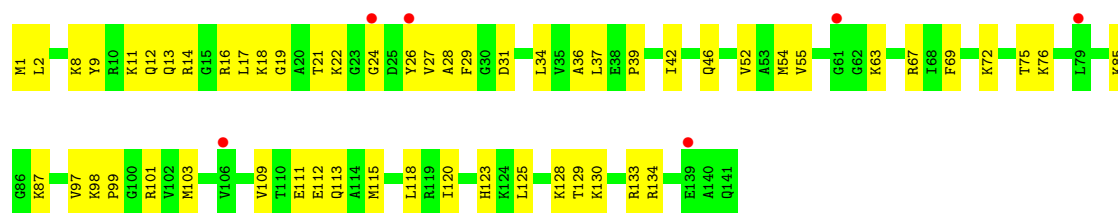


- Molecule 12: 50S Ribosomal Protein L16



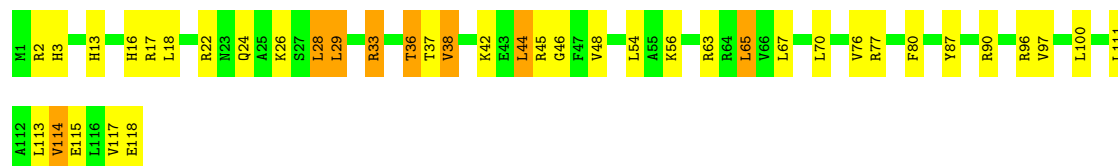
- Molecule 12: 50S Ribosomal Protein L16





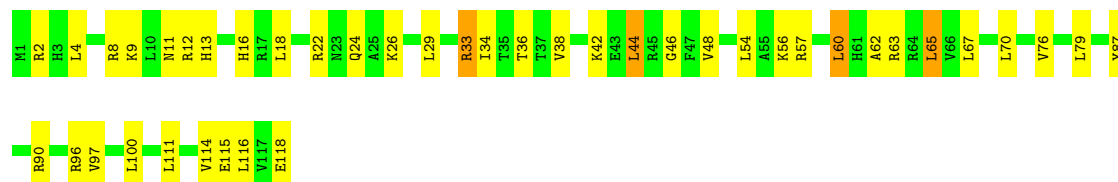
• Molecule 13: 50S Ribosomal Protein L17

Chain 1R: 66% 27% 7%



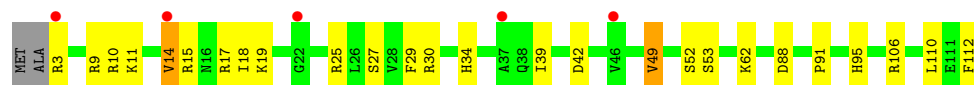
• Molecule 13: 50S Ribosomal Protein L17

Chain 2R: 64% 32% 4%



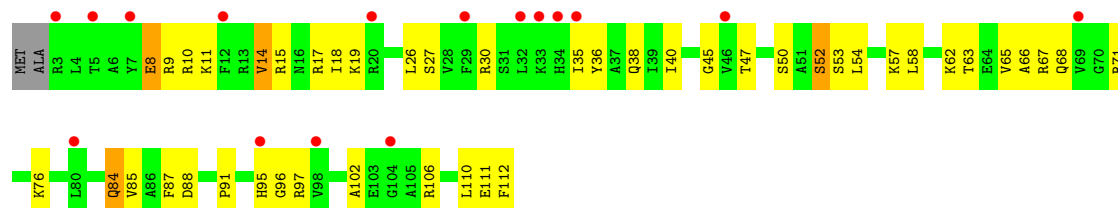
• Molecule 14: 50S Ribosomal Protein L18

Chain 1S: 75% 21% 4%



• Molecule 14: 50S Ribosomal Protein L18

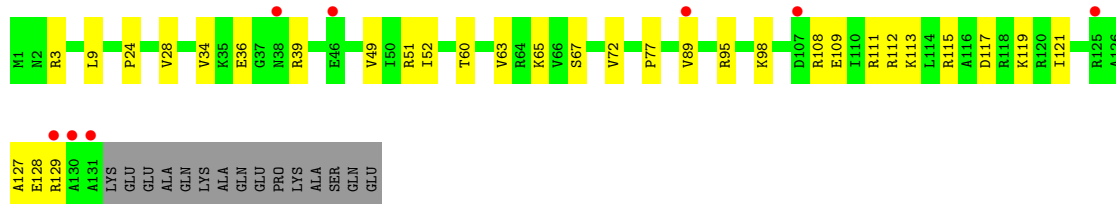
Chain 2S: 58% 37% 14%



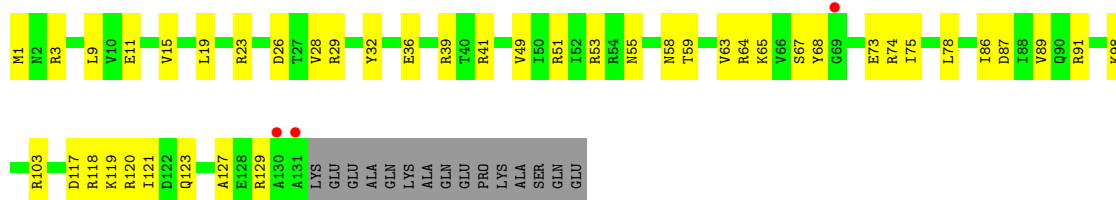
• Molecule 15: 50S Ribosomal Protein L19

Chain 1T: 68% 21% 10%

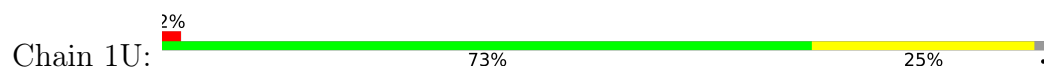




• Molecule 15: 50S Ribosomal Protein L19



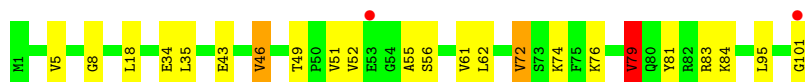
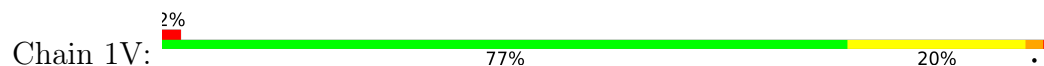
• Molecule 16: 50S Ribosomal Protein L20



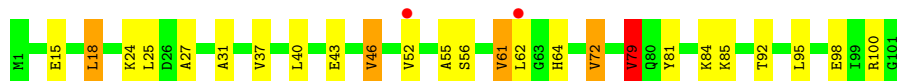
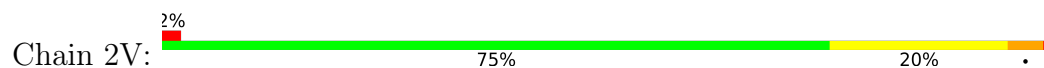
• Molecule 16: 50S Ribosomal Protein L20



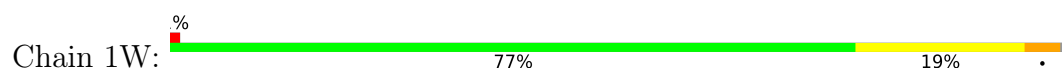
• Molecule 17: 50S Ribosomal Protein L21



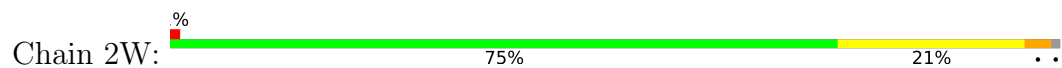
• Molecule 17: 50S Ribosomal Protein L21



• Molecule 18: 50S Ribosomal Protein L22



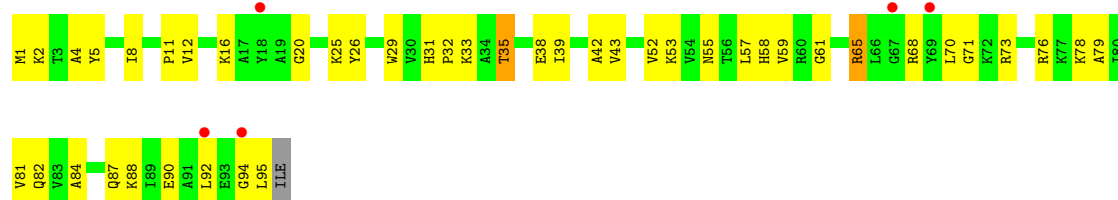
• Molecule 18: 50S Ribosomal Protein L22



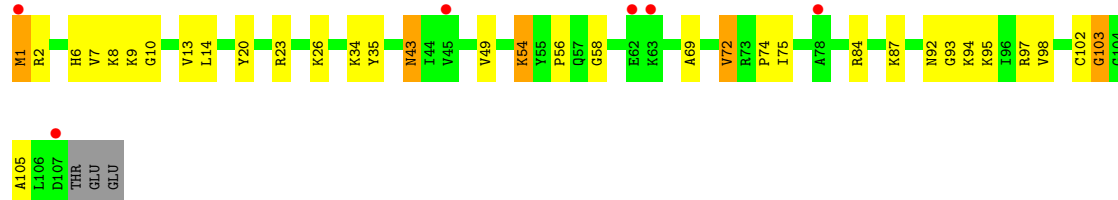
• Molecule 19: 50S Ribosomal Protein L23



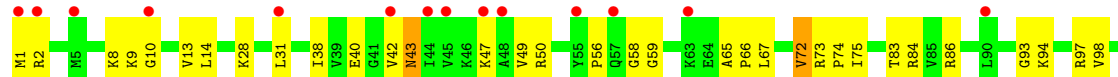
• Molecule 19: 50S Ribosomal Protein L23

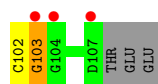


• Molecule 20: 50S Ribosomal Protein L24

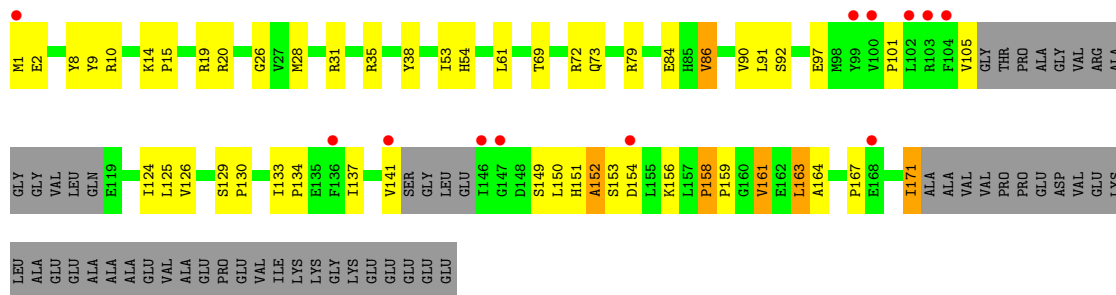


• Molecule 20: 50S Ribosomal Protein L24

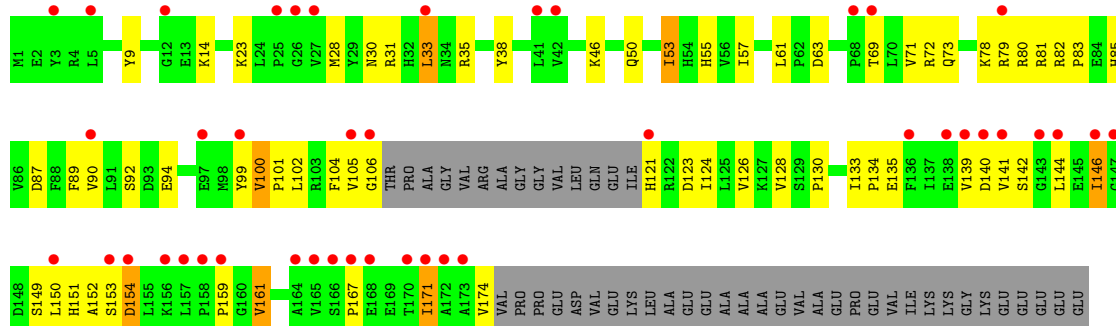




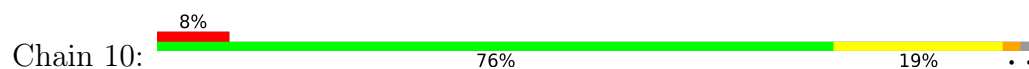
• Molecule 21: 50S Ribosomal Protein L25



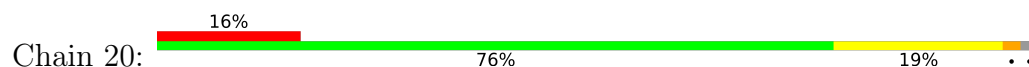
• Molecule 21: 50S Ribosomal Protein L25



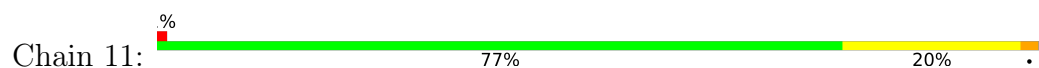
• Molecule 22: 50S Ribosomal Protein L27



• Molecule 22: 50S Ribosomal Protein L27

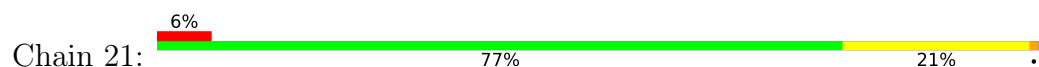


• Molecule 23: 50S Ribosomal Protein L28

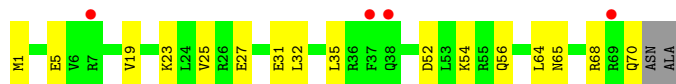
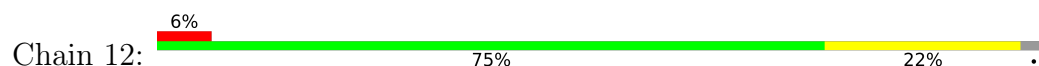




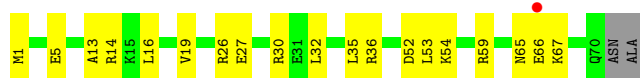
• Molecule 23: 50S Ribosomal Protein L28



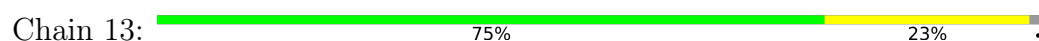
• Molecule 24: 50S Ribosomal Protein L29



• Molecule 24: 50S Ribosomal Protein L29



• Molecule 25: 50S Ribosomal Protein L30



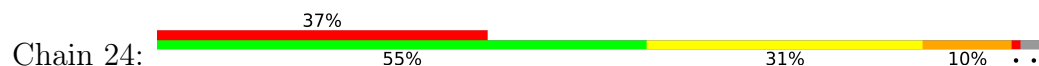
• Molecule 25: 50S Ribosomal Protein L30



• Molecule 26: 50S Ribosomal Protein L31



• Molecule 26: 50S Ribosomal Protein L31





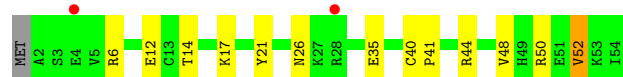
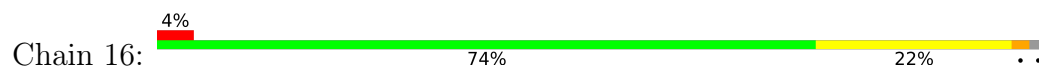
● Molecule 27: 50S Ribosomal Protein L32



● Molecule 27: 50S Ribosomal Protein L32



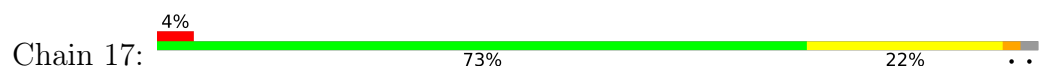
● Molecule 28: 50S Ribosomal Protein L33



● Molecule 28: 50S Ribosomal Protein L33



● Molecule 29: 50S Ribosomal Protein L34



● Molecule 29: 50S Ribosomal Protein L34



● Molecule 30: 50S Ribosomal Protein L35

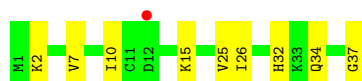
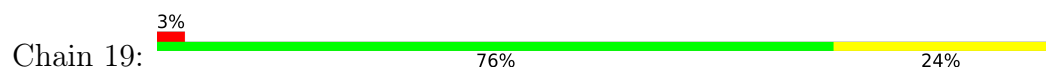




- Molecule 30: 50S Ribosomal Protein L35



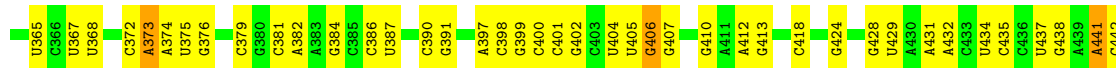
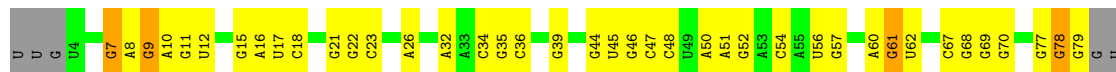
- Molecule 31: 50S Ribosomal Protein L36



- Molecule 31: 50S Ribosomal Protein L36

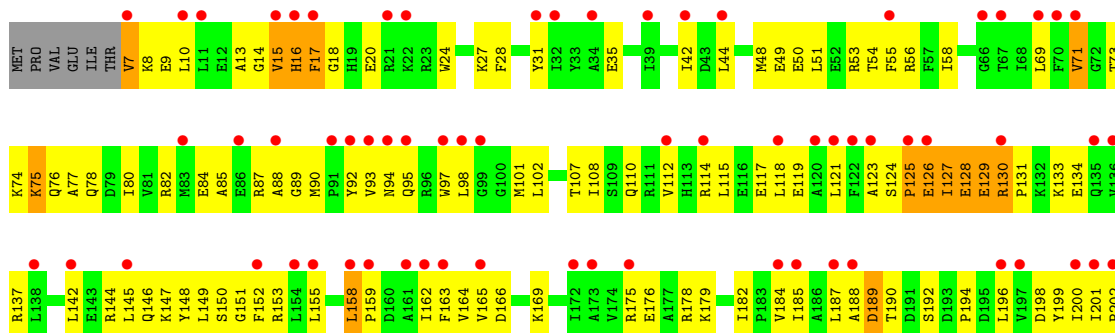


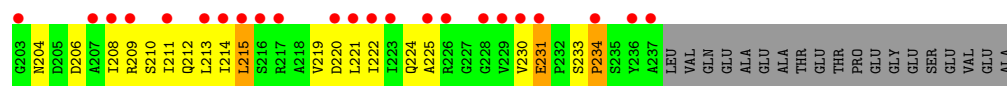
- Molecule 32: 16S Ribosomal RNA



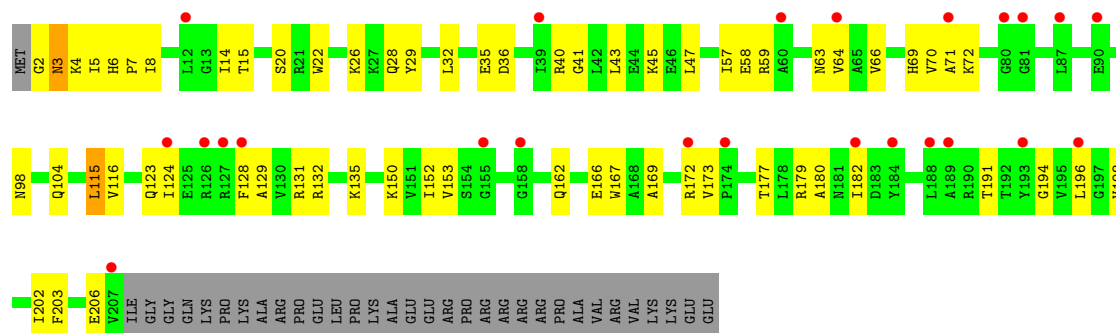




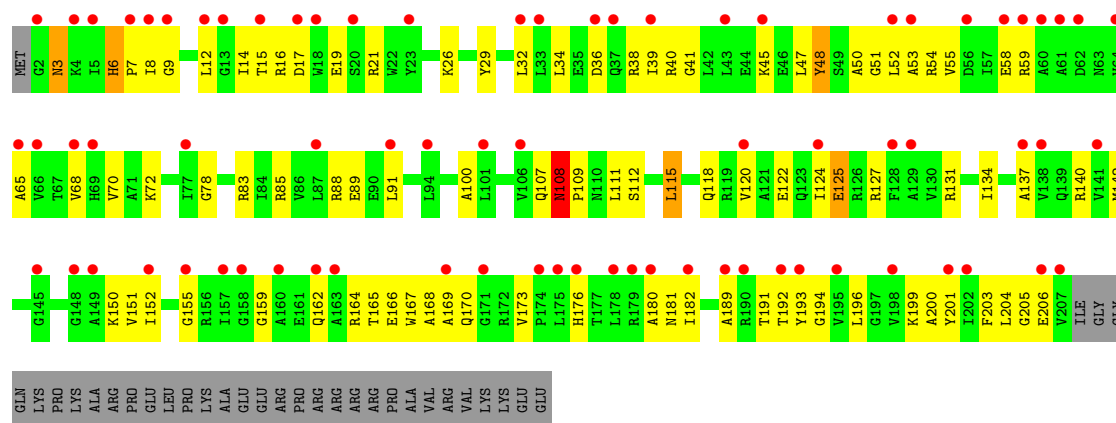




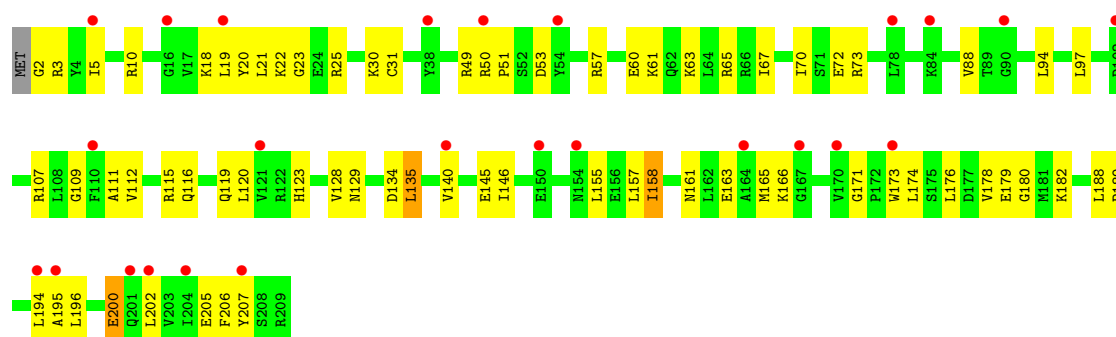
• Molecule 34: 30S Ribosomal Protein S3



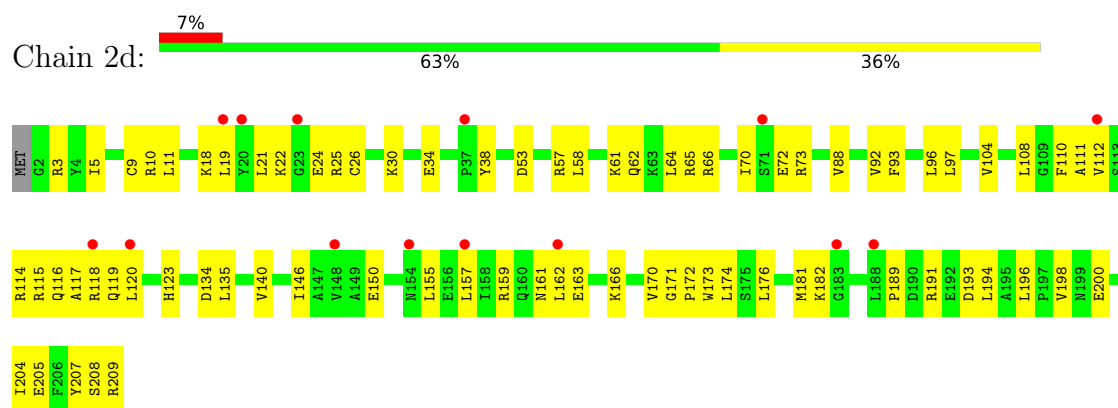
• Molecule 34: 30S Ribosomal Protein S3



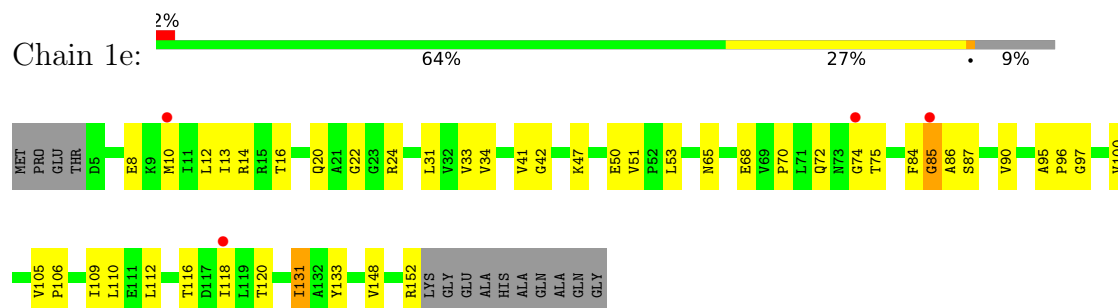
• Molecule 35: 30S Ribosomal Protein S4



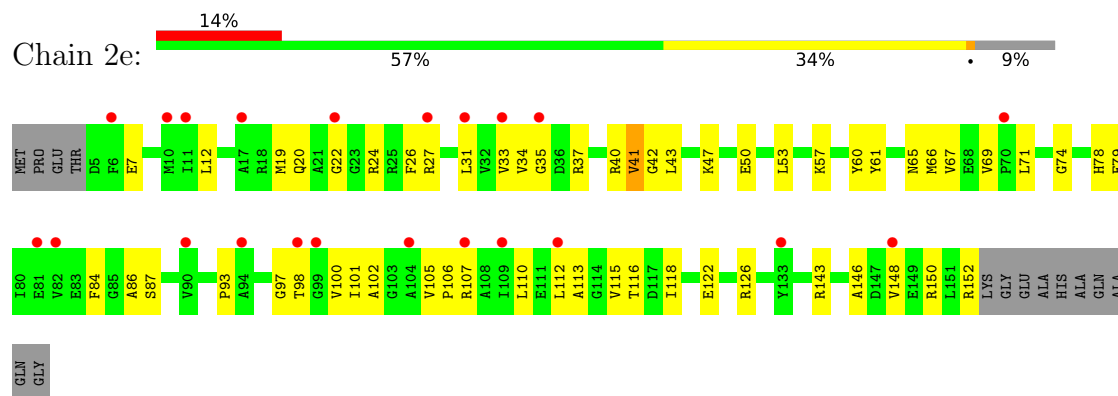
• Molecule 35: 30S Ribosomal Protein S4



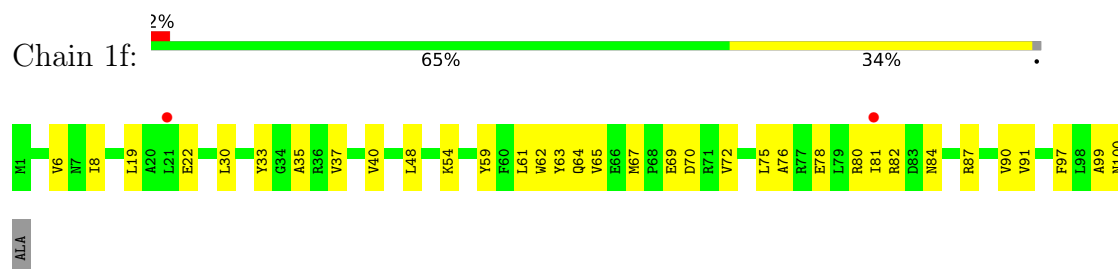
- Molecule 36: 30S Ribosomal Protein S5



- Molecule 36: 30S Ribosomal Protein S5



- Molecule 37: 30S Ribosomal Protein S6

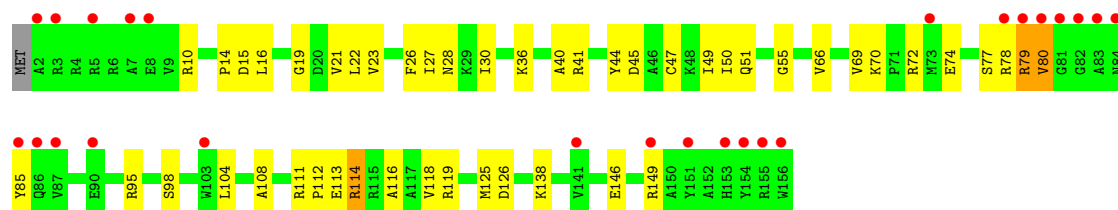


- Molecule 37: 30S Ribosomal Protein S6

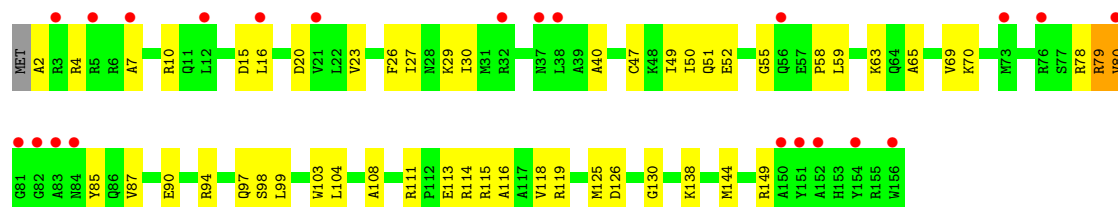




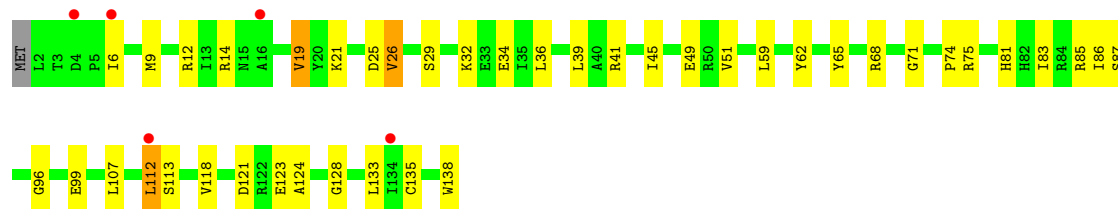
• Molecule 38: 30S Ribosomal Protein S7



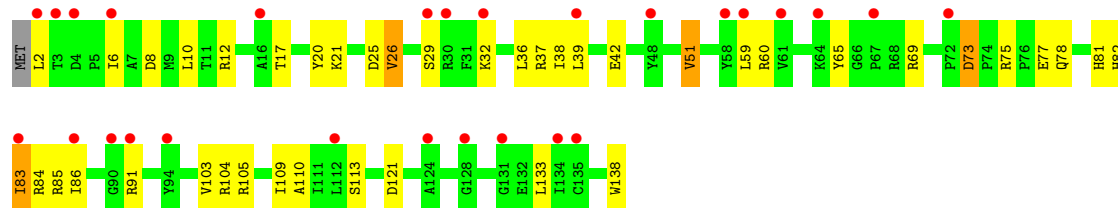
• Molecule 38: 30S Ribosomal Protein S7



• Molecule 39: 30S Ribosomal Protein S8

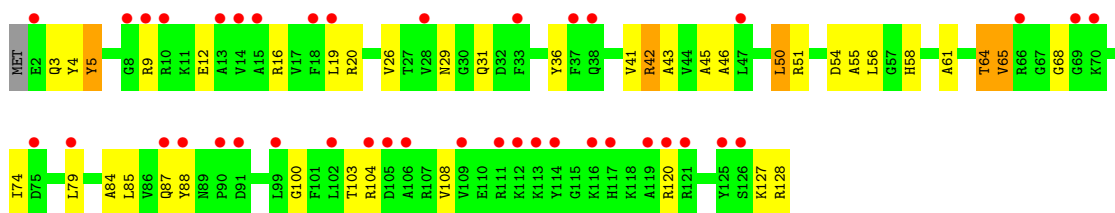


• Molecule 39: 30S Ribosomal Protein S8

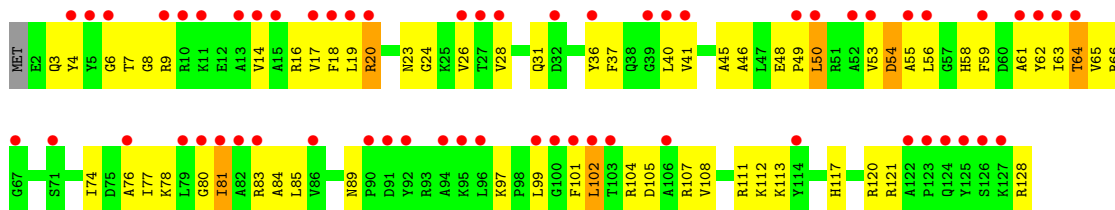


• Molecule 40: 30S Ribosomal Protein S9

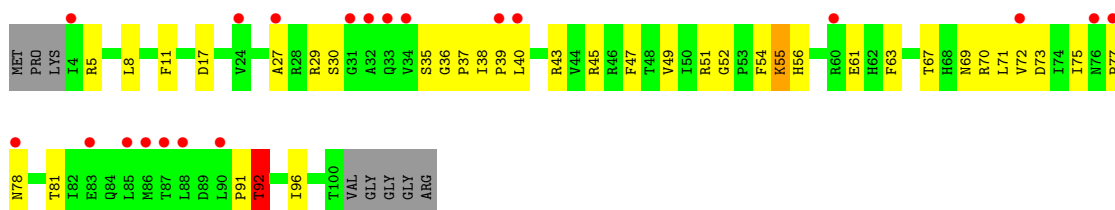




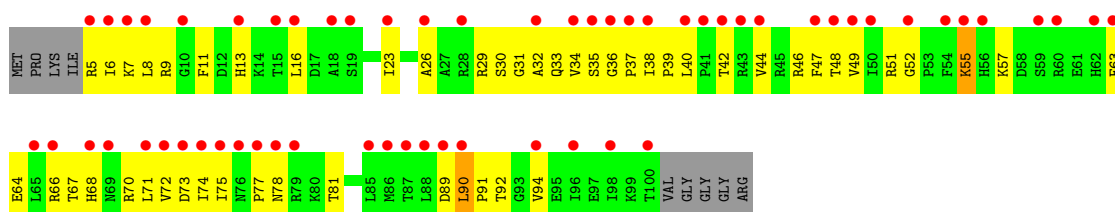
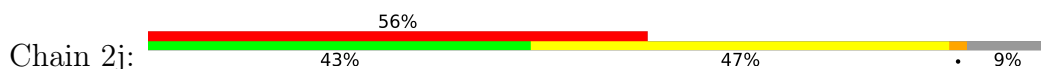
• Molecule 40: 30S Ribosomal Protein S9



• Molecule 41: 30S Ribosomal Protein S10



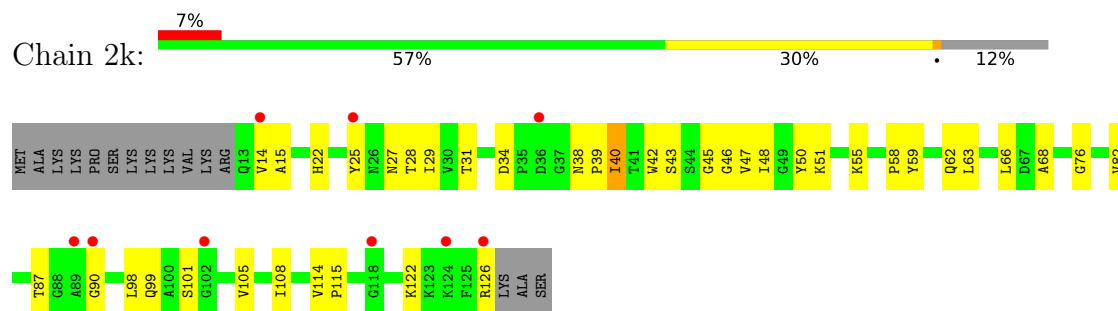
• Molecule 41: 30S Ribosomal Protein S10



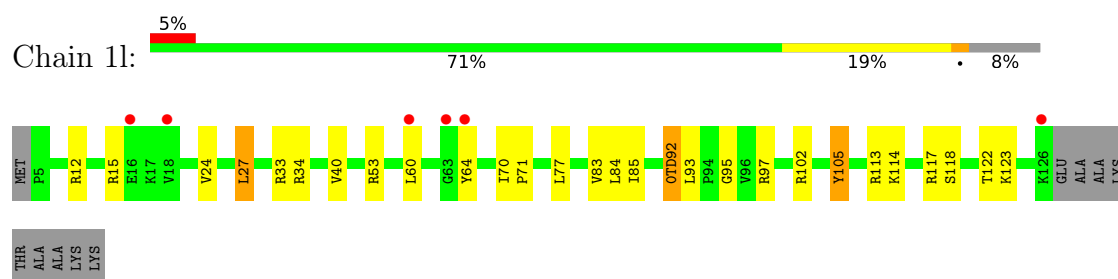
• Molecule 42: 30S Ribosomal Protein S11



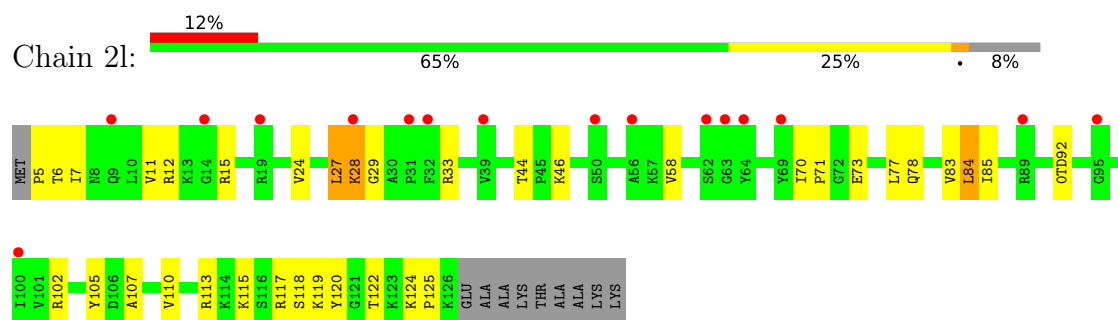
- Molecule 42: 30S Ribosomal Protein S11



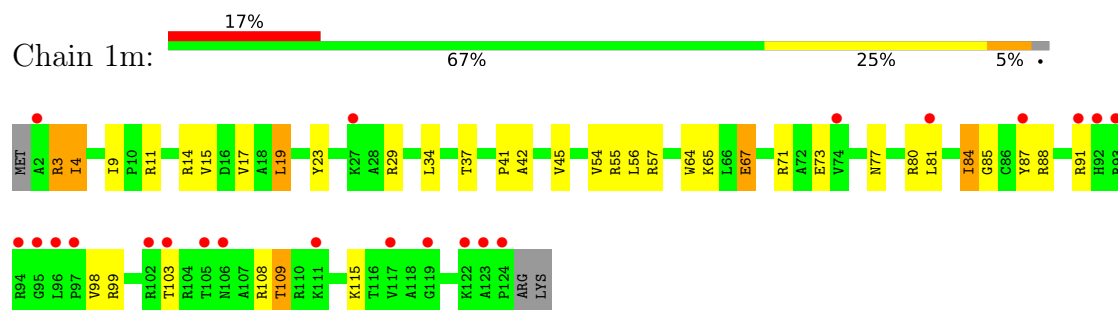
- Molecule 43: 30S Ribosomal Protein S12



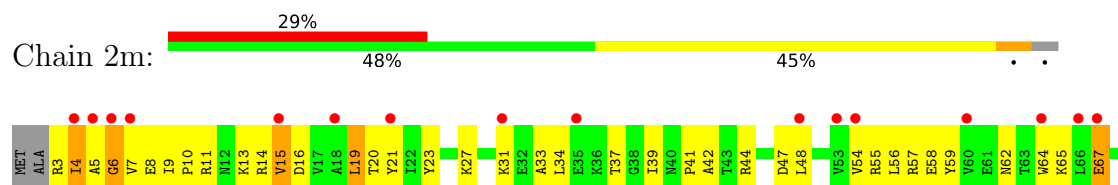
- Molecule 43: 30S Ribosomal Protein S12



- Molecule 44: 30S Ribosomal Protein S13



- Molecule 44: 30S Ribosomal Protein S13

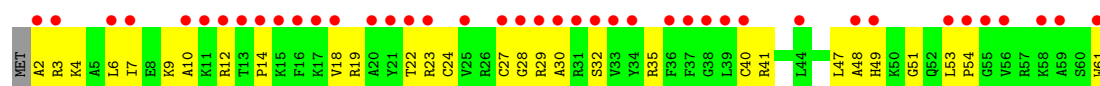




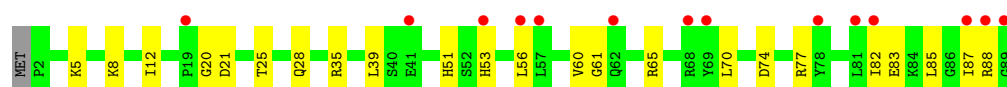
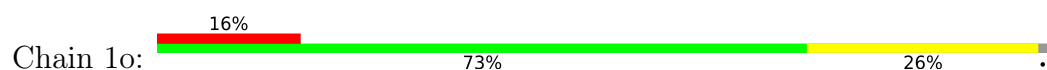
• Molecule 45: 30S Ribosomal Protein S14



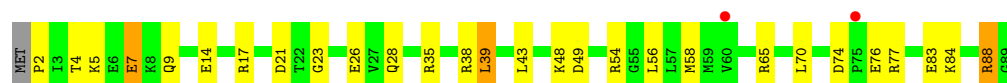
• Molecule 45: 30S Ribosomal Protein S14



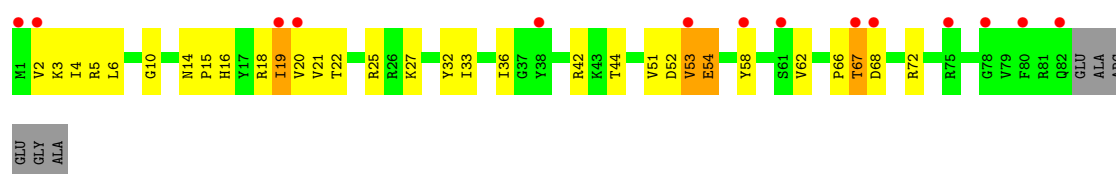
• Molecule 46: 30S Ribosomal Protein S15



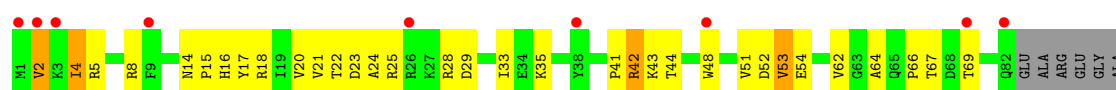
• Molecule 46: 30S Ribosomal Protein S15



• Molecule 47: 30S Ribosomal Protein S16

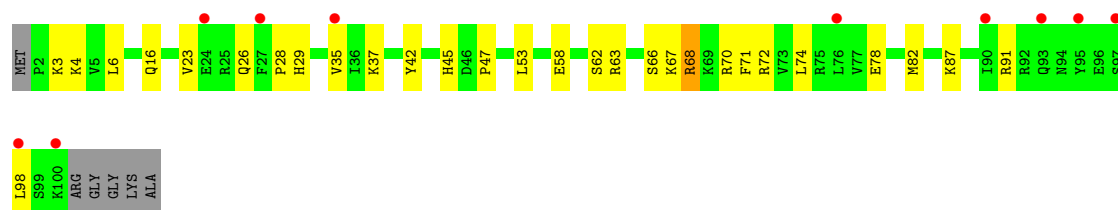


• Molecule 47: 30S Ribosomal Protein S16



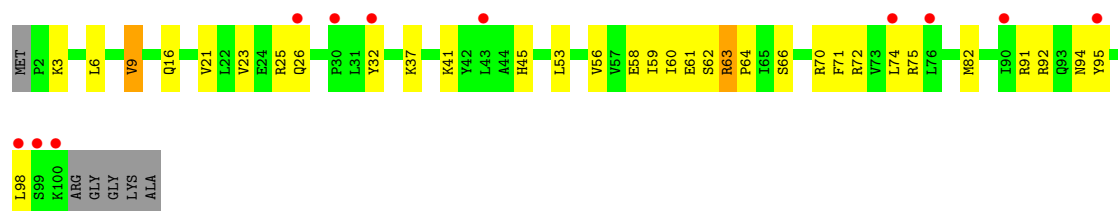
- Molecule 48: 30S Ribosomal Protein S17

Chain 1q: 



- Molecule 48: 30S Ribosomal Protein S17

Chain 2q: 



- Molecule 49: 30S Ribosomal Protein S18

Chain 1r: 



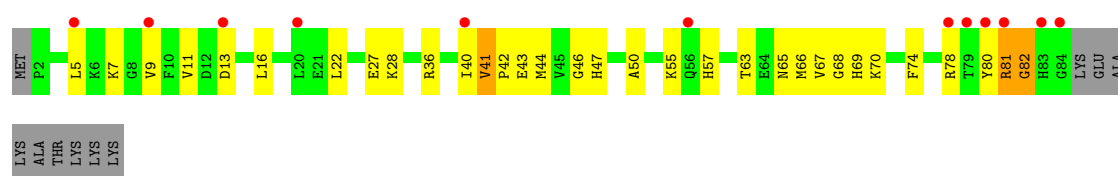
- Molecule 49: 30S Ribosomal Protein S18

Chain 2r: 

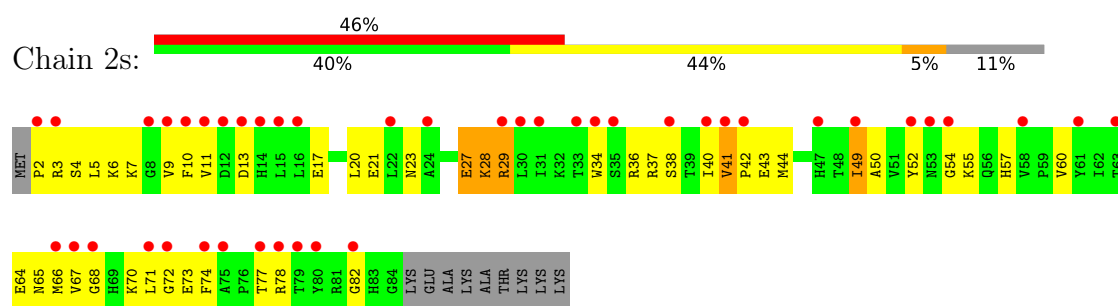


- Molecule 50: 30S Ribosomal Protein S19

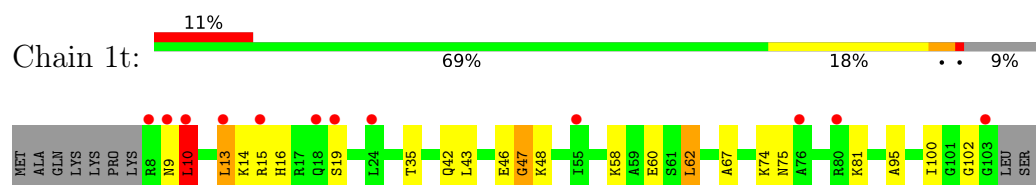
Chain 1s: 



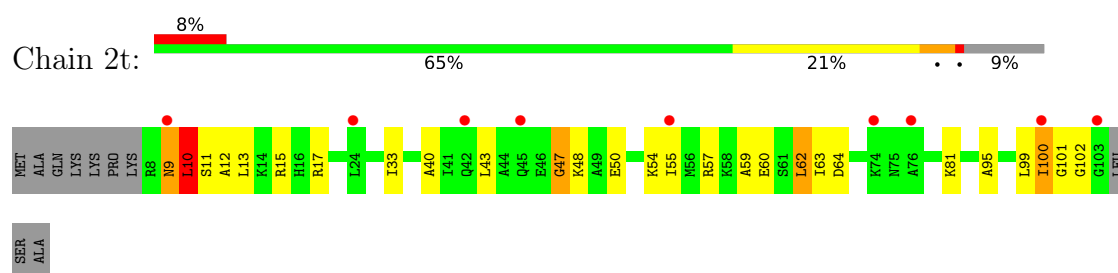
- Molecule 50: 30S Ribosomal Protein S19



• Molecule 51: 30S Ribosomal Protein S20



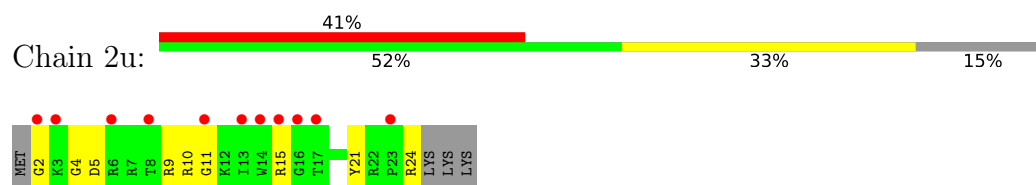
• Molecule 51: 30S Ribosomal Protein S20



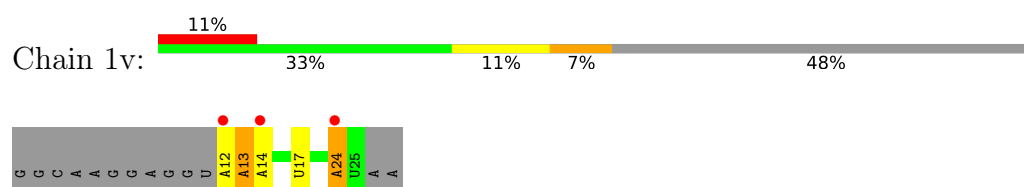
• Molecule 52: 30S Ribosomal Protein THX



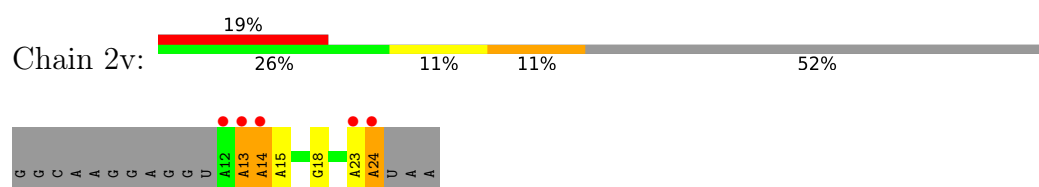
• Molecule 52: 30S Ribosomal Protein THX



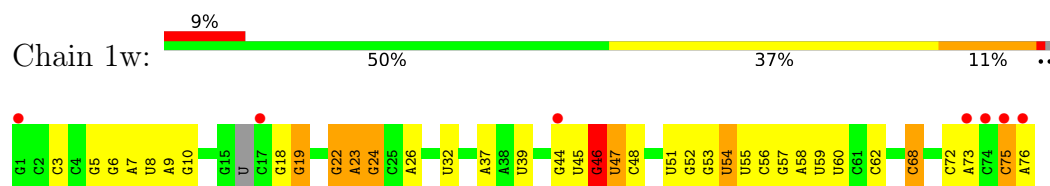
• Molecule 53: mRNA



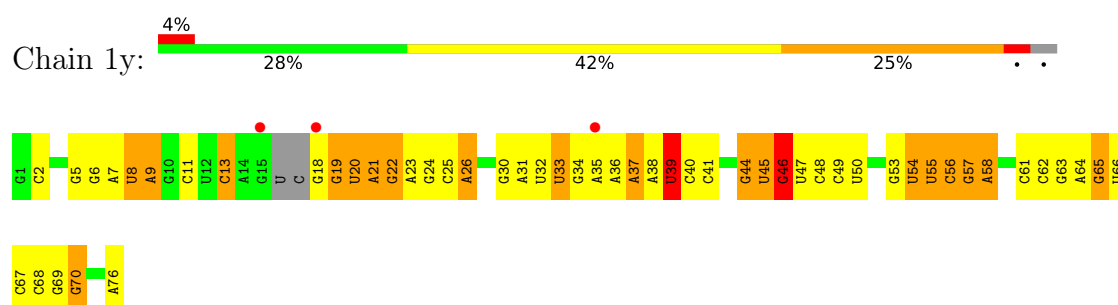
• Molecule 53: mRNA



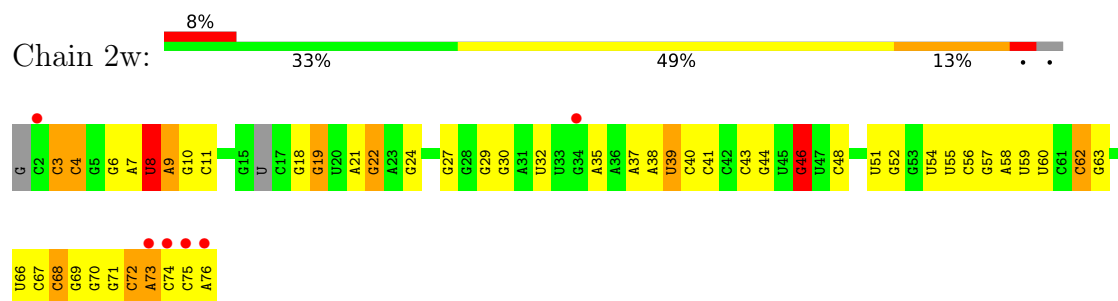
- Molecule 54: A-site and E-site tRNAs



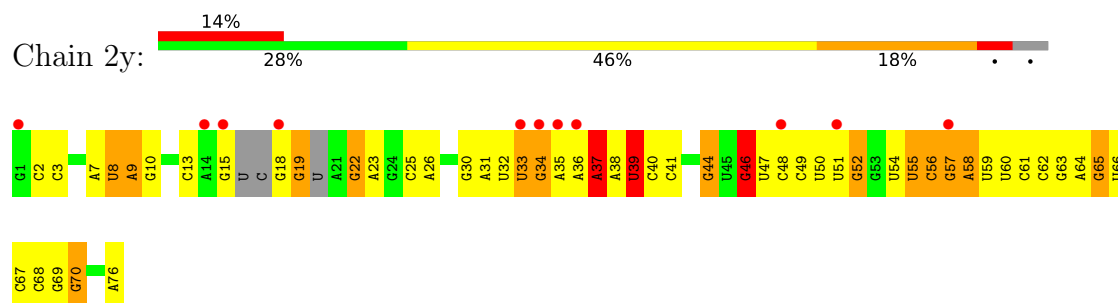
- Molecule 54: A-site and E-site tRNAs



- Molecule 54: A-site and E-site tRNAs

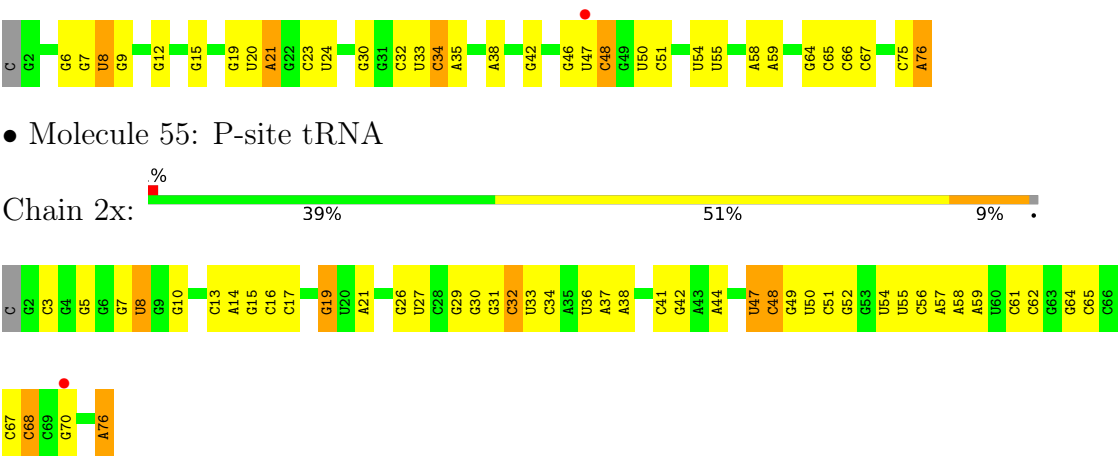


- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.39Å 444.58Å 619.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	361.14 – 2.60 361.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (361.14-2.60) 99.3 (361.14-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.283 0.239 , 0.285	Depositor DCC
R_{free} test set	86608 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.7	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	298925	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: FME, UR3, 7MG, HGR, K, 5MU, PSU, 0TD, 2MA, SF4, MA6, MG, 4OC, MIA, 2MU, 4SU, OMG, 5MC, M2G, 2MG, ZN

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	0.29	0/69009	0.46	2/107712 (0.0%)
1	2A	0.24	0/67293	0.44	1/105034 (0.0%)
2	1B	0.23	0/2882	0.39	0/4494
2	2B	0.24	0/2879	0.42	0/4487
3	1D	0.50	0/2186	0.88	2/2944 (0.1%)
3	2D	0.44	0/2186	0.91	5/2944 (0.2%)
4	1E	0.49	0/1592	0.90	2/2149 (0.1%)
4	2E	0.43	0/1592	0.90	4/2149 (0.2%)
5	1F	0.47	0/1619	0.88	5/2193 (0.2%)
5	2F	0.40	0/1615	0.94	4/2188 (0.2%)
6	1G	0.42	0/1454	0.85	3/1964 (0.2%)
6	2G	0.39	0/1453	0.93	4/1963 (0.2%)
7	1H	0.45	0/1356	0.89	4/1834 (0.2%)
7	2H	0.41	0/1356	0.90	0/1834
8	1I	0.39	0/1112	0.92	5/1514 (0.3%)
8	2I	0.37	0/1079	0.92	3/1475 (0.2%)
9	1N	0.45	0/1144	0.87	2/1543 (0.1%)
9	2N	0.37	0/1144	0.91	6/1543 (0.4%)
10	1O	0.48	0/943	0.81	0/1269
10	2O	0.42	0/943	0.79	0/1269
11	1P	0.46	0/1152	0.82	3/1533 (0.2%)
11	2P	0.40	0/1152	0.94	3/1533 (0.2%)
12	1Q	0.51	0/1143	0.82	0/1527
12	2Q	0.42	0/1143	0.86	0/1527
13	1R	0.50	0/982	0.85	1/1312 (0.1%)
13	2R	0.44	0/982	0.82	1/1312 (0.1%)
14	1S	0.42	0/883	0.84	0/1176
14	2S	0.38	0/880	0.91	1/1172 (0.1%)
15	1T	0.44	0/1105	0.80	0/1477
15	2T	0.38	0/1097	0.84	0/1468
16	1U	0.54	0/977	0.80	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.42	0/977	0.85	0/1301
17	1V	0.49	0/782	0.80	0/1049
17	2V	0.40	0/782	0.82	0/1049
18	1W	0.53	0/897	0.86	2/1205 (0.2%)
18	2W	0.47	0/897	0.87	2/1205 (0.2%)
19	1X	0.51	0/764	0.89	2/1025 (0.2%)
19	2X	0.42	0/764	0.82	0/1025
20	1Y	0.45	0/819	0.88	0/1095
20	2Y	0.37	0/819	0.87	3/1095 (0.3%)
21	1Z	0.41	0/1267	0.91	3/1717 (0.2%)
21	2Z	0.38	0/1299	0.92	6/1763 (0.3%)
22	10	0.44	0/662	0.85	1/881 (0.1%)
22	20	0.36	0/662	0.91	2/881 (0.2%)
23	11	0.46	0/762	0.86	0/1014
23	21	0.40	0/762	0.84	0/1014
24	12	0.44	0/590	0.80	0/781
24	22	0.36	0/590	0.77	0/781
25	13	0.48	0/474	0.84	0/635
25	23	0.40	0/469	0.89	0/630
26	14	0.40	0/565	1.08	4/761 (0.5%)
26	24	0.45	0/545	1.08	3/737 (0.4%)
27	15	0.52	0/469	0.83	1/635 (0.2%)
27	25	0.43	0/469	0.86	0/635
28	16	0.47	0/460	0.75	0/613
28	26	0.37	0/456	0.75	0/608
29	17	0.52	0/426	0.78	0/561
29	27	0.46	0/426	0.86	0/561
30	18	0.49	0/525	0.87	2/691 (0.3%)
30	28	0.41	0/525	0.82	0/691
31	19	0.44	0/310	0.82	0/407
31	29	0.37	0/310	0.92	0/407
32	1a	0.22	0/35795	0.41	0/55864
32	2a	0.21	0/35886	0.42	2/56005 (0.0%)
33	1b	0.38	0/1881	0.97	6/2542 (0.2%)
33	2b	0.41	0/1860	0.99	9/2518 (0.4%)
34	1c	0.38	0/1572	0.85	2/2126 (0.1%)
34	2c	0.41	0/1566	0.95	8/2119 (0.4%)
35	1d	0.38	0/1685	0.84	2/2262 (0.1%)
35	2d	0.36	0/1704	0.81	2/2284 (0.1%)
36	1e	0.43	0/1145	0.90	0/1543
36	2e	0.39	0/1149	0.96	4/1548 (0.3%)
37	1f	0.39	0/823	0.78	0/1115
37	2f	0.38	0/829	0.79	1/1123 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.40	0/1250	0.88	1/1679 (0.1%)
38	2g	0.37	0/1254	0.96	1/1683 (0.1%)
39	1h	0.37	0/1108	0.94	5/1494 (0.3%)
39	2h	0.35	0/1108	0.87	2/1494 (0.1%)
40	1i	0.37	0/1002	0.94	2/1346 (0.1%)
40	2i	0.36	0/997	0.87	2/1343 (0.1%)
41	1j	0.36	0/722	0.99	3/982 (0.3%)
41	2j	0.40	0/727	0.99	2/988 (0.2%)
42	1k	0.39	0/844	0.84	0/1145
42	2k	0.37	0/848	0.83	1/1149 (0.1%)
43	1l	0.38	0/937	0.81	1/1260 (0.1%)
43	2l	0.40	0/937	0.98	6/1260 (0.5%)
44	1m	0.41	0/969	0.90	1/1302 (0.1%)
44	2m	0.41	0/961	0.91	1/1291 (0.1%)
45	1n	0.37	0/501	0.81	2/664 (0.3%)
45	2n	0.37	0/501	0.83	0/664
46	1o	0.39	0/739	0.84	1/985 (0.1%)
46	2o	0.36	0/739	0.86	0/985
47	1p	0.37	0/697	0.80	0/939
47	2p	0.40	0/693	0.85	1/935 (0.1%)
48	1q	0.36	0/836	0.86	2/1117 (0.2%)
48	2q	0.35	0/836	0.83	0/1117
49	1r	0.38	0/560	0.80	0/746
49	2r	0.36	0/560	0.84	0/746
50	1s	0.37	0/667	0.95	3/900 (0.3%)
50	2s	0.44	0/661	1.05	4/893 (0.4%)
51	1t	0.37	0/730	0.90	0/965
51	2t	0.38	0/729	0.89	2/965 (0.2%)
52	1u	0.33	0/203	0.77	0/266
52	2u	0.37	0/203	0.86	0/266
53	1v	0.22	0/314	0.35	0/487
53	2v	0.22	0/310	0.41	0/480
54	1w	0.28	0/1585	0.52	0/2468
54	1y	0.25	1/1602 (0.1%)	0.44	0/2493
54	2w	0.30	1/1562 (0.1%)	0.52	0/2431
54	2y	0.26	0/1579	0.45	0/2455
55	1x	0.34	1/1725 (0.1%)	0.49	2/2689 (0.1%)
55	2x	0.29	1/1725 (0.1%)	0.46	1/2689 (0.0%)
All	All	0.31	4/316673 (0.0%)	0.59	174/474103 (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
26	14	0	1
50	2s	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	76	A	N7-C5	-5.73	1.27	1.39
54	1y	8	4SU	O3'-P	5.38	1.61	1.56
55	2x	8	4SU	O3'-P	5.26	1.61	1.56
54	2w	8	4SU	O3'-P	5.21	1.61	1.56

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1420	C	OP1-P-O3'	-9.41	79.77	108.00
40	1i	51	ARG	N-CA-C	-9.39	103.91	114.62
21	1Z	158	PRO	CA-C-N	8.93	131.01	119.84
21	1Z	158	PRO	C-N-CA	8.93	131.01	119.84
26	14	59	PHE	N-CA-C	-8.65	101.49	114.64

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
50	2s	28	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31191	825	0
1	2A	60322	0	30426	1087	0
2	1B	2577	0	1305	34	0
2	2B	2575	0	1303	79	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	61	0
3	2D	2136	0	2218	64	0
4	1E	1559	0	1618	42	0
4	2E	1559	0	1618	40	0
5	1F	1584	0	1625	43	0
5	2F	1580	0	1619	52	0
6	1G	1429	0	1447	40	0
6	2G	1428	0	1438	73	0
7	1H	1330	0	1407	37	0
7	2H	1330	0	1407	49	0
8	1I	1097	0	1140	35	0
8	2I	1064	0	1082	33	1
9	1N	1117	0	1184	26	0
9	2N	1117	0	1184	29	0
10	1O	933	0	996	21	0
10	2O	933	0	996	36	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	49	0
12	1Q	1122	0	1179	24	0
12	2Q	1122	0	1179	46	0
13	1R	968	0	1033	31	0
13	2R	968	0	1033	33	0
14	1S	873	0	927	22	0
14	2S	870	0	923	41	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	35	0
16	1U	959	0	1019	28	0
16	2U	959	0	1019	37	0
17	1V	771	0	830	15	0
17	2V	771	0	829	23	0
18	1W	886	0	940	15	0
18	2W	886	0	940	16	0
19	1X	750	0	814	21	0
19	2X	750	0	814	33	0
20	1Y	806	0	881	25	0
20	2Y	806	0	881	26	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	49	0
22	10	653	0	674	20	0
22	20	653	0	674	15	0
23	11	755	0	826	19	0
23	21	755	0	826	17	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	8	0
24	22	588	0	643	15	0
25	13	469	0	518	9	0
25	23	464	0	514	12	0
26	14	552	0	533	29	0
26	24	532	0	503	29	0
27	15	455	0	465	14	0
27	25	455	0	465	17	0
28	16	453	0	472	8	0
28	26	449	0	469	11	0
29	17	418	0	467	8	0
29	27	418	0	467	10	0
30	18	517	0	582	18	0
30	28	517	0	582	20	0
31	19	307	0	335	8	0
31	29	307	0	335	15	0
32	1a	32246	0	16296	544	1
32	2a	32327	0	16340	684	0
33	1b	1846	0	1867	78	0
33	2b	1825	0	1828	107	0
34	1c	1548	0	1535	44	0
34	2c	1542	0	1517	65	0
35	1d	1655	0	1671	60	0
35	2d	1674	0	1714	61	0
36	1e	1129	0	1185	27	0
36	2e	1133	0	1191	43	0
37	1f	810	0	804	25	0
37	2f	816	0	808	27	0
38	1g	1231	0	1238	35	0
38	2g	1235	0	1249	41	0
39	1h	1088	0	1126	28	0
39	2h	1088	0	1126	33	0
40	1i	983	0	986	31	0
40	2i	978	0	966	51	0
41	1j	709	0	650	29	0
41	2j	714	0	672	39	0
42	1k	829	0	825	19	0
42	2k	833	0	836	27	0
43	1l	932	0	981	20	0
43	2l	932	0	980	25	0
44	1m	958	0	1002	32	0
44	2m	950	0	988	52	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	25	0
45	2n	492	0	529	29	0
46	1o	728	0	760	16	0
46	2o	728	0	760	20	0
47	1p	681	0	697	24	0
47	2p	677	0	686	25	0
48	1q	823	0	891	25	0
48	2q	823	0	891	28	0
49	1r	555	0	618	14	0
49	2r	555	0	618	23	0
50	1s	652	0	662	25	0
50	2s	646	0	644	39	0
51	1t	728	0	798	16	0
51	2t	727	0	796	19	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	281	0	139	4	0
53	2v	277	0	140	6	0
54	1w	1574	0	810	28	0
54	1y	1581	0	805	44	0
54	2w	1547	0	783	38	0
54	2y	1561	0	796	48	0
55	1x	1625	0	828	18	0
55	2x	1625	0	828	29	0
56	10	4	0	0	0	0
56	11	3	0	0	0	0
56	12	1	0	0	0	0
56	13	3	0	0	0	0
56	15	2	0	0	0	0
56	16	1	0	0	0	0
56	17	2	0	0	0	0
56	18	2	0	0	0	0
56	19	2	0	0	0	0
56	1A	963	0	0	1	0
56	1B	29	0	0	0	0
56	1D	5	0	0	0	0
56	1E	6	0	0	0	0
56	1F	7	0	0	0	0
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	7	0	0	0	0
56	1O	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1P	4	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	3	0	0	0	0
56	1S	2	0	0	0	0
56	1T	3	0	0	0	0
56	1U	5	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	4	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	5	0	0	0	0
56	1a	239	0	0	0	0
56	1b	2	0	0	0	0
56	1d	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	2	0	0	0	0
56	1l	3	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	6	0	0	0	0
56	1x	10	0	0	0	0
56	1y	2	0	0	0	0
56	20	3	0	0	0	0
56	23	1	0	0	0	0
56	26	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	673	0	0	0	0
56	2B	18	0	0	0	0
56	2D	4	0	0	0	0
56	2E	5	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	1	0	0	0	0
56	2T	1	0	0	0	0
56	2U	4	0	0	0	0
56	2V	1	0	0	0	0
56	2X	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	196	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	2	0	0	0	0
56	2p	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2w	3	0	0	0	0
56	2x	2	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	36	0	29	2	0
58	2A	36	0	29	5	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	2	0
60	2d	8	0	0	0	0
61	1x	10	0	10	0	0
61	2x	10	0	10	0	0
62	10	9	0	0	2	0
62	11	3	0	0	0	0
62	12	4	0	0	0	0
62	13	3	0	0	0	0
62	14	1	0	0	0	0
62	15	4	0	0	0	0
62	16	2	0	0	0	0
62	17	5	0	0	0	0
62	18	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	19	1	0	0	0	0
62	1A	1577	0	0	94	0
62	1B	43	0	0	2	0
62	1D	23	0	0	0	0
62	1E	25	0	0	2	0
62	1F	17	0	0	0	0
62	1G	3	0	0	1	0
62	1H	1	0	0	0	0
62	1N	3	0	0	1	0
62	1O	4	0	0	1	0
62	1P	20	0	0	3	0
62	1Q	4	0	0	0	0
62	1R	5	0	0	0	0
62	1S	3	0	0	0	0
62	1T	4	0	0	0	0
62	1U	9	0	0	0	0
62	1V	5	0	0	0	0
62	1W	8	0	0	2	0
62	1X	7	0	0	0	0
62	1Y	2	0	0	1	0
62	1Z	1	0	0	0	0
62	1a	287	0	0	24	0
62	1e	1	0	0	0	0
62	1h	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	4	0	0	0	0
62	1m	1	0	0	0	0
62	1n	1	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	1	0	0	0	0
62	1s	1	0	0	0	0
62	1v	3	0	0	0	0
62	1w	8	0	0	0	0
62	1x	6	0	0	0	0
62	1y	1	0	0	0	0
62	20	4	0	0	0	0
62	21	3	0	0	0	0
62	23	1	0	0	0	0
62	25	2	0	0	0	0
62	26	2	0	0	1	0
62	28	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	29	1	0	0	0	0
62	2A	1063	0	0	90	0
62	2B	10	0	0	1	0
62	2D	20	0	0	0	0
62	2E	9	0	0	1	0
62	2F	7	0	0	0	0
62	2I	1	0	0	0	0
62	2N	2	0	0	1	0
62	2O	1	0	0	0	0
62	2P	14	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	3	0	0	0	0
62	2T	2	0	0	0	0
62	2U	1	0	0	0	0
62	2V	2	0	0	0	0
62	2W	2	0	0	0	0
62	2X	3	0	0	0	0
62	2Y	1	0	0	1	0
62	2Z	1	0	0	0	0
62	2a	213	0	0	18	0
62	2d	3	0	0	0	0
62	2g	2	0	0	0	0
62	2i	2	0	0	0	0
62	2j	5	0	0	2	0
62	2l	3	0	0	1	0
62	2n	1	0	0	0	0
62	2o	1	0	0	0	0
62	2p	3	0	0	0	0
62	2r	1	0	0	0	0
62	2t	2	0	0	0	0
62	2v	1	0	0	0	0
62	2w	2	0	0	0	0
62	2x	6	0	0	2	0
All	All	298925	0	196763	5536	1

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 12.

The worst 5 of 5536 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.44	1.14
54:2w:4:C:N4	54:2w:69:G:H1	1.55	1.04
54:2y:7:A:N6	54:2y:66:U:H3	1.55	1.03
32:2a:79:G:H1	32:2a:90:U:H3	1.07	1.03
54:1y:53:G:H1	54:1y:61:C:H42	1.06	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:358:U:OP1	8:2I:121:LYS:NZ[2_655]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	30	51
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	46
4	2E	202/206 (98%)	194 (96%)	6 (3%)	2 (1%)	12	28
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	46
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	12	28
6	1G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	11	25
6	2G	179/182 (98%)	165 (92%)	12 (7%)	2 (1%)	11	25
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	42
8	1I	144/148 (97%)	126 (88%)	13 (9%)	5 (4%)	3	4
8	2I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	18	38
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2N	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	34
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	18	38
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	19
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	38
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	14	30
15	1T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	16	34
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	28
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	25
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	13
20	2Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12	28
21	1Z	148/206 (72%)	128 (86%)	16 (11%)	4 (3%)	4	7
21	2Z	156/206 (76%)	131 (84%)	22 (14%)	3 (2%)	6	13
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	76 (94%)	3 (4%)	2 (2%)	4	8
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	25
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	8 (12%)	6 (9%)	0	0
26	24	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	10
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	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%)	197 (86%)	27 (12%)	5 (2%)	5	10
33	2b	229/256 (90%)	199 (87%)	21 (9%)	9 (4%)	2	3
34	1c	204/239 (85%)	183 (90%)	19 (9%)	2 (1%)	12	28
34	2c	204/239 (85%)	181 (89%)	20 (10%)	3 (2%)	8	18
35	1d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100	100
36	1e	146/162 (90%)	142 (97%)	2 (1%)	2 (1%)	9	19
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9	21
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9	21
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	18	38
40	1i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
40	2i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	34
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	2j	94/105 (90%)	80 (85%)	9 (10%)	5 (5%)	1	1
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	2k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	6 (5%)	2 (2%)	7	15
44	2m	120/126 (95%)	110 (92%)	7 (6%)	3 (2%)	4	8
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	9
47	1p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	9	21
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	21
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	28
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	4	8
50	2s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	4	8
51	1t	94/106 (89%)	87 (93%)	2 (2%)	5 (5%)	1	1
51	2t	94/106 (89%)	87 (93%)	1 (1%)	6 (6%)	1	1
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10613 (93%)	636 (6%)	121 (1%)	11	25

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1D	275	LYS
5	1F	130	ALA
6	1G	47	LYS
6	1G	51	ARG
7	1H	126	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	26	52
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26	52
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	26
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10	22
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	16
5	2F	159/166 (96%)	146 (92%)	13 (8%)	10	24
6	1G	144/156 (92%)	134 (93%)	10 (7%)	14	32
6	2G	143/156 (92%)	132 (92%)	11 (8%)	12	27
7	1H	144/148 (97%)	140 (97%)	4 (3%)	38	66
7	2H	144/148 (97%)	137 (95%)	7 (5%)	22	47
8	1I	113/124 (91%)	107 (95%)	6 (5%)	20	43
8	2I	105/124 (85%)	97 (92%)	8 (8%)	12	27
9	1N	118/119 (99%)	112 (95%)	6 (5%)	21	45
9	2N	118/119 (99%)	113 (96%)	5 (4%)	26	52
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	64
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	64
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	51
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	59
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	51	76
12	2Q	111/111 (100%)	110 (99%)	1 (1%)	70	87
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	13
13	2R	101/101 (100%)	91 (90%)	10 (10%)	7	16
14	1S	86/88 (98%)	83 (96%)	3 (4%)	32	59
14	2S	85/88 (97%)	82 (96%)	3 (4%)	32	59
15	1T	115/127 (91%)	113 (98%)	2 (2%)	53	78
15	2T	113/127 (89%)	111 (98%)	2 (2%)	51	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	62
16	2U	93/94 (99%)	91 (98%)	2 (2%)	45	72
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	28
17	2V	80/82 (98%)	75 (94%)	5 (6%)	16	36
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	26
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	40
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	23	48
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	43	70
21	1Z	135/179 (75%)	129 (96%)	6 (4%)	25	50
21	2Z	137/179 (76%)	132 (96%)	5 (4%)	31	58
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	63
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	80
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	82
23	21	80/83 (96%)	79 (99%)	1 (1%)	61	82
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	63
24	22	65/67 (97%)	62 (95%)	3 (5%)	24	49
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	55
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	25
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	15
26	24	53/63 (84%)	49 (92%)	4 (8%)	12	28
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	37
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	37
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	55
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	55
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	40 (98%)	1 (2%)	43	70
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	40
31	19	34/34 (100%)	34 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	192/220 (87%)	182 (95%)	10 (5%)	21	44
33	2b	187/220 (85%)	179 (96%)	8 (4%)	26	51
34	1c	142/188 (76%)	138 (97%)	4 (3%)	38	66
34	2c	140/188 (74%)	138 (99%)	2 (1%)	59	81
35	1d	169/181 (93%)	166 (98%)	3 (2%)	51	76
35	2d	173/181 (96%)	170 (98%)	3 (2%)	53	78
36	1e	113/123 (92%)	108 (96%)	5 (4%)	25	50
36	2e	114/123 (93%)	112 (98%)	2 (2%)	51	76
37	1f	84/90 (93%)	83 (99%)	1 (1%)	63	83
37	2f	85/90 (94%)	84 (99%)	1 (1%)	63	83
38	1g	119/127 (94%)	119 (100%)	0	100	100
38	2g	120/127 (94%)	118 (98%)	2 (2%)	53	78
39	1h	114/119 (96%)	111 (97%)	3 (3%)	40	68
39	2h	114/119 (96%)	111 (97%)	3 (3%)	40	68
40	1i	90/99 (91%)	85 (94%)	5 (6%)	19	40
40	2i	89/99 (90%)	82 (92%)	7 (8%)	11	26
41	1j	66/92 (72%)	65 (98%)	1 (2%)	57	80
41	2j	69/92 (75%)	68 (99%)	1 (1%)	59	81
42	1k	82/99 (83%)	79 (96%)	3 (4%)	30	57
42	2k	83/99 (84%)	81 (98%)	2 (2%)	43	70
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	52
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	63
44	1m	93/101 (92%)	89 (96%)	4 (4%)	26	51
44	2m	92/101 (91%)	88 (96%)	4 (4%)	26	51
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	37
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	37
46	1o	78/80 (98%)	77 (99%)	1 (1%)	61	82
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	45
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	15
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	93 (99%)	1 (1%)	65	84
48	2q	94/97 (97%)	92 (98%)	2 (2%)	47	73
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	32
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	45
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59	81
50	2s	67/80 (84%)	65 (97%)	2 (3%)	36	64
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26	51
51	2t	70/82 (85%)	68 (97%)	2 (3%)	37	65
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9304/10064 (92%)	8905 (96%)	399 (4%)	26	51

5 of 399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	2F	70	THR
13	2R	65	LEU
5	2F	183	VAL
8	2I	15	VAL
17	2V	72	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
51	1t	42	GLN
39	2h	78	GLN
9	2N	131	GLN
38	2g	28	ASN
44	2m	106	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	443 (15%)	33 (1%)
1	2A	2791/2915 (95%)	515 (18%)	30 (1%)
2	1B	120/121 (99%)	8 (6%)	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2B	118/121 (97%)	36 (30%)	0
32	1a	1497/1521 (98%)	228 (15%)	0
32	2a	1501/1521 (98%)	242 (16%)	0
53	1v	12/27 (44%)	3 (25%)	0
53	2v	12/27 (44%)	3 (25%)	0
54	1w	70/76 (92%)	17 (24%)	0
54	1y	72/76 (94%)	23 (31%)	0
54	2w	69/76 (90%)	19 (27%)	0
54	2y	70/76 (92%)	18 (25%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9346/9626 (97%)	1574 (16%)	64 (0%)

5 of 1574 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C

5 of 64 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1913	A
1	2A	2126	A
1	1A	1653	G
1	1A	1608	A
1	2A	2156	G

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

84 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
32	5MC	2a	1407	32	19,22,23	1.62	3 (15%)	26,32,35	1.22	3 (11%)
32	PSU	2a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.97	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.15	2 (7%)
32	2MG	1a	1207	32	23,26,27	1.26	2 (8%)	33,38,41	2.11	7 (21%)
32	MA6	2a	1519	32	23,26,27	1.59	4 (17%)	33,38,41	2.30	11 (33%)
54	MIA	1w	37	54	28,31,32	2.32	6 (21%)	38,44,47	2.70	12 (31%)
55	5MU	2x	54	55	19,22,23	1.38	4 (21%)	27,32,35	2.21	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	2.02	4 (19%)
54	7MG	1y	46	54	23,26,27	1.34	5 (21%)	27,39,42	2.62	6 (22%)
54	PSU	2y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.90	3 (14%)
1	4OC	2A	1920	1	19,22,24	0.78	0	25,31,35	0.78	0
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.90	4 (19%)
1	5MC	1A	1962	1	19,22,23	1.69	3 (15%)	26,32,35	1.12	3 (11%)
54	PSU	2w	39	54	18,21,22	1.45	2 (11%)	21,30,33	1.68	4 (19%)
55	4SU	2x	8	55	18,21,22	2.00	6 (33%)	25,30,33	1.61	7 (28%)
32	PSU	1a	516	32,56	18,21,22	1.41	2 (11%)	21,30,33	2.06	4 (19%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.78	5 (15%)
32	5MC	2a	967	32,56	19,22,23	1.68	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.82	3 (15%)	26,32,35	1.10	2 (7%)
54	PSU	2y	39	54	18,21,22	1.36	1 (5%)	21,30,33	2.41	3 (14%)
55	5MU	1x	54	56,55	19,22,23	1.41	6 (31%)	27,32,35	1.84	6 (22%)
54	5MU	2w	54	54	19,22,23	1.39	6 (31%)	27,32,35	1.81	6 (22%)
1	2MU	1A	2552	1,56	19,22,24	1.26	3 (15%)	25,31,36	1.96	5 (20%)
55	4SU	1x	8	55	18,21,22	2.09	5 (27%)	25,30,33	1.48	6 (24%)
1	5MC	1A	1942	1	19,22,23	1.41	3 (15%)	26,32,35	1.10	2 (7%)
32	7MG	1a	527	32,56	23,26,27	1.39	4 (17%)	27,39,42	2.61	7 (25%)
54	4SU	1y	8	54	18,21,22	1.91	4 (22%)	25,30,33	2.02	4 (16%)
43	0TD	1l	92	43	8,9,10	4.71	1 (12%)	6,11,13	8.27	3 (50%)
54	5MU	2y	54	54	19,22,23	1.45	4 (21%)	27,32,35	1.98	7 (25%)
54	PSU	1w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
1	2MA	2A	2503	1,56	22,25,26	1.44	5 (22%)	32,37,40	2.25	9 (28%)
1	5MU	2A	1915	1	19,22,23	1.50	6 (31%)	27,32,35	2.08	6 (22%)
1	PSU	2A	2605	1	18,21,22	1.24	2 (11%)	21,30,33	2.31	5 (23%)
32	2MG	2a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.12	7 (21%)
1	5MU	1A	1939	1,56	19,22,23	1.33	3 (15%)	27,32,35	2.31	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MU	2A	2552	1,56	19,22,24	1.38	4 (21%)	25,31,36	1.78	5 (20%)
32	UR3	1a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.87	5 (19%)
1	PSU	2A	1911	1	18,21,22	1.33	2 (11%)	21,30,33	1.98	3 (14%)
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.88	6 (18%)
54	PSU	1w	55	54	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
54	7MG	1w	46	54	23,26,27	1.43	3 (13%)	27,39,42	2.55	7 (25%)
1	PSU	1A	2605	1	18,21,22	1.42	3 (16%)	21,30,33	2.02	5 (23%)
1	OMG	1A	2251	1,56,55	23,26,27	1.25	3 (13%)	32,38,41	2.00	6 (18%)
32	5MC	1a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.13	3 (11%)
1	5MC	2A	1962	1,56	19,22,23	1.55	3 (15%)	26,32,35	1.18	3 (11%)
54	4SU	1w	8	54	18,21,22	1.71	4 (22%)	25,30,33	2.14	5 (20%)
54	PSU	1w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.95	3 (14%)
1	5MU	2A	1939	1,56	19,22,23	1.37	6 (31%)	27,32,35	2.34	6 (22%)
32	MA6	1a	1518	32	23,26,27	1.53	4 (17%)	33,38,41	2.30	14 (42%)
54	MIA	1y	37	54	21,24,32	1.60	3 (14%)	30,35,47	2.06	8 (26%)
32	MA6	1a	1519	32	23,26,27	1.56	4 (17%)	33,38,41	2.30	11 (33%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
54	5MU	1w	54	54	19,22,23	1.35	5 (26%)	27,32,35	1.96	6 (22%)
54	PSU	1y	39	54	18,21,22	1.50	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	1A	1917	1	18,21,22	1.41	3 (16%)	21,30,33	2.03	4 (19%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.96	4 (19%)
32	MA6	2a	1518	32	23,26,27	1.56	5 (21%)	33,38,41	2.28	12 (36%)
54	7MG	2w	46	54	23,26,27	1.35	4 (17%)	27,39,42	2.59	7 (25%)
1	OMG	2A	2251	1,56,55	23,26,27	1.24	3 (13%)	32,38,41	1.99	7 (21%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.15	7 (25%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	1.92	3 (14%)
54	7MG	2y	46	54	23,26,27	1.34	4 (17%)	27,39,42	2.67	9 (33%)
54	5MU	1y	54	54	19,22,23	1.44	5 (26%)	27,32,35	1.55	6 (22%)
1	2MA	1A	2503	1,56	22,25,26	1.47	4 (18%)	32,37,40	2.37	8 (25%)
32	5MC	2a	1400	32	19,22,23	1.53	3 (15%)	26,32,35	1.27	5 (19%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
54	MIA	2w	37	54	21,24,32	1.59	4 (19%)	30,35,47	2.00	7 (23%)
1	4OC	1A	1920	1	19,22,24	0.80	0	25,31,35	1.05	2 (8%)
54	PSU	2y	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.98	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MC	1x	32	55	19,22,23	1.71	3 (15%)	26,32,35	1.22	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.53	3 (15%)	26,32,35	1.05	2 (7%)
32	7MG	2a	527	32,56	23,26,27	1.35	4 (17%)	27,39,42	2.60	7 (25%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	25,32,35	1.05	1 (4%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.73	3 (11%)
54	MIA	2y	37	54	21,24,32	1.65	4 (19%)	30,35,47	2.07	7 (23%)
43	0TD	2l	92	43	8,9,10	4.73	1 (12%)	6,11,13	5.50	3 (50%)
55	PSU	1x	55	55	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
54	PSU	1y	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.92	3 (14%)
55	5MC	2x	32	55	19,22,23	1.59	3 (15%)	26,32,35	1.25	4 (15%)
32	4OC	1a	1402	32	20,23,24	0.73	0	25,32,35	0.92	1 (4%)
54	4SU	2w	8	54,56	18,21,22	1.75	5 (27%)	25,30,33	1.94	4 (16%)
32	5MC	1a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.11	2 (7%)
54	4SU	2y	8	54	18,21,22	1.85	4 (22%)	25,30,33	2.35	6 (24%)

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
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	6/11/29/30	0/3/3/3
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32,56	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	2/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	0/7/25/26	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,56,55	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/11/29/30	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	7MG	2w	46	54	-	1/7/37/38	0/3/3/3
1	OMG	2A	2251	1,56,55	-	1/9/27/28	0/3/3/3
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	4/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	1/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/25/34	0/3/3/3
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	1/7/37/38	0/3/3/3
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	2/7/25/34	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	4SU	2w	8	54,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2

The worst 5 of 265 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-13.01	1.69	1.82
43	1l	92	0TD	CB-SB	-12.93	1.69	1.82
54	1w	37	MIA	C2-S10	-6.93	1.70	1.75
54	1w	37	MIA	C13-C14	6.88	1.53	1.32
32	1a	1400	5MC	C5-C4	6.84	1.49	1.44

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	19.86	138.07	102.36
43	2l	92	0TD	CSB-SB-CB	-12.59	79.73	102.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	N9-C4-N3	9.12	138.82	125.46
54	1y	46	7MG	N9-C4-N3	9.08	138.76	125.46
32	2a	527	7MG	N9-C4-N3	8.70	138.21	125.46

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
32	2a	1400	5MC	C4'-C5'-O5'-P
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

44 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1207	2MG	1	0
32	2a	1519	MA6	2	0
54	1y	46	7MG	1	0
54	2w	39	PSU	1	0
55	2x	8	4SU	1	0
32	1a	966	M2G	1	0
32	2a	967	5MC	1	0
54	2y	39	PSU	1	0
1	1A	2552	2MU	1	0
55	1x	8	4SU	2	0
54	1y	8	4SU	1	0
43	1l	92	0TD	1	0
1	2A	2503	2MA	1	0
32	2a	1207	2MG	3	0
1	1A	1939	5MU	2	0
1	2A	2552	2MU	2	0
32	1a	1498	UR3	1	0
32	2a	966	M2G	1	0
54	1w	46	7MG	3	0
32	2a	1404	5MC	1	0
1	2A	1939	5MU	1	0
32	1a	1518	MA6	2	0
54	1y	37	MIA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1519	MA6	2	0
54	1w	54	5MU	1	0
54	1y	39	PSU	2	0
32	2a	1518	MA6	4	0
54	2w	46	7MG	1	0
1	2A	2251	OMG	1	0
1	1A	1915	5MU	1	0
54	2y	46	7MG	3	0
54	1y	54	5MU	2	0
1	1A	2503	2MA	1	0
32	2a	1400	5MC	2	0
54	1y	55	PSU	1	0
1	1A	1920	4OC	1	0
54	2y	55	PSU	3	0
32	2a	1402	4OC	2	0
32	2a	1498	UR3	2	0
54	2y	37	MIA	2	0
55	2x	32	5MC	1	0
32	1a	1402	4OC	2	0
54	2w	8	4SU	1	0
54	2y	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2321 ligands modelled in this entry, 2315 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	1d	501	35	0,12,12	-	-	-		
61	FME	2x	103	55	8,9,10	0.45	0	8,9,11	1.24	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	HGR	2A	3652	-	39,39,39	2.38	8 (20%)	48,58,58	1.72	13 (27%)
58	HGR	1A	3915	56	39,39,39	2.39	7 (17%)	48,58,58	1.79	13 (27%)
61	FME	1x	3011	55	8,9,10	0.35	0	8,9,11	1.26	2 (25%)
60	SF4	2d	301	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	1d	501	35	-	-	0/6/5/5
61	FME	2x	103	55	-	5/7/9/11	-
58	HGR	2A	3652	-	-	7/20/79/79	0/4/4/4
58	HGR	1A	3915	56	-	7/20/79/79	0/4/4/4
61	FME	1x	3011	55	-	5/7/9/11	-
60	SF4	2d	301	35	-	-	0/6/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3652	HGR	C12-C14	9.21	1.55	1.33
58	1A	3915	HGR	C12-C14	8.76	1.54	1.33
58	2A	3652	HGR	C5-C4	-5.59	1.39	1.49
58	1A	3915	HGR	C5-C4	-5.50	1.39	1.49
58	1A	3915	HGR	C5-C6	-5.29	1.39	1.50

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3652	HGR	C10-C9-C8	-4.65	96.50	102.29
58	2A	3652	HGR	C4-C5-C6	4.37	121.68	112.35
58	1A	3915	HGR	C23-O9-C22	-4.22	99.88	106.31
58	1A	3915	HGR	C12-C6-C1	-3.93	114.97	119.35
58	1A	3915	HGR	C4-C5-C6	3.88	120.63	112.35

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

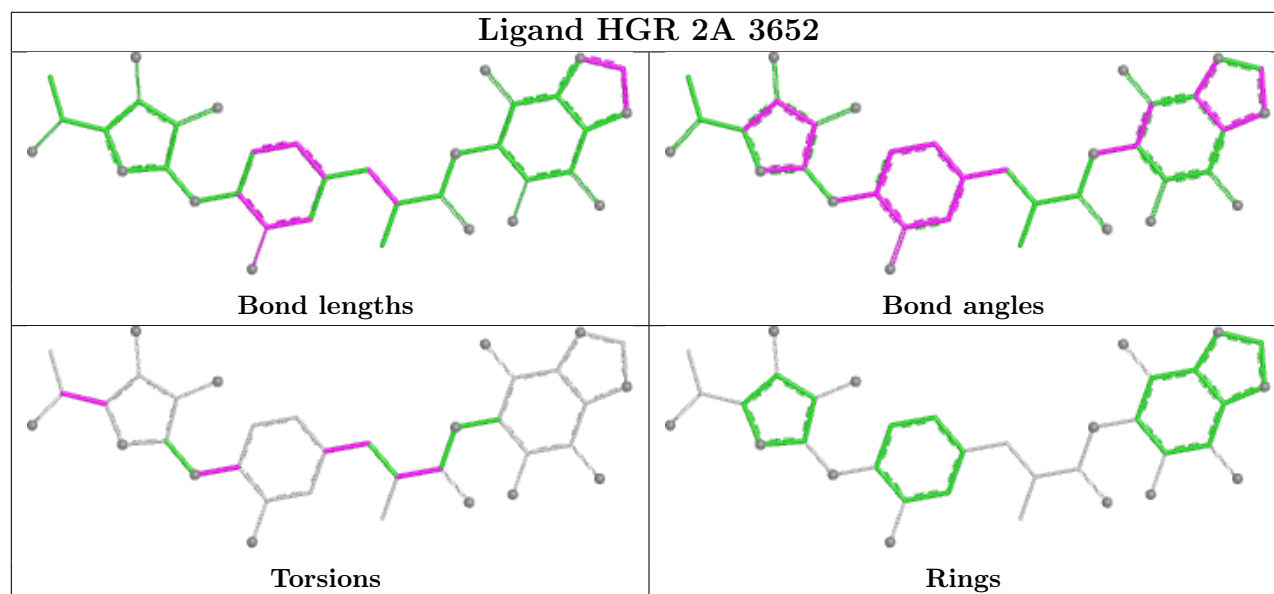
Mol	Chain	Res	Type	Atoms
58	1A	3915	HGR	C14-C12-C6-C1
61	1x	3011	FME	O1-CN-N-CA
61	1x	3011	FME	N-CA-CB-CG
61	1x	3011	FME	C-CA-CB-CG
61	1x	3011	FME	O-C-CA-CB

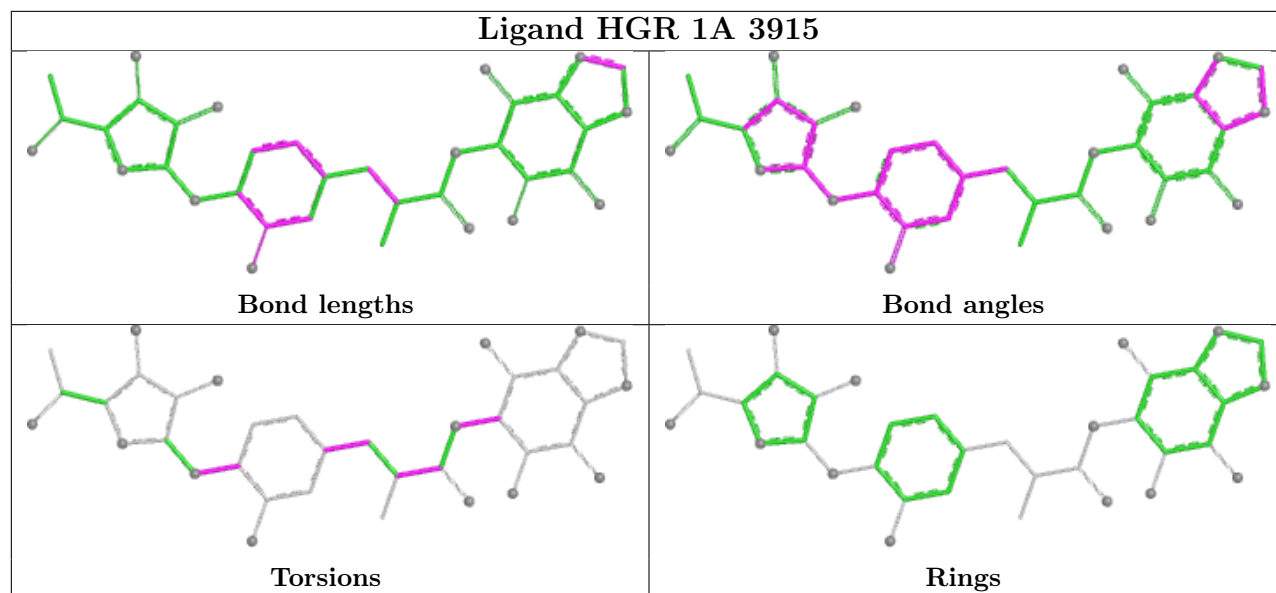
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	501	SF4	2	0
58	2A	3652	HGR	5	0
58	1A	3915	HGR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.16	84 (2%)	53	48	22, 42, 90, 106	0
1	2A	2789/2915 (95%)	-0.07	57 (2%)	65	60	26, 45, 87, 104	0
2	1B	120/121 (99%)	0.25	0	100	100	37, 58, 69, 86	0
2	2B	120/121 (99%)	0.86	5 (4%)	40	35	44, 65, 74, 87	0
3	1D	275/276 (99%)	0.10	3 (1%)	78	74	21, 41, 58, 73	0
3	2D	275/276 (99%)	0.13	3 (1%)	78	74	25, 42, 61, 72	0
4	1E	204/206 (99%)	0.23	1 (0%)	87	85	22, 46, 65, 78	0
4	2E	204/206 (99%)	0.39	4 (1%)	65	60	25, 49, 66, 79	0
5	1F	203/210 (96%)	0.43	4 (1%)	65	60	21, 50, 72, 83	0
5	2F	203/210 (96%)	0.49	6 (2%)	52	47	24, 54, 74, 85	0
6	1G	181/182 (99%)	1.01	19 (10%)	11	9	49, 66, 77, 91	0
6	2G	181/182 (99%)	1.32	31 (17%)	4	3	53, 69, 80, 93	0
7	1H	174/180 (96%)	0.95	8 (4%)	37	32	47, 63, 73, 81	0
7	2H	174/180 (96%)	1.07	17 (9%)	13	10	53, 67, 76, 82	0
8	1I	146/148 (98%)	0.84	6 (4%)	41	36	44, 72, 81, 85	0
8	2I	146/148 (98%)	1.01	10 (6%)	23	19	47, 72, 81, 84	0
9	1N	140/140 (100%)	-0.03	1 (0%)	84	82	23, 37, 59, 69	0
9	2N	140/140 (100%)	0.80	6 (4%)	40	34	37, 64, 76, 84	0
10	1O	122/122 (100%)	-0.02	1 (0%)	82	80	26, 39, 58, 66	0
10	2O	122/122 (100%)	0.47	0	100	100	39, 56, 68, 78	0
11	1P	149/150 (99%)	0.35	4 (2%)	56	50	22, 52, 71, 81	0
11	2P	149/150 (99%)	0.79	10 (6%)	24	19	27, 55, 77, 82	0
12	1Q	141/141 (100%)	0.44	1 (0%)	84	82	32, 49, 63, 76	0
12	2Q	141/141 (100%)	0.72	6 (4%)	40	34	36, 53, 66, 77	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%)	0.15	0 100 100	28, 39, 54, 64	0
13	2R	118/118 (100%)	0.13	0 100 100	31, 41, 57, 64	0
14	1S	110/112 (98%)	0.71	5 (4%) 38 32	46, 58, 70, 74	0
14	2S	110/112 (98%)	1.19	16 (14%) 6 4	51, 61, 73, 77	0
15	1T	131/146 (89%)	0.60	8 (6%) 27 22	39, 51, 69, 75	0
15	2T	131/146 (89%)	0.48	3 (2%) 61 55	41, 53, 70, 74	0
16	1U	116/118 (98%)	0.27	2 (1%) 69 64	26, 39, 57, 71	0
16	2U	116/118 (98%)	0.28	0 100 100	29, 44, 63, 72	0
17	1V	101/101 (100%)	0.53	2 (1%) 65 60	26, 49, 66, 70	0
17	2V	101/101 (100%)	0.53	2 (1%) 65 60	30, 54, 69, 73	0
18	1W	112/113 (99%)	0.07	1 (0%) 81 78	26, 36, 55, 83	0
18	2W	112/113 (99%)	0.06	1 (0%) 81 78	29, 39, 59, 86	0
19	1X	95/96 (98%)	0.35	3 (3%) 50 44	30, 43, 63, 80	0
19	2X	95/96 (98%)	0.46	5 (5%) 32 26	34, 47, 65, 80	0
20	1Y	107/110 (97%)	0.90	6 (5%) 30 24	44, 55, 71, 79	0
20	2Y	107/110 (97%)	1.10	17 (15%) 5 4	49, 59, 73, 81	0
21	1Z	154/206 (74%)	0.71	12 (7%) 19 15	37, 61, 82, 94	0
21	2Z	160/206 (77%)	1.63	43 (26%) 1 1	65, 80, 91, 97	0
22	10	83/85 (97%)	0.17	7 (8%) 17 13	24, 36, 65, 88	0
22	20	83/85 (97%)	1.44	14 (16%) 4 3	48, 64, 80, 89	0
23	11	97/98 (98%)	0.36	1 (1%) 79 76	23, 43, 67, 74	0
23	21	97/98 (98%)	0.75	6 (6%) 26 21	35, 55, 72, 76	0
24	12	70/72 (97%)	0.64	4 (5%) 29 24	41, 56, 65, 68	0
24	22	70/72 (97%)	0.68	1 (1%) 73 69	45, 59, 68, 78	0
25	13	59/60 (98%)	0.26	0 100 100	28, 44, 65, 72	0
25	23	59/60 (98%)	0.42	1 (1%) 69 64	36, 49, 69, 76	0
26	14	69/71 (97%)	0.88	7 (10%) 12 9	49, 71, 85, 89	0
26	24	69/71 (97%)	1.76	26 (37%) 1 0	72, 83, 93, 97	0
27	15	59/60 (98%)	-0.32	1 (1%) 69 64	17, 28, 46, 72	0
27	25	59/60 (98%)	0.24	0 100 100	32, 49, 63, 72	0
28	16	53/54 (98%)	0.30	2 (3%) 44 38	33, 47, 60, 64	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%)	0.58	1 (1%) 66 61	35, 51, 61, 67	0
29	17	48/49 (97%)	-0.20	2 (4%) 40 35	16, 25, 49, 72	0
29	27	48/49 (97%)	0.07	1 (2%) 63 58	31, 38, 63, 69	0
30	18	64/65 (98%)	0.23	1 (1%) 70 66	32, 40, 49, 60	0
30	28	64/65 (98%)	0.35	0 100 100	36, 44, 52, 61	0
31	19	37/37 (100%)	0.25	1 (2%) 56 50	36, 47, 61, 70	0
31	29	37/37 (100%)	0.53	0 100 100	42, 52, 64, 74	0
32	1a	1488/1521 (97%)	0.65	52 (3%) 47 41	39, 70, 90, 105	0
32	2a	1491/1521 (98%)	0.80	116 (7%) 19 15	42, 72, 91, 104	0
33	1b	231/256 (90%)	1.49	62 (26%) 1 1	67, 79, 88, 92	0
33	2b	231/256 (90%)	1.85	90 (38%) 1 0	67, 81, 88, 93	0
34	1c	206/239 (86%)	1.20	24 (11%) 9 7	66, 76, 83, 92	0
34	2c	206/239 (86%)	1.76	75 (36%) 1 0	69, 78, 85, 92	0
35	1d	208/209 (99%)	1.14	25 (12%) 9 7	57, 71, 79, 84	0
35	2d	208/209 (99%)	1.04	14 (6%) 24 19	58, 71, 79, 84	0
36	1e	148/162 (91%)	0.76	4 (2%) 56 50	48, 63, 73, 83	0
36	2e	148/162 (91%)	1.42	22 (14%) 5 4	67, 78, 85, 90	0
37	1f	100/101 (99%)	0.62	2 (2%) 65 60	46, 65, 74, 76	0
37	2f	100/101 (99%)	0.82	2 (2%) 65 60	55, 70, 79, 87	0
38	1g	155/156 (99%)	1.25	25 (16%) 4 3	61, 72, 81, 88	0
38	2g	155/156 (99%)	1.24	22 (14%) 6 5	64, 74, 82, 87	0
39	1h	137/138 (99%)	0.78	5 (3%) 46 40	52, 64, 73, 86	0
39	2h	137/138 (99%)	1.40	27 (19%) 3 2	60, 77, 84, 89	0
40	1i	127/128 (99%)	1.70	40 (31%) 1 1	59, 77, 85, 88	0
40	2i	127/128 (99%)	2.00	60 (47%) 0 0	64, 79, 86, 89	0
41	1j	97/105 (92%)	1.42	20 (20%) 2 2	56, 75, 85, 92	0
41	2j	96/105 (91%)	2.33	59 (61%) 0 0	68, 85, 92, 94	0
42	1k	114/129 (88%)	0.48	1 (0%) 81 78	37, 64, 73, 77	0
42	2k	114/129 (88%)	0.91	9 (7%) 18 14	44, 73, 81, 85	0
43	1l	121/132 (91%)	0.36	6 (4%) 34 28	41, 55, 68, 75	0
43	2l	121/132 (91%)	1.23	16 (13%) 7 5	50, 70, 79, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.29	22 (17%) 3 3	58, 73, 81, 84	0
44	2m	122/126 (96%)	1.78	37 (30%) 1 1	63, 76, 82, 85	0
45	1n	60/61 (98%)	0.89	2 (3%) 49 43	55, 64, 74, 80	0
45	2n	60/61 (98%)	2.60	41 (68%) 0 0	73, 85, 90, 94	0
46	1o	88/89 (98%)	1.20	14 (15%) 5 4	52, 66, 76, 83	0
46	2o	88/89 (98%)	0.84	2 (2%) 61 55	56, 68, 78, 85	0
47	1p	82/88 (93%)	1.34	14 (17%) 4 3	56, 68, 76, 81	0
47	2p	82/88 (93%)	1.16	9 (10%) 10 8	58, 68, 76, 82	0
48	1q	99/105 (94%)	1.12	10 (10%) 12 9	59, 68, 76, 78	0
48	2q	99/105 (94%)	1.11	11 (11%) 10 8	60, 69, 77, 80	0
49	1r	68/88 (77%)	0.76	5 (7%) 20 16	57, 67, 76, 82	0
49	2r	68/88 (77%)	0.78	6 (8%) 15 12	57, 68, 77, 83	0
50	1s	83/93 (89%)	1.30	12 (14%) 6 4	64, 76, 84, 91	0
50	2s	83/93 (89%)	2.03	43 (51%) 0 0	67, 79, 86, 93	0
51	1t	96/106 (90%)	1.07	12 (12%) 8 6	56, 67, 77, 81	0
51	2t	96/106 (90%)	1.22	9 (9%) 14 11	56, 68, 78, 80	0
52	1u	23/27 (85%)	1.39	5 (21%) 2 2	62, 70, 74, 75	0
52	2u	23/27 (85%)	2.01	11 (47%) 0 0	65, 72, 76, 76	0
53	1v	14/27 (51%)	1.04	3 (21%) 2 2	55, 73, 97, 105	0
53	2v	13/27 (48%)	1.76	5 (38%) 1 0	60, 75, 89, 98	0
54	1w	68/76 (89%)	0.95	7 (10%) 12 9	67, 86, 97, 105	0
54	1y	67/76 (88%)	0.77	3 (4%) 38 32	40, 91, 97, 99	0
54	2w	67/76 (88%)	1.06	6 (8%) 15 11	73, 88, 97, 99	0
54	2y	66/76 (86%)	1.21	11 (16%) 4 3	43, 93, 97, 99	0
55	1x	72/77 (93%)	0.16	1 (1%) 73 69	27, 56, 81, 85	0
55	2x	72/77 (93%)	0.44	1 (1%) 73 69	44, 77, 88, 94	0
All	All	20879/21754 (95%)	0.57	1569 (7%) 20 16	16, 61, 86, 106	0

The worst 5 of 1569 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	9.1
44	2m	123	ALA	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	888	C	7.0
38	1g	82	GLY	6.5
22	20	2	ALA	6.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	7MG	2y	46	24/25	0.43	0.18	84,98,104,130	0
54	7MG	1y	46	24/25	0.56	0.13	81,96,103,124	0
54	4SU	2y	8	20/21	0.61	0.16	80,97,107,114	0
54	PSU	2y	55	20/21	0.63	0.16	80,96,106,120	0
54	7MG	1w	46	24/25	0.66	0.14	66,84,103,123	0
54	7MG	2w	46	24/25	0.66	0.12	73,93,103,114	0
54	5MU	2y	54	21/22	0.70	0.14	81,94,101,117	0
54	PSU	1y	55	20/21	0.73	0.12	80,96,105,117	0
54	MIA	2y	37	22/30	0.74	0.14	68,84,93,122	0
54	4SU	2w	8	20/21	0.77	0.12	68,89,101,117	0
54	PSU	2y	32	20/21	0.77	0.13	74,85,99,103	0
54	5MU	1y	54	21/22	0.78	0.12	70,86,99,113	0
54	PSU	2y	39	20/21	0.79	0.13	75,83,94,99	0
54	PSU	2w	55	20/21	0.80	0.12	63,84,92,92	0
54	5MU	2w	54	21/22	0.80	0.14	55,78,91,98	0
54	PSU	1y	32	20/21	0.82	0.13	72,86,96,100	0
54	4SU	1y	8	20/21	0.84	0.10	79,87,95,95	0
54	PSU	2w	32	20/21	0.85	0.13	69,80,91,97	0
32	2MG	2a	1207	24/25	0.85	0.14	69,80,93,94	0
54	MIA	1y	37	22/30	0.85	0.11	64,78,83,86	0
54	PSU	1w	55	20/21	0.86	0.11	61,81,88,95	0
55	4SU	2x	8	20/21	0.86	0.12	65,81,88,92	0
55	5MU	2x	54	21/22	0.86	0.11	68,79,84,102	0
55	PSU	2x	55	20/21	0.86	0.11	63,74,87,92	0
54	PSU	1y	39	20/21	0.87	0.12	73,83,89,90	0
32	M2G	2a	966	25/26	0.87	0.17	52,72,85,96	0
54	MIA	2w	37	22/30	0.88	0.12	60,78,83,89	0
1	5MU	2A	1915	21/22	0.88	0.12	59,69,77,91	0
54	PSU	1w	32	20/21	0.90	0.10	67,79,90,93	0
43	0TD	1l	92	10/11	0.90	0.10	48,55,61,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	2w	39	20/21	0.90	0.10	68,76,83,83	0
32	PSU	2a	516	20/21	0.91	0.10	56,70,76,84	0
43	0TD	2l	92	10/11	0.91	0.12	62,70,72,90	0
54	4SU	1w	8	20/21	0.91	0.10	63,75,89,89	0
32	5MC	2a	1400	21/22	0.91	0.15	61,73,83,87	0
32	4OC	2a	1402	22/23	0.91	0.13	48,64,76,83	0
32	5MC	2a	1404	21/22	0.91	0.12	50,61,68,76	0
1	PSU	2A	1917	20/21	0.92	0.10	48,61,71,72	0
32	5MC	2a	967	21/22	0.92	0.12	61,67,75,87	0
55	PSU	1x	55	20/21	0.92	0.09	48,55,72,72	0
1	PSU	2A	1911	20/21	0.92	0.10	40,58,64,67	0
54	5MU	1w	54	21/22	0.93	0.08	48,66,72,87	0
55	5MC	2x	32	21/22	0.93	0.12	63,73,82,83	0
55	5MU	1x	54	21/22	0.93	0.09	40,62,68,69	0
32	7MG	2a	527	24/25	0.93	0.11	54,66,75,89	0
32	PSU	1a	516	20/21	0.93	0.10	58,67,74,78	0
1	4OC	2A	1920	21/23	0.93	0.11	46,54,60,72	0
54	MIA	1w	37	29/30	0.94	0.12	41,59,74,84	0
55	4SU	1x	8	20/21	0.94	0.10	41,59,76,88	0
1	5MU	1A	1915	21/22	0.94	0.11	54,67,70,77	0
32	2MG	1a	1207	24/25	0.94	0.10	49,69,77,81	0
32	UR3	2a	1498	21/22	0.95	0.12	36,56,67,69	0
32	MA6	2a	1519	24/25	0.95	0.14	48,62,68,73	0
1	PSU	1A	1917	20/21	0.95	0.11	44,58,66,67	0
1	5MC	1A	1942	21/22	0.95	0.12	37,49,54,58	0
32	7MG	1a	527	24/25	0.95	0.08	35,51,55,62	0
1	5MC	2A	1942	21/22	0.95	0.09	41,51,58,67	0
32	M2G	1a	966	25/26	0.95	0.10	39,49,58,74	0
54	PSU	1w	39	20/21	0.95	0.09	65,73,79,81	0
1	5MC	2A	1962	21/22	0.95	0.08	27,40,49,52	0
32	5MC	2a	1407	21/22	0.95	0.10	38,51,59,70	0
32	5MC	1a	1400	21/22	0.96	0.10	36,52,62,67	0
1	5MU	2A	1939	21/22	0.96	0.08	25,32,39,43	0
32	MA6	2a	1518	24/25	0.96	0.11	44,63,70,76	0
32	MA6	1a	1519	24/25	0.96	0.11	24,42,50,65	0
1	PSU	1A	1911	20/21	0.96	0.11	41,51,62,64	0
1	OMG	2A	2251	24/25	0.96	0.09	28,33,40,42	0
1	PSU	2A	2605	20/21	0.97	0.06	20,31,35,36	0
32	5MC	1a	1404	21/22	0.97	0.09	30,40,45,48	0
32	5MC	1a	967	21/22	0.97	0.09	42,52,66,70	0
32	5MC	1a	1407	21/22	0.97	0.09	32,46,51,62	0
1	5MU	1A	1939	21/22	0.97	0.08	24,31,38,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UR3	1a	1498	21/22	0.97	0.10	35,43,51,52	0
1	4OC	1A	1920	21/23	0.97	0.11	37,52,60,63	0
55	5MC	1x	32	21/22	0.97	0.10	44,53,60,62	0
32	MA6	1a	1518	24/25	0.97	0.10	28,42,50,51	0
1	2MA	2A	2503	23/24	0.97	0.08	21,28,35,40	0
1	2MU	1A	2552	21/23	0.97	0.07	24,30,37,41	0
1	2MU	2A	2552	21/23	0.97	0.07	26,32,38,49	0
32	4OC	1a	1402	22/23	0.97	0.09	35,45,57,62	0
1	PSU	1A	2605	20/21	0.98	0.06	19,24,34,35	0
1	OMG	1A	2251	24/25	0.98	0.07	25,29,37,40	0
1	5MC	1A	1962	21/22	0.98	0.08	25,36,43,50	0
1	2MA	1A	2503	23/24	0.98	0.07	18,26,31,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2O	8002	1/1	0.53	0.19	112,112,112,112	0
56	MG	2a	1740	1/1	0.57	0.27	82,82,82,82	0
56	MG	1A	3720	1/1	0.60	0.28	71,71,71,71	0
56	MG	2B	3001	1/1	0.62	0.33	69,69,69,69	0
56	MG	2A	3585	1/1	0.63	0.17	44,44,44,44	0
56	MG	1A	3770	1/1	0.66	0.26	63,63,63,63	0
56	MG	1a	1717	1/1	0.66	0.25	80,80,80,80	0
56	MG	2a	1767	1/1	0.68	0.22	74,74,74,74	0
56	MG	1a	1761	1/1	0.69	0.33	72,72,72,72	0
56	MG	2a	1730	1/1	0.70	0.19	71,71,71,71	0
56	MG	1A	3891	1/1	0.70	0.36	76,76,76,76	0
56	MG	2a	1667	1/1	0.70	0.24	73,73,73,73	0
56	MG	1A	3932	1/1	0.71	0.20	56,56,56,56	0
56	MG	2A	3438	1/1	0.71	0.12	44,44,44,44	0
56	MG	1A	3836	1/1	0.71	0.22	54,54,54,54	0
56	MG	1a	1807	1/1	0.72	0.19	84,84,84,84	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	3429	1/1	0.73	0.23	53,53,53,53	0
56	MG	1a	1746	1/1	0.73	0.16	85,85,85,85	0
56	MG	1A	3649	1/1	0.74	0.18	58,58,58,58	0
56	MG	2A	3636	1/1	0.74	0.23	55,55,55,55	0
56	MG	1a	1826	1/1	0.74	0.28	72,72,72,72	0
56	MG	1a	1799	1/1	0.74	0.17	85,85,85,85	0
56	MG	2a	1783	1/1	0.74	0.16	60,60,60,60	0
56	MG	1A	3592	1/1	0.75	0.11	32,32,32,32	0
56	MG	2A	3341	1/1	0.75	0.15	45,45,45,45	0
56	MG	2a	1774	1/1	0.75	0.24	72,72,72,72	0
56	MG	1A	3779	1/1	0.75	0.17	44,44,44,44	0
56	MG	1a	1808	1/1	0.76	0.17	67,67,67,67	0
56	MG	1a	1795	1/1	0.76	0.13	64,64,64,64	0
56	MG	2A	3538	1/1	0.76	0.17	53,53,53,53	0
56	MG	2A	3550	1/1	0.76	0.19	52,52,52,52	0
56	MG	2A	3578	1/1	0.76	0.20	65,65,65,65	0
56	MG	1a	1691	1/1	0.77	0.26	66,66,66,66	0
56	MG	1a	1798	1/1	0.77	0.14	71,71,71,71	0
56	MG	2a	1779	1/1	0.77	0.19	74,74,74,74	0
56	MG	2a	1782	1/1	0.77	0.20	71,71,71,71	0
56	MG	1A	3334	1/1	0.77	0.24	54,54,54,54	0
56	MG	2Z	8001	1/1	0.78	0.13	70,70,70,70	0
56	MG	1A	3784	1/1	0.78	0.17	63,63,63,63	0
56	MG	2a	1680	1/1	0.78	0.16	73,73,73,73	0
56	MG	1A	3815	1/1	0.78	0.19	60,60,60,60	0
56	MG	1A	3705	1/1	0.78	0.19	52,52,52,52	0
56	MG	1A	3874	1/1	0.79	0.27	63,63,63,63	0
56	MG	1A	3503	1/1	0.79	0.14	33,33,33,33	0
56	MG	1a	1815	1/1	0.79	0.15	76,76,76,76	0
56	MG	2A	3579	1/1	0.79	0.19	65,65,65,65	0
56	MG	2a	1621	1/1	0.79	0.16	74,74,74,74	0
56	MG	2a	1625	1/1	0.79	0.24	71,71,71,71	0
56	MG	2a	1647	1/1	0.79	0.16	64,64,64,64	0
56	MG	2A	3530	1/1	0.79	0.14	52,52,52,52	0
56	MG	2A	3587	1/1	0.80	0.22	48,48,48,48	0
56	MG	2a	1734	1/1	0.80	0.23	70,70,70,70	0
56	MG	1B	3012	1/1	0.80	0.20	66,66,66,66	0
56	MG	2A	3399	1/1	0.80	0.19	47,47,47,47	0
56	MG	2B	3009	1/1	0.80	0.26	62,62,62,62	0
56	MG	2a	1661	1/1	0.80	0.26	65,65,65,65	0
56	MG	2F	303	1/1	0.80	0.15	58,58,58,58	0
56	MG	2A	3328	1/1	0.80	0.13	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1788	1/1	0.80	0.18	68,68,68,68	0
56	MG	2a	1649	1/1	0.81	0.26	71,71,71,71	0
56	MG	1A	3183	1/1	0.81	0.20	50,50,50,50	0
56	MG	1A	3960	1/1	0.81	0.11	38,38,38,38	0
56	MG	1B	3010	1/1	0.81	0.18	68,68,68,68	0
56	MG	1A	3257	1/1	0.81	0.24	65,65,65,65	0
56	MG	2a	1731	1/1	0.81	0.14	65,65,65,65	0
56	MG	2B	3016	1/1	0.81	0.38	66,66,66,66	0
56	MG	1a	1624	1/1	0.81	0.22	65,65,65,65	0
56	MG	1A	3761	1/1	0.81	0.12	56,56,56,56	0
56	MG	1A	3271	1/1	0.81	0.22	71,71,71,71	0
56	MG	28	101	1/1	0.81	0.22	57,57,57,57	0
56	MG	1A	3023	1/1	0.81	0.13	57,57,57,57	0
56	MG	1a	1828	1/1	0.81	0.16	62,62,62,62	0
56	MG	2A	3218	1/1	0.81	0.26	49,49,49,49	0
56	MG	1A	3660	1/1	0.82	0.18	50,50,50,50	0
56	MG	2A	3577	1/1	0.82	0.13	61,61,61,61	0
56	MG	1B	3014	1/1	0.82	0.14	63,63,63,63	0
56	MG	1a	1616	1/1	0.82	0.12	62,62,62,62	0
56	MG	1A	3819	1/1	0.82	0.10	51,51,51,51	0
56	MG	1A	3512	1/1	0.82	0.16	53,53,53,53	0
56	MG	2a	1706	1/1	0.82	0.12	75,75,75,75	0
56	MG	2A	3632	1/1	0.82	0.24	58,58,58,58	0
56	MG	1A	3844	1/1	0.82	0.18	64,64,64,64	0
56	MG	2A	3241	1/1	0.82	0.10	42,42,42,42	0
56	MG	1A	3558	1/1	0.82	0.12	51,51,51,51	0
56	MG	1A	3570	1/1	0.82	0.15	43,43,43,43	0
56	MG	2a	1771	1/1	0.82	0.22	63,63,63,63	0
56	MG	1a	1776	1/1	0.82	0.16	63,63,63,63	0
56	MG	1A	3462	1/1	0.82	0.13	53,53,53,53	0
56	MG	2A	3497	1/1	0.82	0.17	56,56,56,56	0
56	MG	1A	3608	1/1	0.82	0.13	40,40,40,40	0
56	MG	1A	3095	1/1	0.82	0.22	54,54,54,54	0
56	MG	1a	1809	1/1	0.83	0.38	83,83,83,83	0
56	MG	1a	1811	1/1	0.83	0.15	57,57,57,57	0
56	MG	2A	3504	1/1	0.83	0.12	45,45,45,45	0
56	MG	2A	3509	1/1	0.83	0.19	50,50,50,50	0
56	MG	2a	1628	1/1	0.83	0.20	65,65,65,65	0
56	MG	1A	3755	1/1	0.83	0.14	55,55,55,55	0
56	MG	1A	3904	1/1	0.83	0.11	55,55,55,55	0
56	MG	2a	1659	1/1	0.83	0.20	66,66,66,66	0
56	MG	1A	3780	1/1	0.83	0.12	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	2A	3570	1/1	0.83	0.15	57,57,57,57	0
56	MG	2A	3097	1/1	0.83	0.19	57,57,57,57	0
56	MG	1A	3697	1/1	0.83	0.18	57,57,57,57	0
56	MG	2A	3222	1/1	0.83	0.08	47,47,47,47	0
56	MG	1a	1676	1/1	0.83	0.25	64,64,64,64	0
56	MG	2A	3242	1/1	0.83	0.11	54,54,54,54	0
56	MG	2A	3627	1/1	0.83	0.18	56,56,56,56	0
56	MG	2a	1745	1/1	0.83	0.29	78,78,78,78	0
56	MG	2A	3298	1/1	0.83	0.11	39,39,39,39	0
56	MG	1B	3004	1/1	0.83	0.29	68,68,68,68	0
56	MG	1A	3723	1/1	0.83	0.19	62,62,62,62	0
56	MG	2a	1775	1/1	0.83	0.25	71,71,71,71	0
56	MG	2A	3373	1/1	0.83	0.10	27,27,27,27	0
56	MG	2a	1781	1/1	0.83	0.12	66,66,66,66	0
56	MG	2A	3389	1/1	0.83	0.18	52,52,52,52	0
56	MG	1a	1721	1/1	0.83	0.13	66,66,66,66	0
56	MG	2A	3402	1/1	0.83	0.16	53,53,53,53	0
56	MG	2l	202	1/1	0.83	0.09	62,62,62,62	0
56	MG	2a	1633	1/1	0.84	0.26	61,61,61,61	0
56	MG	1w	3003	1/1	0.84	0.10	78,78,78,78	0
56	MG	2A	3025	1/1	0.84	0.20	61,61,61,61	0
56	MG	2A	3391	1/1	0.84	0.20	53,53,53,53	0
56	MG	1A	3597	1/1	0.84	0.16	50,50,50,50	0
56	MG	2a	1664	1/1	0.84	0.23	71,71,71,71	0
56	MG	1A	3674	1/1	0.84	0.09	53,53,53,53	0
56	MG	2a	1673	1/1	0.84	0.26	60,60,60,60	0
56	MG	2A	3607	1/1	0.84	0.16	60,60,60,60	0
56	MG	2a	1683	1/1	0.84	0.23	57,57,57,57	0
56	MG	2A	3610	1/1	0.84	0.12	32,32,32,32	0
56	MG	2A	3625	1/1	0.84	0.13	56,56,56,56	0
56	MG	1A	3888	1/1	0.84	0.11	89,89,89,89	0
56	MG	2A	3458	1/1	0.84	0.15	57,57,57,57	0
56	MG	2A	3490	1/1	0.84	0.15	48,48,48,48	0
56	MG	2A	3675	1/1	0.84	0.12	55,55,55,55	0
56	MG	2A	3230	1/1	0.84	0.22	57,57,57,57	0
56	MG	1A	3098	1/1	0.84	0.15	56,56,56,56	0
56	MG	1a	1821	1/1	0.84	0.15	68,68,68,68	0
56	MG	2A	3520	1/1	0.84	0.13	51,51,51,51	0
56	MG	2A	3528	1/1	0.84	0.09	55,55,55,55	0
56	MG	2A	3529	1/1	0.84	0.12	57,57,57,57	0
56	MG	1A	3644	1/1	0.84	0.10	57,57,57,57	0
56	MG	1A	3210	1/1	0.84	0.11	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1w	3002	1/1	0.84	0.10	56,56,56,56	0
56	MG	2A	3347	1/1	0.84	0.12	45,45,45,45	0
56	MG	2A	3547	1/1	0.85	0.13	37,37,37,37	0
56	MG	2A	3549	1/1	0.85	0.11	45,45,45,45	0
56	MG	1A	3587	1/1	0.85	0.12	25,25,25,25	0
56	MG	1A	3214	1/1	0.85	0.10	59,59,59,59	0
56	MG	2A	3370	1/1	0.85	0.08	42,42,42,42	0
56	MG	2a	1657	1/1	0.85	0.14	54,54,54,54	0
56	MG	1A	3726	1/1	0.85	0.11	62,62,62,62	0
56	MG	1l	203	1/1	0.85	0.12	58,58,58,58	0
56	MG	1a	1759	1/1	0.85	0.18	57,57,57,57	0
56	MG	1A	3522	1/1	0.85	0.16	38,38,38,38	0
56	MG	2A	3592	1/1	0.85	0.16	57,57,57,57	0
56	MG	2A	3603	1/1	0.85	0.18	65,65,65,65	0
56	MG	1A	3675	1/1	0.85	0.20	56,56,56,56	0
56	MG	2A	3074	1/1	0.85	0.16	54,54,54,54	0
56	MG	1A	3851	1/1	0.85	0.18	45,45,45,45	0
56	MG	2A	3474	1/1	0.85	0.09	44,44,44,44	0
56	MG	2A	3122	1/1	0.85	0.18	60,60,60,60	0
56	MG	2a	1736	1/1	0.85	0.12	68,68,68,68	0
56	MG	2a	1738	1/1	0.85	0.13	76,76,76,76	0
56	MG	2A	3127	1/1	0.85	0.12	50,50,50,50	0
56	MG	2A	3669	1/1	0.85	0.20	44,44,44,44	0
56	MG	1A	3762	1/1	0.85	0.17	31,31,31,31	0
56	MG	2A	3506	1/1	0.85	0.20	50,50,50,50	0
56	MG	2B	3004	1/1	0.85	0.23	62,62,62,62	0
56	MG	1A	3683	1/1	0.85	0.12	50,50,50,50	0
56	MG	2A	3514	1/1	0.85	0.20	59,59,59,59	0
56	MG	2a	1780	1/1	0.85	0.19	64,64,64,64	0
56	MG	1a	1657	1/1	0.85	0.23	56,56,56,56	0
56	MG	1a	1661	1/1	0.85	0.12	56,56,56,56	0
56	MG	1A	3259	1/1	0.85	0.18	61,61,61,61	0
56	MG	2a	1786	1/1	0.85	0.18	59,59,59,59	0
56	MG	1A	3352	1/1	0.85	0.31	58,58,58,58	0
56	MG	1a	1709	1/1	0.85	0.20	60,60,60,60	0
56	MG	2w	3003	1/1	0.85	0.11	70,70,70,70	0
56	MG	2A	3201	1/1	0.86	0.21	61,61,61,61	0
56	MG	1a	1618	1/1	0.86	0.12	64,64,64,64	0
56	MG	1A	3879	1/1	0.86	0.15	54,54,54,54	0
56	MG	1A	3373	1/1	0.86	0.16	53,53,53,53	0
56	MG	2a	1637	1/1	0.86	0.16	60,60,60,60	0
56	MG	1A	3605	1/1	0.86	0.09	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3403	1/1	0.86	0.15	52,52,52,52	0
56	MG	2A	3243	1/1	0.86	0.13	53,53,53,53	0
56	MG	2A	3285	1/1	0.86	0.13	64,64,64,64	0
56	MG	2A	3555	1/1	0.86	0.12	53,53,53,53	0
56	MG	1a	1810	1/1	0.86	0.11	90,90,90,90	0
56	MG	1a	1683	1/1	0.86	0.22	64,64,64,64	0
56	MG	2a	1672	1/1	0.86	0.28	72,72,72,72	0
56	MG	1a	1813	1/1	0.86	0.15	72,72,72,72	0
56	MG	2A	3345	1/1	0.86	0.13	40,40,40,40	0
56	MG	1A	3816	1/1	0.86	0.21	62,62,62,62	0
56	MG	1a	1694	1/1	0.86	0.29	66,66,66,66	0
56	MG	2a	1726	1/1	0.86	0.17	64,64,64,64	0
56	MG	1a	1702	1/1	0.86	0.21	60,60,60,60	0
56	MG	2A	3382	1/1	0.86	0.09	48,48,48,48	0
56	MG	1A	3640	1/1	0.86	0.11	21,21,21,21	0
56	MG	1b	3002	1/1	0.86	0.26	74,74,74,74	0
56	MG	1A	3831	1/1	0.86	0.17	62,62,62,62	0
56	MG	1A	3479	1/1	0.86	0.14	48,48,48,48	0
56	MG	2A	3424	1/1	0.86	0.16	43,43,43,43	0
56	MG	2a	1750	1/1	0.86	0.18	72,72,72,72	0
56	MG	1A	3532	1/1	0.86	0.13	59,59,59,59	0
56	MG	2A	3667	1/1	0.86	0.14	53,53,53,53	0
56	MG	2a	1773	1/1	0.86	0.14	66,66,66,66	0
56	MG	1A	3709	1/1	0.86	0.12	43,43,43,43	0
56	MG	2A	3469	1/1	0.86	0.15	46,46,46,46	0
56	MG	2A	3051	1/1	0.86	0.20	61,61,61,61	0
56	MG	1F	307	1/1	0.86	0.18	57,57,57,57	0
56	MG	2A	3491	1/1	0.86	0.15	49,49,49,49	0
56	MG	2A	3078	1/1	0.86	0.13	47,47,47,47	0
56	MG	1N	3006	1/1	0.86	0.22	50,50,50,50	0
56	MG	2A	3120	1/1	0.86	0.11	53,53,53,53	0
56	MG	1a	1778	1/1	0.86	0.22	66,66,66,66	0
56	MG	1A	3718	1/1	0.86	0.14	69,69,69,69	0
56	MG	2a	1605	1/1	0.86	0.26	81,81,81,81	0
56	MG	1A	3439	1/1	0.87	0.12	43,43,43,43	0
56	MG	2a	1611	1/1	0.87	0.15	62,62,62,62	0
56	MG	2a	1617	1/1	0.87	0.18	52,52,52,52	0
56	MG	1A	3264	1/1	0.87	0.19	64,64,64,64	0
56	MG	1a	1696	1/1	0.87	0.18	66,66,66,66	0
56	MG	1A	3883	1/1	0.87	0.20	60,60,60,60	0
56	MG	1A	3747	1/1	0.87	0.14	49,49,49,49	0
56	MG	2a	1634	1/1	0.87	0.21	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3200	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	3638	1/1	0.87	0.17	27,27,27,27	0
56	MG	2A	3125	1/1	0.87	0.10	56,56,56,56	0
56	MG	1A	3486	1/1	0.87	0.16	46,46,46,46	0
56	MG	2A	3128	1/1	0.87	0.14	49,49,49,49	0
56	MG	1a	1752	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3208	1/1	0.87	0.08	45,45,45,45	0
56	MG	1A	3498	1/1	0.87	0.09	50,50,50,50	0
56	MG	1A	3124	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3212	1/1	0.87	0.20	67,67,67,67	0
56	MG	1A	3143	1/1	0.87	0.11	30,30,30,30	0
56	MG	1a	1782	1/1	0.87	0.09	44,44,44,44	0
56	MG	2a	1689	1/1	0.87	0.24	61,61,61,61	0
56	MG	1a	1794	1/1	0.87	0.10	45,45,45,45	0
56	MG	2a	1710	1/1	0.87	0.22	61,61,61,61	0
56	MG	2a	1715	1/1	0.87	0.19	53,53,53,53	0
56	MG	2a	1722	1/1	0.87	0.20	57,57,57,57	0
56	MG	2a	1724	1/1	0.87	0.12	83,83,83,83	0
56	MG	2A	3245	1/1	0.87	0.13	42,42,42,42	0
56	MG	2a	1729	1/1	0.87	0.16	65,65,65,65	0
56	MG	1A	3798	1/1	0.87	0.11	43,43,43,43	0
56	MG	1A	3381	1/1	0.87	0.12	57,57,57,57	0
56	MG	2A	3305	1/1	0.87	0.10	37,37,37,37	0
56	MG	1A	3384	1/1	0.87	0.18	52,52,52,52	0
56	MG	2A	3330	1/1	0.87	0.12	44,44,44,44	0
56	MG	1O	204	1/1	0.87	0.14	52,52,52,52	0
56	MG	1R	203	1/1	0.87	0.14	44,44,44,44	0
56	MG	1a	1602	1/1	0.87	0.21	68,68,68,68	0
56	MG	2a	1756	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	3817	1/1	0.87	0.13	45,45,45,45	0
56	MG	1A	3057	1/1	0.87	0.09	44,44,44,44	0
56	MG	1A	3584	1/1	0.87	0.12	19,19,19,19	0
56	MG	1A	3416	1/1	0.87	0.12	54,54,54,54	0
56	MG	1a	1660	1/1	0.87	0.08	47,47,47,47	0
56	MG	2a	1776	1/1	0.87	0.22	66,66,66,66	0
56	MG	2A	3398	1/1	0.87	0.09	47,47,47,47	0
56	MG	1A	3187	1/1	0.87	0.14	60,60,60,60	0
56	MG	1a	1665	1/1	0.87	0.13	56,56,56,56	0
56	MG	1a	1668	1/1	0.87	0.18	52,52,52,52	0
56	MG	1A	3847	1/1	0.87	0.13	74,74,74,74	0
56	MG	2A	3441	1/1	0.87	0.12	33,33,33,33	0
56	MG	1a	1682	1/1	0.87	0.17	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1796	1/1	0.87	0.20	60,60,60,60	0
56	MG	1A	3593	1/1	0.87	0.10	29,29,29,29	0
56	MG	1w	3004	1/1	0.87	0.14	51,51,51,51	0
56	MG	1A	3722	1/1	0.88	0.28	48,48,48,48	0
56	MG	1a	1645	1/1	0.88	0.10	56,56,56,56	0
56	MG	2A	3368	1/1	0.88	0.09	38,38,38,38	0
56	MG	1a	1649	1/1	0.88	0.16	56,56,56,56	0
56	MG	1a	1651	1/1	0.88	0.22	62,62,62,62	0
56	MG	1a	1652	1/1	0.88	0.10	51,51,51,51	0
56	MG	1A	3524	1/1	0.88	0.14	50,50,50,50	0
56	MG	2Q	201	1/1	0.88	0.43	61,61,61,61	0
56	MG	1a	1820	1/1	0.88	0.18	62,62,62,62	0
56	MG	1A	3639	1/1	0.88	0.10	39,39,39,39	0
56	MG	1A	3732	1/1	0.88	0.10	60,60,60,60	0
56	MG	1A	3866	1/1	0.88	0.10	44,44,44,44	0
56	MG	2A	3414	1/1	0.88	0.10	40,40,40,40	0
56	MG	2A	3416	1/1	0.88	0.17	44,44,44,44	0
56	MG	2a	1623	1/1	0.88	0.21	65,65,65,65	0
56	MG	1A	3742	1/1	0.88	0.15	37,37,37,37	0
56	MG	1A	3876	1/1	0.88	0.18	55,55,55,55	0
56	MG	1A	3529	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3643	1/1	0.88	0.14	30,30,30,30	0
56	MG	2A	3461	1/1	0.88	0.11	39,39,39,39	0
56	MG	2A	3463	1/1	0.88	0.13	45,45,45,45	0
56	MG	1A	3062	1/1	0.88	0.14	50,50,50,50	0
56	MG	1a	1692	1/1	0.88	0.14	60,60,60,60	0
56	MG	1a	1693	1/1	0.88	0.24	60,60,60,60	0
56	MG	1A	3386	1/1	0.88	0.12	42,42,42,42	0
56	MG	2A	3495	1/1	0.88	0.25	61,61,61,61	0
56	MG	2a	1665	1/1	0.88	0.11	55,55,55,55	0
56	MG	1A	3128	1/1	0.88	0.15	49,49,49,49	0
56	MG	2A	3499	1/1	0.88	0.11	52,52,52,52	0
56	MG	1A	3481	1/1	0.88	0.12	26,26,26,26	0
56	MG	2a	1677	1/1	0.88	0.16	51,51,51,51	0
56	MG	2a	1678	1/1	0.88	0.21	64,64,64,64	0
56	MG	1A	3121	1/1	0.88	0.15	55,55,55,55	0
56	MG	1A	3783	1/1	0.88	0.10	27,27,27,27	0
56	MG	1a	1718	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3419	1/1	0.88	0.12	43,43,43,43	0
56	MG	2A	3523	1/1	0.88	0.15	54,54,54,54	0
56	MG	2A	3527	1/1	0.88	0.17	53,53,53,53	0
56	MG	1a	1730	1/1	0.88	0.11	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3138	1/1	0.88	0.15	47,47,47,47	0
56	MG	2A	3150	1/1	0.88	0.14	35,35,35,35	0
56	MG	2A	3534	1/1	0.88	0.11	62,62,62,62	0
56	MG	2A	3172	1/1	0.88	0.15	59,59,59,59	0
56	MG	2A	3179	1/1	0.88	0.09	45,45,45,45	0
56	MG	2A	3197	1/1	0.88	0.10	50,50,50,50	0
56	MG	1a	1735	1/1	0.88	0.12	58,58,58,58	0
56	MG	1A	3788	1/1	0.88	0.12	24,24,24,24	0
56	MG	2A	3557	1/1	0.88	0.11	49,49,49,49	0
56	MG	2a	1742	1/1	0.88	0.22	62,62,62,62	0
56	MG	2A	3559	1/1	0.88	0.17	59,59,59,59	0
56	MG	1A	3426	1/1	0.88	0.14	51,51,51,51	0
56	MG	1B	3020	1/1	0.88	0.10	48,48,48,48	0
56	MG	2a	1761	1/1	0.88	0.17	82,82,82,82	0
56	MG	2A	3225	1/1	0.88	0.25	53,53,53,53	0
56	MG	2a	1768	1/1	0.88	0.13	54,54,54,54	0
56	MG	1A	3806	1/1	0.88	0.12	73,73,73,73	0
56	MG	1A	3810	1/1	0.88	0.08	36,36,36,36	0
56	MG	1A	3221	1/1	0.88	0.11	48,48,48,48	0
56	MG	1A	3602	1/1	0.88	0.11	22,22,22,22	0
56	MG	1a	1787	1/1	0.88	0.12	48,48,48,48	0
56	MG	2A	3259	1/1	0.88	0.12	43,43,43,43	0
56	MG	2A	3281	1/1	0.88	0.13	40,40,40,40	0
56	MG	1Z	3003	1/1	0.88	0.07	61,61,61,61	0
56	MG	1A	3717	1/1	0.88	0.12	60,60,60,60	0
56	MG	2A	3628	1/1	0.88	0.12	46,46,46,46	0
56	MG	2A	3629	1/1	0.88	0.10	56,56,56,56	0
56	MG	1a	1612	1/1	0.88	0.18	63,63,63,63	0
56	MG	1A	3521	1/1	0.88	0.08	35,35,35,35	0
56	MG	1a	1806	1/1	0.88	0.14	68,68,68,68	0
56	MG	2t	3001	1/1	0.88	0.22	48,48,48,48	0
56	MG	1A	3437	1/1	0.88	0.09	28,28,28,28	0
56	MG	1a	1644	1/1	0.89	0.26	56,56,56,56	0
56	MG	1A	3687	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3371	1/1	0.89	0.09	49,49,49,49	0
56	MG	1A	3371	1/1	0.89	0.27	56,56,56,56	0
56	MG	1A	3568	1/1	0.89	0.19	53,53,53,53	0
56	MG	2A	3386	1/1	0.89	0.09	50,50,50,50	0
56	MG	1A	3041	1/1	0.89	0.10	35,35,35,35	0
56	MG	2B	3017	1/1	0.89	0.38	63,63,63,63	0
56	MG	1A	3207	1/1	0.89	0.09	52,52,52,52	0
56	MG	2F	304	1/1	0.89	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3393	1/1	0.89	0.08	21,21,21,21	0
56	MG	1A	3484	1/1	0.89	0.12	30,30,30,30	0
56	MG	1A	3044	1/1	0.89	0.07	23,23,23,23	0
56	MG	1A	3491	1/1	0.89	0.14	53,53,53,53	0
56	MG	1a	1667	1/1	0.89	0.22	68,68,68,68	0
56	MG	1A	3497	1/1	0.89	0.07	29,29,29,29	0
56	MG	2a	1614	1/1	0.89	0.25	71,71,71,71	0
56	MG	1A	3074	1/1	0.89	0.11	45,45,45,45	0
56	MG	2a	1618	1/1	0.89	0.24	67,67,67,67	0
56	MG	1y	102	1/1	0.89	0.11	63,63,63,63	0
56	MG	1A	3871	1/1	0.89	0.09	18,18,18,18	0
56	MG	2A	3447	1/1	0.89	0.10	46,46,46,46	0
56	MG	2A	3039	1/1	0.89	0.13	46,46,46,46	0
56	MG	2a	1629	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3280	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3738	1/1	0.89	0.26	44,44,44,44	0
56	MG	2A	3467	1/1	0.89	0.09	65,65,65,65	0
56	MG	2a	1642	1/1	0.89	0.21	66,66,66,66	0
56	MG	1A	3505	1/1	0.89	0.09	28,28,28,28	0
56	MG	2A	3470	1/1	0.89	0.09	30,30,30,30	0
56	MG	2a	1651	1/1	0.89	0.27	70,70,70,70	0
56	MG	1A	3745	1/1	0.89	0.15	61,61,61,61	0
56	MG	2A	3483	1/1	0.89	0.13	61,61,61,61	0
56	MG	2A	3487	1/1	0.89	0.12	56,56,56,56	0
56	MG	1A	3630	1/1	0.89	0.12	35,35,35,35	0
56	MG	1A	3750	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3124	1/1	0.89	0.07	50,50,50,50	0
56	MG	2A	3496	1/1	0.89	0.14	53,53,53,53	0
56	MG	1A	3900	1/1	0.89	0.16	28,28,28,28	0
56	MG	1a	1706	1/1	0.89	0.28	66,66,66,66	0
56	MG	1A	3903	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3308	1/1	0.89	0.21	58,58,58,58	0
56	MG	2a	1681	1/1	0.89	0.24	47,47,47,47	0
56	MG	1A	3910	1/1	0.89	0.15	40,40,40,40	0
56	MG	1A	3757	1/1	0.89	0.09	44,44,44,44	0
56	MG	1A	3938	1/1	0.89	0.23	43,43,43,43	0
56	MG	2A	3521	1/1	0.89	0.17	63,63,63,63	0
56	MG	2A	3522	1/1	0.89	0.08	53,53,53,53	0
56	MG	1A	3515	1/1	0.89	0.09	37,37,37,37	0
56	MG	2A	3198	1/1	0.89	0.08	42,42,42,42	0
56	MG	1a	1740	1/1	0.89	0.09	45,45,45,45	0
56	MG	1A	3322	1/1	0.89	0.15	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	3084	1/1	0.89	0.12	42,42,42,42	0
56	MG	1A	3774	1/1	0.89	0.12	42,42,42,42	0
56	MG	1A	3341	1/1	0.89	0.17	60,60,60,60	0
56	MG	2A	3229	1/1	0.89	0.18	53,53,53,53	0
56	MG	1A	3347	1/1	0.89	0.26	54,54,54,54	0
56	MG	2A	3234	1/1	0.89	0.13	54,54,54,54	0
56	MG	2A	3551	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3531	1/1	0.89	0.08	53,53,53,53	0
56	MG	1a	1781	1/1	0.89	0.21	63,63,63,63	0
56	MG	2a	1751	1/1	0.89	0.16	65,65,65,65	0
56	MG	1A	3667	1/1	0.89	0.09	45,45,45,45	0
56	MG	1A	3673	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3251	1/1	0.89	0.09	27,27,27,27	0
56	MG	1R	201	1/1	0.89	0.07	34,34,34,34	0
56	MG	2A	3263	1/1	0.89	0.10	45,45,45,45	0
56	MG	2A	3264	1/1	0.89	0.19	40,40,40,40	0
56	MG	1A	3197	1/1	0.89	0.19	51,51,51,51	0
56	MG	2A	3588	1/1	0.89	0.19	60,60,60,60	0
56	MG	1A	3800	1/1	0.89	0.10	54,54,54,54	0
56	MG	2A	3296	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3604	1/1	0.89	0.12	45,45,45,45	0
56	MG	1A	3805	1/1	0.89	0.14	64,64,64,64	0
56	MG	2A	3302	1/1	0.89	0.13	38,38,38,38	0
56	MG	2A	3612	1/1	0.89	0.15	57,57,57,57	0
56	MG	1a	1803	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3548	1/1	0.89	0.17	47,47,47,47	0
56	MG	2a	1791	1/1	0.89	0.22	63,63,63,63	0
56	MG	1A	3809	1/1	0.89	0.09	42,42,42,42	0
56	MG	2d	302	1/1	0.89	0.10	67,67,67,67	0
56	MG	2j	8001	1/1	0.89	0.18	69,69,69,69	0
56	MG	2j	8002	1/1	0.89	0.08	66,66,66,66	0
56	MG	1A	3555	1/1	0.89	0.10	55,55,55,55	0
56	MG	2p	3001	1/1	0.89	0.10	52,52,52,52	0
56	MG	2r	101	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	3811	1/1	0.89	0.17	64,64,64,64	0
56	MG	1a	1642	1/1	0.89	0.09	42,42,42,42	0
56	MG	2A	3250	1/1	0.90	0.11	43,43,43,43	0
56	MG	1O	205	1/1	0.90	0.13	55,55,55,55	0
56	MG	1P	201	1/1	0.90	0.09	50,50,50,50	0
56	MG	1P	204	1/1	0.90	0.18	42,42,42,42	0
56	MG	1Q	206	1/1	0.90	0.21	54,54,54,54	0
56	MG	1A	3350	1/1	0.90	0.14	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3631	1/1	0.90	0.13	51,51,51,51	0
56	MG	1a	1788	1/1	0.90	0.17	64,64,64,64	0
56	MG	1a	1791	1/1	0.90	0.19	62,62,62,62	0
56	MG	2A	3651	1/1	0.90	0.15	55,55,55,55	0
56	MG	1a	1792	1/1	0.90	0.11	75,75,75,75	0
56	MG	1A	3421	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3594	1/1	0.90	0.09	35,35,35,35	0
56	MG	2A	3315	1/1	0.90	0.12	40,40,40,40	0
56	MG	1Z	3004	1/1	0.90	0.15	52,52,52,52	0
56	MG	10	103	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3339	1/1	0.90	0.10	38,38,38,38	0
56	MG	13	102	1/1	0.90	0.16	52,52,52,52	0
56	MG	1A	3273	1/1	0.90	0.10	42,42,42,42	0
56	MG	1a	1611	1/1	0.90	0.10	57,57,57,57	0
56	MG	1A	3600	1/1	0.90	0.10	41,41,41,41	0
56	MG	1A	3719	1/1	0.90	0.12	41,41,41,41	0
56	MG	1A	3366	1/1	0.90	0.30	61,61,61,61	0
56	MG	20	101	1/1	0.90	0.15	57,57,57,57	0
56	MG	20	102	1/1	0.90	0.15	57,57,57,57	0
56	MG	1a	1623	1/1	0.90	0.32	59,59,59,59	0
56	MG	1A	3604	1/1	0.90	0.15	29,29,29,29	0
56	MG	2a	1608	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3275	1/1	0.90	0.08	39,39,39,39	0
56	MG	1A	3253	1/1	0.90	0.08	51,51,51,51	0
56	MG	1A	3618	1/1	0.90	0.07	70,70,70,70	0
56	MG	1A	3620	1/1	0.90	0.09	32,32,32,32	0
56	MG	1A	3440	1/1	0.90	0.14	72,72,72,72	0
56	MG	1A	3859	1/1	0.90	0.13	53,53,53,53	0
56	MG	1a	1655	1/1	0.90	0.31	63,63,63,63	0
56	MG	2A	3407	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3408	1/1	0.90	0.07	50,50,50,50	0
56	MG	1a	1656	1/1	0.90	0.15	46,46,46,46	0
56	MG	1A	3441	1/1	0.90	0.14	48,48,48,48	0
56	MG	2A	3420	1/1	0.90	0.11	43,43,43,43	0
56	MG	1A	3528	1/1	0.90	0.11	64,64,64,64	0
56	MG	2A	3425	1/1	0.90	0.08	38,38,38,38	0
56	MG	2A	3434	1/1	0.90	0.11	39,39,39,39	0
56	MG	1A	3457	1/1	0.90	0.11	30,30,30,30	0
56	MG	2a	1656	1/1	0.90	0.13	62,62,62,62	0
56	MG	1A	3374	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	3473	1/1	0.90	0.08	26,26,26,26	0
56	MG	2A	3041	1/1	0.90	0.16	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	2A	3048	1/1	0.90	0.29	44,44,44,44	0
56	MG	1A	3758	1/1	0.90	0.11	40,40,40,40	0
56	MG	2A	3058	1/1	0.90	0.11	47,47,47,47	0
56	MG	2A	3062	1/1	0.90	0.10	42,42,42,42	0
56	MG	2A	3067	1/1	0.90	0.07	32,32,32,32	0
56	MG	1a	1673	1/1	0.90	0.13	65,65,65,65	0
56	MG	2A	3481	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3534	1/1	0.90	0.09	47,47,47,47	0
56	MG	2A	3083	1/1	0.90	0.10	48,48,48,48	0
56	MG	2a	1682	1/1	0.90	0.28	64,64,64,64	0
56	MG	2A	3084	1/1	0.90	0.08	40,40,40,40	0
56	MG	1A	3053	1/1	0.90	0.16	52,52,52,52	0
56	MG	2a	1694	1/1	0.90	0.24	62,62,62,62	0
56	MG	2A	3493	1/1	0.90	0.10	62,62,62,62	0
56	MG	2A	3113	1/1	0.90	0.22	51,51,51,51	0
56	MG	1A	3662	1/1	0.90	0.22	55,55,55,55	0
56	MG	2a	1720	1/1	0.90	0.08	53,53,53,53	0
56	MG	1A	3901	1/1	0.90	0.15	46,46,46,46	0
56	MG	2A	3498	1/1	0.90	0.07	37,37,37,37	0
56	MG	1A	3773	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3665	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3775	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	3776	1/1	0.90	0.14	45,45,45,45	0
56	MG	1a	1697	1/1	0.90	0.14	63,63,63,63	0
56	MG	1a	1701	1/1	0.90	0.18	52,52,52,52	0
56	MG	2A	3169	1/1	0.90	0.10	41,41,41,41	0
56	MG	2a	1739	1/1	0.90	0.18	74,74,74,74	0
56	MG	1A	3050	1/1	0.90	0.10	46,46,46,46	0
56	MG	2A	3176	1/1	0.90	0.27	52,52,52,52	0
56	MG	1a	1704	1/1	0.90	0.39	73,73,73,73	0
56	MG	2a	1747	1/1	0.90	0.20	72,72,72,72	0
56	MG	2a	1748	1/1	0.90	0.16	77,77,77,77	0
56	MG	2A	3190	1/1	0.90	0.10	44,44,44,44	0
56	MG	1A	3958	1/1	0.90	0.29	49,49,49,49	0
56	MG	2a	1752	1/1	0.90	0.12	68,68,68,68	0
56	MG	1a	1707	1/1	0.90	0.19	62,62,62,62	0
56	MG	1A	3670	1/1	0.90	0.21	58,58,58,58	0
56	MG	2a	1765	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3536	1/1	0.90	0.12	46,46,46,46	0
56	MG	2A	3204	1/1	0.90	0.15	47,47,47,47	0
56	MG	1A	3237	1/1	0.90	0.08	44,44,44,44	0
56	MG	2A	3212	1/1	0.90	0.21	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3213	1/1	0.90	0.10	45,45,45,45	0
56	MG	1A	3397	1/1	0.90	0.14	56,56,56,56	0
56	MG	1A	3266	1/1	0.90	0.15	61,61,61,61	0
56	MG	1A	3679	1/1	0.90	0.11	52,52,52,52	0
56	MG	2A	3227	1/1	0.90	0.12	48,48,48,48	0
56	MG	2A	3228	1/1	0.90	0.07	43,43,43,43	0
56	MG	2A	3572	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3574	1/1	0.90	0.16	43,43,43,43	0
56	MG	2A	3576	1/1	0.90	0.07	59,59,59,59	0
56	MG	1A	3494	1/1	0.90	0.09	47,47,47,47	0
56	MG	1B	3021	1/1	0.90	0.08	48,48,48,48	0
56	MG	2a	1795	1/1	0.90	0.14	55,55,55,55	0
56	MG	2A	3231	1/1	0.90	0.11	49,49,49,49	0
56	MG	1A	3802	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3240	1/1	0.90	0.09	46,46,46,46	0
56	MG	1G	203	1/1	0.90	0.07	71,71,71,71	0
56	MG	1a	1758	1/1	0.90	0.10	55,55,55,55	0
56	MG	1A	3803	1/1	0.90	0.18	60,60,60,60	0
56	MG	1A	3239	1/1	0.90	0.13	56,56,56,56	0
56	MG	2A	3605	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3246	1/1	0.90	0.16	56,56,56,56	0
59	ZN	24	501	1/1	0.90	0.10	143,143,143,143	0
61	FME	2x	103	10/11	0.90	0.21	36,58,64,90	10
56	MG	16	502	1/1	0.91	0.24	51,51,51,51	0
56	MG	17	101	1/1	0.91	0.11	48,48,48,48	0
56	MG	2A	3274	1/1	0.91	0.12	48,48,48,48	0
56	MG	2A	3613	1/1	0.91	0.19	64,64,64,64	0
56	MG	2A	3617	1/1	0.91	0.09	54,54,54,54	0
56	MG	17	102	1/1	0.91	0.08	50,50,50,50	0
56	MG	2A	3626	1/1	0.91	0.09	49,49,49,49	0
56	MG	1A	3846	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3287	1/1	0.91	0.13	31,31,31,31	0
56	MG	2A	3289	1/1	0.91	0.23	60,60,60,60	0
56	MG	2A	3292	1/1	0.91	0.12	45,45,45,45	0
56	MG	1a	1603	1/1	0.91	0.14	66,66,66,66	0
56	MG	2A	3297	1/1	0.91	0.08	32,32,32,32	0
56	MG	2A	3643	1/1	0.91	0.09	38,38,38,38	0
56	MG	1A	3116	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3848	1/1	0.91	0.10	29,29,29,29	0
56	MG	1a	1613	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3311	1/1	0.91	0.15	45,45,45,45	0
56	MG	2A	3312	1/1	0.91	0.10	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	3581	1/1	0.91	0.12	50,50,50,50	0
56	MG	1A	3323	1/1	0.91	0.18	50,50,50,50	0
56	MG	1A	3409	1/1	0.91	0.06	34,34,34,34	0
56	MG	1A	3868	1/1	0.91	0.07	48,48,48,48	0
56	MG	2F	301	1/1	0.91	0.11	37,37,37,37	0
56	MG	1a	1634	1/1	0.91	0.28	61,61,61,61	0
56	MG	2A	3343	1/1	0.91	0.07	33,33,33,33	0
56	MG	2O	8001	1/1	0.91	0.10	52,52,52,52	0
56	MG	1a	1637	1/1	0.91	0.08	47,47,47,47	0
56	MG	1a	1641	1/1	0.91	0.09	50,50,50,50	0
56	MG	2A	3357	1/1	0.91	0.13	49,49,49,49	0
56	MG	1a	1837	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3766	1/1	0.91	0.12	57,57,57,57	0
56	MG	1d	502	1/1	0.91	0.23	51,51,51,51	0
56	MG	1d	503	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3262	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3335	1/1	0.91	0.18	47,47,47,47	0
56	MG	1A	3018	1/1	0.91	0.20	52,52,52,52	0
56	MG	2a	1615	1/1	0.91	0.18	63,63,63,63	0
56	MG	1A	3880	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3392	1/1	0.91	0.15	55,55,55,55	0
56	MG	1w	3006	1/1	0.91	0.09	67,67,67,67	0
56	MG	1x	3005	1/1	0.91	0.18	66,66,66,66	0
56	MG	2a	1624	1/1	0.91	0.18	54,54,54,54	0
56	MG	1x	3007	1/1	0.91	0.26	51,51,51,51	0
56	MG	1x	3010	1/1	0.91	0.10	74,74,74,74	0
56	MG	2A	3404	1/1	0.91	0.10	37,37,37,37	0
56	MG	2a	1631	1/1	0.91	0.23	58,58,58,58	0
56	MG	1A	3236	1/1	0.91	0.19	52,52,52,52	0
56	MG	2A	3006	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3008	1/1	0.91	0.09	39,39,39,39	0
56	MG	2a	1638	1/1	0.91	0.08	50,50,50,50	0
56	MG	1A	3887	1/1	0.91	0.09	49,49,49,49	0
56	MG	2a	1644	1/1	0.91	0.09	66,66,66,66	0
56	MG	2a	1646	1/1	0.91	0.18	55,55,55,55	0
56	MG	1A	3148	1/1	0.91	0.24	31,31,31,31	0
56	MG	1A	3777	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3171	1/1	0.91	0.11	43,43,43,43	0
56	MG	2a	1652	1/1	0.91	0.16	62,62,62,62	0
56	MG	2a	1655	1/1	0.91	0.19	64,64,64,64	0
56	MG	1A	3689	1/1	0.91	0.10	35,35,35,35	0
56	MG	1A	3782	1/1	0.91	0.10	34,34,34,34	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	1658	1/1	0.91	0.16	69,69,69,69	0
56	MG	1A	3274	1/1	0.91	0.17	66,66,66,66	0
56	MG	2A	3444	1/1	0.91	0.08	50,50,50,50	0
56	MG	2A	3065	1/1	0.91	0.11	43,43,43,43	0
56	MG	2A	3452	1/1	0.91	0.29	54,54,54,54	0
56	MG	2A	3066	1/1	0.91	0.09	46,46,46,46	0
56	MG	2a	1671	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3702	1/1	0.91	0.07	45,45,45,45	0
56	MG	1A	3914	1/1	0.91	0.11	38,38,38,38	0
56	MG	1A	3370	1/1	0.91	0.12	42,42,42,42	0
56	MG	2A	3082	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3790	1/1	0.91	0.07	49,49,49,49	0
56	MG	1A	3793	1/1	0.91	0.09	28,28,28,28	0
56	MG	2A	3476	1/1	0.91	0.16	47,47,47,47	0
56	MG	2A	3087	1/1	0.91	0.13	55,55,55,55	0
56	MG	2a	1686	1/1	0.91	0.30	66,66,66,66	0
56	MG	2a	1688	1/1	0.91	0.18	56,56,56,56	0
56	MG	2A	3090	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3093	1/1	0.91	0.08	51,51,51,51	0
56	MG	2a	1702	1/1	0.91	0.12	60,60,60,60	0
56	MG	2a	1705	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3488	1/1	0.91	0.11	52,52,52,52	0
56	MG	1A	3796	1/1	0.91	0.13	47,47,47,47	0
56	MG	2A	3102	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3103	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3963	1/1	0.91	0.11	34,34,34,34	0
56	MG	1B	3002	1/1	0.91	0.13	48,48,48,48	0
56	MG	1A	3180	1/1	0.91	0.17	56,56,56,56	0
56	MG	2a	1727	1/1	0.91	0.11	62,62,62,62	0
56	MG	2a	1728	1/1	0.91	0.15	52,52,52,52	0
56	MG	1B	3007	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	3799	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3501	1/1	0.91	0.08	46,46,46,46	0
56	MG	1A	3279	1/1	0.91	0.14	52,52,52,52	0
56	MG	1A	3801	1/1	0.91	0.13	45,45,45,45	0
56	MG	1A	3461	1/1	0.91	0.09	27,27,27,27	0
56	MG	1A	3624	1/1	0.91	0.11	57,57,57,57	0
56	MG	2A	3518	1/1	0.91	0.09	50,50,50,50	0
56	MG	2a	1741	1/1	0.91	0.21	48,48,48,48	0
56	MG	1B	3022	1/1	0.91	0.13	53,53,53,53	0
56	MG	1B	3023	1/1	0.91	0.16	51,51,51,51	0
56	MG	2a	1746	1/1	0.91	0.15	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	1710	1/1	0.91	0.22	61,61,61,61	0
56	MG	2A	3178	1/1	0.91	0.16	43,43,43,43	0
56	MG	1a	1711	1/1	0.91	0.16	49,49,49,49	0
56	MG	1B	3024	1/1	0.91	0.11	63,63,63,63	0
56	MG	1B	3025	1/1	0.91	0.08	49,49,49,49	0
56	MG	1a	1720	1/1	0.91	0.26	64,64,64,64	0
56	MG	2A	3533	1/1	0.91	0.12	26,26,26,26	0
56	MG	1B	3026	1/1	0.91	0.10	62,62,62,62	0
56	MG	1a	1722	1/1	0.91	0.12	50,50,50,50	0
56	MG	2A	3537	1/1	0.91	0.12	57,57,57,57	0
56	MG	1a	1723	1/1	0.91	0.16	62,62,62,62	0
56	MG	2a	1772	1/1	0.91	0.08	52,52,52,52	0
56	MG	1D	304	1/1	0.91	0.14	44,44,44,44	0
56	MG	1A	3628	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3629	1/1	0.91	0.10	42,42,42,42	0
56	MG	1N	3002	1/1	0.91	0.07	49,49,49,49	0
56	MG	1A	3254	1/1	0.91	0.12	58,58,58,58	0
56	MG	1O	202	1/1	0.91	0.09	63,63,63,63	0
56	MG	2A	3558	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3632	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3464	1/1	0.91	0.11	35,35,35,35	0
56	MG	2a	1785	1/1	0.91	0.15	66,66,66,66	0
56	MG	1a	1766	1/1	0.91	0.17	59,59,59,59	0
56	MG	2a	1787	1/1	0.91	0.14	51,51,51,51	0
56	MG	1a	1772	1/1	0.91	0.09	60,60,60,60	0
56	MG	2a	1790	1/1	0.91	0.30	66,66,66,66	0
56	MG	1A	3737	1/1	0.91	0.15	50,50,50,50	0
56	MG	1A	3465	1/1	0.91	0.08	32,32,32,32	0
56	MG	1A	3468	1/1	0.91	0.09	44,44,44,44	0
56	MG	1A	3470	1/1	0.91	0.12	27,27,27,27	0
56	MG	2A	3582	1/1	0.91	0.15	47,47,47,47	0
56	MG	1R	202	1/1	0.91	0.14	36,36,36,36	0
56	MG	1A	3823	1/1	0.91	0.08	67,67,67,67	0
56	MG	1A	3282	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3835	1/1	0.91	0.12	30,30,30,30	0
56	MG	2A	3598	1/1	0.91	0.16	45,45,45,45	0
56	MG	1A	3056	1/1	0.91	0.20	48,48,48,48	0
57	K	1A	3321	1/1	0.91	0.17	84,84,84,84	0
56	MG	1A	3313	1/1	0.91	0.21	41,41,41,41	0
56	MG	2A	3260	1/1	0.91	0.10	52,52,52,52	0
56	MG	2a	1601	1/1	0.92	0.10	45,45,45,45	0
56	MG	2a	1602	1/1	0.92	0.10	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1604	1/1	0.92	0.08	60,60,60,60	0
56	MG	1A	3884	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3480	1/1	0.92	0.14	72,72,72,72	0
56	MG	2a	1609	1/1	0.92	0.11	60,60,60,60	0
56	MG	2a	1610	1/1	0.92	0.27	52,52,52,52	0
56	MG	1a	1829	1/1	0.92	0.27	57,57,57,57	0
56	MG	1A	3380	1/1	0.92	0.12	30,30,30,30	0
56	MG	1A	3518	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3049	1/1	0.92	0.24	60,60,60,60	0
56	MG	1a	1699	1/1	0.92	0.08	46,46,46,46	0
56	MG	1f	3002	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3233	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3892	1/1	0.92	0.10	41,41,41,41	0
56	MG	2A	3236	1/1	0.92	0.15	55,55,55,55	0
56	MG	2a	1626	1/1	0.92	0.19	50,50,50,50	0
56	MG	1A	3181	1/1	0.92	0.19	48,48,48,48	0
56	MG	1Z	3002	1/1	0.92	0.11	56,56,56,56	0
56	MG	1a	1705	1/1	0.92	0.17	56,56,56,56	0
56	MG	2a	1632	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3333	1/1	0.92	0.16	51,51,51,51	0
56	MG	1x	3004	1/1	0.92	0.15	47,47,47,47	0
56	MG	2A	3505	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3671	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3603	1/1	0.92	0.10	31,31,31,31	0
56	MG	1A	3182	1/1	0.92	0.23	65,65,65,65	0
56	MG	1A	3099	1/1	0.92	0.11	51,51,51,51	0
56	MG	1a	1713	1/1	0.92	0.24	53,53,53,53	0
56	MG	1A	3112	1/1	0.92	0.16	43,43,43,43	0
56	MG	1A	3765	1/1	0.92	0.23	46,46,46,46	0
56	MG	2A	3033	1/1	0.92	0.06	29,29,29,29	0
56	MG	2a	1654	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3524	1/1	0.92	0.08	56,56,56,56	0
56	MG	2A	3525	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3275	1/1	0.92	0.12	46,46,46,46	0
56	MG	19	101	1/1	0.92	0.08	41,41,41,41	0
56	MG	1A	3943	1/1	0.92	0.07	42,42,42,42	0
56	MG	1A	3344	1/1	0.92	0.12	48,48,48,48	0
56	MG	2a	1663	1/1	0.92	0.21	62,62,62,62	0
56	MG	2A	3049	1/1	0.92	0.07	42,42,42,42	0
56	MG	2A	3050	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3959	1/1	0.92	0.18	53,53,53,53	0
56	MG	2a	1668	1/1	0.92	0.19	64,64,64,64	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	3055	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3056	1/1	0.92	0.16	54,54,54,54	0
56	MG	2A	3544	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3545	1/1	0.92	0.16	47,47,47,47	0
56	MG	1a	1725	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3769	1/1	0.92	0.28	39,39,39,39	0
56	MG	2A	3064	1/1	0.92	0.14	58,58,58,58	0
56	MG	1A	3225	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3830	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3556	1/1	0.92	0.08	49,49,49,49	0
56	MG	2A	3321	1/1	0.92	0.10	53,53,53,53	0
56	MG	1B	3003	1/1	0.92	0.34	62,62,62,62	0
56	MG	2a	1691	1/1	0.92	0.20	57,57,57,57	0
56	MG	2A	3071	1/1	0.92	0.25	34,34,34,34	0
56	MG	2a	1698	1/1	0.92	0.14	57,57,57,57	0
56	MG	2A	3561	1/1	0.92	0.07	71,71,71,71	0
56	MG	2A	3569	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3334	1/1	0.92	0.07	44,44,44,44	0
56	MG	1a	1621	1/1	0.92	0.06	49,49,49,49	0
56	MG	2a	1711	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3544	1/1	0.92	0.06	54,54,54,54	0
56	MG	2a	1718	1/1	0.92	0.06	51,51,51,51	0
56	MG	1B	3006	1/1	0.92	0.11	44,44,44,44	0
56	MG	2a	1721	1/1	0.92	0.14	61,61,61,61	0
56	MG	1A	3281	1/1	0.92	0.09	48,48,48,48	0
56	MG	2a	1723	1/1	0.92	0.11	54,54,54,54	0
56	MG	1a	1636	1/1	0.92	0.10	53,53,53,53	0
56	MG	1a	1768	1/1	0.92	0.08	56,56,56,56	0
56	MG	2A	3580	1/1	0.92	0.13	38,38,38,38	0
56	MG	2A	3581	1/1	0.92	0.17	66,66,66,66	0
56	MG	2A	3358	1/1	0.92	0.08	52,52,52,52	0
56	MG	2A	3367	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3025	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3842	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3096	1/1	0.92	0.19	56,56,56,56	0
56	MG	1A	3287	1/1	0.92	0.09	47,47,47,47	0
56	MG	2A	3599	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3379	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3434	1/1	0.92	0.07	39,39,39,39	0
56	MG	2A	3385	1/1	0.92	0.07	43,43,43,43	0
56	MG	1A	3635	1/1	0.92	0.07	49,49,49,49	0
56	MG	2A	3111	1/1	0.92	0.10	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3390	1/1	0.92	0.08	30,30,30,30	0
56	MG	1A	3306	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3614	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3850	1/1	0.92	0.12	60,60,60,60	0
56	MG	2A	3618	1/1	0.92	0.07	44,44,44,44	0
56	MG	2a	1755	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3622	1/1	0.92	0.17	41,41,41,41	0
56	MG	2a	1760	1/1	0.92	0.12	54,54,54,54	0
56	MG	1a	1789	1/1	0.92	0.12	45,45,45,45	0
56	MG	2a	1764	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3397	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3265	1/1	0.92	0.11	40,40,40,40	0
56	MG	1A	3852	1/1	0.92	0.07	38,38,38,38	0
56	MG	1A	3582	1/1	0.92	0.10	45,45,45,45	0
56	MG	1D	302	1/1	0.92	0.08	21,21,21,21	0
56	MG	2A	3406	1/1	0.92	0.10	47,47,47,47	0
56	MG	2A	3137	1/1	0.92	0.13	42,42,42,42	0
56	MG	2A	3637	1/1	0.92	0.10	41,41,41,41	0
56	MG	1a	1659	1/1	0.92	0.21	55,55,55,55	0
56	MG	1A	3641	1/1	0.92	0.17	35,35,35,35	0
56	MG	2A	3161	1/1	0.92	0.23	49,49,49,49	0
56	MG	1E	302	1/1	0.92	0.16	43,43,43,43	0
56	MG	2A	3673	1/1	0.92	0.09	33,33,33,33	0
56	MG	1a	1664	1/1	0.92	0.15	57,57,57,57	0
56	MG	1F	302	1/1	0.92	0.11	54,54,54,54	0
56	MG	1A	3036	1/1	0.92	0.15	49,49,49,49	0
56	MG	1A	3318	1/1	0.92	0.22	53,53,53,53	0
56	MG	2A	3185	1/1	0.92	0.12	55,55,55,55	0
56	MG	2A	3443	1/1	0.92	0.07	36,36,36,36	0
56	MG	2A	3188	1/1	0.92	0.09	50,50,50,50	0
56	MG	1A	3376	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3733	1/1	0.92	0.07	25,25,25,25	0
56	MG	2G	3001	1/1	0.92	0.18	54,54,54,54	0
56	MG	1A	3797	1/1	0.92	0.11	57,57,57,57	0
56	MG	1a	1814	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3734	1/1	0.92	0.17	48,48,48,48	0
56	MG	2Q	204	1/1	0.92	0.16	44,44,44,44	0
56	MG	1a	1689	1/1	0.92	0.19	63,63,63,63	0
56	MG	1A	3659	1/1	0.92	0.10	64,64,64,64	0
56	MG	1O	206	1/1	0.92	0.11	62,62,62,62	0
56	MG	20	103	1/1	0.92	0.08	49,49,49,49	0
56	MG	26	502	1/1	0.92	0.14	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1827	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3339	1/1	0.93	0.20	46,46,46,46	0
56	MG	1A	3861	1/1	0.93	0.08	26,26,26,26	0
56	MG	2A	3665	1/1	0.93	0.09	57,57,57,57	0
56	MG	1A	3340	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3215	1/1	0.93	0.11	56,56,56,56	0
56	MG	1a	1627	1/1	0.93	0.25	58,58,58,58	0
56	MG	1a	1632	1/1	0.93	0.12	54,54,54,54	0
56	MG	2A	3348	1/1	0.93	0.13	55,55,55,55	0
56	MG	2B	3002	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3352	1/1	0.93	0.17	55,55,55,55	0
56	MG	2B	3005	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3355	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3588	1/1	0.93	0.20	39,39,39,39	0
56	MG	1A	3731	1/1	0.93	0.09	58,58,58,58	0
56	MG	2D	301	1/1	0.93	0.35	39,39,39,39	0
56	MG	2E	301	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3366	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3217	1/1	0.93	0.08	42,42,42,42	0
56	MG	1x	3009	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3452	1/1	0.93	0.07	43,43,43,43	0
56	MG	1y	101	1/1	0.93	0.17	38,38,38,38	0
56	MG	1A	3117	1/1	0.93	0.16	38,38,38,38	0
56	MG	2P	201	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3736	1/1	0.93	0.15	38,38,38,38	0
56	MG	1A	3595	1/1	0.93	0.13	26,26,26,26	0
56	MG	2R	201	1/1	0.93	0.11	48,48,48,48	0
56	MG	1a	1648	1/1	0.93	0.15	43,43,43,43	0
56	MG	2A	3027	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	3348	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3739	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3741	1/1	0.93	0.11	58,58,58,58	0
56	MG	2A	3043	1/1	0.93	0.20	39,39,39,39	0
56	MG	1A	3349	1/1	0.93	0.11	38,38,38,38	0
56	MG	1A	3893	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3894	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3899	1/1	0.93	0.07	14,14,14,14	0
56	MG	1A	3601	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	3746	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3085	1/1	0.93	0.14	51,51,51,51	0
56	MG	2A	3060	1/1	0.93	0.14	42,42,42,42	0
56	MG	1A	3749	1/1	0.93	0.10	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	3278	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3754	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3931	1/1	0.93	0.18	57,57,57,57	0
56	MG	2A	3421	1/1	0.93	0.17	52,52,52,52	0
56	MG	2a	1622	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3354	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3068	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3363	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3939	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3440	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3940	1/1	0.93	0.15	33,33,33,33	0
56	MG	2A	3081	1/1	0.93	0.13	39,39,39,39	0
56	MG	1A	3235	1/1	0.93	0.22	32,32,32,32	0
56	MG	1A	3952	1/1	0.93	0.15	33,33,33,33	0
56	MG	2A	3449	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3760	1/1	0.93	0.08	57,57,57,57	0
56	MG	1A	3614	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3459	1/1	0.93	0.14	49,49,49,49	0
56	MG	2a	1643	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3367	1/1	0.93	0.22	55,55,55,55	0
56	MG	1A	3369	1/1	0.93	0.06	40,40,40,40	0
56	MG	2A	3464	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3465	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3964	1/1	0.93	0.07	26,26,26,26	0
56	MG	1A	3622	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3091	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3063	1/1	0.93	0.19	36,36,36,36	0
56	MG	2A	3105	1/1	0.93	0.16	49,49,49,49	0
56	MG	1A	3372	1/1	0.93	0.16	52,52,52,52	0
56	MG	2A	3112	1/1	0.93	0.24	49,49,49,49	0
56	MG	1A	3192	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3116	1/1	0.93	0.20	56,56,56,56	0
56	MG	1B	3008	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3489	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3631	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3015	1/1	0.93	0.13	43,43,43,43	0
56	MG	2A	3492	1/1	0.93	0.07	50,50,50,50	0
56	MG	1A	3633	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	3375	1/1	0.93	0.10	32,32,32,32	0
56	MG	1a	1716	1/1	0.93	0.11	62,62,62,62	0
56	MG	2a	1676	1/1	0.93	0.21	40,40,40,40	0
56	MG	1A	3502	1/1	0.93	0.12	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3288	1/1	0.93	0.05	36,36,36,36	0
56	MG	2a	1679	1/1	0.93	0.19	64,64,64,64	0
56	MG	1A	3305	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3507	1/1	0.93	0.12	34,34,34,34	0
56	MG	2A	3503	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3166	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3511	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3080	1/1	0.93	0.19	31,31,31,31	0
56	MG	2A	3173	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3383	1/1	0.93	0.12	33,33,33,33	0
56	MG	1a	1727	1/1	0.93	0.07	65,65,65,65	0
56	MG	2a	1695	1/1	0.93	0.16	54,54,54,54	0
56	MG	1a	1728	1/1	0.93	0.09	49,49,49,49	0
56	MG	2a	1699	1/1	0.93	0.07	38,38,38,38	0
56	MG	2A	3182	1/1	0.93	0.09	53,53,53,53	0
56	MG	1a	1729	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3307	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3157	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3194	1/1	0.93	0.15	40,40,40,40	0
56	MG	1a	1739	1/1	0.93	0.09	51,51,51,51	0
56	MG	1E	304	1/1	0.93	0.09	57,57,57,57	0
56	MG	2a	1719	1/1	0.93	0.14	44,44,44,44	0
56	MG	1a	1743	1/1	0.93	0.27	63,63,63,63	0
56	MG	1E	306	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3531	1/1	0.93	0.10	45,45,45,45	0
56	MG	2A	3532	1/1	0.93	0.11	69,69,69,69	0
56	MG	2A	3206	1/1	0.93	0.11	38,38,38,38	0
56	MG	1A	3661	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3535	1/1	0.93	0.07	62,62,62,62	0
56	MG	1F	303	1/1	0.93	0.07	34,34,34,34	0
56	MG	1F	305	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	3388	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3542	1/1	0.93	0.17	37,37,37,37	0
56	MG	1A	3389	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3224	1/1	0.93	0.07	46,46,46,46	0
56	MG	2a	1737	1/1	0.93	0.13	51,51,51,51	0
56	MG	1A	3666	1/1	0.93	0.24	44,44,44,44	0
56	MG	1A	3208	1/1	0.93	0.14	24,24,24,24	0
56	MG	1a	1774	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3170	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3320	1/1	0.93	0.27	59,59,59,59	0
56	MG	1A	3672	1/1	0.93	0.07	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3412	1/1	0.93	0.07	35,35,35,35	0
56	MG	1a	1784	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	3414	1/1	0.93	0.08	31,31,31,31	0
56	MG	1A	3537	1/1	0.93	0.07	40,40,40,40	0
56	MG	1Q	205	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3676	1/1	0.93	0.24	50,50,50,50	0
56	MG	2a	1753	1/1	0.93	0.07	80,80,80,80	0
56	MG	2a	1754	1/1	0.93	0.13	67,67,67,67	0
56	MG	1A	3539	1/1	0.93	0.19	51,51,51,51	0
56	MG	2A	3573	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3244	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	3543	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	1762	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3684	1/1	0.93	0.08	29,29,29,29	0
56	MG	2A	3248	1/1	0.93	0.11	52,52,52,52	0
56	MG	1Z	3001	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3263	1/1	0.93	0.17	41,41,41,41	0
56	MG	1a	1801	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3081	1/1	0.93	0.14	43,43,43,43	0
56	MG	1A	3690	1/1	0.93	0.10	48,48,48,48	0
56	MG	1Z	3005	1/1	0.93	0.20	56,56,56,56	0
56	MG	2A	3266	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3589	1/1	0.93	0.08	41,41,41,41	0
56	MG	2A	3273	1/1	0.93	0.11	35,35,35,35	0
56	MG	2A	3593	1/1	0.93	0.11	56,56,56,56	0
56	MG	10	101	1/1	0.93	0.13	59,59,59,59	0
56	MG	10	102	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3331	1/1	0.93	0.24	53,53,53,53	0
56	MG	12	3001	1/1	0.93	0.15	53,53,53,53	0
56	MG	1A	3698	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3841	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3699	1/1	0.93	0.10	66,66,66,66	0
56	MG	2a	1789	1/1	0.93	0.11	58,58,58,58	0
56	MG	2A	3293	1/1	0.93	0.06	33,33,33,33	0
56	MG	1A	3843	1/1	0.93	0.08	33,33,33,33	0
56	MG	1A	3213	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3561	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3706	1/1	0.93	0.10	51,51,51,51	0
56	MG	2f	3002	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3304	1/1	0.93	0.22	53,53,53,53	0
56	MG	1a	1605	1/1	0.93	0.09	50,50,50,50	0
56	MG	1a	1606	1/1	0.93	0.12	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1835	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3051	1/1	0.93	0.07	38,38,38,38	0
56	MG	2A	3318	1/1	0.93	0.15	38,38,38,38	0
56	MG	2w	3001	1/1	0.93	0.08	67,67,67,67	0
56	MG	1A	3430	1/1	0.93	0.06	21,21,21,21	0
56	MG	2x	102	1/1	0.93	0.07	58,58,58,58	0
56	MG	2A	3326	1/1	0.93	0.06	42,42,42,42	0
56	MG	1A	3572	1/1	0.93	0.08	33,33,33,33	0
61	FME	1x	3011	10/11	0.93	0.18	37,40,51,79	10
56	MG	1A	3267	1/1	0.93	0.08	53,53,53,53	0
56	MG	2A	3584	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3270	1/1	0.94	0.11	57,57,57,57	0
56	MG	1a	1760	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3431	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3818	1/1	0.94	0.07	30,30,30,30	0
56	MG	1A	3686	1/1	0.94	0.09	29,29,29,29	0
56	MG	1A	3820	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3595	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3597	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3556	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	3827	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3602	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3238	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3829	1/1	0.94	0.19	59,59,59,59	0
56	MG	1A	3158	1/1	0.94	0.07	49,49,49,49	0
56	MG	1V	201	1/1	0.94	0.18	52,52,52,52	0
56	MG	1a	1783	1/1	0.94	0.13	63,63,63,63	0
56	MG	2A	3611	1/1	0.94	0.09	60,60,60,60	0
56	MG	1X	3004	1/1	0.94	0.08	64,64,64,64	0
56	MG	1A	3436	1/1	0.94	0.07	31,31,31,31	0
56	MG	1A	3691	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3693	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3564	1/1	0.94	0.12	24,24,24,24	0
56	MG	2A	3619	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	3164	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3253	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3255	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3165	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3168	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3575	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3169	1/1	0.94	0.10	44,44,44,44	0
56	MG	2A	3265	1/1	0.94	0.08	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3634	1/1	0.94	0.10	38,38,38,38	0
56	MG	1a	1800	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3451	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3638	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3640	1/1	0.94	0.07	45,45,45,45	0
56	MG	1a	1802	1/1	0.94	0.10	50,50,50,50	0
56	MG	13	103	1/1	0.94	0.13	50,50,50,50	0
56	MG	2A	3656	1/1	0.94	0.27	44,44,44,44	0
56	MG	2A	3659	1/1	0.94	0.25	43,43,43,43	0
56	MG	2A	3276	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3278	1/1	0.94	0.08	31,31,31,31	0
56	MG	15	103	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3282	1/1	0.94	0.09	33,33,33,33	0
56	MG	2A	3284	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3583	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3101	1/1	0.94	0.22	47,47,47,47	0
56	MG	2B	3003	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3357	1/1	0.94	0.19	52,52,52,52	0
56	MG	2A	3290	1/1	0.94	0.07	40,40,40,40	0
56	MG	2B	3007	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3458	1/1	0.94	0.08	42,42,42,42	0
56	MG	2B	3014	1/1	0.94	0.32	65,65,65,65	0
56	MG	19	102	1/1	0.94	0.09	50,50,50,50	0
56	MG	1a	1812	1/1	0.94	0.10	51,51,51,51	0
56	MG	2B	3018	1/1	0.94	0.06	57,57,57,57	0
56	MG	1A	3460	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3864	1/1	0.94	0.08	38,38,38,38	0
56	MG	1A	3360	1/1	0.94	0.19	50,50,50,50	0
56	MG	2A	3303	1/1	0.94	0.23	60,60,60,60	0
56	MG	1A	3223	1/1	0.94	0.15	42,42,42,42	0
56	MG	1a	1607	1/1	0.94	0.22	68,68,68,68	0
56	MG	1a	1824	1/1	0.94	0.10	48,48,48,48	0
56	MG	1a	1608	1/1	0.94	0.16	57,57,57,57	0
56	MG	1a	1609	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3364	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3872	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3102	1/1	0.94	0.09	44,44,44,44	0
56	MG	2U	204	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3231	1/1	0.94	0.26	53,53,53,53	0
56	MG	1A	3234	1/1	0.94	0.16	34,34,34,34	0
56	MG	2A	3332	1/1	0.94	0.06	37,37,37,37	0
56	MG	2A	3333	1/1	0.94	0.15	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	23	3001	1/1	0.94	0.20	54,54,54,54	0
56	MG	1A	3471	1/1	0.94	0.06	26,26,26,26	0
56	MG	2A	3335	1/1	0.94	0.07	25,25,25,25	0
56	MG	1A	3882	1/1	0.94	0.10	52,52,52,52	0
56	MG	1e	201	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3177	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3475	1/1	0.94	0.08	37,37,37,37	0
56	MG	1v	3001	1/1	0.94	0.08	56,56,56,56	0
56	MG	1a	1630	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3349	1/1	0.94	0.07	18,18,18,18	0
56	MG	1a	1631	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	3886	1/1	0.94	0.10	50,50,50,50	0
56	MG	1w	3005	1/1	0.94	0.09	82,82,82,82	0
56	MG	1a	1633	1/1	0.94	0.21	52,52,52,52	0
56	MG	2A	3361	1/1	0.94	0.06	58,58,58,58	0
56	MG	1x	3002	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3290	1/1	0.94	0.20	33,33,33,33	0
56	MG	1A	3292	1/1	0.94	0.08	49,49,49,49	0
56	MG	1x	3006	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3483	1/1	0.94	0.09	29,29,29,29	0
56	MG	1a	1638	1/1	0.94	0.21	42,42,42,42	0
56	MG	1a	1639	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3381	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3295	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3619	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3002	1/1	0.94	0.26	53,53,53,53	0
56	MG	2A	3388	1/1	0.94	0.07	52,52,52,52	0
56	MG	2a	1635	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3485	1/1	0.94	0.13	38,38,38,38	0
56	MG	1A	3897	1/1	0.94	0.20	38,38,38,38	0
56	MG	2A	3019	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3023	1/1	0.94	0.28	49,49,49,49	0
56	MG	2A	3024	1/1	0.94	0.09	33,33,33,33	0
56	MG	2A	3394	1/1	0.94	0.11	45,45,45,45	0
56	MG	1a	1647	1/1	0.94	0.17	60,60,60,60	0
56	MG	2a	1648	1/1	0.94	0.12	61,61,61,61	0
56	MG	1A	3898	1/1	0.94	0.09	25,25,25,25	0
56	MG	2A	3028	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3031	1/1	0.94	0.05	24,24,24,24	0
56	MG	2A	3403	1/1	0.94	0.11	37,37,37,37	0
56	MG	2A	3032	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3405	1/1	0.94	0.15	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	1A	3748	1/1	0.94	0.06	29,29,29,29	0
56	MG	1a	1650	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3040	1/1	0.94	0.09	43,43,43,43	0
56	MG	2A	3411	1/1	0.94	0.18	50,50,50,50	0
56	MG	2A	3412	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3296	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3623	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3047	1/1	0.94	0.05	22,22,22,22	0
56	MG	1a	1653	1/1	0.94	0.19	59,59,59,59	0
56	MG	1A	3002	1/1	0.94	0.09	61,61,61,61	0
56	MG	1A	3006	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3088	1/1	0.94	0.18	54,54,54,54	0
56	MG	2a	1674	1/1	0.94	0.14	58,58,58,58	0
56	MG	2a	1675	1/1	0.94	0.10	66,66,66,66	0
56	MG	2A	3054	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3031	1/1	0.94	0.07	31,31,31,31	0
56	MG	1A	3311	1/1	0.94	0.17	50,50,50,50	0
56	MG	2A	3057	1/1	0.94	0.21	57,57,57,57	0
56	MG	1A	3185	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3316	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3061	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3764	1/1	0.94	0.08	40,40,40,40	0
56	MG	2A	3453	1/1	0.94	0.07	37,37,37,37	0
56	MG	2A	3455	1/1	0.94	0.15	44,44,44,44	0
56	MG	1A	3634	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3387	1/1	0.94	0.09	38,38,38,38	0
56	MG	1a	1669	1/1	0.94	0.21	58,58,58,58	0
56	MG	1A	3948	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3768	1/1	0.94	0.20	50,50,50,50	0
56	MG	1a	1680	1/1	0.94	0.20	56,56,56,56	0
56	MG	2A	3073	1/1	0.94	0.09	46,46,46,46	0
56	MG	1a	1681	1/1	0.94	0.32	54,54,54,54	0
56	MG	1A	3255	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3471	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3473	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3079	1/1	0.94	0.11	49,49,49,49	0
56	MG	2A	3475	1/1	0.94	0.08	52,52,52,52	0
56	MG	2A	3080	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3094	1/1	0.94	0.19	58,58,58,58	0
56	MG	1a	1684	1/1	0.94	0.11	54,54,54,54	0
56	MG	1a	1686	1/1	0.94	0.11	47,47,47,47	0
56	MG	1a	1688	1/1	0.94	0.07	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3771	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3961	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	3772	1/1	0.94	0.17	29,29,29,29	0
56	MG	1A	3513	1/1	0.94	0.13	29,29,29,29	0
56	MG	1A	3514	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3642	1/1	0.94	0.06	39,39,39,39	0
56	MG	1A	3396	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3258	1/1	0.94	0.08	32,32,32,32	0
56	MG	2A	3110	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3778	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3646	1/1	0.94	0.17	36,36,36,36	0
56	MG	1a	1703	1/1	0.94	0.14	50,50,50,50	0
56	MG	1B	3009	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3648	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3121	1/1	0.94	0.15	41,41,41,41	0
56	MG	2a	1743	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3519	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3123	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3512	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3655	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3516	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3658	1/1	0.94	0.20	35,35,35,35	0
56	MG	1A	3021	1/1	0.94	0.21	50,50,50,50	0
56	MG	1A	3326	1/1	0.94	0.18	43,43,43,43	0
56	MG	2A	3130	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3131	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3132	1/1	0.94	0.14	44,44,44,44	0
56	MG	2a	1759	1/1	0.94	0.13	76,76,76,76	0
56	MG	2A	3134	1/1	0.94	0.07	44,44,44,44	0
56	MG	1a	1712	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	3523	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1714	1/1	0.94	0.20	42,42,42,42	0
56	MG	2A	3155	1/1	0.94	0.11	43,43,43,43	0
56	MG	2A	3159	1/1	0.94	0.16	41,41,41,41	0
56	MG	1a	1715	1/1	0.94	0.17	51,51,51,51	0
56	MG	2a	1769	1/1	0.94	0.10	73,73,73,73	0
56	MG	1A	3411	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3664	1/1	0.94	0.10	39,39,39,39	0
56	MG	2A	3170	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3171	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3525	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3526	1/1	0.94	0.08	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	1777	1/1	0.94	0.13	77,77,77,77	0
56	MG	1A	3135	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3177	1/1	0.94	0.05	37,37,37,37	0
56	MG	1E	301	1/1	0.94	0.10	27,27,27,27	0
56	MG	2A	3546	1/1	0.94	0.10	33,33,33,33	0
56	MG	1A	3669	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3548	1/1	0.94	0.08	35,35,35,35	0
56	MG	2A	3181	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3413	1/1	0.94	0.10	30,30,30,30	0
56	MG	1A	3058	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3186	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3203	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3147	1/1	0.94	0.07	34,34,34,34	0
56	MG	2A	3191	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3082	1/1	0.94	0.07	41,41,41,41	0
56	MG	1a	1733	1/1	0.94	0.06	33,33,33,33	0
56	MG	2A	3564	1/1	0.94	0.10	45,45,45,45	0
56	MG	2g	8001	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3567	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3422	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3100	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3812	1/1	0.94	0.09	41,41,41,41	0
56	MG	1a	1742	1/1	0.94	0.09	68,68,68,68	0
56	MG	1N	3004	1/1	0.94	0.12	56,56,56,56	0
56	MG	2A	3209	1/1	0.94	0.07	41,41,41,41	0
56	MG	2w	3002	1/1	0.94	0.09	63,63,63,63	0
56	MG	1A	3813	1/1	0.94	0.11	40,40,40,40	0
56	MG	2x	101	1/1	0.94	0.09	56,56,56,56	0
56	MG	1a	1749	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3814	1/1	0.94	0.20	16,16,16,16	0
57	K	2A	3207	1/1	0.94	0.16	75,75,75,75	0
56	MG	1a	1753	1/1	0.94	0.10	58,58,58,58	0
56	MG	1a	1755	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3269	1/1	0.94	0.11	30,30,30,30	0
56	MG	1A	3232	1/1	0.95	0.05	49,49,49,49	0
56	MG	1A	3233	1/1	0.95	0.21	35,35,35,35	0
56	MG	1A	3908	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3090	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3504	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3280	1/1	0.95	0.14	42,42,42,42	0
56	MG	1x	3001	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3922	1/1	0.95	0.05	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3283	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3925	1/1	0.95	0.05	59,59,59,59	0
56	MG	1A	3928	1/1	0.95	0.06	24,24,24,24	0
56	MG	2A	3616	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3286	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3929	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3390	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3620	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3621	1/1	0.95	0.09	57,57,57,57	0
56	MG	1x	3008	1/1	0.95	0.25	61,61,61,61	0
56	MG	1A	3506	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3934	1/1	0.95	0.18	30,30,30,30	0
56	MG	2A	3295	1/1	0.95	0.06	39,39,39,39	0
56	MG	1a	1654	1/1	0.95	0.06	54,54,54,54	0
56	MG	1A	3394	1/1	0.95	0.12	12,12,12,12	0
56	MG	2A	3630	1/1	0.95	0.13	41,41,41,41	0
56	MG	1A	3039	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3300	1/1	0.95	0.07	29,29,29,29	0
56	MG	2A	3633	1/1	0.95	0.07	49,49,49,49	0
56	MG	2A	3301	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3635	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3175	1/1	0.95	0.08	31,31,31,31	0
56	MG	1A	3941	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3011	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3639	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3014	1/1	0.95	0.06	38,38,38,38	0
56	MG	2A	3641	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3642	1/1	0.95	0.08	32,32,32,32	0
56	MG	2A	3306	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3648	1/1	0.95	0.22	47,47,47,47	0
56	MG	2A	3015	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3655	1/1	0.95	0.05	31,31,31,31	0
56	MG	1A	3401	1/1	0.95	0.11	38,38,38,38	0
56	MG	2A	3314	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3662	1/1	0.95	0.17	29,29,29,29	0
56	MG	1A	3119	1/1	0.95	0.19	36,36,36,36	0
56	MG	1A	3179	1/1	0.95	0.12	31,31,31,31	0
56	MG	1A	3953	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3516	1/1	0.95	0.09	25,25,25,25	0
56	MG	1A	3093	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3076	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3331	1/1	0.95	0.08	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1671	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3048	1/1	0.95	0.16	32,32,32,32	0
56	MG	2A	3034	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3037	1/1	0.95	0.14	42,42,42,42	0
56	MG	2B	3008	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3327	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3329	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3965	1/1	0.95	0.24	38,38,38,38	0
56	MG	1A	3256	1/1	0.95	0.15	49,49,49,49	0
56	MG	2A	3045	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3420	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3130	1/1	0.95	0.05	50,50,50,50	0
56	MG	2E	304	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3663	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3353	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3354	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3131	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3786	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3052	1/1	0.95	0.07	50,50,50,50	0
56	MG	2A	3053	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3363	1/1	0.95	0.05	30,30,30,30	0
56	MG	2Q	202	1/1	0.95	0.05	46,46,46,46	0
56	MG	1A	3132	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3789	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3427	1/1	0.95	0.08	39,39,39,39	0
56	MG	2V	201	1/1	0.95	0.08	44,44,44,44	0
56	MG	2X	101	1/1	0.95	0.09	37,37,37,37	0
56	MG	1B	3013	1/1	0.95	0.07	53,53,53,53	0
56	MG	1a	1695	1/1	0.95	0.05	55,55,55,55	0
56	MG	2A	3059	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3374	1/1	0.95	0.15	54,54,54,54	0
56	MG	2A	3375	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3791	1/1	0.95	0.11	43,43,43,43	0
56	MG	1B	3016	1/1	0.95	0.21	61,61,61,61	0
56	MG	1a	1698	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3428	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3794	1/1	0.95	0.08	21,21,21,21	0
56	MG	1A	3336	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3190	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3052	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3433	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3196	1/1	0.95	0.13	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	2a	1612	1/1	0.95	0.10	54,54,54,54	0
56	MG	2a	1613	1/1	0.95	0.09	58,58,58,58	0
56	MG	1B	3027	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3075	1/1	0.95	0.13	41,41,41,41	0
56	MG	2a	1616	1/1	0.95	0.14	52,52,52,52	0
56	MG	2A	3395	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3077	1/1	0.95	0.07	43,43,43,43	0
56	MG	1D	301	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3140	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3400	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3198	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	3199	1/1	0.95	0.20	35,35,35,35	0
56	MG	1A	3677	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3059	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3681	1/1	0.95	0.06	32,32,32,32	0
56	MG	2a	1630	1/1	0.95	0.20	55,55,55,55	0
56	MG	2A	3086	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3560	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3144	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3563	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3446	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3566	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3417	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3099	1/1	0.95	0.07	24,24,24,24	0
56	MG	2A	3101	1/1	0.95	0.20	53,53,53,53	0
56	MG	1I	3001	1/1	0.95	0.08	58,58,58,58	0
56	MG	1N	3001	1/1	0.95	0.23	38,38,38,38	0
56	MG	2A	3429	1/1	0.95	0.06	29,29,29,29	0
56	MG	2A	3433	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3449	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3435	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3351	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3692	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3146	1/1	0.95	0.07	31,31,31,31	0
56	MG	1O	203	1/1	0.95	0.06	52,52,52,52	0
56	MG	1a	1731	1/1	0.95	0.09	61,61,61,61	0
56	MG	2A	3446	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3117	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3448	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3694	1/1	0.95	0.16	47,47,47,47	0
56	MG	2A	3451	1/1	0.95	0.14	36,36,36,36	0
56	MG	1A	3455	1/1	0.95	0.12	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	3821	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3577	1/1	0.95	0.09	47,47,47,47	0
56	MG	2a	1670	1/1	0.95	0.17	53,53,53,53	0
56	MG	2A	3456	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3826	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3272	1/1	0.95	0.12	38,38,38,38	0
56	MG	1a	1744	1/1	0.95	0.09	53,53,53,53	0
56	MG	2A	3462	1/1	0.95	0.09	57,57,57,57	0
56	MG	1a	1745	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3701	1/1	0.95	0.10	47,47,47,47	0
56	MG	1a	1747	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3083	1/1	0.95	0.09	27,27,27,27	0
56	MG	1a	1751	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	3703	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	3704	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3141	1/1	0.95	0.09	29,29,29,29	0
56	MG	2a	1685	1/1	0.95	0.16	53,53,53,53	0
56	MG	2A	3143	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3144	1/1	0.95	0.10	43,43,43,43	0
56	MG	2A	3148	1/1	0.95	0.19	43,43,43,43	0
56	MG	2a	1690	1/1	0.95	0.22	50,50,50,50	0
56	MG	2A	3478	1/1	0.95	0.12	56,56,56,56	0
56	MG	1S	3001	1/1	0.95	0.19	52,52,52,52	0
56	MG	1S	3002	1/1	0.95	0.06	53,53,53,53	0
56	MG	2a	1696	1/1	0.95	0.17	50,50,50,50	0
56	MG	2A	3482	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3158	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3486	1/1	0.95	0.10	54,54,54,54	0
56	MG	2a	1704	1/1	0.95	0.07	40,40,40,40	0
56	MG	1T	201	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3160	1/1	0.95	0.08	47,47,47,47	0
56	MG	2a	1708	1/1	0.95	0.09	52,52,52,52	0
56	MG	1T	203	1/1	0.95	0.06	42,42,42,42	0
56	MG	2A	3165	1/1	0.95	0.12	36,36,36,36	0
56	MG	2a	1714	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3004	1/1	0.95	0.07	28,28,28,28	0
56	MG	2a	1717	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3168	1/1	0.95	0.09	46,46,46,46	0
56	MG	1a	1765	1/1	0.95	0.23	69,69,69,69	0
56	MG	2A	3494	1/1	0.95	0.09	45,45,45,45	0
56	MG	1W	3001	1/1	0.95	0.14	43,43,43,43	0
56	MG	1a	1767	1/1	0.95	0.11	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	1X	3002	1/1	0.95	0.06	45,45,45,45	0
56	MG	1a	1769	1/1	0.95	0.08	69,69,69,69	0
56	MG	2a	1725	1/1	0.95	0.07	69,69,69,69	0
56	MG	1A	3839	1/1	0.95	0.09	70,70,70,70	0
56	MG	1Y	502	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3211	1/1	0.95	0.08	38,38,38,38	0
56	MG	1A	3152	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	3710	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	3713	1/1	0.95	0.08	36,36,36,36	0
56	MG	2a	1732	1/1	0.95	0.06	45,45,45,45	0
56	MG	2a	1733	1/1	0.95	0.21	61,61,61,61	0
56	MG	1A	3845	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3463	1/1	0.95	0.06	25,25,25,25	0
56	MG	1A	3589	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3155	1/1	0.95	0.10	48,48,48,48	0
56	MG	1l	103	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3519	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3055	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3721	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3466	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3199	1/1	0.95	0.14	43,43,43,43	0
56	MG	15	102	1/1	0.95	0.07	37,37,37,37	0
56	MG	1a	1796	1/1	0.95	0.11	40,40,40,40	0
56	MG	1a	1797	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3857	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3103	1/1	0.95	0.10	36,36,36,36	0
56	MG	2A	3210	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3211	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3105	1/1	0.95	0.09	31,31,31,31	0
56	MG	1A	3730	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3217	1/1	0.95	0.28	60,60,60,60	0
56	MG	1A	3865	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3221	1/1	0.95	0.19	43,43,43,43	0
56	MG	1A	3286	1/1	0.95	0.13	41,41,41,41	0
56	MG	2A	3223	1/1	0.95	0.13	51,51,51,51	0
56	MG	2A	3540	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3541	1/1	0.95	0.13	51,51,51,51	0
56	MG	1a	1804	1/1	0.95	0.15	65,65,65,65	0
56	MG	1A	3220	1/1	0.95	0.07	48,48,48,48	0
56	MG	2A	3226	1/1	0.95	0.24	42,42,42,42	0
56	MG	1A	3108	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3222	1/1	0.95	0.18	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	3480	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3167	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3606	1/1	0.95	0.09	19,19,19,19	0
56	MG	2A	3232	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3552	1/1	0.95	0.12	57,57,57,57	0
56	MG	2A	3554	1/1	0.95	0.06	45,45,45,45	0
56	MG	1A	3068	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3611	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	3379	1/1	0.95	0.13	52,52,52,52	0
56	MG	2A	3237	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3227	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3885	1/1	0.95	0.10	44,44,44,44	0
56	MG	1a	1617	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3566	1/1	0.95	0.06	38,38,38,38	0
56	MG	1a	1822	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3568	1/1	0.95	0.05	54,54,54,54	0
56	MG	1A	3300	1/1	0.95	0.13	31,31,31,31	0
56	MG	1A	3488	1/1	0.95	0.06	28,28,28,28	0
56	MG	1a	1622	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3489	1/1	0.95	0.13	40,40,40,40	0
56	MG	2A	3247	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3490	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3303	1/1	0.95	0.10	34,34,34,34	0
56	MG	1A	3751	1/1	0.95	0.08	63,63,63,63	0
56	MG	1a	1838	1/1	0.95	0.06	51,51,51,51	0
56	MG	2A	3254	1/1	0.95	0.08	38,38,38,38	0
56	MG	2q	3001	1/1	0.95	0.05	66,66,66,66	0
56	MG	2q	3002	1/1	0.95	0.15	63,63,63,63	0
56	MG	1A	3752	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3257	1/1	0.95	0.11	47,47,47,47	0
56	MG	2v	3001	1/1	0.95	0.22	56,56,56,56	0
56	MG	1A	3896	1/1	0.95	0.09	13,13,13,13	0
56	MG	1A	3753	1/1	0.95	0.07	49,49,49,49	0
56	MG	2A	3261	1/1	0.95	0.12	34,34,34,34	0
56	MG	2A	3262	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3229	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3495	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3756	1/1	0.95	0.07	39,39,39,39	0
58	HGR	2A	3652	36/36	0.95	0.10	21,36,48,50	0
56	MG	1A	3113	1/1	0.95	0.08	40,40,40,40	0
56	MG	2A	3271	1/1	0.95	0.06	34,34,34,34	0
56	MG	2A	3272	1/1	0.95	0.10	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	3912	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3285	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3918	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3920	1/1	0.96	0.13	33,33,33,33	0
56	MG	2A	3606	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3134	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3608	1/1	0.96	0.07	27,27,27,27	0
56	MG	1a	1643	1/1	0.96	0.35	51,51,51,51	0
56	MG	1A	3224	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3109	1/1	0.96	0.20	34,34,34,34	0
56	MG	2A	3001	1/1	0.96	0.14	28,28,28,28	0
56	MG	1A	3625	1/1	0.96	0.08	51,51,51,51	0
56	MG	2A	3003	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3005	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	3930	1/1	0.96	0.29	36,36,36,36	0
56	MG	2A	3007	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3378	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3763	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3178	1/1	0.96	0.19	36,36,36,36	0
56	MG	1A	3138	1/1	0.96	0.19	32,32,32,32	0
56	MG	1A	3047	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3022	1/1	0.96	0.24	43,43,43,43	0
56	MG	1A	3492	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3382	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3142	1/1	0.96	0.10	17,17,17,17	0
56	MG	1A	3944	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3307	1/1	0.96	0.06	31,31,31,31	0
56	MG	2A	3308	1/1	0.96	0.05	45,45,45,45	0
56	MG	2A	3309	1/1	0.96	0.12	31,31,31,31	0
56	MG	2A	3310	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3945	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3029	1/1	0.96	0.12	47,47,47,47	0
56	MG	2A	3313	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3946	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3947	1/1	0.96	0.06	49,49,49,49	0
56	MG	2A	3316	1/1	0.96	0.07	25,25,25,25	0
56	MG	2A	3317	1/1	0.96	0.10	38,38,38,38	0
56	MG	1a	1662	1/1	0.96	0.18	51,51,51,51	0
56	MG	2A	3319	1/1	0.96	0.09	29,29,29,29	0
56	MG	2A	3649	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3496	1/1	0.96	0.05	28,28,28,28	0
56	MG	2A	3323	1/1	0.96	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	2A	3324	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3036	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3660	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3661	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3949	1/1	0.96	0.23	28,28,28,28	0
56	MG	2A	3664	1/1	0.96	0.30	46,46,46,46	0
56	MG	1A	3096	1/1	0.96	0.09	22,22,22,22	0
56	MG	1A	3385	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3668	1/1	0.96	0.44	48,48,48,48	0
56	MG	1A	3954	1/1	0.96	0.07	28,28,28,28	0
56	MG	1a	1670	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3674	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3044	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3955	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3957	1/1	0.96	0.07	37,37,37,37	0
56	MG	2A	3340	1/1	0.96	0.05	27,27,27,27	0
56	MG	1A	3501	1/1	0.96	0.08	32,32,32,32	0
56	MG	1a	1677	1/1	0.96	0.07	56,56,56,56	0
56	MG	2B	3006	1/1	0.96	0.06	51,51,51,51	0
56	MG	1a	1679	1/1	0.96	0.13	48,48,48,48	0
56	MG	1A	3114	1/1	0.96	0.20	32,32,32,32	0
56	MG	1A	3304	1/1	0.96	0.06	48,48,48,48	0
56	MG	2B	3012	1/1	0.96	0.09	51,51,51,51	0
56	MG	2B	3013	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3145	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3350	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3962	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3115	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3054	1/1	0.96	0.20	54,54,54,54	0
56	MG	1a	1687	1/1	0.96	0.08	55,55,55,55	0
56	MG	2E	303	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3392	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3510	1/1	0.96	0.08	25,25,25,25	0
56	MG	2A	3360	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3653	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3362	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3238	1/1	0.96	0.10	28,28,28,28	0
56	MG	1B	3005	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3309	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3026	1/1	0.96	0.08	29,29,29,29	0
56	MG	2A	3369	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3398	1/1	0.96	0.07	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3240	1/1	0.96	0.16	40,40,40,40	0
56	MG	2U	203	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3314	1/1	0.96	0.20	42,42,42,42	0
56	MG	2A	3069	1/1	0.96	0.04	30,30,30,30	0
56	MG	1A	3404	1/1	0.96	0.06	44,44,44,44	0
56	MG	2A	3378	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3407	1/1	0.96	0.04	34,34,34,34	0
56	MG	2A	3380	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3520	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3242	1/1	0.96	0.08	47,47,47,47	0
56	MG	1B	3018	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3410	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3387	1/1	0.96	0.21	50,50,50,50	0
56	MG	1A	3668	1/1	0.96	0.08	35,35,35,35	0
56	MG	2a	1603	1/1	0.96	0.18	65,65,65,65	0
56	MG	1A	3317	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	3244	1/1	0.96	0.18	39,39,39,39	0
56	MG	2a	1606	1/1	0.96	0.08	61,61,61,61	0
56	MG	2a	1607	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3319	1/1	0.96	0.29	28,28,28,28	0
56	MG	1A	3246	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3527	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3248	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3808	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3396	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3088	1/1	0.96	0.19	53,53,53,53	0
56	MG	2A	3089	1/1	0.96	0.06	27,27,27,27	0
56	MG	1A	3252	1/1	0.96	0.05	41,41,41,41	0
56	MG	2A	3091	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3401	1/1	0.96	0.08	45,45,45,45	0
56	MG	2a	1619	1/1	0.96	0.07	46,46,46,46	0
56	MG	2a	1620	1/1	0.96	0.17	58,58,58,58	0
56	MG	2A	3092	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3530	1/1	0.96	0.04	14,14,14,14	0
56	MG	1A	3325	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3193	1/1	0.96	0.08	33,33,33,33	0
56	MG	1a	1719	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3100	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3680	1/1	0.96	0.28	36,36,36,36	0
56	MG	1E	305	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3195	1/1	0.96	0.07	39,39,39,39	0
56	MG	1F	301	1/1	0.96	0.10	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3107	1/1	0.96	0.08	47,47,47,47	0
56	MG	2A	3108	1/1	0.96	0.07	30,30,30,30	0
56	MG	2A	3418	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3109	1/1	0.96	0.05	49,49,49,49	0
56	MG	2a	1636	1/1	0.96	0.12	60,60,60,60	0
56	MG	1a	1724	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3536	1/1	0.96	0.07	48,48,48,48	0
56	MG	2a	1641	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	3423	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3427	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3428	1/1	0.96	0.06	27,27,27,27	0
56	MG	1A	3685	1/1	0.96	0.05	26,26,26,26	0
56	MG	2A	3430	1/1	0.96	0.07	56,56,56,56	0
56	MG	2A	3432	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3114	1/1	0.96	0.24	51,51,51,51	0
56	MG	2a	1650	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3425	1/1	0.96	0.07	36,36,36,36	0
56	MG	1G	202	1/1	0.96	0.12	45,45,45,45	0
56	MG	2a	1653	1/1	0.96	0.14	51,51,51,51	0
56	MG	2A	3436	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3119	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3540	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3688	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3541	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3822	1/1	0.96	0.06	52,52,52,52	0
56	MG	2a	1660	1/1	0.96	0.06	61,61,61,61	0
56	MG	2A	3445	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3542	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3149	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3330	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3546	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3129	1/1	0.96	0.19	41,41,41,41	0
56	MG	1A	3150	1/1	0.96	0.22	41,41,41,41	0
56	MG	1A	3695	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3832	1/1	0.96	0.11	57,57,57,57	0
56	MG	1a	1748	1/1	0.96	0.05	58,58,58,58	0
56	MG	1A	3833	1/1	0.96	0.09	54,54,54,54	0
56	MG	1P	202	1/1	0.96	0.13	33,33,33,33	0
56	MG	2A	3140	1/1	0.96	0.04	50,50,50,50	0
56	MG	1A	3834	1/1	0.96	0.12	46,46,46,46	0
56	MG	1Q	203	1/1	0.96	0.10	33,33,33,33	0
56	MG	1a	1754	1/1	0.96	0.06	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	1Q	204	1/1	0.96	0.12	55,55,55,55	0
56	MG	2A	3466	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3149	1/1	0.96	0.16	49,49,49,49	0
56	MG	1a	1757	1/1	0.96	0.07	39,39,39,39	0
56	MG	2a	1684	1/1	0.96	0.23	48,48,48,48	0
56	MG	1A	3332	1/1	0.96	0.07	31,31,31,31	0
56	MG	1A	3073	1/1	0.96	0.11	29,29,29,29	0
56	MG	2A	3472	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3153	1/1	0.96	0.16	31,31,31,31	0
56	MG	1A	3700	1/1	0.96	0.11	40,40,40,40	0
56	MG	1a	1762	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3163	1/1	0.96	0.12	32,32,32,32	0
56	MG	2A	3164	1/1	0.96	0.08	47,47,47,47	0
56	MG	2A	3479	1/1	0.96	0.07	39,39,39,39	0
56	MG	1a	1763	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3154	1/1	0.96	0.18	36,36,36,36	0
56	MG	2a	1700	1/1	0.96	0.06	60,60,60,60	0
56	MG	2a	1701	1/1	0.96	0.18	62,62,62,62	0
56	MG	2A	3167	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3260	1/1	0.96	0.08	40,40,40,40	0
56	MG	2A	3484	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3435	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3337	1/1	0.96	0.07	39,39,39,39	0
56	MG	2a	1709	1/1	0.96	0.07	68,68,68,68	0
56	MG	1A	3338	1/1	0.96	0.05	36,36,36,36	0
56	MG	1a	1770	1/1	0.96	0.10	44,44,44,44	0
56	MG	2a	1712	1/1	0.96	0.18	58,58,58,58	0
56	MG	1U	201	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3174	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3567	1/1	0.96	0.05	15,15,15,15	0
56	MG	1A	3708	1/1	0.96	0.10	47,47,47,47	0
56	MG	1W	3002	1/1	0.96	0.15	49,49,49,49	0
56	MG	1W	3004	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3180	1/1	0.96	0.14	39,39,39,39	0
56	MG	1W	3006	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3849	1/1	0.96	0.08	29,29,29,29	0
56	MG	2A	3184	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3261	1/1	0.96	0.17	51,51,51,51	0
56	MG	1a	1785	1/1	0.96	0.14	41,41,41,41	0
56	MG	1a	1786	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3201	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3712	1/1	0.96	0.08	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3507	1/1	0.96	0.04	19,19,19,19	0
56	MG	1A	3120	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3510	1/1	0.96	0.04	31,31,31,31	0
56	MG	2A	3511	1/1	0.96	0.05	68,68,68,68	0
56	MG	2A	3195	1/1	0.96	0.07	47,47,47,47	0
56	MG	2a	1735	1/1	0.96	0.18	42,42,42,42	0
56	MG	1A	3714	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3574	1/1	0.96	0.10	47,47,47,47	0
56	MG	1a	1793	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3206	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3447	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3345	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3346	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3037	1/1	0.96	0.06	38,38,38,38	0
56	MG	2a	1744	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3122	1/1	0.96	0.18	40,40,40,40	0
56	MG	13	101	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3209	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3875	1/1	0.96	0.07	32,32,32,32	0
56	MG	2A	3214	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3216	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3728	1/1	0.96	0.18	50,50,50,50	0
56	MG	1A	3878	1/1	0.96	0.08	40,40,40,40	0
56	MG	2A	3220	1/1	0.96	0.13	55,55,55,55	0
56	MG	1A	3162	1/1	0.96	0.42	33,33,33,33	0
56	MG	1A	3459	1/1	0.96	0.10	40,40,40,40	0
56	MG	2a	1758	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3163	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3028	1/1	0.96	0.06	20,20,20,20	0
56	MG	1A	3127	1/1	0.96	0.17	47,47,47,47	0
56	MG	1a	1601	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3077	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3129	1/1	0.96	0.14	38,38,38,38	0
56	MG	2a	1766	1/1	0.96	0.10	56,56,56,56	0
56	MG	1a	1604	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3599	1/1	0.96	0.14	28,28,28,28	0
56	MG	1a	1816	1/1	0.96	0.11	49,49,49,49	0
56	MG	1a	1817	1/1	0.96	0.12	48,48,48,48	0
56	MG	1a	1818	1/1	0.96	0.07	55,55,55,55	0
56	MG	1a	1819	1/1	0.96	0.09	61,61,61,61	0
56	MG	2A	3235	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3362	1/1	0.96	0.20	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	3889	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3016	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3277	1/1	0.96	0.26	57,57,57,57	0
56	MG	1a	1825	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3744	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3218	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3895	1/1	0.96	0.08	40,40,40,40	0
56	MG	1a	1614	1/1	0.96	0.10	37,37,37,37	0
56	MG	1a	1830	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3565	1/1	0.96	0.10	50,50,50,50	0
56	MG	1a	1832	1/1	0.96	0.12	47,47,47,47	0
56	MG	1a	1615	1/1	0.96	0.08	65,65,65,65	0
56	MG	2A	3249	1/1	0.96	0.09	30,30,30,30	0
56	MG	1A	3219	1/1	0.96	0.11	40,40,40,40	0
56	MG	2a	1794	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3368	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3106	1/1	0.96	0.08	37,37,37,37	0
56	MG	1a	1619	1/1	0.96	0.08	56,56,56,56	0
56	MG	2e	3001	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3477	1/1	0.96	0.12	23,23,23,23	0
56	MG	1A	3610	1/1	0.96	0.06	56,56,56,56	0
56	MG	1f	3001	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3478	1/1	0.96	0.06	20,20,20,20	0
56	MG	2l	201	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3902	1/1	0.96	0.12	28,28,28,28	0
56	MG	1t	3001	1/1	0.96	0.17	47,47,47,47	0
56	MG	1a	1625	1/1	0.96	0.20	53,53,53,53	0
56	MG	1w	3001	1/1	0.96	0.06	44,44,44,44	0
56	MG	1a	1626	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3613	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3586	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3267	1/1	0.96	0.12	53,53,53,53	0
56	MG	2A	3269	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3270	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3032	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3905	1/1	0.96	0.12	35,35,35,35	0
56	MG	2A	3594	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3906	1/1	0.96	0.10	42,42,42,42	0
58	HGR	1A	3915	36/36	0.96	0.08	15,30,37,44	0
56	MG	1A	3173	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3283	1/1	0.96	0.05	37,37,37,37	0
59	ZN	2n	501	1/1	0.96	0.06	108,108,108,108	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	3911	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3600	1/1	0.96	0.07	42,42,42,42	0
56	MG	1b	3001	1/1	0.97	0.05	75,75,75,75	0
56	MG	2A	3183	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3358	1/1	0.97	0.05	33,33,33,33	0
56	MG	2B	3010	1/1	0.97	0.05	50,50,50,50	0
56	MG	2B	3011	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3359	1/1	0.97	0.06	44,44,44,44	0
56	MG	2A	3422	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3423	1/1	0.97	0.15	47,47,47,47	0
56	MG	2B	3015	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	1663	1/1	0.97	0.13	59,59,59,59	0
56	MG	2A	3187	1/1	0.97	0.23	60,60,60,60	0
56	MG	2A	3426	1/1	0.97	0.09	38,38,38,38	0
56	MG	1D	303	1/1	0.97	0.19	25,25,25,25	0
56	MG	2D	304	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3299	1/1	0.97	0.17	40,40,40,40	0
56	MG	2E	302	1/1	0.97	0.06	39,39,39,39	0
56	MG	1D	305	1/1	0.97	0.17	31,31,31,31	0
56	MG	2A	3192	1/1	0.97	0.15	51,51,51,51	0
56	MG	2A	3431	1/1	0.97	0.16	52,52,52,52	0
56	MG	2F	302	1/1	0.97	0.15	50,50,50,50	0
56	MG	2A	3193	1/1	0.97	0.07	40,40,40,40	0
56	MG	1l	201	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3856	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3740	1/1	0.97	0.08	39,39,39,39	0
56	MG	1E	303	1/1	0.97	0.05	26,26,26,26	0
56	MG	1A	3858	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3200	1/1	0.97	0.06	46,46,46,46	0
56	MG	1a	1672	1/1	0.97	0.12	55,55,55,55	0
56	MG	2Q	203	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3203	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3361	1/1	0.97	0.08	33,33,33,33	0
56	MG	2T	3001	1/1	0.97	0.11	50,50,50,50	0
56	MG	2U	202	1/1	0.97	0.03	35,35,35,35	0
56	MG	1a	1675	1/1	0.97	0.04	40,40,40,40	0
56	MG	1A	3860	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3030	1/1	0.97	0.23	33,33,33,33	0
56	MG	1A	3862	1/1	0.97	0.06	19,19,19,19	0
56	MG	1A	3743	1/1	0.97	0.11	38,38,38,38	0
56	MG	1x	3003	1/1	0.97	0.05	53,53,53,53	0
56	MG	1A	3301	1/1	0.97	0.32	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1F	306	1/1	0.97	0.09	46,46,46,46	0
56	MG	2A	3215	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3636	1/1	0.97	0.06	53,53,53,53	0
56	MG	1G	201	1/1	0.97	0.05	37,37,37,37	0
56	MG	1a	1685	1/1	0.97	0.16	66,66,66,66	0
56	MG	2A	3460	1/1	0.97	0.11	40,40,40,40	0
56	MG	2A	3219	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3867	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3438	1/1	0.97	0.04	30,30,30,30	0
56	MG	1G	204	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3869	1/1	0.97	0.16	52,52,52,52	0
56	MG	1a	1690	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3870	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3302	1/1	0.97	0.20	30,30,30,30	0
56	MG	2A	3004	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3365	1/1	0.97	0.20	48,48,48,48	0
56	MG	1A	3873	1/1	0.97	0.05	39,39,39,39	0
56	MG	1O	201	1/1	0.97	0.03	39,39,39,39	0
56	MG	1A	3133	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3442	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3013	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3086	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3877	1/1	0.97	0.07	49,49,49,49	0
56	MG	2A	3018	1/1	0.97	0.09	52,52,52,52	0
56	MG	1a	1700	1/1	0.97	0.19	51,51,51,51	0
56	MG	2A	3020	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3021	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3535	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3485	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3087	1/1	0.97	0.06	20,20,20,20	0
56	MG	1A	3137	1/1	0.97	0.19	32,32,32,32	0
56	MG	1P	203	1/1	0.97	0.16	27,27,27,27	0
56	MG	1A	3538	1/1	0.97	0.09	40,40,40,40	0
56	MG	1Q	201	1/1	0.97	0.10	30,30,30,30	0
56	MG	1Q	202	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3651	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3652	1/1	0.97	0.08	25,25,25,25	0
56	MG	1A	3111	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3759	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3035	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3174	1/1	0.97	0.07	34,34,34,34	0
56	MG	2a	1639	1/1	0.97	0.08	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	2a	1640	1/1	0.97	0.14	56,56,56,56	0
56	MG	1A	3656	1/1	0.97	0.11	48,48,48,48	0
56	MG	2A	3038	1/1	0.97	0.15	48,48,48,48	0
56	MG	2A	3258	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3453	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3139	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3310	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	3216	1/1	0.97	0.28	36,36,36,36	0
56	MG	1T	202	1/1	0.97	0.09	46,46,46,46	0
56	MG	2A	3508	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3545	1/1	0.97	0.05	57,57,57,57	0
56	MG	1A	3312	1/1	0.97	0.10	41,41,41,41	0
56	MG	1U	204	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3176	1/1	0.97	0.06	27,27,27,27	0
56	MG	2A	3513	1/1	0.97	0.06	50,50,50,50	0
56	MG	2A	3268	1/1	0.97	0.05	37,37,37,37	0
56	MG	1V	202	1/1	0.97	0.07	59,59,59,59	0
56	MG	2A	3517	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3550	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3377	1/1	0.97	0.11	36,36,36,36	0
56	MG	1A	3066	1/1	0.97	0.29	31,31,31,31	0
56	MG	2a	1662	1/1	0.97	0.19	42,42,42,42	0
56	MG	1W	3005	1/1	0.97	0.06	30,30,30,30	0
56	MG	1A	3315	1/1	0.97	0.13	37,37,37,37	0
56	MG	1A	3559	1/1	0.97	0.04	41,41,41,41	0
56	MG	2a	1666	1/1	0.97	0.15	49,49,49,49	0
56	MG	1a	1732	1/1	0.97	0.16	42,42,42,42	0
56	MG	2A	3277	1/1	0.97	0.07	35,35,35,35	0
56	MG	1X	3003	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3279	1/1	0.97	0.07	43,43,43,43	0
56	MG	1a	1734	1/1	0.97	0.06	30,30,30,30	0
56	MG	1A	3067	1/1	0.97	0.08	18,18,18,18	0
56	MG	1A	3042	1/1	0.97	0.04	27,27,27,27	0
56	MG	1A	3069	1/1	0.97	0.04	27,27,27,27	0
56	MG	2A	3063	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3467	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3001	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	3045	1/1	0.97	0.08	19,19,19,19	0
56	MG	2A	3288	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3118	1/1	0.97	0.07	30,30,30,30	0
56	MG	2A	3539	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3569	1/1	0.97	0.06	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	3075	1/1	0.97	0.17	43,43,43,43	0
56	MG	1A	3186	1/1	0.97	0.23	56,56,56,56	0
56	MG	2A	3072	1/1	0.97	0.08	40,40,40,40	0
56	MG	2a	1687	1/1	0.97	0.15	52,52,52,52	0
56	MG	10	104	1/1	0.97	0.04	55,55,55,55	0
56	MG	11	101	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3917	1/1	0.97	0.31	40,40,40,40	0
56	MG	2A	3076	1/1	0.97	0.11	31,31,31,31	0
56	MG	2a	1693	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3228	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3682	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3097	1/1	0.97	0.09	16,16,16,16	0
56	MG	2a	1697	1/1	0.97	0.05	37,37,37,37	0
56	MG	1a	1756	1/1	0.97	0.04	65,65,65,65	0
56	MG	1A	3230	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3927	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3580	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3391	1/1	0.97	0.07	18,18,18,18	0
56	MG	2a	1703	1/1	0.97	0.10	61,61,61,61	0
56	MG	2A	3085	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3795	1/1	0.97	0.08	20,20,20,20	0
56	MG	1A	3003	1/1	0.97	0.05	32,32,32,32	0
56	MG	2a	1707	1/1	0.97	0.06	60,60,60,60	0
56	MG	2A	3562	1/1	0.97	0.09	42,42,42,42	0
56	MG	18	101	1/1	0.97	0.09	45,45,45,45	0
56	MG	18	102	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3276	1/1	0.97	0.23	51,51,51,51	0
56	MG	1A	3191	1/1	0.97	0.04	38,38,38,38	0
56	MG	2a	1713	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3937	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3585	1/1	0.97	0.06	49,49,49,49	0
56	MG	2a	1716	1/1	0.97	0.06	52,52,52,52	0
56	MG	2A	3094	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3571	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3151	1/1	0.97	0.07	34,34,34,34	0
56	MG	1a	1771	1/1	0.97	0.09	54,54,54,54	0
56	MG	2A	3322	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3098	1/1	0.97	0.03	37,37,37,37	0
56	MG	1A	3034	1/1	0.97	0.17	35,35,35,35	0
56	MG	1a	1773	1/1	0.97	0.07	64,64,64,64	0
56	MG	1A	3399	1/1	0.97	0.13	42,42,42,42	0
56	MG	2A	3329	1/1	0.97	0.04	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	3590	1/1	0.97	0.07	24,24,24,24	0
56	MG	1a	1777	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3583	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3123	1/1	0.97	0.09	43,43,43,43	0
56	MG	1a	1779	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3696	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3807	1/1	0.97	0.12	49,49,49,49	0
56	MG	2A	3336	1/1	0.97	0.07	47,47,47,47	0
56	MG	2A	3337	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3590	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3591	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3338	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3402	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3017	1/1	0.97	0.14	31,31,31,31	0
56	MG	1A	3125	1/1	0.97	0.23	36,36,36,36	0
56	MG	2A	3596	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3342	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3950	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3951	1/1	0.97	0.13	33,33,33,33	0
56	MG	2A	3346	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3601	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3406	1/1	0.97	0.07	23,23,23,23	0
56	MG	1A	3598	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3126	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3408	1/1	0.97	0.04	43,43,43,43	0
56	MG	2A	3351	1/1	0.97	0.09	46,46,46,46	0
56	MG	1a	1620	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3956	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3011	1/1	0.97	0.15	41,41,41,41	0
56	MG	2a	1757	1/1	0.97	0.08	70,70,70,70	0
56	MG	1A	3060	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3061	1/1	0.97	0.08	36,36,36,36	0
56	MG	2A	3126	1/1	0.97	0.18	53,53,53,53	0
56	MG	1A	3707	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3342	1/1	0.97	0.07	33,33,33,33	0
56	MG	2a	1763	1/1	0.97	0.11	46,46,46,46	0
56	MG	1A	3243	1/1	0.97	0.08	56,56,56,56	0
56	MG	1a	1629	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3289	1/1	0.97	0.11	29,29,29,29	0
56	MG	1A	3711	1/1	0.97	0.08	41,41,41,41	0
56	MG	2A	3133	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3607	1/1	0.97	0.10	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1770	1/1	0.97	0.15	41,41,41,41	0
56	MG	2A	3623	1/1	0.97	0.12	46,46,46,46	0
56	MG	2A	3136	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3825	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3415	1/1	0.97	0.07	28,28,28,28	0
56	MG	1a	1635	1/1	0.97	0.21	50,50,50,50	0
56	MG	1A	3104	1/1	0.97	0.18	33,33,33,33	0
56	MG	2A	3376	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3828	1/1	0.97	0.07	58,58,58,58	0
56	MG	1A	3716	1/1	0.97	0.14	59,59,59,59	0
56	MG	2A	3145	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3417	1/1	0.97	0.14	32,32,32,32	0
56	MG	1a	1640	1/1	0.97	0.11	41,41,41,41	0
56	MG	2a	1784	1/1	0.97	0.12	56,56,56,56	0
56	MG	2A	3384	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3291	1/1	0.97	0.23	28,28,28,28	0
56	MG	2A	3153	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3245	1/1	0.97	0.17	29,29,29,29	0
56	MG	2A	3156	1/1	0.97	0.13	31,31,31,31	0
56	MG	1A	3617	1/1	0.97	0.10	26,26,26,26	0
56	MG	1B	3011	1/1	0.97	0.13	54,54,54,54	0
56	MG	2a	1792	1/1	0.97	0.08	50,50,50,50	0
56	MG	1A	3293	1/1	0.97	0.20	26,26,26,26	0
56	MG	2A	3644	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3645	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3647	1/1	0.97	0.13	41,41,41,41	0
56	MG	1a	1646	1/1	0.97	0.07	25,25,25,25	0
56	MG	2A	3162	1/1	0.97	0.04	45,45,45,45	0
56	MG	2A	3650	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3294	1/1	0.97	0.05	32,32,32,32	0
56	MG	2A	3653	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3020	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3166	1/1	0.97	0.08	44,44,44,44	0
56	MG	1B	3017	1/1	0.97	0.04	44,44,44,44	0
56	MG	1A	3727	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3353	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3729	1/1	0.97	0.11	39,39,39,39	0
56	MG	2A	3663	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	3297	1/1	0.97	0.19	19,19,19,19	0
56	MG	1A	3355	1/1	0.97	0.17	46,46,46,46	0
56	MG	1A	3626	1/1	0.97	0.07	56,56,56,56	0
56	MG	1a	1831	1/1	0.97	0.07	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3627	1/1	0.97	0.04	44,44,44,44	0
56	MG	2A	3175	1/1	0.97	0.23	54,54,54,54	0
56	MG	1a	1833	1/1	0.97	0.26	52,52,52,52	0
56	MG	1a	1658	1/1	0.97	0.21	51,51,51,51	0
56	MG	2A	3409	1/1	0.97	0.15	42,42,42,42	0
56	MG	1a	1836	1/1	0.97	0.19	60,60,60,60	0
59	ZN	14	501	1/1	0.97	0.04	97,97,97,97	0
56	MG	1A	3356	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3413	1/1	0.97	0.11	50,50,50,50	0
60	SF4	1d	501	8/8	0.97	0.06	55,66,73,80	0
56	MG	1A	3298	1/1	0.97	0.18	33,33,33,33	0
56	MG	1a	1839	1/1	0.97	0.05	37,37,37,37	0
56	MG	1a	1823	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	3863	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3089	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3107	1/1	0.98	0.04	26,26,26,26	0
56	MG	11	102	1/1	0.98	0.08	38,38,38,38	0
56	MG	1B	3001	1/1	0.98	0.15	39,39,39,39	0
56	MG	1A	3448	1/1	0.98	0.07	57,57,57,57	0
56	MG	1A	3010	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3637	1/1	0.98	0.11	39,39,39,39	0
56	MG	2A	3410	1/1	0.98	0.04	43,43,43,43	0
56	MG	2a	1645	1/1	0.98	0.08	50,50,50,50	0
56	MG	1A	3450	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3785	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3005	1/1	0.98	0.06	43,43,43,43	0
56	MG	2A	3252	1/1	0.98	0.04	58,58,58,58	0
56	MG	2A	3415	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3787	1/1	0.98	0.03	34,34,34,34	0
56	MG	1A	3226	1/1	0.98	0.17	35,35,35,35	0
56	MG	1A	3571	1/1	0.98	0.12	39,39,39,39	0
56	MG	2A	3419	1/1	0.98	0.07	37,37,37,37	0
56	MG	2A	3256	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3104	1/1	0.98	0.17	46,46,46,46	0
56	MG	1A	3508	1/1	0.98	0.06	38,38,38,38	0
56	MG	2A	3106	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3715	1/1	0.98	0.04	50,50,50,50	0
56	MG	1A	3792	1/1	0.98	0.04	17,17,17,17	0
56	MG	1A	3509	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3172	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3576	1/1	0.98	0.04	41,41,41,41	0
56	MG	1A	3881	1/1	0.98	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	1A	3092	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3578	1/1	0.98	0.04	39,39,39,39	0
56	MG	2A	3115	1/1	0.98	0.08	38,38,38,38	0
56	MG	2A	3609	1/1	0.98	0.05	36,36,36,36	0
56	MG	2a	1669	1/1	0.98	0.07	44,44,44,44	0
56	MG	1l	202	1/1	0.98	0.12	52,52,52,52	0
56	MG	1A	3650	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3456	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3038	1/1	0.98	0.09	36,36,36,36	0
56	MG	2A	3437	1/1	0.98	0.09	34,34,34,34	0
56	MG	2A	3615	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	3724	1/1	0.98	0.07	23,23,23,23	0
56	MG	1a	1726	1/1	0.98	0.04	57,57,57,57	0
56	MG	1a	1610	1/1	0.98	0.04	22,22,22,22	0
56	MG	2A	3442	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3725	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3027	1/1	0.98	0.19	33,33,33,33	0
56	MG	1B	3028	1/1	0.98	0.04	39,39,39,39	0
56	MG	1B	3029	1/1	0.98	0.03	28,28,28,28	0
56	MG	2A	3624	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	3804	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3202	1/1	0.98	0.21	31,31,31,31	0
56	MG	1A	3078	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3204	1/1	0.98	0.10	24,24,24,24	0
56	MG	1a	1737	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3079	1/1	0.98	0.14	30,30,30,30	0
56	MG	1A	3268	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3135	1/1	0.98	0.03	33,33,33,33	0
56	MG	2A	3457	1/1	0.98	0.04	48,48,48,48	0
56	MG	1a	1741	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3019	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3064	1/1	0.98	0.12	35,35,35,35	0
56	MG	2A	3291	1/1	0.98	0.10	49,49,49,49	0
56	MG	2A	3139	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3591	1/1	0.98	0.09	49,49,49,49	0
56	MG	2A	3294	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3735	1/1	0.98	0.08	25,25,25,25	0
56	MG	2A	3142	1/1	0.98	0.11	37,37,37,37	0
56	MG	1A	3136	1/1	0.98	0.05	39,39,39,39	0
56	MG	2A	3468	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3343	1/1	0.98	0.15	54,54,54,54	0
56	MG	2A	3646	1/1	0.98	0.04	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3299	1/1	0.98	0.04	36,36,36,36	0
56	MG	1A	3013	1/1	0.98	0.15	24,24,24,24	0
56	MG	2A	3146	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3147	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3160	1/1	0.98	0.07	26,26,26,26	0
56	MG	1a	1750	1/1	0.98	0.04	41,41,41,41	0
56	MG	2A	3654	1/1	0.98	0.07	34,34,34,34	0
56	MG	1F	304	1/1	0.98	0.10	37,37,37,37	0
56	MG	2A	3477	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3657	1/1	0.98	0.04	36,36,36,36	0
56	MG	2A	3658	1/1	0.98	0.04	39,39,39,39	0
56	MG	2A	3151	1/1	0.98	0.08	31,31,31,31	0
56	MG	1A	3161	1/1	0.98	0.05	41,41,41,41	0
56	MG	2A	3154	1/1	0.98	0.11	41,41,41,41	0
56	MG	2A	3009	1/1	0.98	0.12	41,41,41,41	0
56	MG	2A	3010	1/1	0.98	0.09	30,30,30,30	0
56	MG	2A	3157	1/1	0.98	0.03	29,29,29,29	0
56	MG	1A	3472	1/1	0.98	0.07	32,32,32,32	0
56	MG	2A	3666	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3907	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3241	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3909	1/1	0.98	0.05	36,36,36,36	0
56	MG	2A	3670	1/1	0.98	0.15	57,57,57,57	0
56	MG	2A	3671	1/1	0.98	0.05	51,51,51,51	0
56	MG	2A	3672	1/1	0.98	0.15	41,41,41,41	0
56	MG	2A	3016	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3017	1/1	0.98	0.04	26,26,26,26	0
56	MG	1A	3474	1/1	0.98	0.13	29,29,29,29	0
56	MG	1A	3184	1/1	0.98	0.06	34,34,34,34	0
56	MG	2A	3320	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3008	1/1	0.98	0.09	26,26,26,26	0
56	MG	1A	3913	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3824	1/1	0.98	0.06	36,36,36,36	0
56	MG	1N	3003	1/1	0.98	0.03	36,36,36,36	0
56	MG	1A	3916	1/1	0.98	0.15	34,34,34,34	0
56	MG	1a	1764	1/1	0.98	0.05	38,38,38,38	0
56	MG	2A	3026	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3500	1/1	0.98	0.04	38,38,38,38	0
56	MG	1N	3005	1/1	0.98	0.10	51,51,51,51	0
56	MG	2A	3502	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3533	1/1	0.98	0.04	28,28,28,28	0
56	MG	2a	1749	1/1	0.98	0.16	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	1N	3007	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3030	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3022	1/1	0.98	0.05	27,27,27,27	0
56	MG	1A	3919	1/1	0.98	0.25	33,33,33,33	0
56	MG	1A	3009	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3921	1/1	0.98	0.09	40,40,40,40	0
56	MG	2D	303	1/1	0.98	0.25	45,45,45,45	0
56	MG	1A	3188	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3923	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3924	1/1	0.98	0.17	28,28,28,28	0
56	MG	1A	3678	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3189	1/1	0.98	0.05	32,32,32,32	0
56	MG	2E	305	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3432	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3344	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3609	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3042	1/1	0.98	0.06	37,37,37,37	0
56	MG	1a	1780	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3249	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3250	1/1	0.98	0.14	30,30,30,30	0
56	MG	2A	3046	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3612	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3933	1/1	0.98	0.12	28,28,28,28	0
56	MG	2A	3526	1/1	0.98	0.14	49,49,49,49	0
56	MG	1A	3284	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3935	1/1	0.98	0.06	48,48,48,48	0
56	MG	1A	3936	1/1	0.98	0.12	29,29,29,29	0
56	MG	2U	201	1/1	0.98	0.10	39,39,39,39	0
56	MG	2a	1778	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3837	1/1	0.98	0.05	21,21,21,21	0
56	MG	1A	3838	1/1	0.98	0.06	38,38,38,38	0
56	MG	2A	3359	1/1	0.98	0.04	44,44,44,44	0
56	MG	2A	3202	1/1	0.98	0.12	44,44,44,44	0
56	MG	1a	1790	1/1	0.98	0.04	46,46,46,46	0
56	MG	1a	1666	1/1	0.98	0.12	36,36,36,36	0
56	MG	2A	3205	1/1	0.98	0.10	53,53,53,53	0
56	MG	2A	3364	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3487	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3840	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	3615	1/1	0.98	0.06	45,45,45,45	0
56	MG	1A	3942	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3616	1/1	0.98	0.06	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1U	202	1/1	0.98	0.07	31,31,31,31	0
56	MG	2a	1793	1/1	0.98	0.05	41,41,41,41	0
56	MG	2A	3372	1/1	0.98	0.12	41,41,41,41	0
56	MG	1U	203	1/1	0.98	0.13	27,27,27,27	0
56	MG	1A	3393	1/1	0.98	0.06	35,35,35,35	0
56	MG	1U	205	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3251	1/1	0.98	0.24	25,25,25,25	0
56	MG	2f	3001	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3377	1/1	0.98	0.03	43,43,43,43	0
56	MG	1a	1678	1/1	0.98	0.10	57,57,57,57	0
56	MG	1A	3071	1/1	0.98	0.09	47,47,47,47	0
56	MG	2A	3553	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3072	1/1	0.98	0.05	40,40,40,40	0
56	MG	1a	1805	1/1	0.98	0.09	49,49,49,49	0
56	MG	2A	3070	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3621	1/1	0.98	0.08	48,48,48,48	0
56	MG	1W	3003	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3035	1/1	0.98	0.13	32,32,32,32	0
56	MG	2A	3560	1/1	0.98	0.14	51,51,51,51	0
56	MG	1A	3767	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3324	1/1	0.98	0.05	43,43,43,43	0
56	MG	1X	3001	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3554	1/1	0.98	0.08	32,32,32,32	0
56	MG	1A	3400	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3853	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3854	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3443	1/1	0.98	0.06	26,26,26,26	0
56	MG	2a	1627	1/1	0.98	0.03	46,46,46,46	0
56	MG	1A	3557	1/1	0.98	0.05	44,44,44,44	0
56	MG	1A	3444	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3445	1/1	0.98	0.05	53,53,53,53	0
59	ZN	29	501	1/1	0.98	0.04	62,62,62,62	0
56	MG	1A	3499	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	3500	1/1	0.98	0.04	26,26,26,26	0
60	SF4	2d	301	8/8	0.98	0.05	51,72,83,98	0
56	MG	2A	3575	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3562	1/1	0.98	0.04	42,42,42,42	0
56	MG	2A	3543	1/1	0.99	0.03	28,28,28,28	0
56	MG	2A	3012	1/1	0.99	0.10	40,40,40,40	0
56	MG	2A	3118	1/1	0.99	0.03	37,37,37,37	0
56	MG	2a	1692	1/1	0.99	0.12	54,54,54,54	0
56	MG	1A	3418	1/1	0.99	0.08	34,34,34,34	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	3573	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3065	1/1	0.99	0.06	14,14,14,14	0
56	MG	1A	3040	1/1	0.99	0.04	32,32,32,32	0
56	MG	1a	1834	1/1	0.99	0.12	44,44,44,44	0
56	MG	1A	3328	1/1	0.99	0.06	27,27,27,27	0
56	MG	2A	3356	1/1	0.99	0.03	29,29,29,29	0
56	MG	1A	3194	1/1	0.99	0.09	38,38,38,38	0
56	MG	2A	3239	1/1	0.99	0.03	43,43,43,43	0
56	MG	1A	3654	1/1	0.99	0.03	40,40,40,40	0
56	MG	1a	1736	1/1	0.99	0.04	58,58,58,58	0
56	MG	1A	3517	1/1	0.99	0.03	9,9,9,9	0
56	MG	2D	302	1/1	0.99	0.03	27,27,27,27	0
56	MG	1A	3579	1/1	0.99	0.09	21,21,21,21	0
56	MG	1A	3657	1/1	0.99	0.03	29,29,29,29	0
56	MG	1A	3781	1/1	0.99	0.03	23,23,23,23	0
56	MG	2A	3365	1/1	0.99	0.03	29,29,29,29	0
56	MG	1A	3024	1/1	0.99	0.05	27,27,27,27	0
56	MG	2A	3563	1/1	0.99	0.04	36,36,36,36	0
56	MG	1A	3424	1/1	0.99	0.04	14,14,14,14	0
56	MG	2A	3189	1/1	0.99	0.04	31,31,31,31	0
56	MG	1A	3547	1/1	0.99	0.04	36,36,36,36	0
56	MG	1A	3493	1/1	0.99	0.08	21,21,21,21	0
56	MG	1A	3549	1/1	0.99	0.09	41,41,41,41	0
56	MG	1A	3141	1/1	0.99	0.14	27,27,27,27	0
56	MG	1A	3586	1/1	0.99	0.09	41,41,41,41	0
56	MG	1A	3551	1/1	0.99	0.09	26,26,26,26	0
56	MG	2A	3196	1/1	0.99	0.04	35,35,35,35	0
56	MG	2A	3439	1/1	0.99	0.04	36,36,36,36	0
56	MG	1A	3552	1/1	0.99	0.06	22,22,22,22	0
56	MG	1A	3553	1/1	0.99	0.06	28,28,28,28	0
56	MG	1A	3469	1/1	0.99	0.06	33,33,33,33	0
56	MG	1A	3405	1/1	0.99	0.05	40,40,40,40	0
56	MG	1A	3029	1/1	0.99	0.14	28,28,28,28	0
56	MG	1A	3043	1/1	0.99	0.09	27,27,27,27	0
56	MG	1A	3247	1/1	0.99	0.17	27,27,27,27	0
56	MG	2A	3383	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3156	1/1	0.99	0.06	34,34,34,34	0
56	MG	2A	3515	1/1	0.99	0.06	35,35,35,35	0
56	MG	1a	1708	1/1	0.99	0.12	34,34,34,34	0
56	MG	2A	3095	1/1	0.99	0.04	47,47,47,47	0
56	MG	1A	3596	1/1	0.99	0.06	32,32,32,32	0
56	MG	2A	3325	1/1	0.99	0.03	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	2A	3454	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3110	1/1	0.99	0.07	29,29,29,29	0
56	MG	2A	3327	1/1	0.99	0.04	33,33,33,33	0
56	MG	2A	3152	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3476	1/1	0.99	0.03	31,31,31,31	0
56	MG	1A	3070	1/1	0.99	0.05	33,33,33,33	0
56	MG	1A	3454	1/1	0.99	0.09	35,35,35,35	0
56	MG	1A	3159	1/1	0.99	0.19	34,34,34,34	0
56	MG	1A	3565	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3890	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3012	1/1	0.99	0.03	28,28,28,28	0
56	MG	1B	3015	1/1	0.99	0.04	31,31,31,31	0
56	MG	1A	3007	1/1	0.99	0.07	29,29,29,29	0
56	MG	1A	3482	1/1	0.99	0.03	27,27,27,27	0
56	MG	1A	3205	1/1	0.99	0.04	33,33,33,33	0
59	ZN	1Y	501	1/1	0.99	0.03	67,67,67,67	0
56	MG	1a	1674	1/1	0.99	0.07	42,42,42,42	0
59	ZN	19	103	1/1	0.99	0.11	61,61,61,61	0
59	ZN	1n	501	1/1	0.99	0.03	58,58,58,58	0
59	ZN	2Y	501	1/1	0.99	0.03	83,83,83,83	0
56	MG	1a	1628	1/1	0.99	0.04	43,43,43,43	0
59	ZN	25	101	1/1	0.99	0.04	64,64,64,64	0
56	MG	1B	3019	1/1	0.99	0.03	22,22,22,22	0
56	MG	1a	1775	1/1	0.99	0.03	52,52,52,52	0
56	MG	1A	3014	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3645	1/1	0.99	0.03	23,23,23,23	0
56	MG	1A	3033	1/1	0.99	0.12	22,22,22,22	0
56	MG	1A	3647	1/1	0.99	0.04	45,45,45,45	0
56	MG	2A	3450	1/1	1.00	0.03	24,24,24,24	0
56	MG	1a	1738	1/1	1.00	0.02	43,43,43,43	0
59	ZN	26	501	1/1	1.00	0.03	54,54,54,54	0
56	MG	1A	3855	1/1	1.00	0.05	23,23,23,23	0
59	ZN	15	101	1/1	1.00	0.06	25,25,25,25	0
59	ZN	16	501	1/1	1.00	0.01	35,35,35,35	0
56	MG	1A	3926	1/1	1.00	0.15	29,29,29,29	0
56	MG	1A	3395	1/1	1.00	0.08	31,31,31,31	0
56	MG	1A	3046	1/1	1.00	0.08	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.