



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:19 PM EDT

PDB ID : 9D0J / pdb_00009d0j
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with BT-33, mRNA, deacylated A-site tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.50Å resolution
Authors : Aleksandrova, E.V.; Tresco, B.I.C.; Wu, K.J.Y.; Ramkisson, A.; Purdy, M.; See, D.N.Y.; Liu, R.Y.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2024-08-07
Resolution : 2.50 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](#) ①) 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

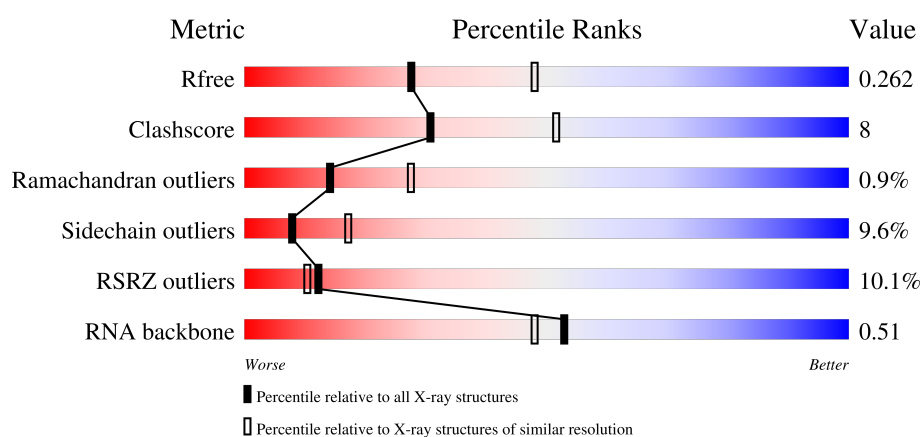
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



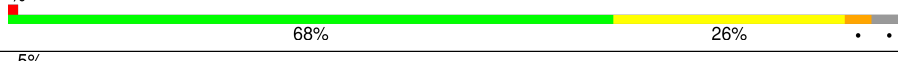
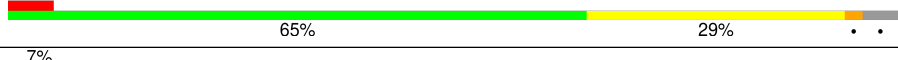
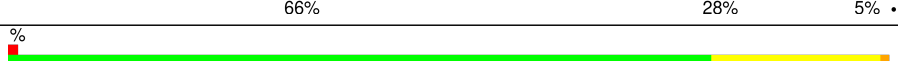
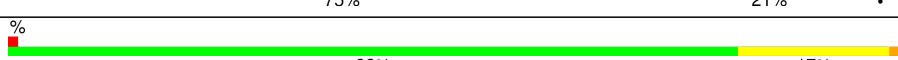
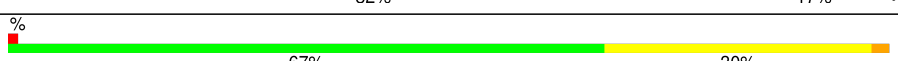
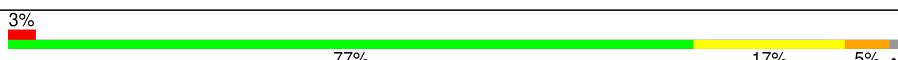
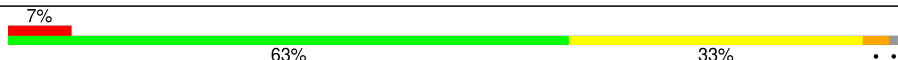
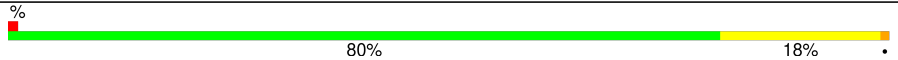
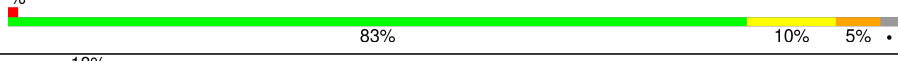
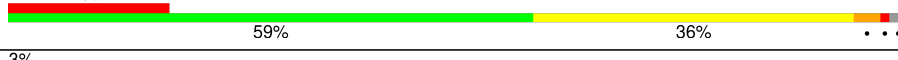
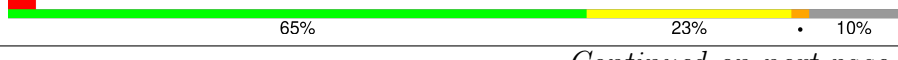
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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

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

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

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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3386	-	-	-	X
56	MG	1A	3391	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299293 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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

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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	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	79	Total	C	N	O	S	0	0	0
			620	383	131	105	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			

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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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0	0
			1530	685	274	498	71	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1059	Total	Mg	0	0
			1059	1059		
56	1B	39	Total	Mg	0	0
			39	39		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	16	Total	Mg	0	0
			16	16		
56	1F	14	Total	Mg	0	0
			14	14		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	6	Total 6	Mg 6	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	6	Total 6	Mg 6	0	0
56	1Q	7	Total 7	Mg 7	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	7	Total 7	Mg 7	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	6	Total 6	Mg 6	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	8	Total 8	Mg 8	0	0
56	16	3	Total 3	Mg 3	0	0
56	17	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	18	4	Total 4	Mg 4	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	198	Total 198	Mg 198	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	2	Total 2	Mg 2	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1u	1	Total 1	Mg 1	0	0
56	1w	4	Total 4	Mg 4	0	0
56	1x	12	Total 12	Mg 12	0	0
56	2A	782	Total 782	Mg 782	0	0
56	2B	18	Total 18	Mg 18	0	0
56	2D	8	Total 8	Mg 8	0	0
56	2E	9	Total 9	Mg 9	0	0
56	2F	6	Total 6	Mg 6	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0

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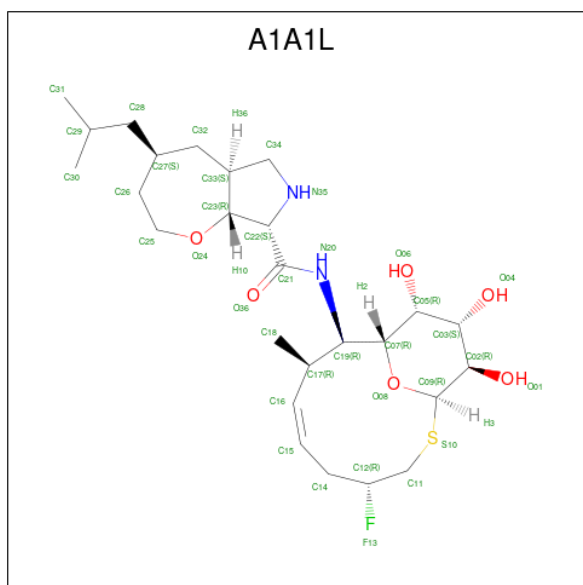
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2O	2	Total 2	Mg 2	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	5	Total 5	Mg 5	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	2	Total 2	Mg 2	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	5	Total 5	Mg 5	0	0
56	27	4	Total 4	Mg 4	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	202	Total 202	Mg 202	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2j	1	Total	Mg	0	0
			1	1		
56	2k	1	Total	Mg	0	0
			1	1		
56	2l	5	Total	Mg	0	0
			5	5		
56	2q	2	Total	Mg	0	0
			2	2		
56	2r	2	Total	Mg	0	0
			2	2		
56	2t	2	Total	Mg	0	0
			2	2		
56	2v	1	Total	Mg	0	0
			1	1		
56	2w	3	Total	Mg	0	0
			3	3		
56	2x	6	Total	Mg	0	0
			6	6		

- Molecule 57 is (4S,5aS,8S,8aR)-N-[(1R,4R,6Z,8R,9R,10R,11R,12S,13R)-4-fluoro-11,12,13-trihydroxy-8-methyl-14-oxa-2-thiabicyclo[8.3.1]tetradec-6-en-9-yl]-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: A1A1L) (formula: C₂₆H₄₃FN₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
57	1A	1	Total	C	F	N	O	S	0	0
			36	26	1	2	6	1		

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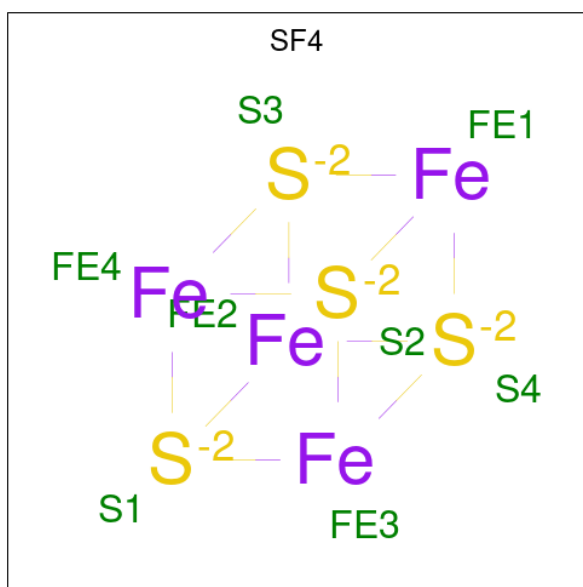
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
57	2A	1	Total	C	F	N	O	S	0	0
			36	26	1	2	6	1		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2x	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1902	Total	O	0	0
			1902	1902		
61	1B	59	Total	O	0	0
			59	59		
61	1D	27	Total	O	0	0
			27	27		
61	1E	31	Total	O	0	0
			31	31		
61	1F	20	Total	O	0	0
			20	20		
61	1G	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	2	Total	O	0	0
			2	2		
61	1N	6	Total	O	0	0
			6	6		
61	1O	6	Total	O	0	0
			6	6		
61	1P	18	Total	O	0	0
			18	18		
61	1Q	8	Total	O	0	0
			8	8		
61	1R	11	Total	O	0	0
			11	11		
61	1S	5	Total	O	0	0
			5	5		
61	1T	7	Total	O	0	0
			7	7		
61	1U	15	Total	O	0	0
			15	15		
61	1V	8	Total	O	0	0
			8	8		
61	1W	8	Total	O	0	0
			8	8		
61	1X	7	Total	O	0	0
			7	7		
61	1Y	3	Total	O	0	0
			3	3		
61	1Z	1	Total	O	0	0
			1	1		
61	10	8	Total	O	0	0
			8	8		
61	11	7	Total	O	0	0
			7	7		
61	12	4	Total	O	0	0
			4	4		
61	13	4	Total	O	0	0
			4	4		
61	14	1	Total	O	0	0
			1	1		
61	15	7	Total	O	0	0
			7	7		
61	16	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	17	8	Total 8	O 8	0	0
61	18	13	Total 13	O 13	0	0
61	1a	298	Total 298	O 298	0	0
61	1b	1	Total 1	O 1	0	0
61	1l	5	Total 5	O 5	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1t	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	4	Total 4	O 4	0	0
61	1x	9	Total 9	O 9	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1002	Total 1002	O 1002	0	0
61	2B	16	Total 16	O 16	0	0
61	2D	23	Total 23	O 23	0	0
61	2E	16	Total 16	O 16	0	0
61	2F	14	Total 14	O 14	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	9	Total 9	O 9	0	0
61	2Q	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	3	Total 3	O 3	0	0
61	20	2	Total 2	O 2	0	0
61	21	3	Total 3	O 3	0	0
61	23	3	Total 3	O 3	0	0
61	25	2	Total 2	O 2	0	0
61	27	4	Total 4	O 4	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	168	Total 168	O 168	0	0
61	2e	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	3	Total 3	O 3	0	0
61	2p	1	Total 1	O 1	0	0
61	2t	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	1	Total 1	O 1	0	0

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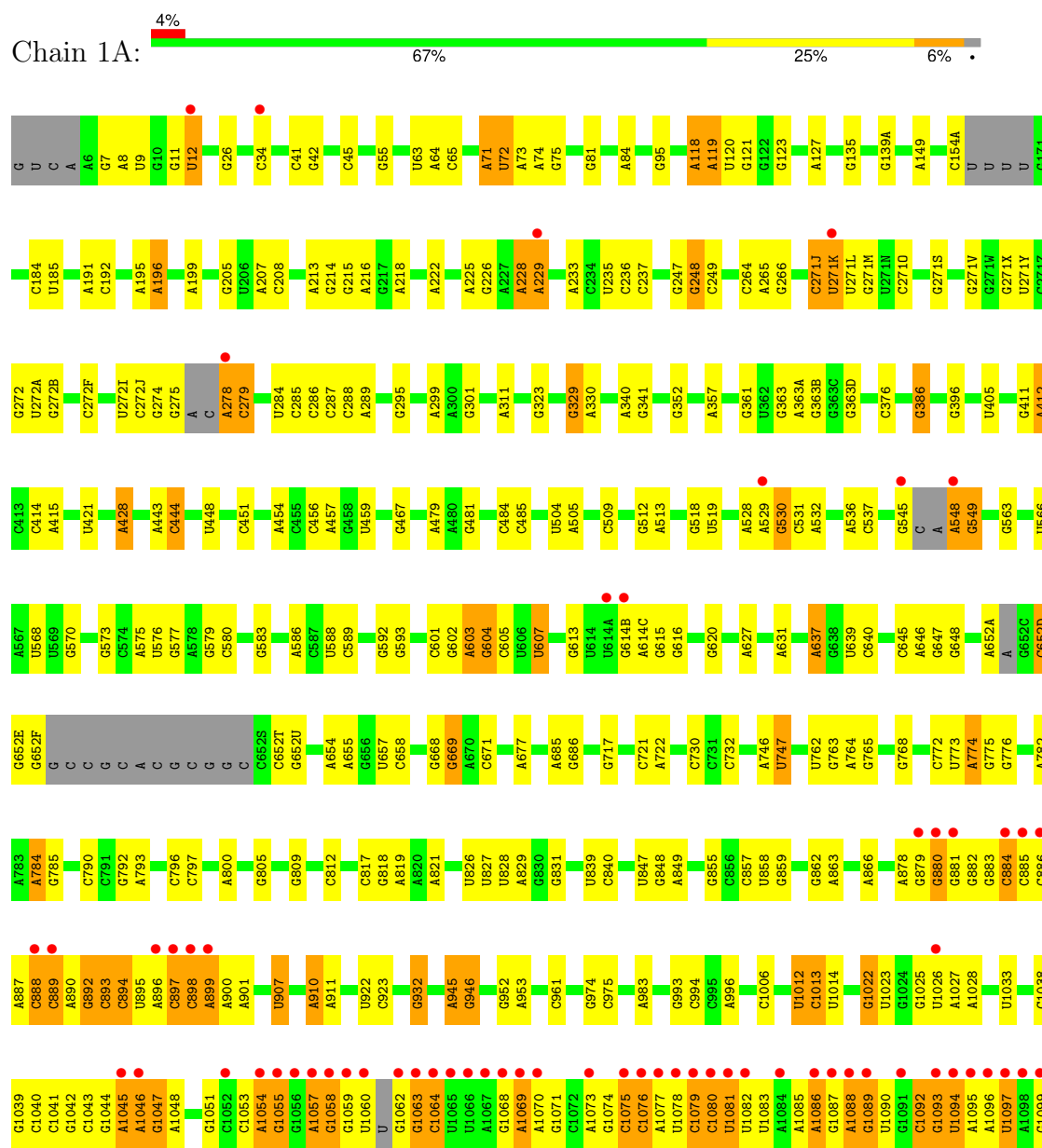
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2x	4	Total	O	0	0
			4	4		

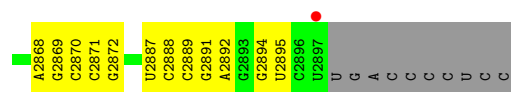
3 Residue-property plots

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

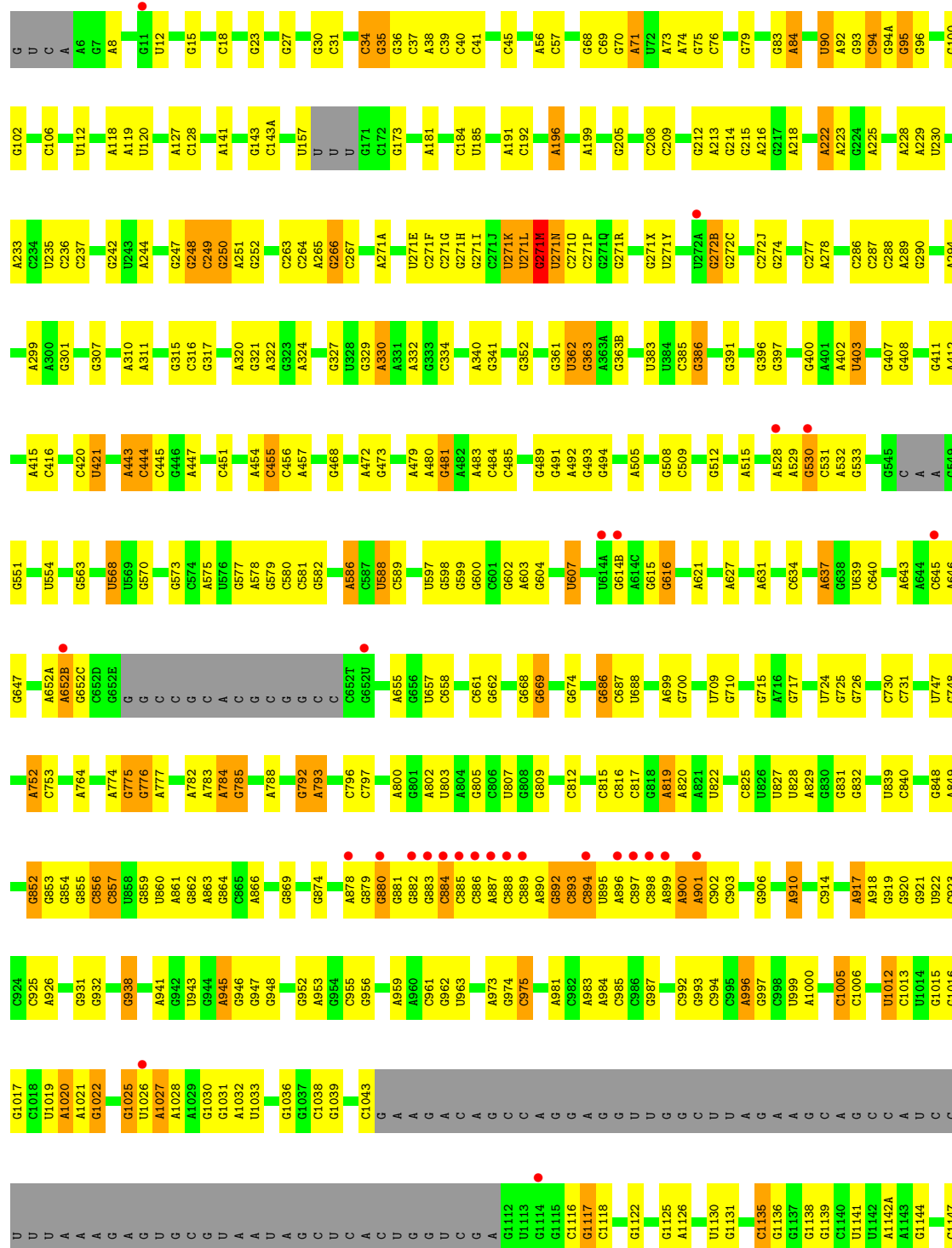
• Molecule 1: 23S Ribosomal RNA



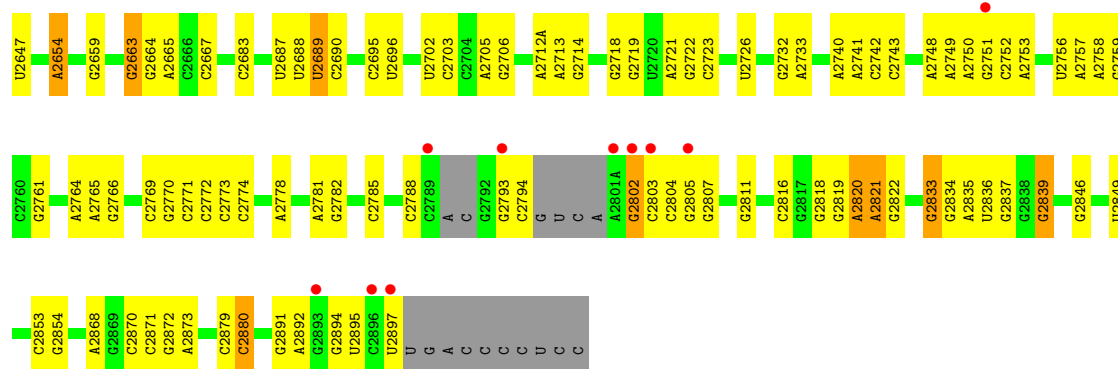
U754	C2628	A2476	C2350	U2233	C2145	C2065	U1951	A1803	G1674	A1509B	C1393	C1202	U1100
C2755	A2629	C2477	G2351	G2234	C2146	C2066	U1952	C1804	C1686	G1510	U1393	G1203	U1101
U2756	G2630	A2478	A2352	G2234	G2147	C2067	A1953	U1805	C1687	C1511	U1395	G1223	C1102
A2757	G2631	C2499	C2355	G2238	G2149	U2068	G1954	A1810	U1688	C1513	U1396	U1226	A1103
A2758	C2646	G2502	C2359	G2239	U2150	G2070	U1955	G1811	U1693	U1518	C1399	U1243	U1105
A2765	U2647	A2503	C2360	U2243	G2152	A2071	C1962	A1812	U1696	G1519	U1405	G1243	U1106
G2766	U2648	G2504	A2361	U2244	G2153	G2080	U1963	G1813	G1696	A1528A	U1406	U1253	U1108
U2649	U2650	G2505	A2366	C2248	G2154	U2086	C1967	A1814	U1700	A1528A	C1407	G1109	G1109
C2771	A2654	G2512	A2366	C2248	G2155	G2087	U1968	A1815	A1700	A1528A	U1407	G1256	A1111
C2772	G2654	G2513	A2375	G2251	G2156	G2087	G1968	A1816	G1702	C1532	G1416	U1268	U1112
A2778	G2663	U2514	G2376	A2268	A2158	G2093	A1970	G1817	G1703	G	C1417	G1286	U1113
A2781	A2664	G2515	A2377	A2268	G2159	G2094	A1971	G1828	G1709	U	G1418	U1287	G1114
G2787	A2665	G2516	A2378	G2271	G2160	C2095	A1972	A1829	C1710	A	G1419	U1268	G1115
C2788	C2666	G2517	A2378	G2271	G2161	U2096	A1986	G1839	C1710	C	U1420	G1116	C1116
C2789	C2667	A2518	G2379	G2271	G2162	U2099	A1986	G1839	C1710	G1537	G1421	G1117	G1117
G2790	G2674	U2522	G2383	G2277	C2163	U2099	U1991	C1843	G1721	U1540	A1427	A1272	G1125
C2791	A2679	G2529	G2384	A2276	G2164	G2100	G1992	A1847	A1722	G1541	C1428	U1273	U1273
G2792	G2679	G2535	C2385	G2280	G2165	G2101	U1993	U1851	A1739	G1541	C1429	A1278	C1135
C2793	C2683	G2535	U2390	G2283	U2167	U2102	G1993	C1852	G1740	A1558	C1430	G1289	G1136
G	U	G2550	U2396	C2284	C2168	C2108	G1996	C1852	C1745A	A1566	U1431	C1290	G1137
U	C	G2551	G2396	C2285	A2169	U2109	G1997	C1852	C1745A	A1567	C1432	C1300	G1138
A	A	G2552	U2406	A2287	A2170	G2110	G1998	G1865	G1750	G1568	U1439	U1300	G1139
A2801A	G2688	G2552	G2407	A2287	U2171	G2111	C1999	C1866	G1750	G1569	G1440	A1301	U1140
G2802	C2690	G2553	G2407	A2287	A2172	G2112	G2012	A1876	G1753	A1570	G1441	U1432	U141
C2803	A2693	U2554	G2414	A2298	C2174	U2113	G2013	G1877	G1753	U1578	G1442	G1303	A1142A
C2804	G2694	A2564	G2414	G2299	C2175	G2115	A2014	A1889	G1756	U1578	U1445	C1315	A1143
G2810	C2701	A2565	C2417	A2305	A2176	G2116	A2020	A1890	A1762	A1579	A1445	C1315	G1144
G2811	U2702	A2566	A2422	C2306	U2180	A2117	C2021	A1890	A1762	A1580	G1448	U1321	C1153
G2817	C2703	C2568	U2423	C2307	C2183	U2118	U2022	G1899	G1764	G1581	A1449	G1332	G1154
A2820	G2706	A2572	C2424	C2308	C2184	G2120	G2023	A1900	A1773	A1584	G1450	U1338	A1155
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Molecule 1: 23S Ribosomal RNA

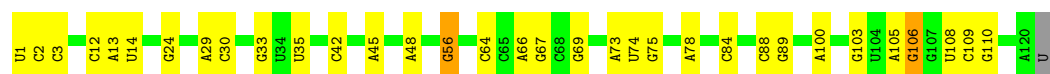


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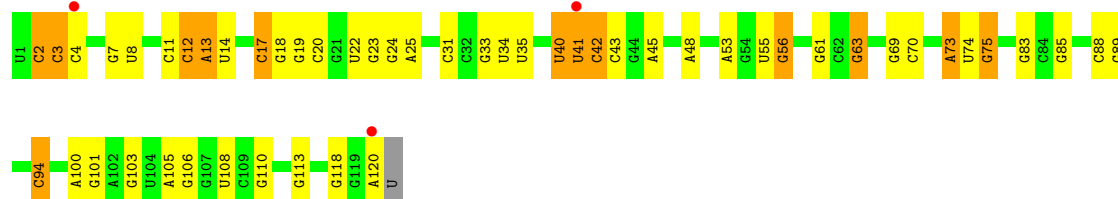
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 72% 26%



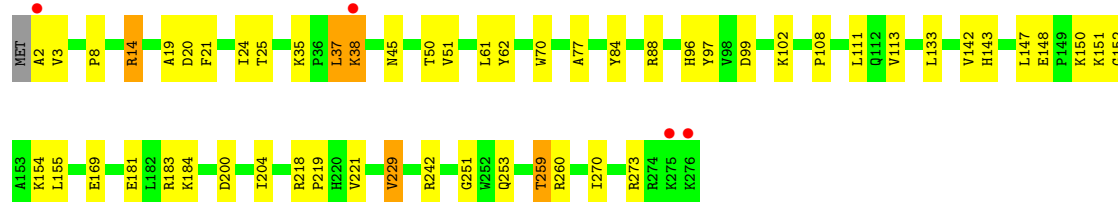
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 2% 56% 32% 11%



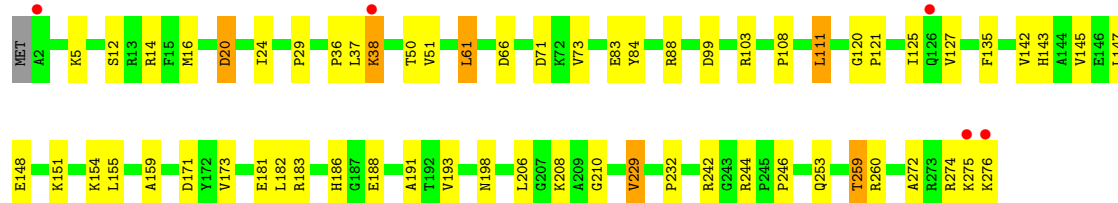
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 80% 18%

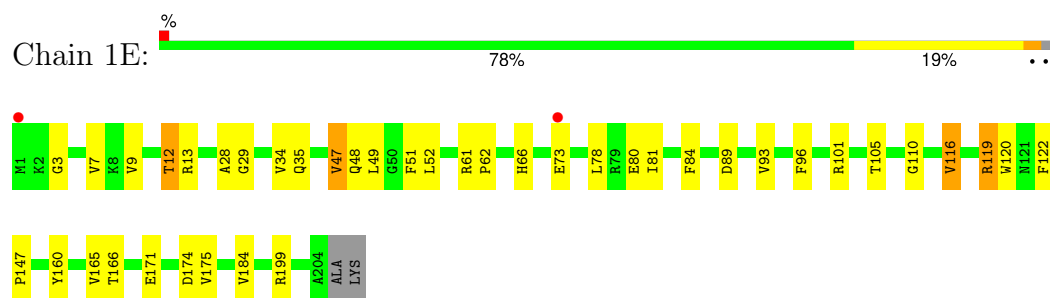


• Molecule 3: 50S ribosomal protein L2

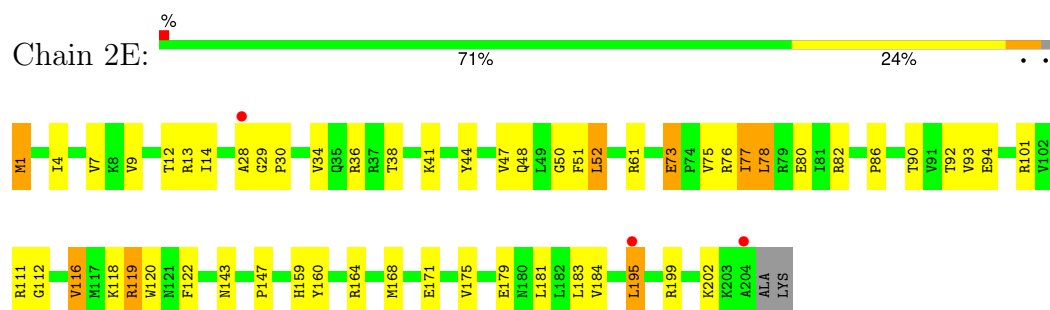
Chain 2D: 2% 77% 20%



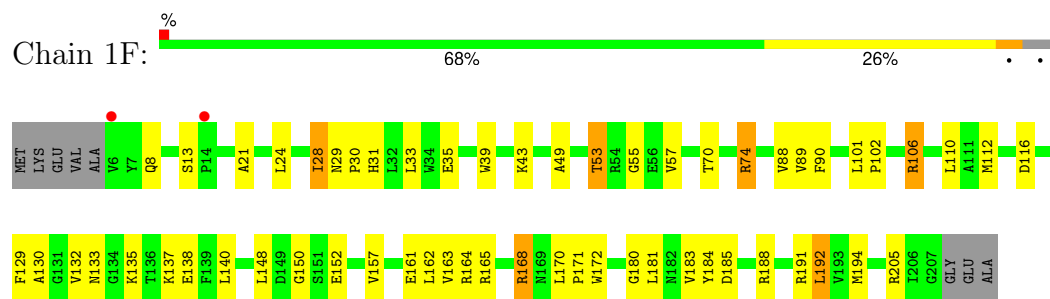
- Molecule 4: 50S ribosomal protein L3



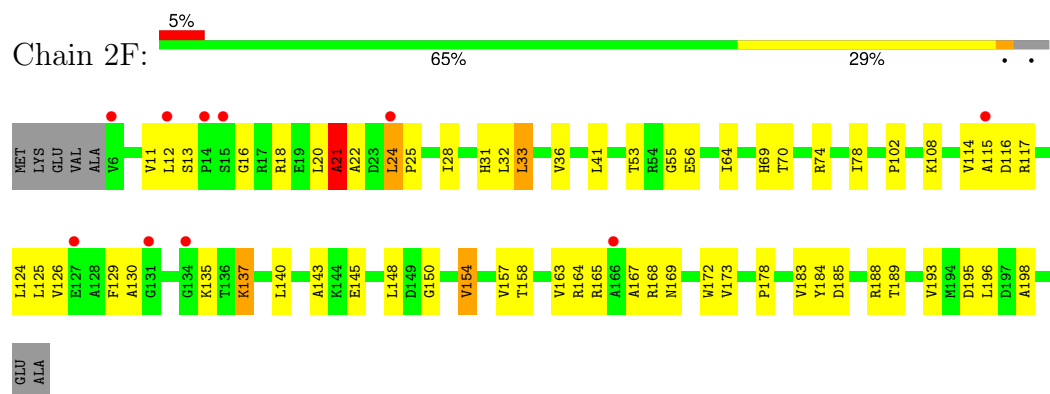
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

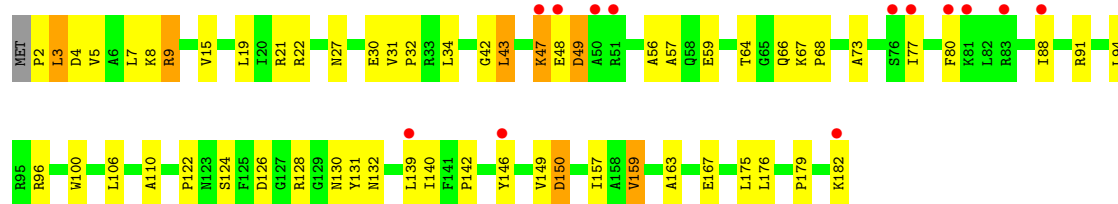


- Molecule 5: 50S ribosomal protein L4



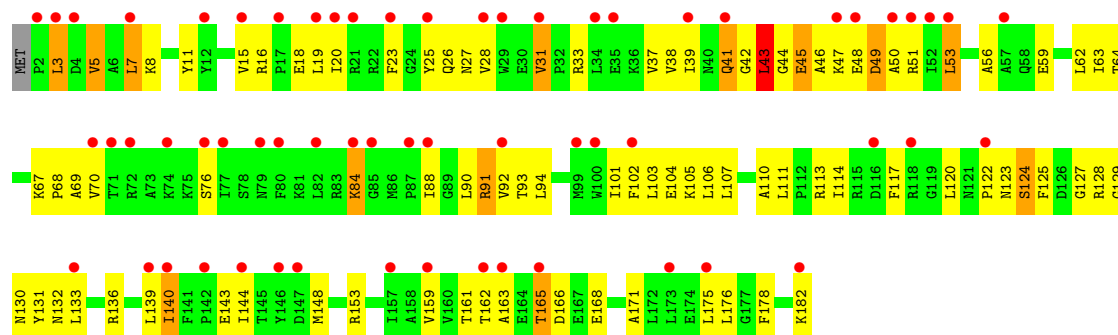
- Molecule 6: 50S ribosomal protein L5





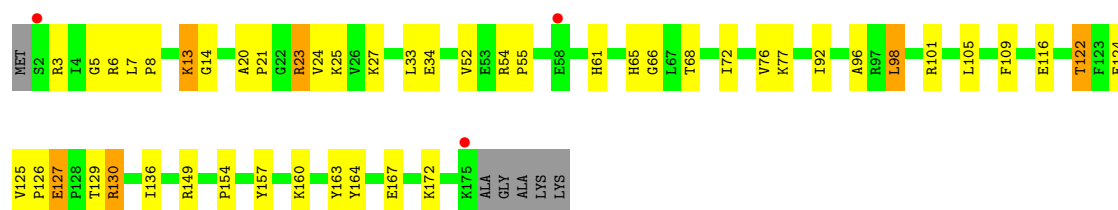
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 34% 49% 43% 7% ..



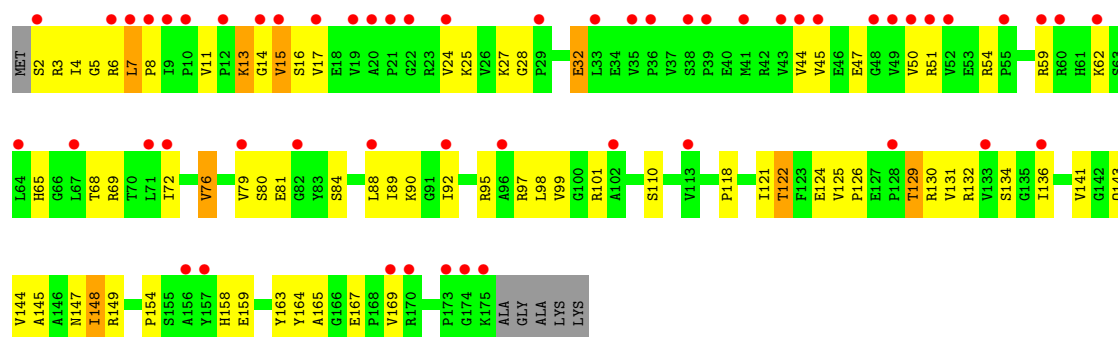
• Molecule 7: 50S ribosomal protein L6

Chain 1H: 2% 70% 23% ..



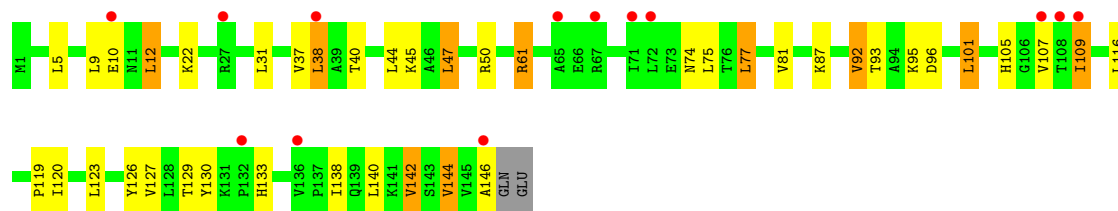
• Molecule 7: 50S ribosomal protein L6

Chain 2H: 31% 57% 36% ..

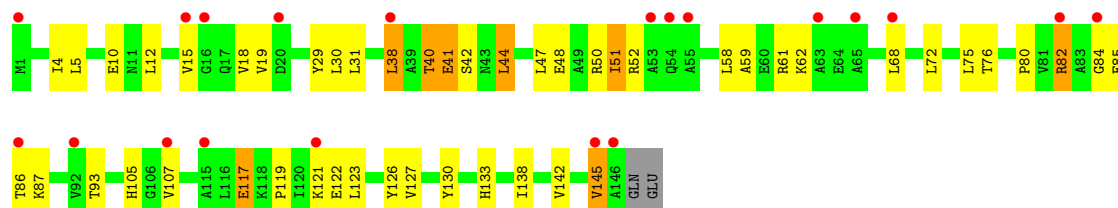


• Molecule 8: 50S ribosomal protein L9

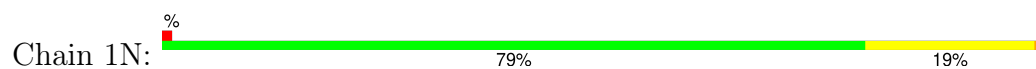
Chain 1I: 9% 71% 21% 7% ..



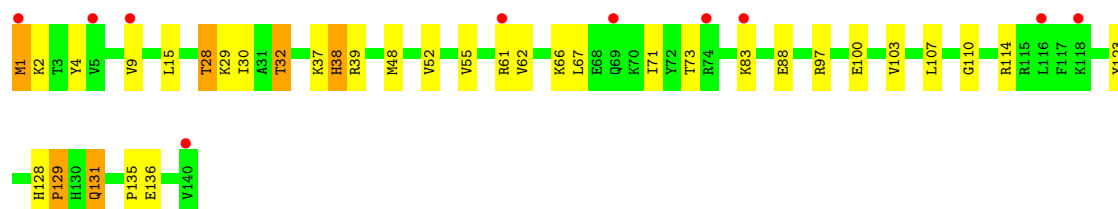
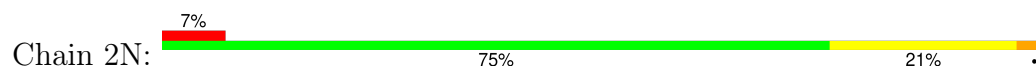
• Molecule 8: 50S ribosomal protein L9



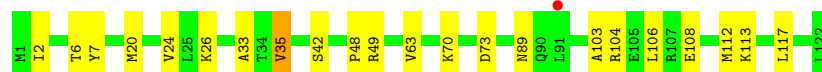
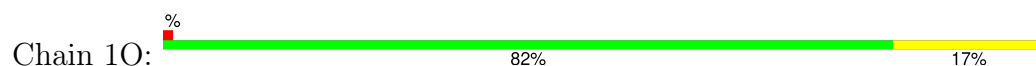
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



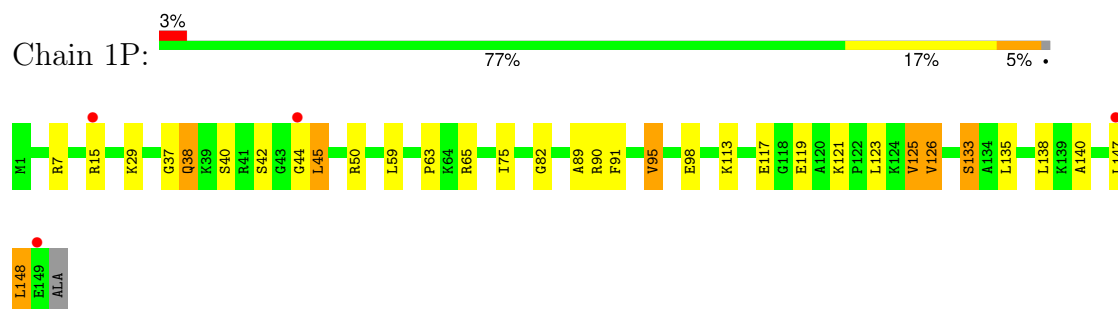
• Molecule 10: 50S ribosomal protein L14



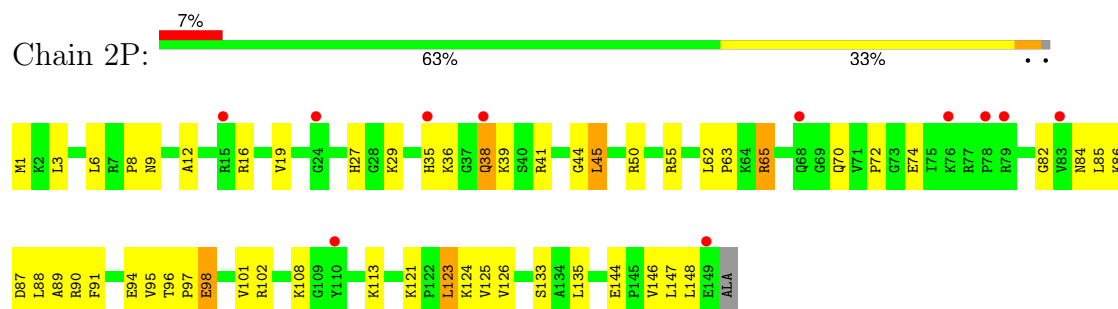
• Molecule 10: 50S ribosomal protein L14



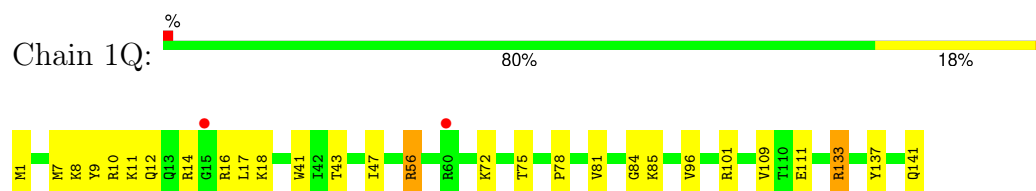
- Molecule 11: 50S ribosomal protein L15



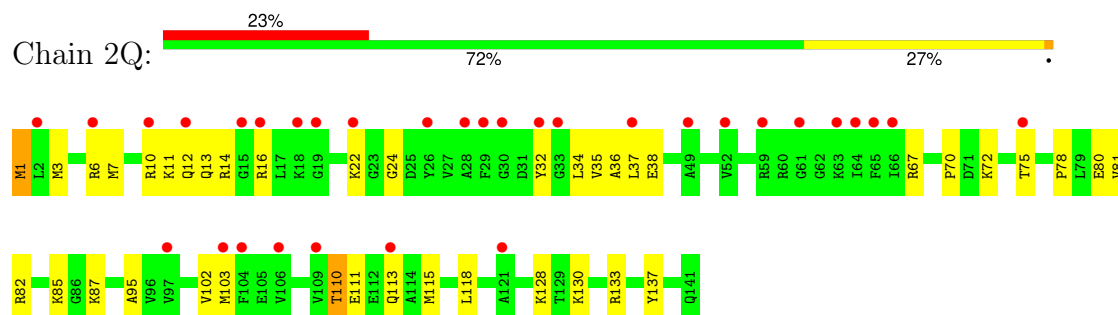
- Molecule 11: 50S ribosomal protein L15



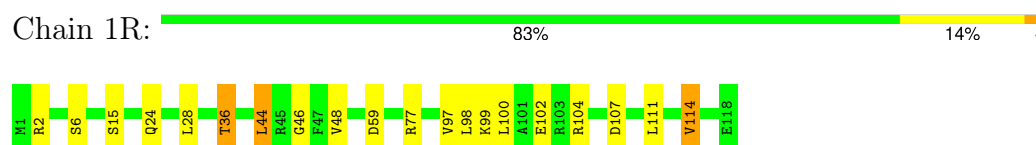
- Molecule 12: 50S ribosomal protein L16



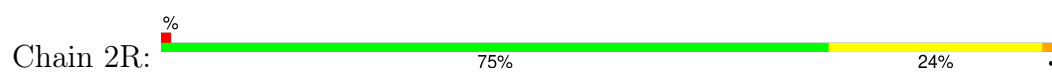
- Molecule 12: 50S ribosomal protein L16



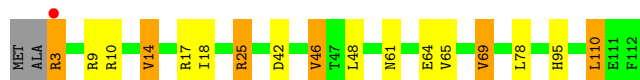
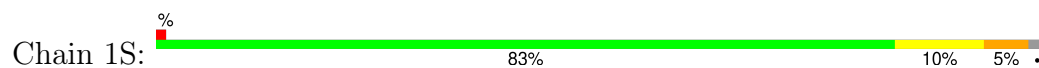
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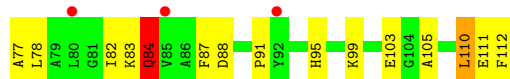
- Molecule 13: 50S ribosomal protein L17



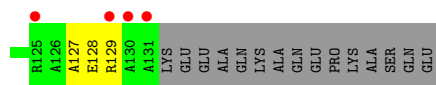
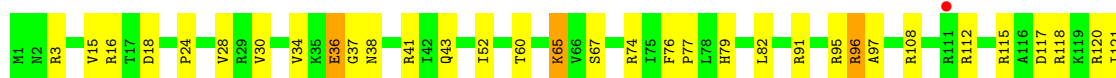
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18



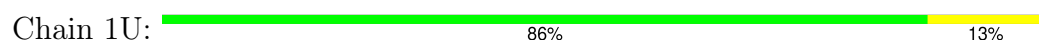
- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

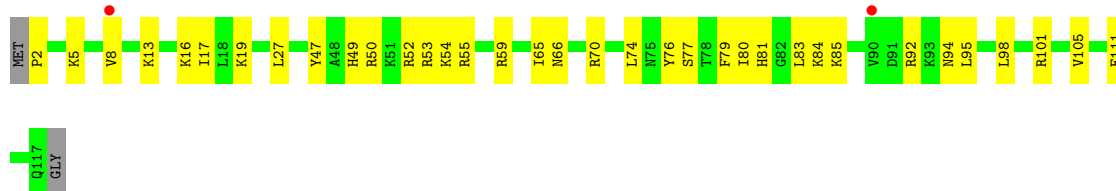


- Molecule 16: 50S ribosomal protein L20

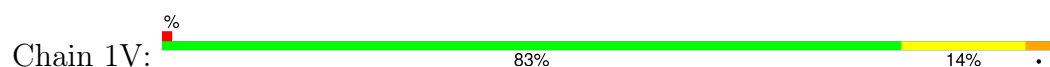




- Molecule 16: 50S ribosomal protein L20



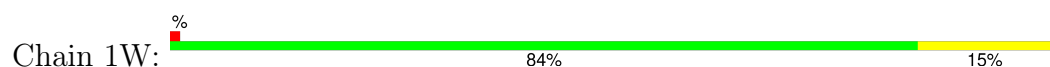
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



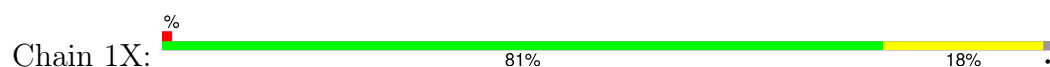
- Molecule 18: 50S ribosomal protein L22



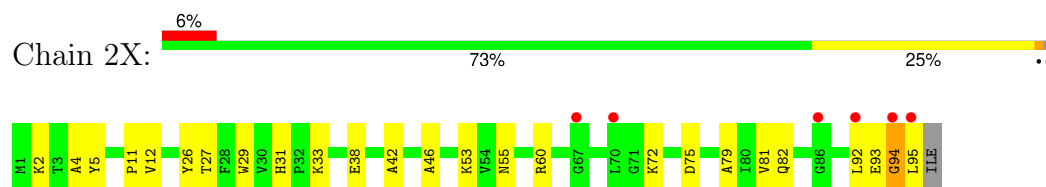
- Molecule 18: 50S ribosomal protein L22



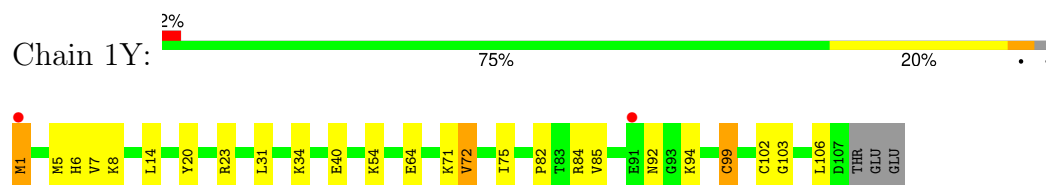
- Molecule 19: 50S ribosomal protein L23



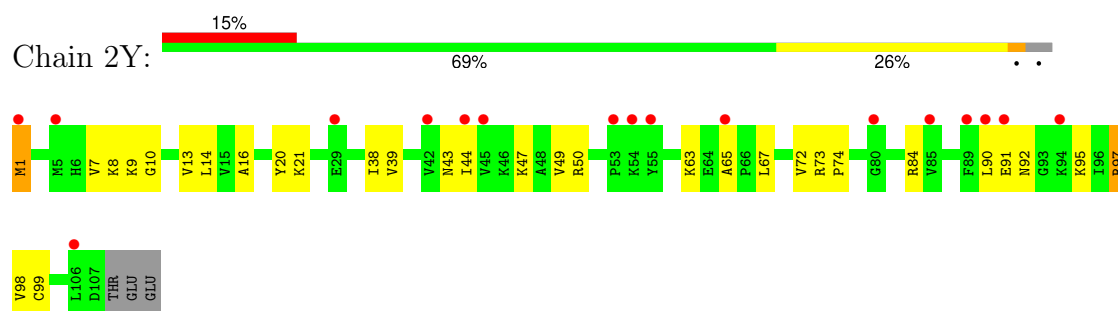
- Molecule 19: 50S ribosomal protein L23



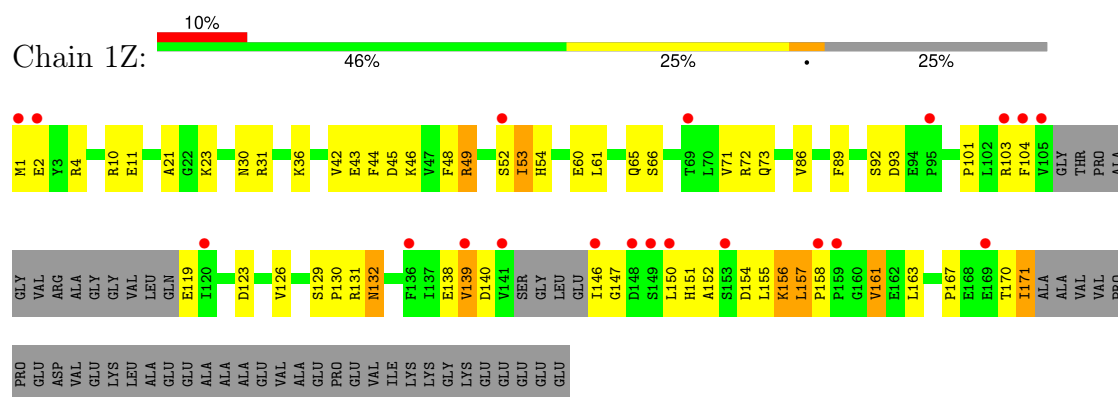
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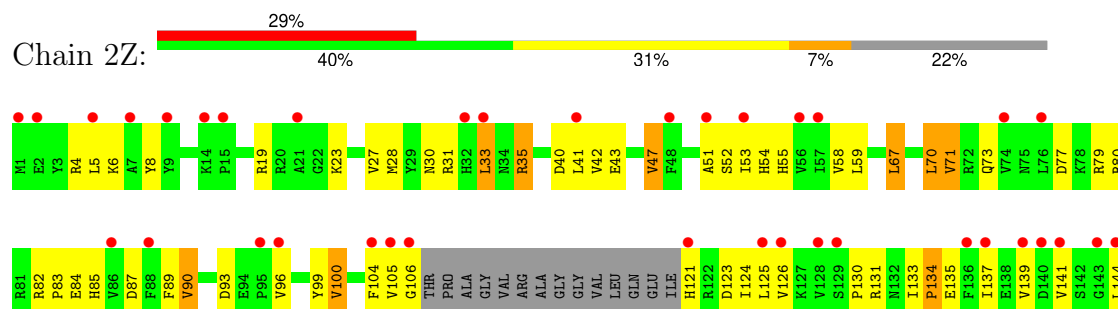
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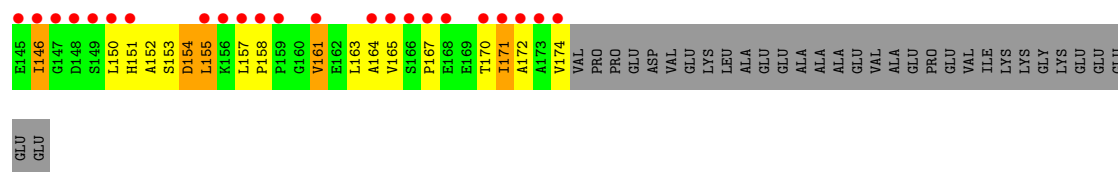


- Molecule 21: 50S ribosomal protein L25

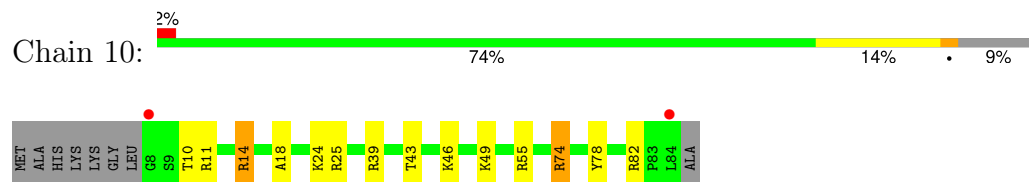


- Molecule 21: 50S ribosomal protein L25

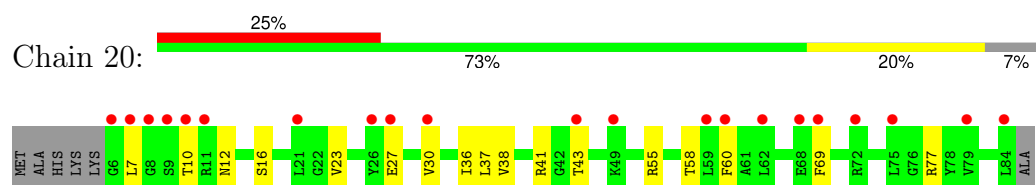




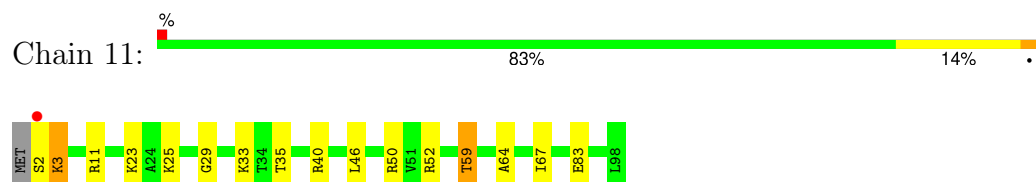
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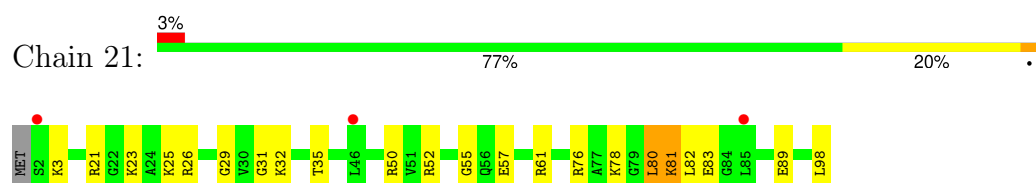
- Molecule 22: 50S ribosomal protein L27



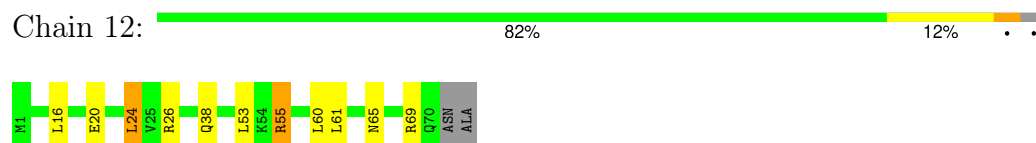
- Molecule 23: 50S ribosomal protein L28



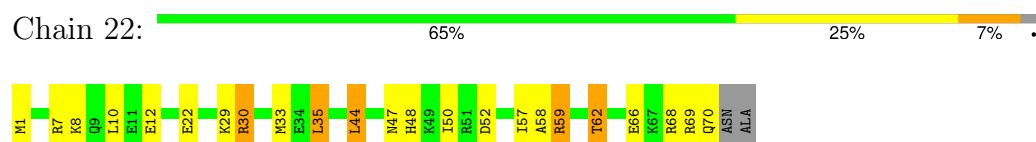
- Molecule 23: 50S ribosomal protein L28



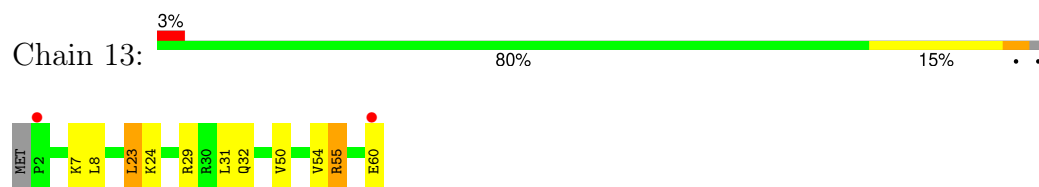
- Molecule 24: 50S ribosomal protein L29



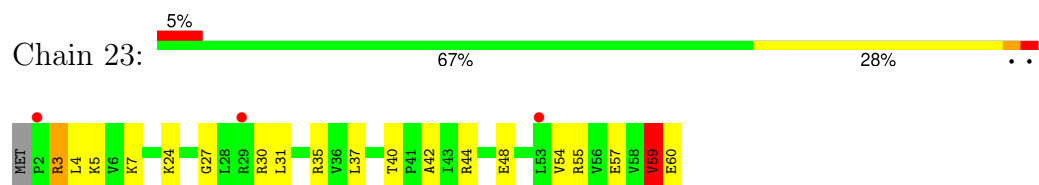
- Molecule 24: 50S ribosomal protein L29



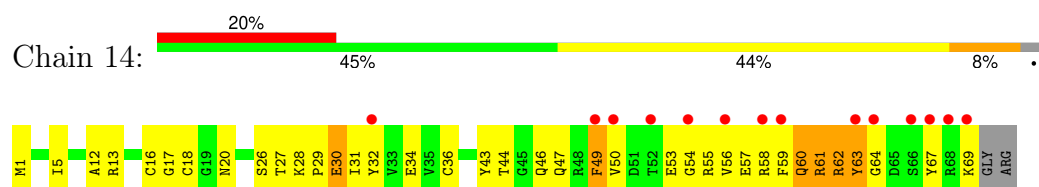
- Molecule 25: 50S ribosomal protein L30



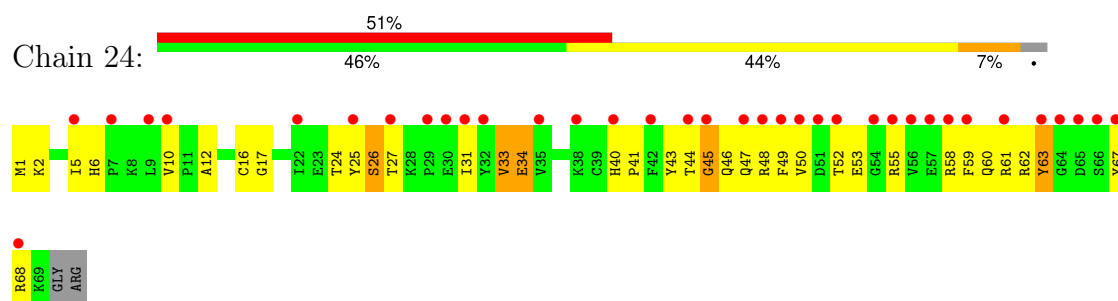
- Molecule 25: 50S ribosomal protein L30



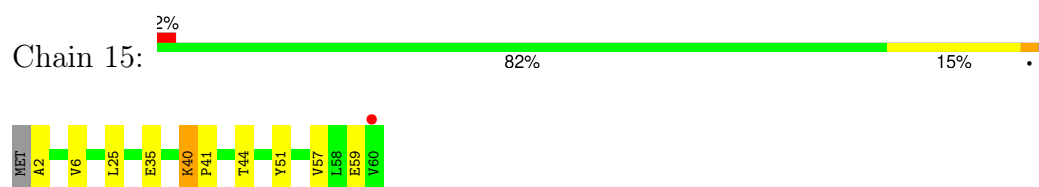
- Molecule 26: 50S ribosomal protein L31



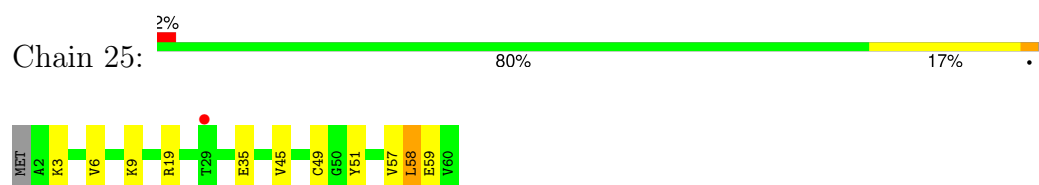
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  63% 33% ..



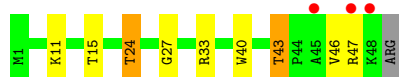
- Molecule 28: 50S ribosomal protein L33

Chain 26:  4% 72% 24% ..



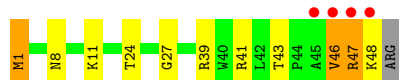
- Molecule 29: 50S ribosomal protein L34

Chain 17:  6% 80% 14% ..



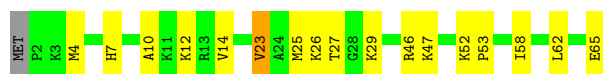
- Molecule 29: 50S ribosomal protein L34

Chain 27:  8% 76% 16% 6% .



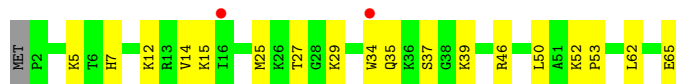
- Molecule 30: 50S ribosomal protein L35

Chain 18:  72% 25% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  3% 71% 28% .



- Molecule 31: 50S ribosomal protein L36

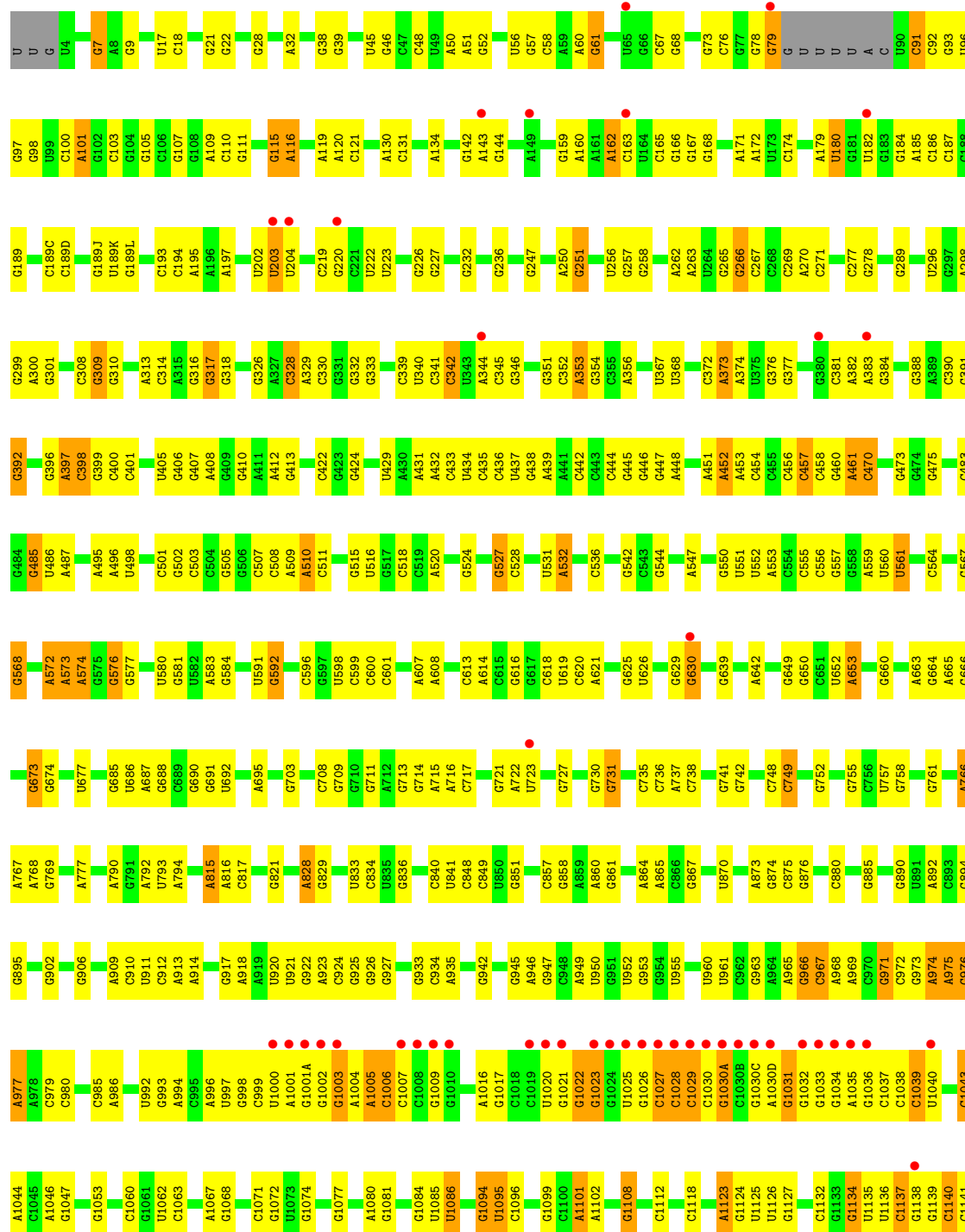
Chain 19:  84% 16%

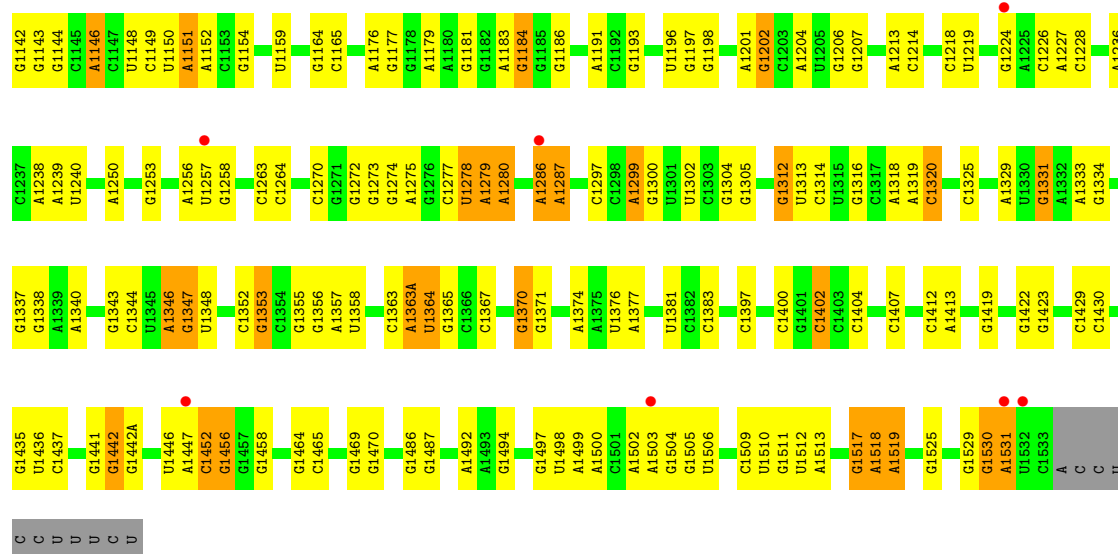


- Molecule 31: 50S ribosomal protein L36

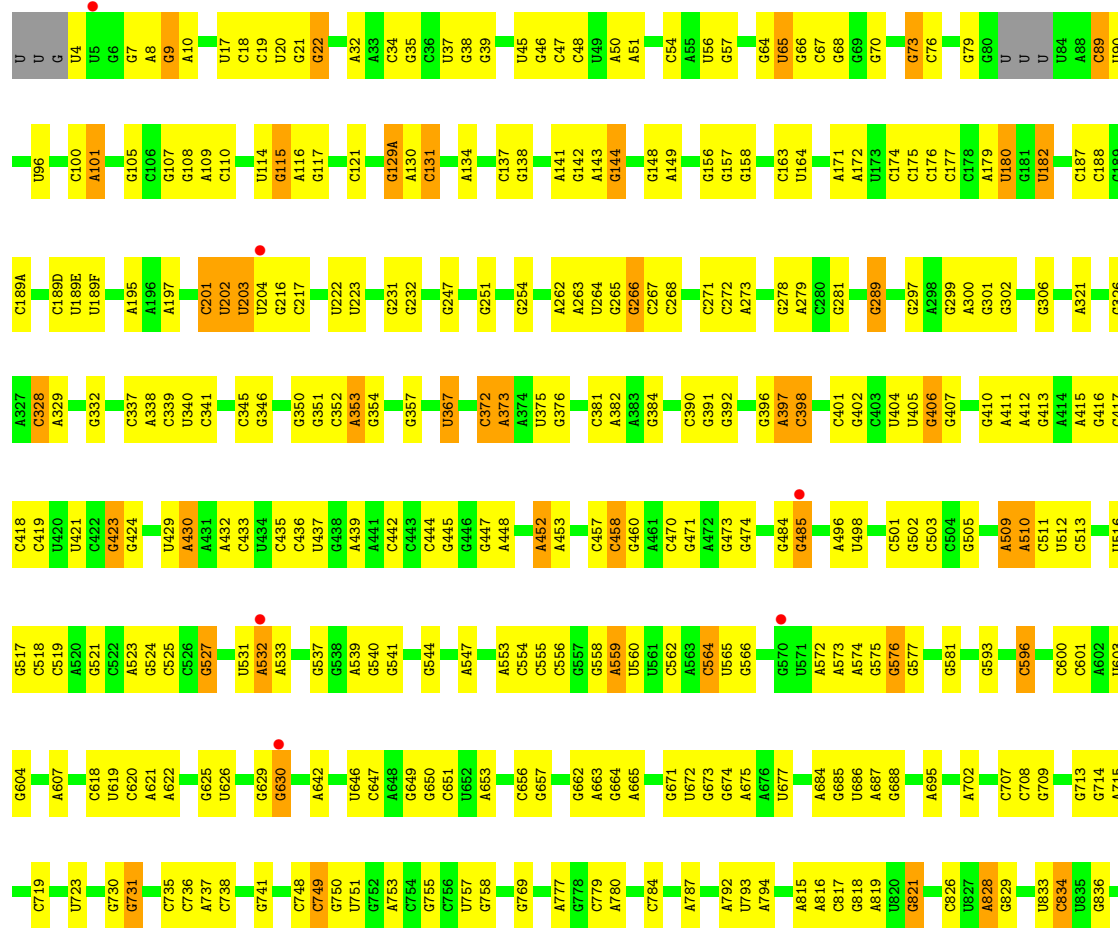


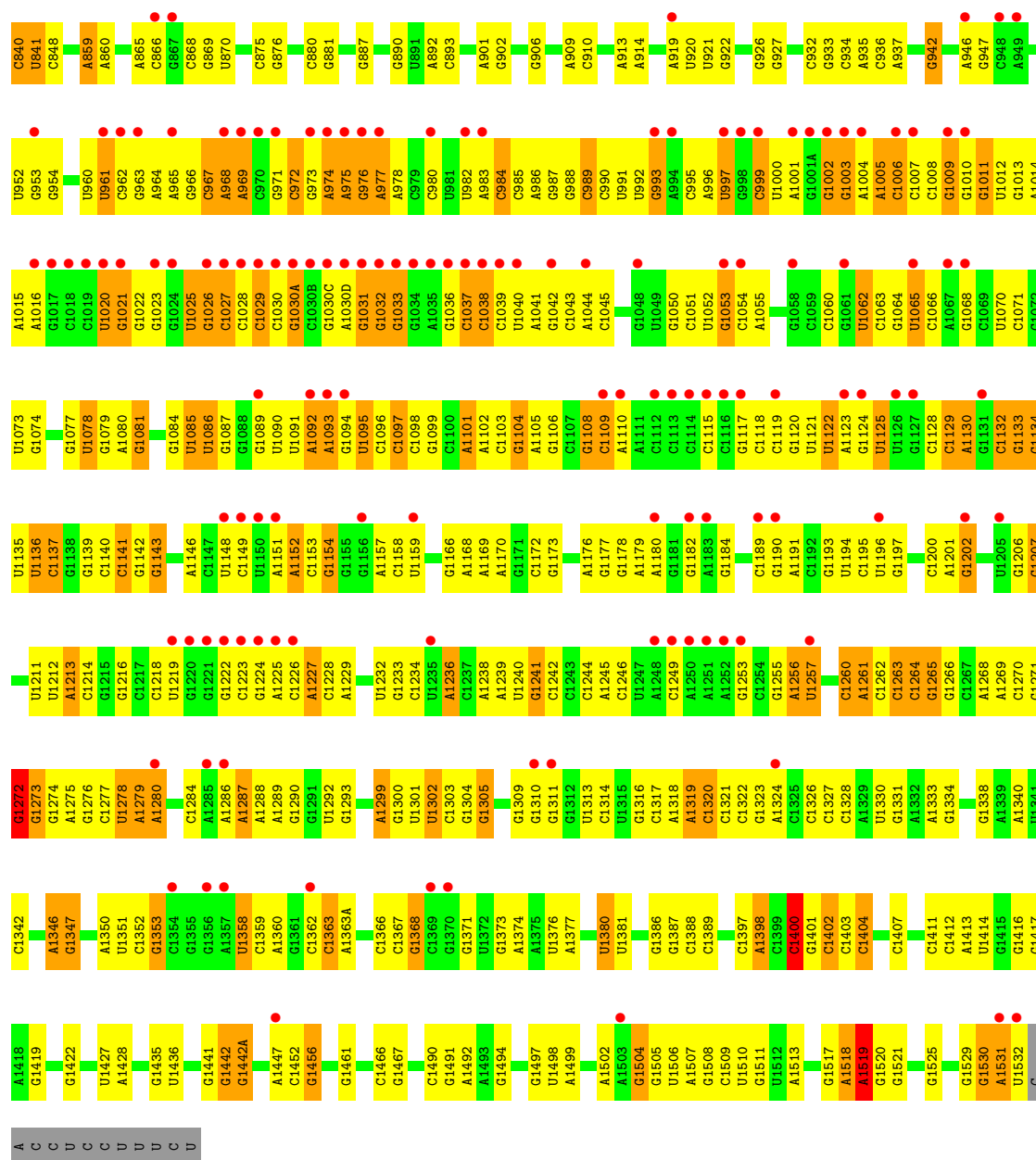
Chain 1a:





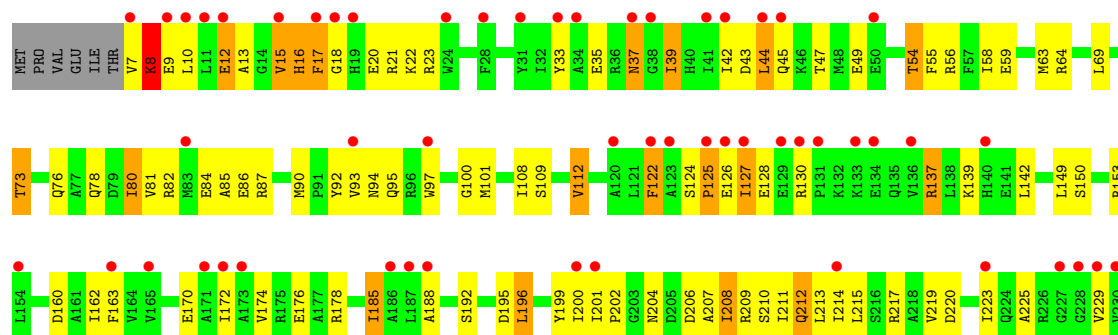
• Molecule 32: 16S Ribosomal RNA

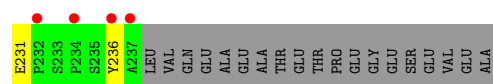




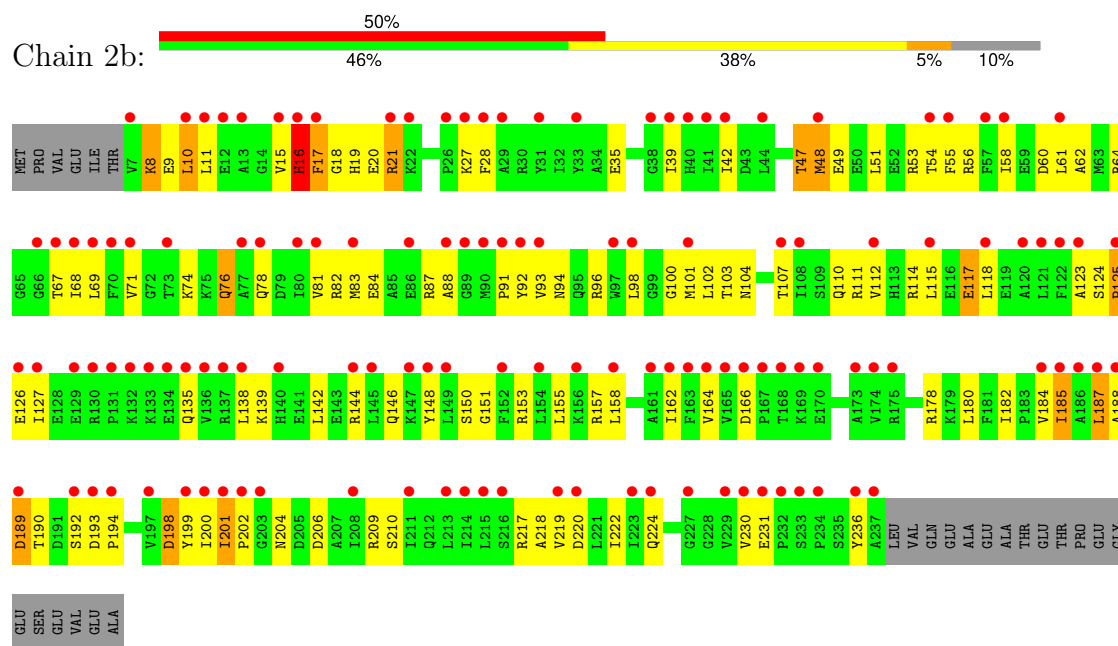
• Molecule 33: 30S ribosomal protein S2

Chain 1b: 23% 50% 32% 7% 10%

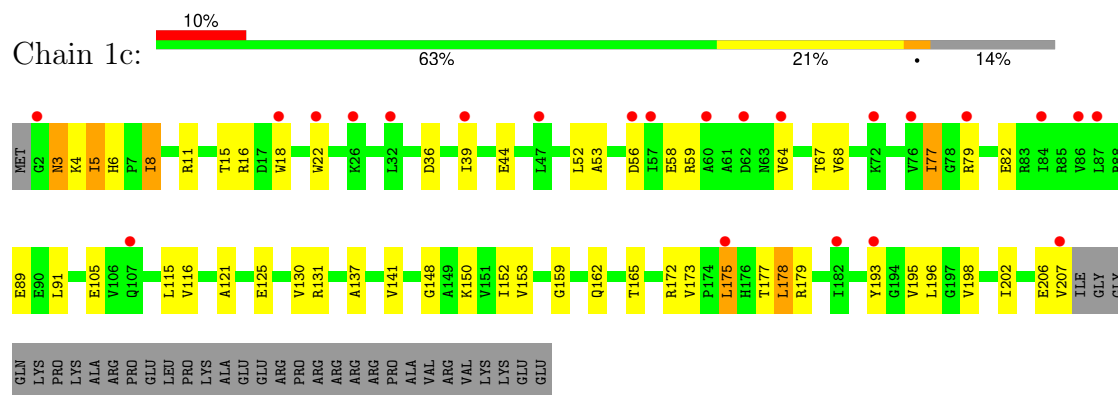




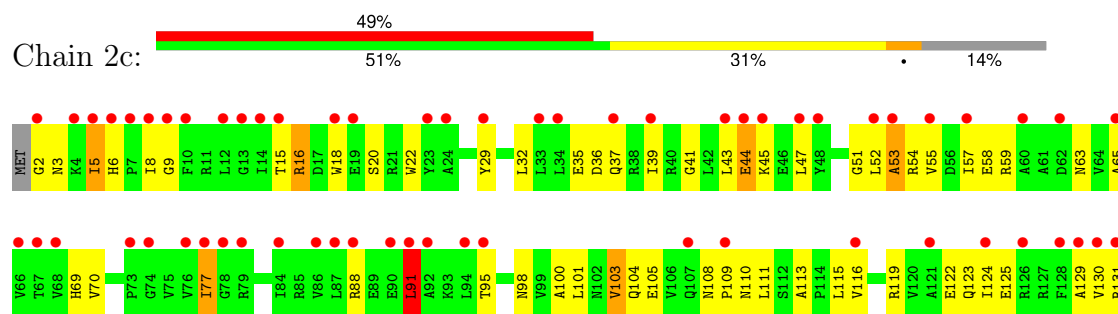
• Molecule 33: 30S ribosomal protein S2

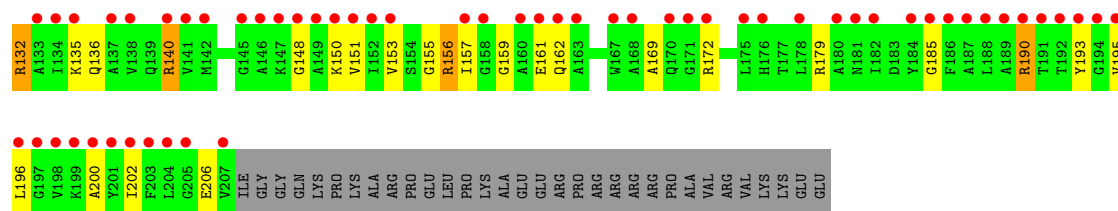


• Molecule 34: 30S ribosomal protein S3

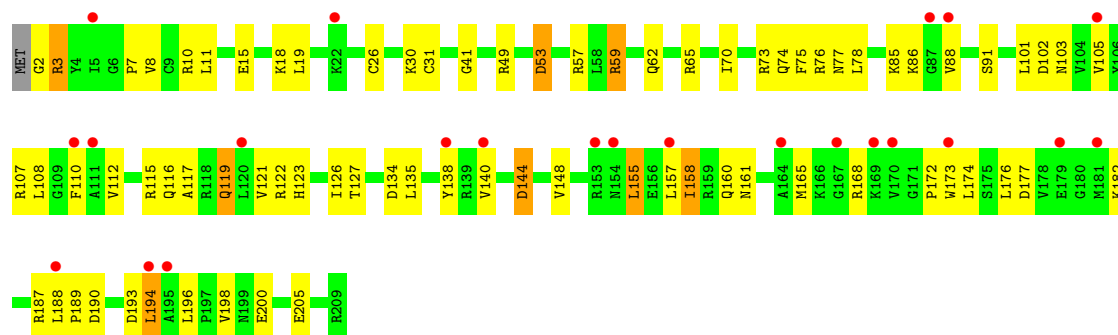


• Molecule 34: 30S ribosomal protein S3

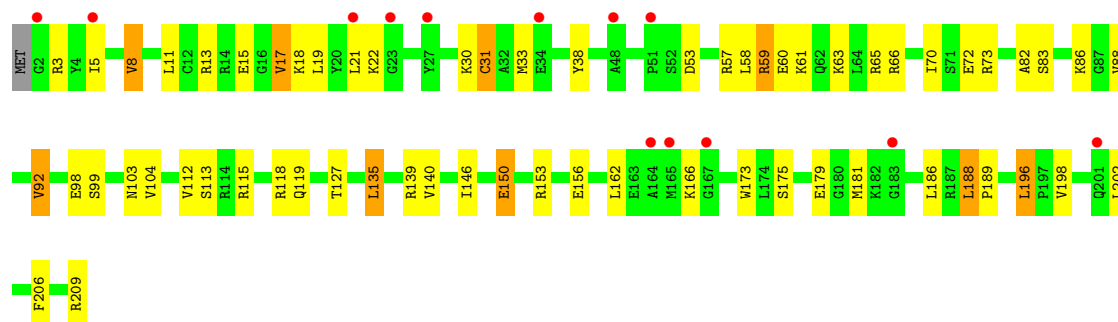




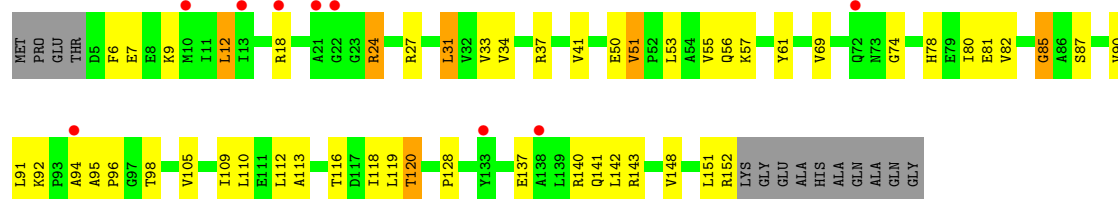
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

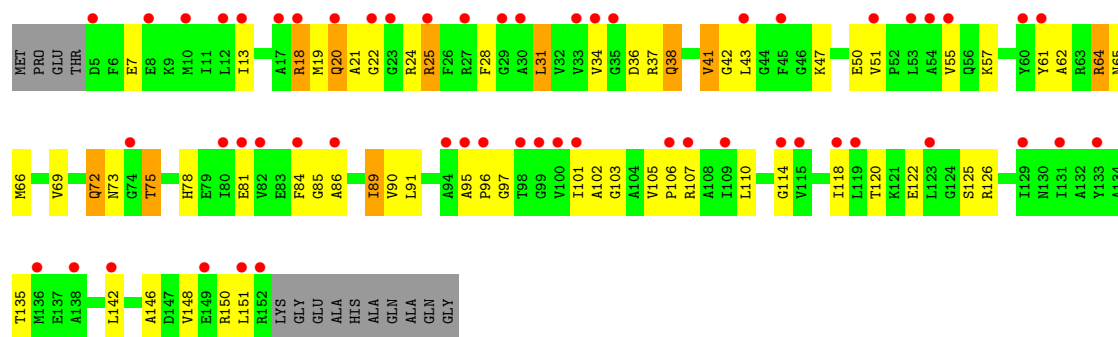


• Molecule 36: 30S ribosomal protein S5

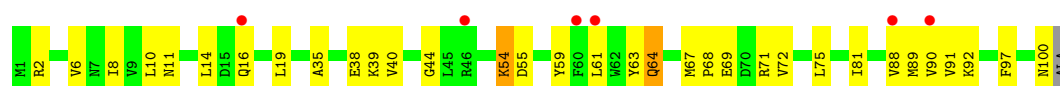


• Molecule 36: 30S ribosomal protein S5

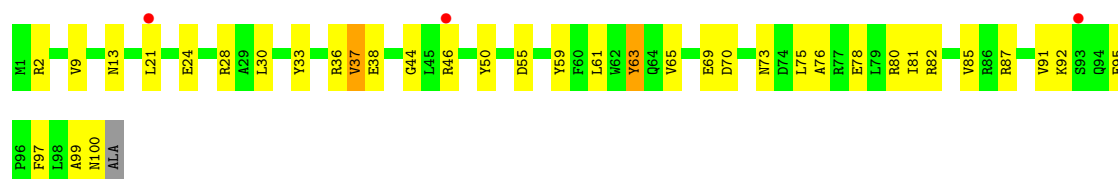




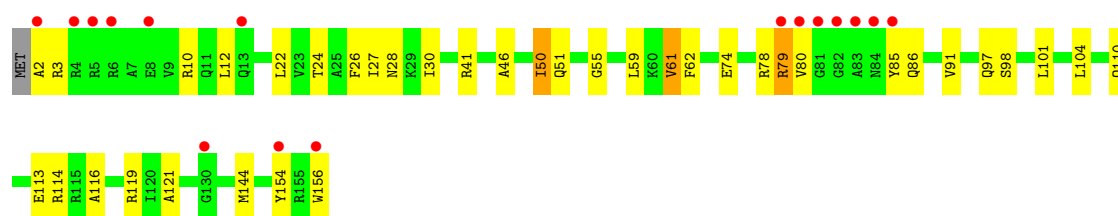
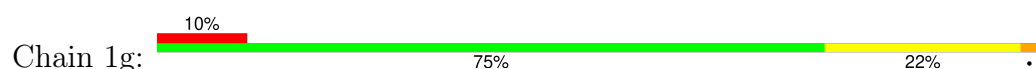
- Molecule 37: 30S ribosomal protein S6



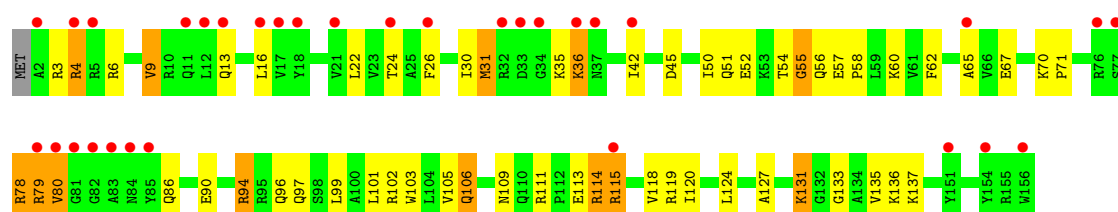
- Molecule 37: 30S ribosomal protein S6



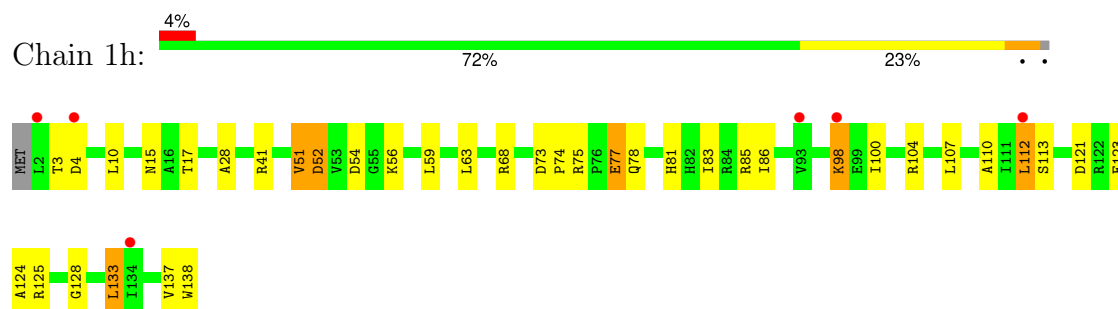
- Molecule 38: 30S ribosomal protein S7



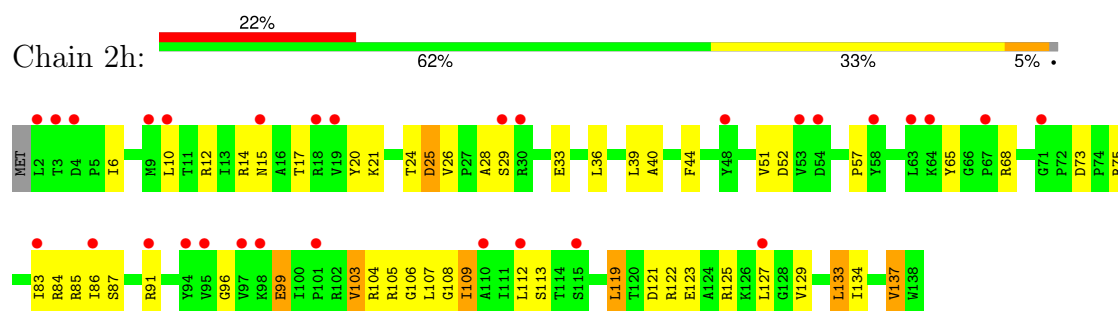
- Molecule 38: 30S ribosomal protein S7



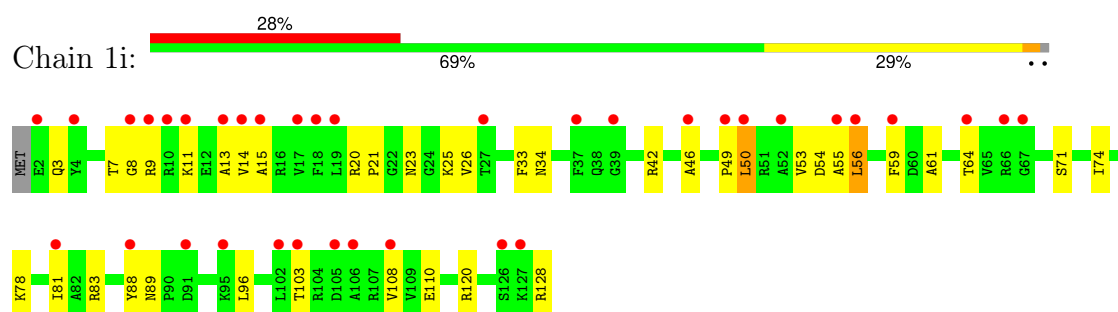
- Molecule 39: 30S ribosomal protein S8



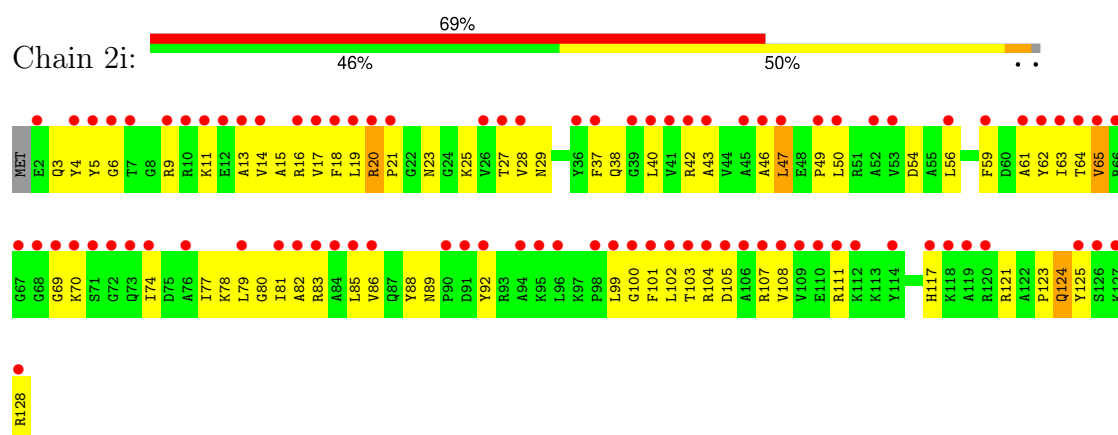
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

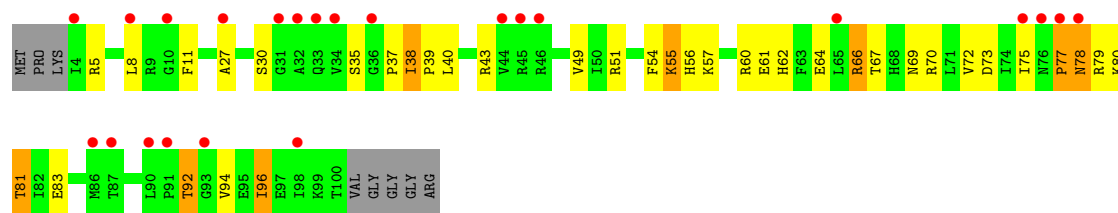


- Molecule 40: 30S ribosomal protein S9

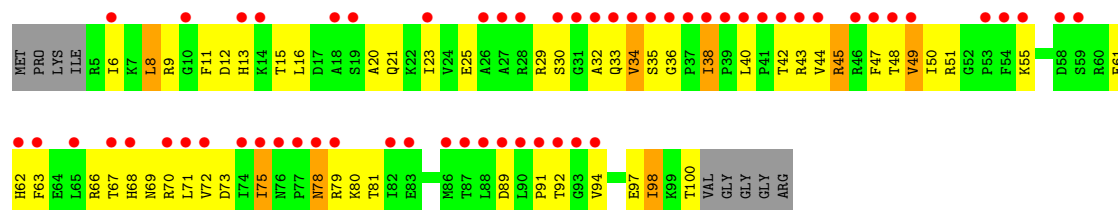
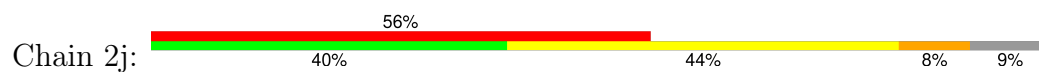


- Molecule 41: 30S ribosomal protein S10

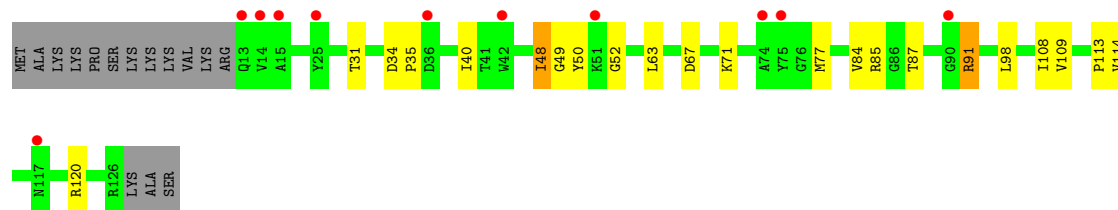




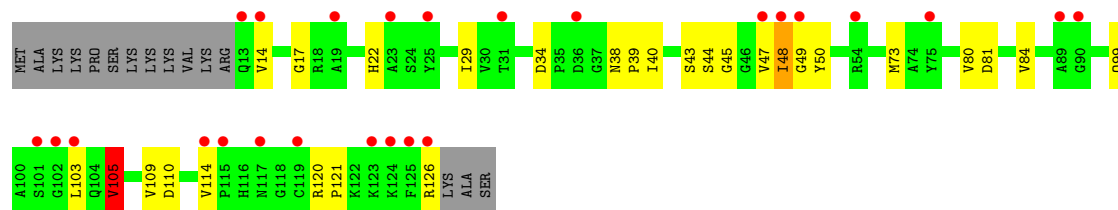
• Molecule 41: 30S ribosomal protein S10



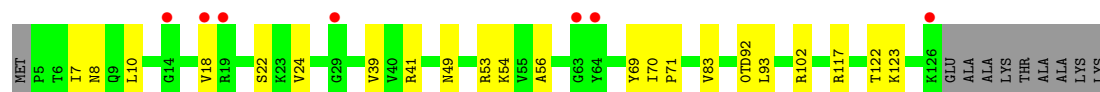
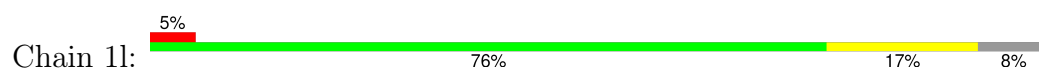
• Molecule 42: 30S ribosomal protein S11



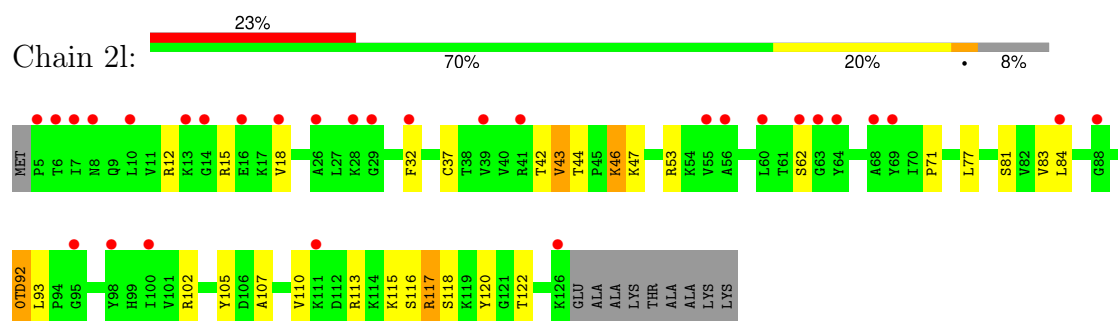
• Molecule 42: 30S ribosomal protein S11



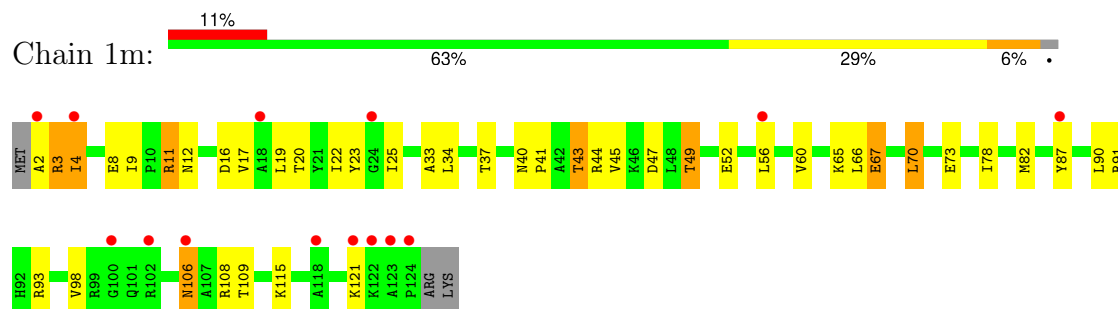
• Molecule 43: 30S ribosomal protein S12



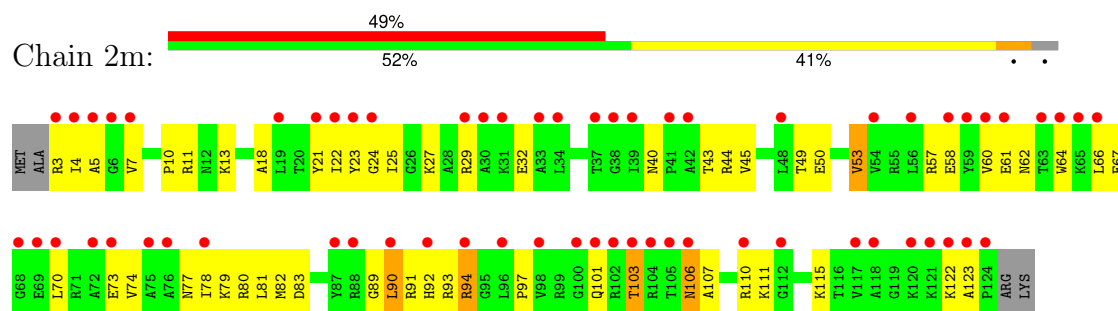
• Molecule 43: 30S ribosomal protein S12



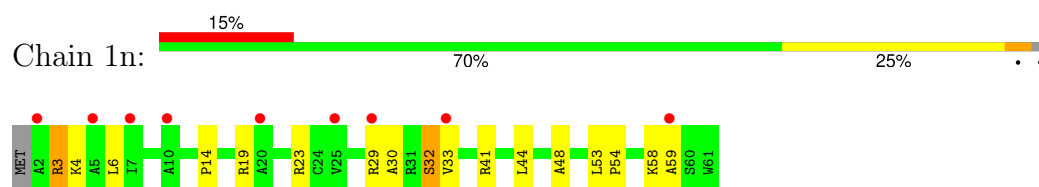
- Molecule 44: 30S ribosomal protein S13



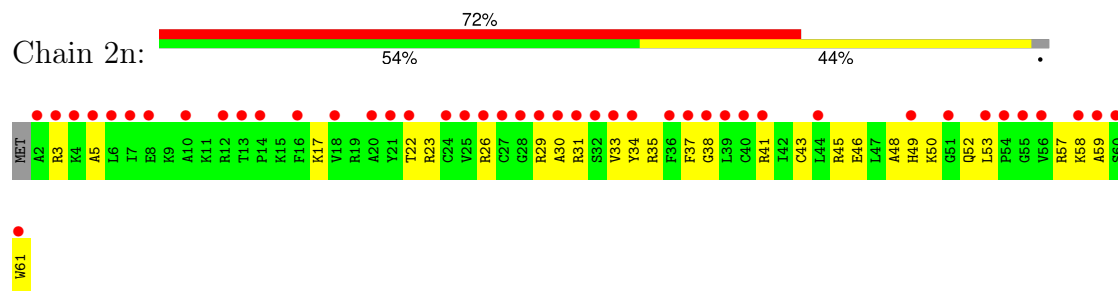
- Molecule 44: 30S ribosomal protein S13



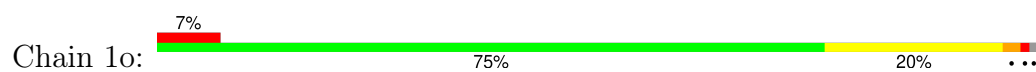
- Molecule 45: 30S ribosomal protein S14 type Z



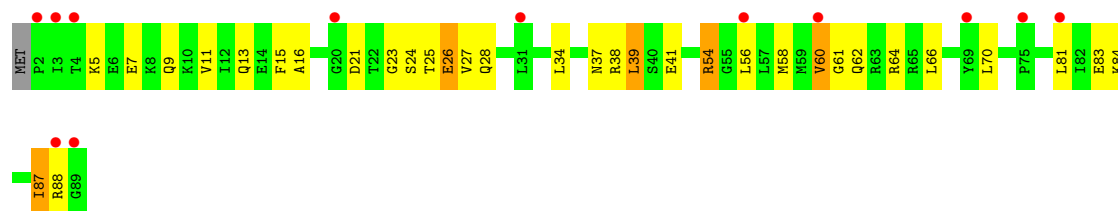
- Molecule 45: 30S ribosomal protein S14 type Z



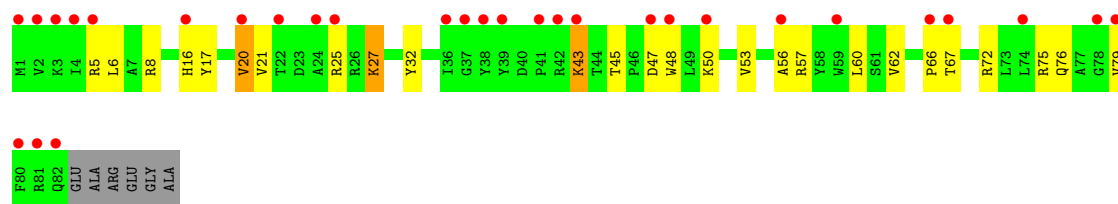
- Molecule 46: 30S ribosomal protein S15



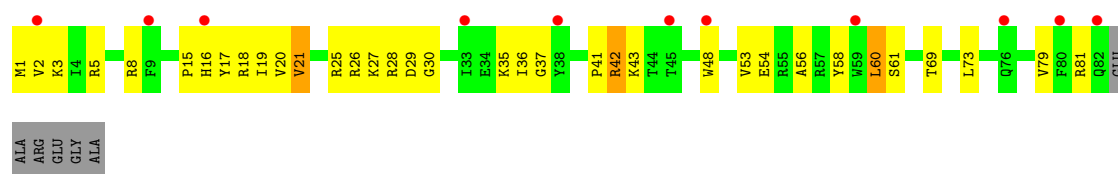
• Molecule 46: 30S ribosomal protein S15



• Molecule 47: 30S ribosomal protein S16



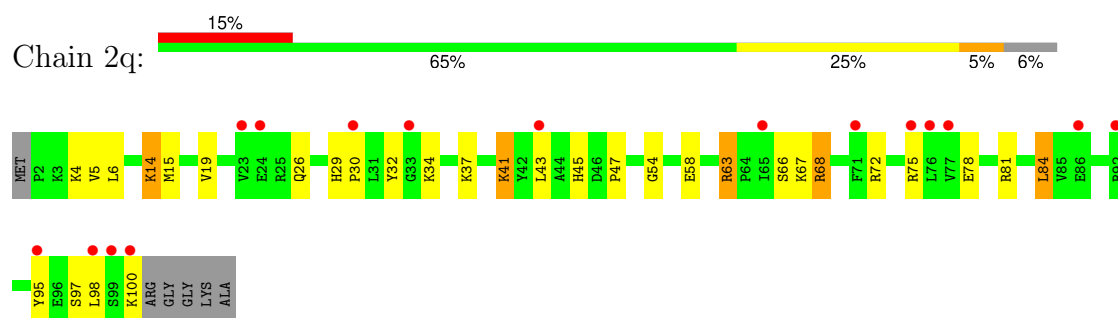
• Molecule 47: 30S ribosomal protein S16



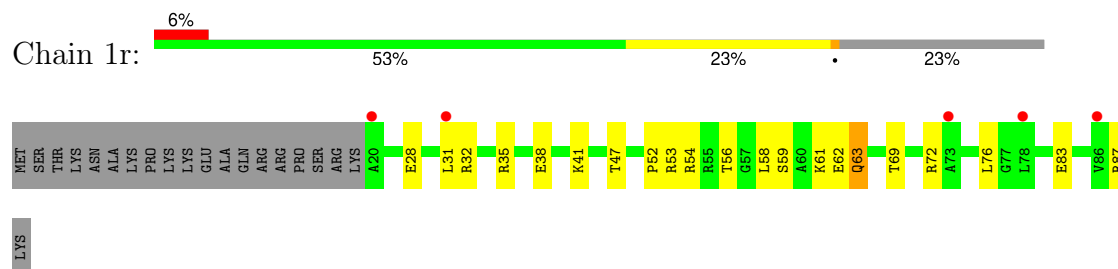
• Molecule 48: 30S ribosomal protein S17



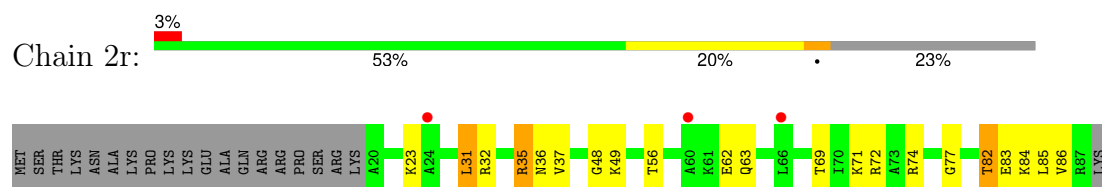
• Molecule 48: 30S ribosomal protein S17



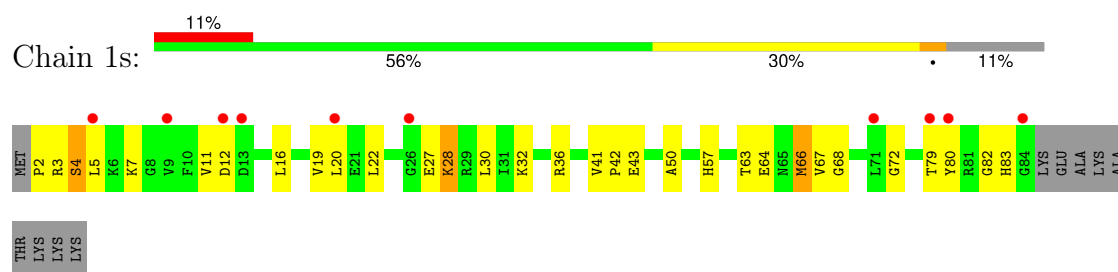
- Molecule 49: 30S ribosomal protein S18



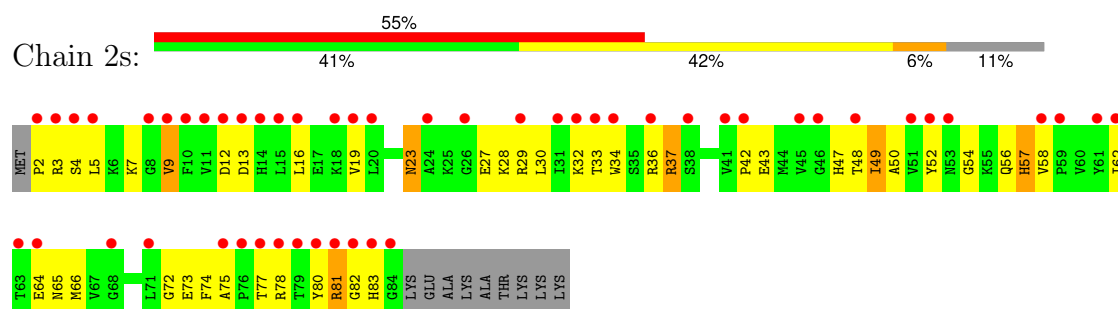
- Molecule 49: 30S ribosomal protein S18



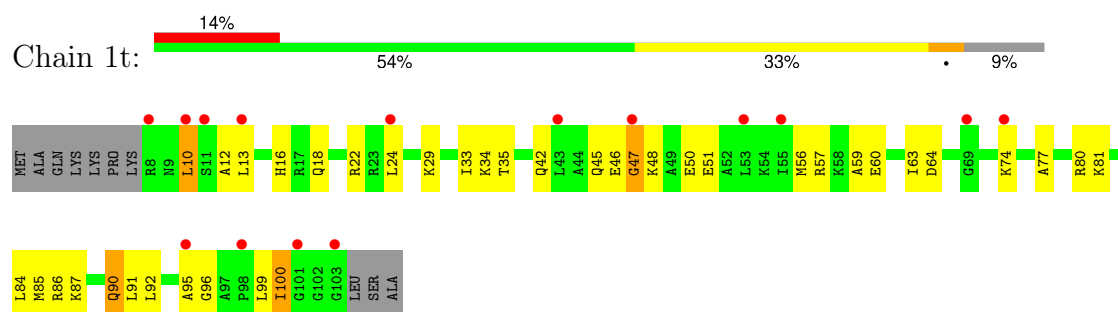
- Molecule 50: 30S ribosomal protein S19



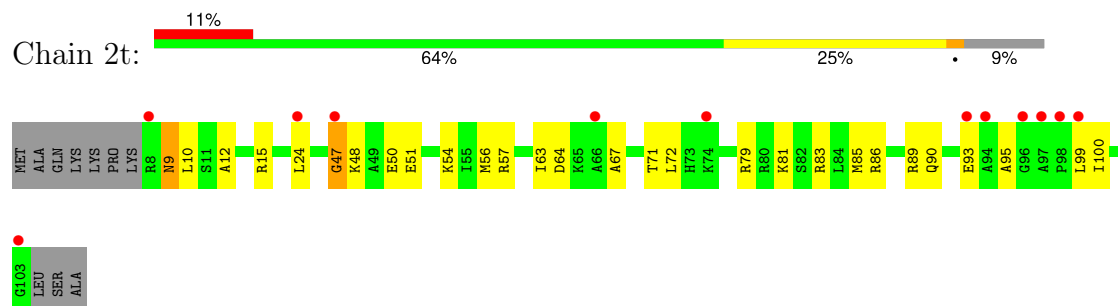
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



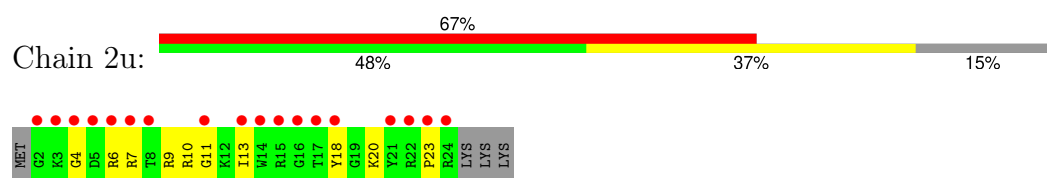
- Molecule 51: 30S ribosomal protein S20



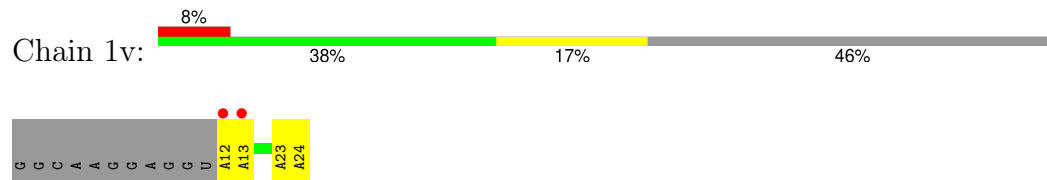
- Molecule 52: 30S ribosomal protein Thx



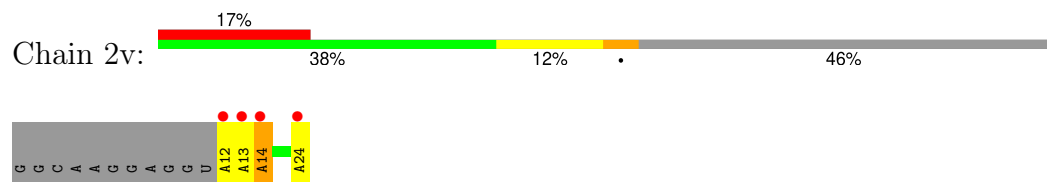
- Molecule 52: 30S ribosomal protein Thx



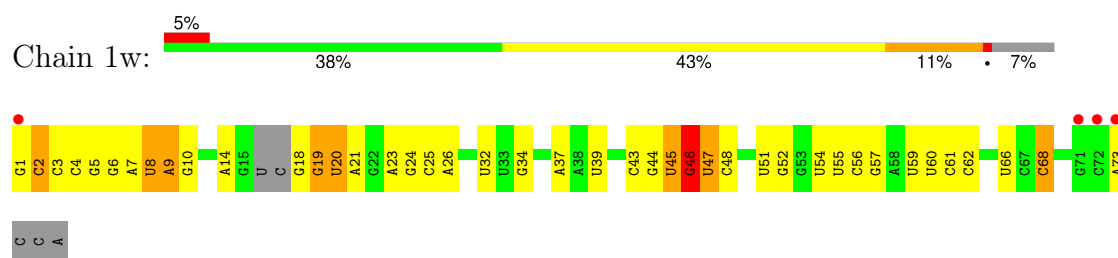
- Molecule 53: MF-mRNA



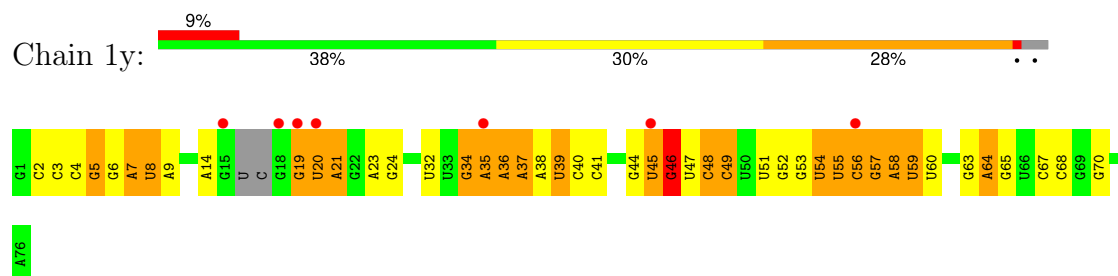
- Molecule 53: MF-mRNA



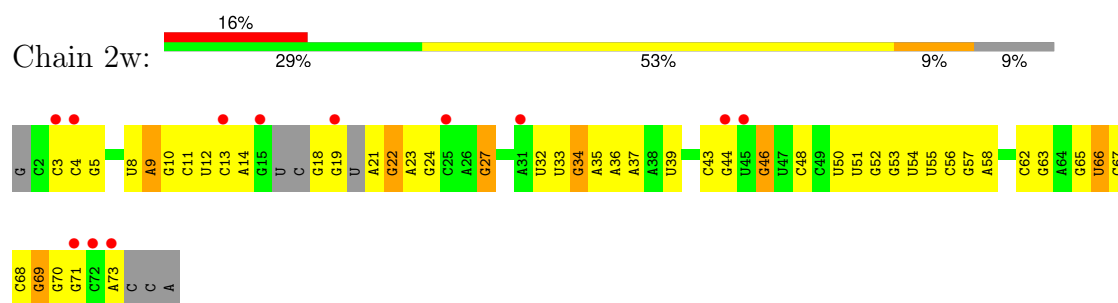
- Molecule 54: A-site and E-site Deacylated tRNAphe



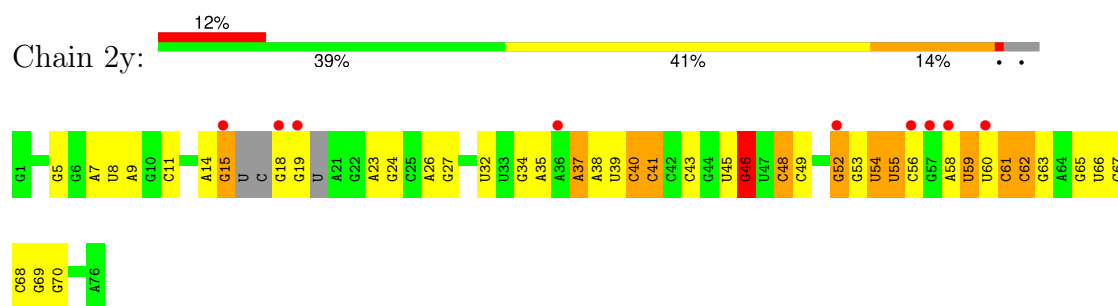
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



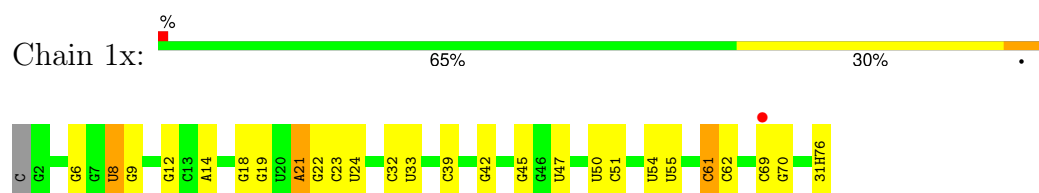
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



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

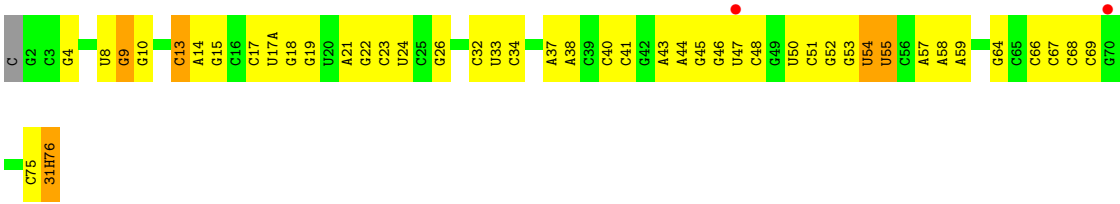


- Molecule 55: P-site Aminoacylated fMet-tRNA^{met}



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.26Å 449.69Å 619.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.86 – 2.50 121.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (121.86-2.50) 99.3 (121.86-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.260 0.220 , 0.262	Depositor DCC
R_{free} test set	98989 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299293	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 31H, OMC, MIA, SF4, 2MA, OMG, A1A1L, MA6, K, MG, 2MG, ZN, PSU, 4SU, 4OC, M2G, 5MU, OMU, UR3, 0TD, G7M

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	0/69011	0.47	3/107720 (0.0%)
1	2A	0.21	0/67295	0.40	3/105042 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.29	0/1592	0.52	0/2149
4	2E	0.20	0/1592	0.45	0/2149
5	1F	0.27	0/1618	0.50	0/2191
5	2F	0.20	0/1614	0.46	2/2186 (0.1%)
6	1G	0.20	0/1448	0.46	1/1957 (0.1%)
6	2G	0.19	0/1453	0.43	0/1963
7	1H	0.22	0/1356	0.41	0/1834
7	2H	0.18	0/1356	0.36	0/1834
8	1I	0.18	0/1112	0.40	0/1514
8	2I	0.18	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.46	0/1269
10	2O	0.20	0/943	0.45	0/1269
11	1P	0.27	0/1152	0.56	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.28	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.50	0/1312
13	2R	0.19	0/982	0.43	0/1312
14	1S	0.21	0/883	0.48	0/1176
14	2S	0.20	0/880	0.43	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.27	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.42	0/1301
17	1V	0.27	0/782	0.51	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.22	0/897	0.42	0/1205
19	1X	0.26	0/764	0.51	0/1025
19	2X	0.21	0/764	0.57	3/1025 (0.3%)
20	1Y	0.23	0/819	0.49	0/1095
20	2Y	0.20	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.43	0/1763
22	10	0.26	0/616	0.49	0/821
22	20	0.19	0/628	0.44	0/837
23	11	0.25	0/762	0.44	0/1014
23	21	0.23	0/762	0.40	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.27	0/474	0.46	0/635
25	23	0.19	0/469	0.43	0/630
26	14	0.28	0/565	0.54	0/761
26	24	0.26	0/545	0.46	0/737
27	15	0.26	0/469	0.49	0/635
27	25	0.22	0/469	0.41	0/635
28	16	0.26	0/460	0.47	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.30	0/426	0.57	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.25	0/525	0.45	0/691
30	28	0.24	0/525	0.41	0/691
31	19	0.25	0/310	0.51	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.38	3/56005 (0.0%)
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.23	0/1860	0.49	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.23	0/1566	0.44	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.21	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.47	0/1548
37	1f	0.20	0/823	0.38	0/1115
37	2f	0.18	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.20	0/1254	0.43	0/1683
39	1h	0.18	0/1108	0.41	0/1494
39	2h	0.20	0/1108	0.42	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.23	0/997	0.46	0/1343
41	1j	0.20	0/722	0.44	0/982
41	2j	0.22	0/727	0.48	0/988
42	1k	0.19	0/844	0.44	0/1145
42	2k	0.19	0/848	0.39	0/1149
43	1l	0.20	0/937	0.42	0/1260
43	2l	0.19	0/937	0.42	0/1260
44	1m	0.20	0/969	0.47	0/1302
44	2m	0.21	0/961	0.46	0/1291
45	1n	0.18	0/501	0.44	0/664
45	2n	0.22	0/501	0.46	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.20	0/697	0.48	0/939
47	2p	0.18	0/693	0.43	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.43	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.17	0/560	0.42	0/746
50	1s	0.20	0/667	0.47	0/900
50	2s	0.25	0/661	0.59	0/893
51	1t	0.18	0/730	0.45	0/965
51	2t	0.20	0/729	0.43	0/965
52	1u	0.18	0/203	0.42	0/266
52	2u	0.22	0/203	0.44	0/266
53	1v	0.22	0/310	0.39	0/480
53	2v	0.20	0/310	0.36	0/480
54	1w	0.28	1/1537 (0.1%)	0.39	0/2390
54	1y	0.28	2/1606 (0.1%)	0.41	0/2497
54	2w	0.32	2/1487 (0.1%)	0.42	0/2311
54	2y	0.29	2/1583 (0.1%)	0.41	0/2459
55	1x	0.26	0/1700	0.41	0/2650
55	2x	0.24	0/1700	0.39	0/2650
All	All	0.23	7/316420 (0.0%)	0.43	15/473729 (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
3	2D	0	1
33	1b	0	1
51	1t	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	46	G7M	O3'-P	5.43	1.61	1.56
54	1y	8	4SU	O3'-P	5.26	1.61	1.56
54	2w	46	G7M	O3'-P	5.26	1.61	1.56
54	1w	46	G7M	O3'-P	5.25	1.61	1.56
54	2y	8	4SU	O3'-P	5.18	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2X	94	GLY	CA-C-N	6.91	134.14	121.70
19	2X	94	GLY	C-N-CA	6.91	134.14	121.70
1	1A	1992	G	C2'-C3'-O3'	6.88	119.83	109.50
1	2A	1992	G	C2'-C3'-O3'	6.12	118.68	109.50
6	1G	96	ARG	CB-CA-C	-5.92	109.73	116.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide
51	1t	99	LEU	Peptide
3	2D	274	ARG	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	31196	538	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	60322	0	30428	632	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	36	0
3	1D	2136	0	2218	38	0
3	2D	2136	0	2218	47	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	36	0
5	1F	1583	0	1625	36	0
5	2F	1579	0	1619	47	0
6	1G	1423	0	1436	35	0
6	2G	1428	0	1438	59	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	46	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	25	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	14	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	29	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	15	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	35	0
16	1U	959	0	1019	9	0
16	2U	959	0	1019	23	0
17	1V	771	0	830	9	0
17	2V	771	0	830	13	0
18	1W	886	0	940	9	0
18	2W	886	0	940	15	0
19	1X	750	0	814	13	0
19	2X	750	0	814	22	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	14	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	54	0
22	10	608	0	622	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	620	0	636	15	0
23	11	755	0	826	12	0
23	21	755	0	826	20	0
24	12	588	0	643	7	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	25	0
26	24	532	0	503	25	0
27	15	455	0	465	6	0
27	25	455	0	465	8	0
28	16	453	0	473	11	0
28	26	449	0	469	6	0
29	17	418	0	467	7	0
29	27	418	0	467	9	0
30	18	517	0	582	15	0
30	28	517	0	582	14	0
31	19	307	0	335	4	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	386	0
32	2a	32327	0	16338	514	0
33	1b	1846	0	1867	61	0
33	2b	1825	0	1828	79	0
34	1c	1548	0	1535	31	0
34	2c	1542	0	1517	62	0
35	1d	1655	0	1672	47	0
35	2d	1674	0	1714	42	0
36	1e	1129	0	1185	33	0
36	2e	1133	0	1191	42	0
37	1f	810	0	804	18	0
37	2f	816	0	808	23	0
38	1g	1231	0	1238	21	0
38	2g	1235	0	1249	37	0
39	1h	1088	0	1126	28	0
39	2h	1088	0	1126	34	0
40	1i	983	0	986	19	0
40	2i	978	0	966	50	0
41	1j	709	0	650	29	0
41	2j	714	0	672	42	0
42	1k	829	0	825	12	0
42	2k	833	0	834	14	0
43	1l	932	0	981	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	19	0
44	1m	958	0	1002	27	0
44	2m	950	0	988	50	0
45	1n	492	0	529	12	0
45	2n	492	0	529	26	0
46	1o	728	0	760	10	0
46	2o	728	0	760	21	0
47	1p	681	0	697	20	0
47	2p	677	0	686	26	0
48	1q	823	0	891	18	0
48	2q	823	0	891	17	0
49	1r	555	0	618	17	0
49	2r	555	0	618	18	0
50	1s	652	0	662	23	0
50	2s	646	0	644	37	0
51	1t	728	0	798	25	0
51	2t	727	0	796	18	0
52	1u	199	0	208	8	0
52	2u	199	0	208	8	0
53	1v	277	0	140	4	0
53	2v	277	0	140	3	0
54	1w	1530	0	785	20	0
54	1y	1585	0	803	29	0
54	2w	1482	0	754	22	0
54	2y	1565	0	793	21	0
55	1x	1635	0	839	9	0
55	2x	1635	0	839	21	0
56	10	7	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	8	0	0	0	0
56	16	3	0	0	0	0
56	17	5	0	0	0	0
56	18	4	0	0	0	0
56	19	1	0	0	0	0
56	1A	1059	0	0	0	0
56	1B	39	0	0	0	0
56	1D	12	0	0	0	0
56	1E	16	0	0	0	0
56	1F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	6	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	7	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	7	0	0	0	0
56	1V	6	0	0	0	0
56	1W	6	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	198	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	2	0	0	0	0
56	1t	1	0	0	0	0
56	1u	1	0	0	0	0
56	1w	4	0	0	0	0
56	1x	12	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	25	5	0	0	0	0
56	27	4	0	0	0	0
56	28	2	0	0	0	0
56	2A	782	0	0	0	0
56	2B	18	0	0	0	0
56	2D	8	0	0	0	0
56	2E	9	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2Q	2	0	0	0	0
56	2R	2	0	0	0	0
56	2T	5	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	1	0	0	0	0
56	2X	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	2	0	0	0	0
56	2a	202	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	5	0	0	0	0
56	2q	2	0	0	0	0
56	2r	2	0	0	0	0
56	2t	2	0	0	0	0
56	2v	1	0	0	0	0
56	2w	3	0	0	0	0
56	2x	6	0	0	0	0
57	1A	36	0	0	1	0
57	2A	36	0	0	1	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	1	0
60	2x	1	0	0	0	0
61	10	8	0	0	0	0
61	11	7	0	0	0	0
61	12	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	13	4	0	0	0	0
61	14	1	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	0	0
61	17	8	0	0	0	0
61	18	13	0	0	0	0
61	1A	1902	0	0	65	0
61	1B	59	0	0	0	0
61	1D	27	0	0	0	0
61	1E	31	0	0	1	0
61	1F	20	0	0	1	0
61	1G	2	0	0	0	0
61	1H	2	0	0	0	0
61	1N	6	0	0	0	0
61	1O	6	0	0	0	0
61	1P	18	0	0	2	0
61	1Q	8	0	0	0	0
61	1R	11	0	0	2	0
61	1S	5	0	0	0	0
61	1T	7	0	0	0	0
61	1U	15	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	0	0
61	1X	7	0	0	0	0
61	1Y	3	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	298	0	0	18	0
61	1b	1	0	0	0	0
61	1l	5	0	0	0	0
61	1m	1	0	0	0	0
61	1o	1	0	0	0	0
61	1q	2	0	0	0	0
61	1t	1	0	0	0	0
61	1v	5	0	0	0	0
61	1w	4	0	0	0	0
61	1x	9	0	0	1	0
61	1y	1	0	0	0	0
61	20	2	0	0	0	0
61	21	3	0	0	0	0
61	23	3	0	0	0	0
61	25	2	0	0	0	0
61	27	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	28	3	0	0	0	0
61	29	1	0	0	0	0
61	2A	1002	0	0	68	0
61	2B	16	0	0	1	0
61	2D	23	0	0	1	0
61	2E	16	0	0	0	0
61	2F	14	0	0	0	0
61	2O	1	0	0	0	0
61	2P	9	0	0	1	0
61	2Q	1	0	0	0	0
61	2R	3	0	0	0	0
61	2T	6	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	2	0	0	1	0
61	2X	3	0	0	0	0
61	2a	168	0	0	14	0
61	2e	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	3	0	0	0	0
61	2p	1	0	0	0	0
61	2t	1	0	0	0	0
61	2v	1	0	0	0	0
61	2w	1	0	0	0	0
61	2x	4	0	0	0	0
All	All	299293	0	196554	3999	0

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

The worst 5 of 3999 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	1.23	1.36
1:1A:1082:U:O4	1:1A:1086:A:N1	1.94	1.00
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.27	0.98
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.44	0.97
20:1Y:92:ASN:HD21	20:1Y:94:LYS:HG2	1.33	0.90

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	24	43
5	2F	200/210 (95%)	187 (94%)	10 (5%)	3 (2%)	8	16
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	11	22
6	2G	179/182 (98%)	149 (83%)	24 (13%)	6 (3%)	3	4
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	38
7	2H	172/180 (96%)	155 (90%)	15 (9%)	2 (1%)	10	20
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	5	9
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	4 (3%)	2 (1%)	9	17
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	31
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	17
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	6
12	1Q	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14	27
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	10
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	24
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5	9
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12	24
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
21	1Z	148/206 (72%)	136 (92%)	9 (6%)	3 (2%)	6	10
21	2Z	156/206 (76%)	128 (82%)	24 (15%)	4 (3%)	4	7
22	10	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
22	20	77/85 (91%)	71 (92%)	5 (6%)	1 (1%)	9	18
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	22
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	6	12
26	14	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	3	5
26	24	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	8	16
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	196 (86%)	26 (11%)	7 (3%)	3	5
33	2b	229/256 (90%)	178 (78%)	44 (19%)	7 (3%)	3	5
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	171 (84%)	28 (14%)	5 (2%)	4	7
35	1d	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
35	2d	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18	34
36	2e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	9
37	1f	98/101 (97%)	97 (99%)	0	1 (1%)	12	24
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	18	34
38	2g	153/156 (98%)	138 (90%)	11 (7%)	4 (3%)	4	7
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	13 (10%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	31
40	2i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	31
41	1j	95/105 (90%)	80 (84%)	11 (12%)	4 (4%)	2	2
41	2j	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	3	4
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	27
42	2k	112/129 (87%)	95 (85%)	15 (13%)	2 (2%)	6	12
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	7	13
44	2m	120/126 (95%)	105 (88%)	14 (12%)	1 (1%)	16	31
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	47 (81%)	11 (19%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	20
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	18
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	24
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	24
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	16
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	4	7
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	4
51	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	9
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11358/12128 (94%)	10454 (92%)	798 (7%)	106 (1%)	14	27

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
11	1P	38	GLN
11	1P	45	LEU
17	1V	43	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	17	36
3	2D	215/218 (99%)	203 (94%)	12 (6%)	19	39
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19	40
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10	22
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	146 (92%)	13 (8%)	10	23
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	19
6	2G	143/156 (92%)	121 (85%)	22 (15%)	2	5
7	1H	144/148 (97%)	130 (90%)	14 (10%)	8	17
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	4
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	4
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	37
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	13
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	44
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	36
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11	24
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	14
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	34
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	34
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	20
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	54
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	23
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	4
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	29
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	24
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	51
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	21
17	1V	80/82 (98%)	75 (94%)	5 (6%)	16	34
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	9
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	31
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	68
19	2X	77/78 (99%)	76 (99%)	1 (1%)	61	82
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	121 (90%)	14 (10%)	7	14
21	2Z	137/179 (76%)	118 (86%)	19 (14%)	3	7
22	10	61/67 (91%)	56 (92%)	5 (8%)	10	23
22	20	62/67 (92%)	60 (97%)	2 (3%)	34	62
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	44
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	26
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	48
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	24
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	24
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	2
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	3
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	36
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	37
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	10
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	27
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	39
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	27
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	11
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	4
33	2b	187/220 (85%)	154 (82%)	33 (18%)	2	3
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	14
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3	6
35	1d	169/181 (93%)	140 (83%)	29 (17%)	2	4
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	20
36	2e	114/123 (93%)	98 (86%)	16 (14%)	3	7
37	1f	84/90 (93%)	74 (88%)	10 (12%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	47
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	15
38	2g	120/127 (94%)	104 (87%)	16 (13%)	4	8
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14	29
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4	8
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	15
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	12
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	10
41	2j	69/92 (75%)	57 (83%)	12 (17%)	2	3
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	16
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	22
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	52
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	18
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4	9
44	2m	92/101 (91%)	85 (92%)	7 (8%)	12	26
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	35
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	35
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	14
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	11
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	11
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	27
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	22
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	43
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	22
50	1s	69/80 (86%)	62 (90%)	7 (10%)	7	15
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	4
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13	29
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	39
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	12
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9296/10064 (92%)	8402 (90%)	894 (10%)	8 17

5 of 894 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	2G	49	ASP
50	2s	58	VAL
16	2U	8	VAL
50	2s	12	ASP
40	2i	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
40	2i	23	ASN
42	2k	22	HIS
50	2s	57	HIS
40	1i	31	GLN
40	1i	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	422 (14%)	29 (1%)
1	2A	2791/2915 (95%)	446 (15%)	28 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	26 (22%)	0
32	1a	1497/1521 (98%)	248 (16%)	0
32	2a	1501/1521 (98%)	309 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	69/76 (90%)	21 (30%)	0
54	1y	72/76 (94%)	24 (33%)	0
54	2w	66/76 (86%)	22 (33%)	0
54	2y	70/76 (92%)	26 (37%)	0
55	1x	74/77 (96%)	12 (16%)	0
55	2x	74/77 (96%)	13 (17%)	0
All	All	9339/9620 (97%)	1581 (16%)	57 (0%)

5 of 1581 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A

5 of 57 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2756	U
1	2A	2689	U
1	2A	277	C
1	2A	2406	U
1	2A	1653	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.10	9 (27%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	27,32,35	1.73	6 (22%)
55	31H	1x	76	56,55	31,34,35	1.22	3 (9%)	35,47,50	1.78	8 (22%)
32	5MC	2a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.20	3 (11%)
32	G7M	2a	527	32,56	23,26,27	1.48	4 (17%)	34,39,42	1.72	4 (11%)
54	PSU	2y	39	42,54	18,21,22	1.37	2 (11%)	21,30,33	1.84	3 (14%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
54	4SU	2w	8	54	18,21,22	1.87	4 (22%)	25,30,33	2.10	5 (20%)
1	PSU	1A	2605	1,56	18,21,22	1.45	3 (16%)	21,30,33	2.18	5 (23%)
1	OMU	2A	2552	1,56	19,22,23	1.15	3 (15%)	25,31,34	1.87	6 (24%)
54	PSU	1w	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.12	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	2.05	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	32	56,54	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
32	UR3	2a	1498	32,56	19,22,23	1.04	2 (10%)	26,32,35	1.77	4 (15%)
54	MIA	2y	37	54	21,24,32	1.62	3 (14%)	30,35,47	2.04	9 (30%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.24	9 (27%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.02	3 (14%)
55	31H	2x	76	56,55	31,34,35	1.23	3 (9%)	35,47,50	2.57	13 (37%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	21,30,33	2.09	5 (23%)
54	G7M	1w	46	54	23,26,27	1.55	4 (17%)	34,39,42	1.59	4 (11%)
54	MIA	2w	37	54	24,27,32	1.98	5 (20%)	32,39,47	2.47	10 (31%)
1	2MA	1A	2503	1,56	22,25,26	1.48	4 (18%)	32,37,40	2.21	9 (28%)
54	G7M	2y	46	54	23,26,27	1.63	3 (13%)	34,39,42	1.77	4 (11%)
54	4SU	1w	8	54	18,21,22	1.79	4 (22%)	25,30,33	1.94	5 (20%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	6.66	2 (33%)
54	PSU	1y	39	54	18,21,22	1.42	3 (16%)	21,30,33	1.77	3 (14%)
55	5MU	1x	54	55	19,22,23	1.48	5 (26%)	27,32,35	1.78	5 (18%)
43	0TD	2l	92	43	8,9,10	4.58	2 (25%)	6,11,13	1.46	1 (16%)
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.97	1 (4%)
55	4SU	2x	8	56,55	18,21,22	2.03	6 (33%)	25,30,33	1.42	4 (16%)
32	PSU	1a	516	32	18,21,22	1.40	2 (11%)	21,30,33	1.96	4 (19%)
54	PSU	2y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.89	3 (14%)
1	5MC	2A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.09	2 (7%)
1	2MA	2A	2503	1,56	22,25,26	1.44	4 (18%)	32,37,40	2.40	9 (28%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.88	6 (18%)
54	5MU	1y	54	54	19,22,23	1.44	6 (31%)	27,32,35	1.92	6 (22%)
32	5MC	1a	1407	32	19,22,23	1.55	2 (10%)	26,32,35	1.12	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.76	4 (15%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.16	3 (11%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.89	3 (14%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.92	3 (14%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.91	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.02	9 (27%)
54	5MU	1w	54	54	19,22,23	1.36	4 (21%)	27,32,35	2.08	6 (22%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.99	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
54	G7M	2w	46	54	23,26,27	1.42	4 (17%)	34,39,42	1.63	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MIA	1w	37	54	28,31,32	2.42	7 (25%)	38,44,47	2.72	12 (31%)
1	5MU	1A	1939	1,56	19,22,23	1.46	5 (26%)	27,32,35	2.27	7 (25%)
1	5MC	1A	1942	1,56	19,22,23	1.61	3 (15%)	26,32,35	1.22	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.20	3 (11%)
54	PSU	1y	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.06	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	2.07	4 (19%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.04	10 (30%)
54	5MU	2y	54	54	19,22,23	1.52	5 (26%)	27,32,35	1.79	8 (29%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
1	5MU	1A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.12	6 (22%)
1	5MC	1A	1962	1,56	19,22,23	1.62	3 (15%)	26,32,35	1.17	4 (15%)
32	5MC	1a	967	32	19,22,23	1.62	2 (10%)	26,32,35	1.07	2 (7%)
54	4SU	2y	8	54	18,21,22	1.76	4 (22%)	25,30,33	2.07	4 (16%)
55	5MC	2x	32	55	19,22,23	1.77	3 (15%)	26,32,35	1.21	3 (11%)
1	5MC	2A	1962	1,56	19,22,23	1.77	3 (15%)	26,32,35	1.14	3 (11%)
54	PSU	2y	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.91	5 (23%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.90	6 (18%)
32	4OC	1a	1402	32	20,23,24	0.71	0	25,32,35	1.00	1 (4%)
1	5MU	2A	1939	1,56	19,22,23	1.39	5 (26%)	27,32,35	2.33	6 (22%)
54	MIA	1y	37	54	21,24,32	1.60	4 (19%)	30,35,47	2.05	8 (26%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
55	5MC	1x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.15	3 (11%)
1	OMG	1A	2251	1,55,56	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
54	G7M	1y	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.72	4 (11%)
1	OMU	1A	2552	1,56	19,22,23	1.23	3 (15%)	25,31,34	1.91	5 (20%)
55	4SU	1x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.64	6 (24%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.26	9 (27%)
32	5MC	1a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.22	4 (15%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.01	2 (8%)
1	5MU	2A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.08	6 (22%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.07	8 (29%)
32	G7M	1a	527	32,56	23,26,27	1.50	4 (17%)	34,39,42	1.62	4 (11%)
32	5MC	2a	967	32	19,22,23	1.80	3 (15%)	26,32,35	1.11	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.89	3 (14%)
54	4SU	1y	8	54	18,21,22	1.81	6 (33%)	25,30,33	1.78	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2A	2251	1,55,56	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.15	3 (11%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.01	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	56,55	-	7/22/40/41	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	2/7/25/26	0/3/3/3
54	PSU	2y	39	42,54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32,56	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	56,55	-	6/22/40/41	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	MIA	2w	37	54	-	4/11/29/34	0/3/3/3
1	2MA	1A	2503	1,56	-	0/7/25/26	0/3/3/3
54	G7M	2y	46	54	-	1/7/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	2x	8	56,55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/7/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	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
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,56	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	1y	46	54	-	2/7/25/26	0/3/3/3
1	OMU	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
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/9/27/28	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2

The worst 5 of 251 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.47	1.69	1.82
43	1l	92	0TD	CB-SB	-12.32	1.69	1.82
54	1w	37	MIA	C2-S10	-7.77	1.69	1.75
54	1w	37	MIA	C13-C14	6.79	1.52	1.32
32	2a	967	5MC	C5-C4	6.69	1.49	1.44

The worst 5 of 423 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.03	73.56	102.36
54	1w	37	MIA	C12-C13-C14	-9.26	110.38	127.01
54	2w	37	MIA	C5-C4-N3	-8.23	118.51	127.18
1	2A	2503	2MA	C5-C4-N3	-8.21	118.53	127.18
55	2x	76	31H	O4'-C1'-N9	7.97	123.39	108.09

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C15

There are no ring outliers.

33 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	2	0
32	2a	1400	5MC	1	0
32	1a	1519	MA6	2	0
54	2y	37	MIA	1	0
32	2a	1207	2MG	2	0
55	2x	76	31H	1	0
54	1w	46	G7M	2	0
1	1A	2503	2MA	2	0
54	2y	46	G7M	2	0
54	1y	39	PSU	1	0
43	2l	92	0TD	2	0
32	1a	966	M2G	1	0
54	1y	54	5MU	1	0
32	2a	1518	MA6	2	0
1	2A	1917	PSU	1	0
54	1y	55	PSU	3	0
32	1a	1518	MA6	2	0
32	1a	967	5MC	1	0
54	2y	55	PSU	4	0
32	1a	1402	4OC	1	0
1	2A	1939	5MU	1	0
54	1y	37	MIA	1	0
1	1A	1917	PSU	1	0
1	1A	2251	OMG	1	0
54	1y	46	G7M	1	0
1	1A	2552	OMU	1	0
55	1x	8	4SU	2	0
32	2a	1402	4OC	2	0
1	2A	1915	5MU	1	0
55	2x	54	5MU	2	0
32	2a	967	5MC	1	0
54	1y	8	4SU	2	0
55	2x	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2581 ligands modelled in this entry, 2577 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SF4	1d	302	35	0,12,12	-	-	-		
59	SF4	2d	302	35	0,12,12	-	-	-		
57	A1A1L	1A	4060	-	34,39,39	3.35	12 (35%)	33,56,56	1.50	6 (18%)
57	A1A1L	2A	3783	-	34,39,39	3.52	10 (29%)	33,56,56	1.41	5 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	302	35	-	-	0/6/5/5
59	SF4	2d	302	35	-	-	0/6/5/5
57	A1A1L	1A	4060	-	-	5/30/74/74	0/3/4/4
57	A1A1L	2A	3783	-	-	6/30/74/74	0/3/4/4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3783	A1A1L	C23-C22	-11.84	1.35	1.53
57	1A	4060	A1A1L	C23-C22	-10.87	1.37	1.53
57	2A	3783	A1A1L	O24-C23	9.74	1.52	1.42
57	1A	4060	A1A1L	C21-N20	9.40	1.54	1.34
57	2A	3783	A1A1L	C21-N20	9.23	1.53	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3783	A1A1L	C09-O08-C07	-3.99	108.94	114.17
57	1A	4060	A1A1L	C12-C14-C15	-3.64	104.92	114.51
57	2A	3783	A1A1L	C11-S10-C09	3.61	106.82	100.12
57	1A	4060	A1A1L	C09-O08-C07	-3.28	109.87	114.17
57	1A	4060	A1A1L	O08-C07-C05	2.86	111.98	107.94

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

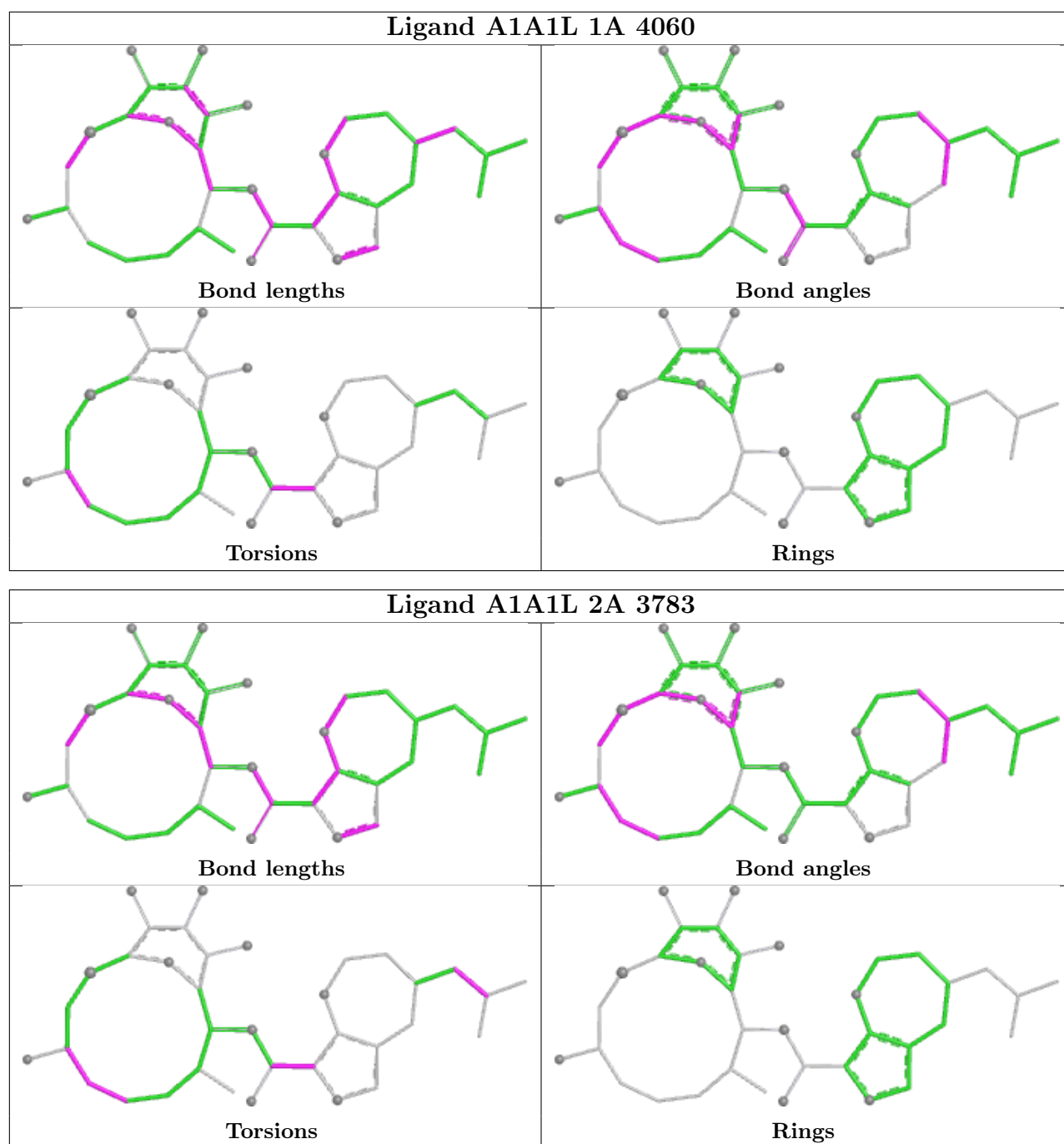
Mol	Chain	Res	Type	Atoms
57	1A	4060	A1A1L	C11-C12-C14-C15
57	1A	4060	A1A1L	F13-C12-C14-C15
57	2A	3783	A1A1L	C11-C12-C14-C15
57	2A	3783	A1A1L	F13-C12-C14-C15
57	1A	4060	A1A1L	O36-C21-C22-C23

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1d	302	SF4	1	0
59	2d	302	SF4	1	0
57	1A	4060	A1A1L	1	0
57	2A	3783	A1A1L	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.47	128 (4%) 38 33	22, 38, 92, 107	0
1	2A	2789/2915 (95%)	0.10	110 (3%) 43 38	34, 59, 92, 104	0
2	1B	120/121 (99%)	-0.31	0 100 100	32, 52, 65, 90	0
2	2B	120/121 (99%)	0.97	3 (2%) 58 54	64, 81, 88, 92	0
3	1D	275/276 (99%)	-0.08	4 (1%) 72 68	23, 38, 52, 76	0
3	2D	275/276 (99%)	0.39	5 (1%) 67 64	32, 52, 63, 80	0
4	1E	204/206 (99%)	-0.06	2 (0%) 79 76	22, 40, 60, 73	0
4	2E	204/206 (99%)	0.58	3 (1%) 72 68	38, 60, 71, 78	0
5	1F	202/210 (96%)	0.09	2 (0%) 79 76	19, 43, 69, 84	0
5	2F	202/210 (96%)	0.77	10 (4%) 34 30	36, 68, 80, 86	0
6	1G	181/182 (99%)	0.75	13 (7%) 21 19	42, 62, 75, 88	0
6	2G	181/182 (99%)	1.75	61 (33%) 1 1	72, 81, 86, 91	0
7	1H	174/180 (96%)	0.32	3 (1%) 69 65	39, 54, 66, 72	0
7	2H	174/180 (96%)	1.65	55 (31%) 1 1	72, 82, 88, 92	0
8	1I	146/148 (98%)	1.05	13 (8%) 15 13	47, 74, 81, 84	0
8	2I	146/148 (98%)	1.30	20 (13%) 6 5	57, 73, 81, 85	0
9	1N	140/140 (100%)	-0.05	1 (0%) 84 81	28, 39, 61, 74	0
9	2N	140/140 (100%)	0.95	10 (7%) 22 19	49, 66, 78, 83	0
10	1O	122/122 (100%)	0.08	1 (0%) 82 80	30, 42, 59, 64	0
10	2O	122/122 (100%)	0.62	1 (0%) 82 80	48, 61, 71, 78	0
11	1P	149/150 (99%)	0.23	4 (2%) 56 51	23, 46, 67, 73	0
11	2P	149/150 (99%)	0.88	11 (7%) 20 18	39, 69, 81, 88	0
12	1Q	141/141 (100%)	0.12	2 (1%) 73 70	28, 43, 59, 75	0
12	2Q	141/141 (100%)	1.41	32 (22%) 2 2	50, 70, 78, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.17	0 100 100	26, 35, 50, 57	0
13	2R	118/118 (100%)	0.31	1 (0%) 82 80	42, 54, 64, 70	0
14	1S	110/112 (98%)	0.36	1 (0%) 81 78	40, 52, 64, 66	0
14	2S	110/112 (98%)	1.50	20 (18%) 3 2	68, 75, 82, 84	0
15	1T	131/146 (89%)	0.24	5 (3%) 44 39	32, 45, 67, 74	0
15	2T	131/146 (89%)	0.75	5 (3%) 44 39	53, 62, 73, 78	0
16	1U	116/118 (98%)	-0.31	0 100 100	23, 31, 46, 64	0
16	2U	116/118 (98%)	0.74	2 (1%) 69 65	48, 63, 76, 81	0
17	1V	101/101 (100%)	-0.20	1 (0%) 79 76	23, 41, 55, 67	0
17	2V	101/101 (100%)	0.91	3 (2%) 52 48	44, 72, 78, 81	0
18	1W	112/113 (99%)	-0.04	1 (0%) 81 78	25, 33, 53, 80	0
18	2W	112/113 (99%)	0.54	4 (3%) 46 41	41, 51, 65, 91	0
19	1X	95/96 (98%)	0.17	1 (1%) 78 75	28, 40, 62, 73	0
19	2X	95/96 (98%)	0.87	6 (6%) 26 23	48, 60, 74, 78	0
20	1Y	107/110 (97%)	0.42	2 (1%) 66 62	36, 51, 67, 78	0
20	2Y	107/110 (97%)	1.35	17 (15%) 5 4	59, 71, 81, 86	0
21	1Z	154/206 (74%)	1.01	20 (12%) 7 6	38, 65, 86, 88	0
21	2Z	160/206 (77%)	1.98	60 (37%) 1 1	71, 83, 91, 95	0
22	10	77/85 (90%)	0.11	2 (2%) 57 52	30, 39, 54, 62	0
22	20	79/85 (92%)	1.67	21 (26%) 1 1	51, 68, 75, 80	0
23	11	97/98 (98%)	0.37	1 (1%) 79 76	28, 45, 69, 77	0
23	21	97/98 (98%)	0.60	3 (3%) 51 47	42, 56, 74, 78	0
24	12	70/72 (97%)	0.22	0 100 100	36, 50, 60, 68	0
24	22	70/72 (97%)	0.92	0 100 100	60, 70, 78, 78	0
25	13	59/60 (98%)	-0.06	2 (3%) 48 43	28, 37, 62, 79	0
25	23	59/60 (98%)	0.91	3 (5%) 33 29	56, 68, 77, 85	0
26	14	69/71 (97%)	1.16	14 (20%) 3 2	57, 75, 87, 91	0
26	24	69/71 (97%)	2.14	36 (52%) 0 0	80, 87, 92, 96	0
27	15	59/60 (98%)	-0.23	1 (1%) 69 65	22, 32, 52, 63	0
27	25	59/60 (98%)	0.42	1 (1%) 69 65	40, 52, 66, 76	0
28	16	53/54 (98%)	0.03	0 100 100	35, 44, 58, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.96	2 (3%) 44 39	55, 64, 71, 76	0
29	17	48/49 (97%)	-0.08	3 (6%) 26 23	22, 29, 55, 65	0
29	27	48/49 (97%)	0.33	4 (8%) 17 15	32, 43, 67, 71	0
30	18	64/65 (98%)	-0.15	0 100 100	27, 35, 42, 62	0
30	28	64/65 (98%)	0.79	2 (3%) 51 47	47, 58, 66, 67	0
31	19	37/37 (100%)	0.17	0 100 100	31, 41, 59, 60	0
31	29	37/37 (100%)	1.16	3 (8%) 18 15	64, 69, 76, 80	0
32	1a	1488/1521 (97%)	0.36	52 (3%) 47 42	37, 68, 92, 104	0
32	2a	1491/1521 (98%)	0.81	144 (9%) 13 11	50, 77, 95, 107	0
33	1b	231/256 (90%)	1.47	58 (25%) 1 1	66, 78, 87, 91	0
33	2b	231/256 (90%)	2.22	129 (55%) 0 0	73, 85, 89, 93	0
34	1c	206/239 (86%)	1.14	23 (11%) 10 8	62, 74, 83, 87	0
34	2c	206/239 (86%)	2.26	118 (57%) 0 0	74, 84, 88, 94	0
35	1d	208/209 (99%)	1.15	23 (11%) 10 8	57, 71, 80, 83	0
35	2d	208/209 (99%)	1.13	13 (6%) 26 23	61, 70, 78, 85	0
36	1e	148/162 (91%)	0.93	9 (6%) 27 23	53, 65, 75, 79	0
36	2e	148/162 (91%)	1.72	55 (37%) 1 1	63, 77, 84, 89	0
37	1f	100/101 (99%)	0.95	6 (6%) 27 24	58, 68, 77, 78	0
37	2f	100/101 (99%)	0.82	3 (3%) 52 48	59, 71, 78, 84	0
38	1g	155/156 (99%)	0.97	16 (10%) 12 10	59, 71, 83, 96	0
38	2g	155/156 (99%)	1.44	32 (20%) 2 2	69, 79, 86, 94	0
39	1h	137/138 (99%)	0.83	6 (4%) 39 34	57, 68, 73, 75	0
39	2h	137/138 (99%)	1.56	30 (21%) 2 2	68, 76, 82, 86	0
40	1i	127/128 (99%)	1.56	36 (28%) 1 1	57, 77, 84, 88	0
40	2i	127/128 (99%)	2.59	88 (69%) 0 0	73, 84, 88, 89	0
41	1j	97/105 (92%)	1.49	23 (23%) 2 1	62, 78, 85, 90	0
41	2j	96/105 (91%)	2.51	59 (61%) 0 0	77, 86, 91, 93	0
42	1k	114/129 (88%)	0.90	11 (9%) 13 11	46, 66, 76, 81	0
42	2k	114/129 (88%)	1.42	25 (21%) 2 2	57, 74, 81, 85	0
43	1l	121/132 (91%)	0.70	7 (5%) 29 25	46, 57, 68, 74	0
43	2l	121/132 (91%)	1.51	30 (24%) 2 1	57, 70, 77, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.15	14 (11%) 10 8	56, 71, 79, 85	0
44	2m	122/126 (96%)	2.28	62 (50%) 0 0	75, 83, 87, 91	0
45	1n	60/61 (98%)	1.35	9 (15%) 5 4	62, 69, 75, 79	0
45	2n	60/61 (98%)	2.84	44 (73%) 0 0	79, 85, 89, 91	0
46	1o	88/89 (98%)	0.79	6 (6%) 23 20	49, 66, 74, 78	0
46	2o	88/89 (98%)	1.27	12 (13%) 7 5	62, 73, 81, 84	0
47	1p	82/88 (93%)	1.76	30 (36%) 1 1	58, 72, 77, 84	0
47	2p	82/88 (93%)	1.24	11 (13%) 7 5	60, 69, 77, 81	0
48	1q	99/105 (94%)	0.96	6 (6%) 27 23	54, 67, 77, 79	0
48	2q	99/105 (94%)	1.26	16 (16%) 4 3	63, 73, 80, 83	0
49	1r	68/88 (77%)	0.86	5 (7%) 20 18	58, 67, 76, 78	0
49	2r	68/88 (77%)	0.90	3 (4%) 39 34	64, 72, 81, 85	0
50	1s	83/93 (89%)	1.07	10 (12%) 9 7	64, 74, 81, 85	0
50	2s	83/93 (89%)	2.29	51 (61%) 0 0	81, 87, 91, 93	0
51	1t	96/106 (90%)	1.28	15 (15%) 5 4	63, 72, 80, 84	0
51	2t	96/106 (90%)	1.14	12 (12%) 8 6	58, 71, 80, 85	0
52	1u	23/27 (85%)	1.42	4 (17%) 4 3	64, 69, 72, 74	0
52	2u	23/27 (85%)	2.77	18 (78%) 0 0	74, 81, 85, 86	0
53	1v	13/24 (54%)	0.84	2 (15%) 5 4	51, 64, 86, 93	0
53	2v	13/24 (54%)	1.76	4 (30%) 1 1	72, 82, 93, 96	0
54	1w	64/76 (84%)	0.99	4 (6%) 26 23	63, 87, 96, 103	0
54	1y	67/76 (88%)	1.03	7 (10%) 11 10	38, 90, 98, 100	0
54	2w	62/76 (81%)	1.43	12 (19%) 3 2	82, 94, 100, 106	0
54	2y	66/76 (86%)	1.27	9 (13%) 7 5	56, 94, 99, 103	0
55	1x	71/77 (92%)	0.34	1 (1%) 73 70	29, 64, 85, 90	0
55	2x	71/77 (92%)	0.73	2 (2%) 55 50	48, 80, 90, 95	0
All	All	20855/21748 (95%)	0.58	2106 (10%) 12 10	19, 65, 89, 107	0

The worst 5 of 2106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	7.8
40	2i	11	LYS	7.4

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Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	7.3
40	2i	102	LEU	7.2
44	1m	2	ALA	7.1

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	G7M	2w	46	24/25	0.48	0.18	86,95,105,115	0
54	PSU	2y	55	20/21	0.56	0.17	92,100,112,113	0
54	G7M	1w	46	24/25	0.57	0.14	81,88,102,122	0
54	5MU	2y	54	21/22	0.59	0.18	90,96,105,123	0
54	G7M	1y	46	24/25	0.63	0.16	87,94,102,112	0
54	G7M	2y	46	24/25	0.63	0.15	91,94,99,119	0
54	MIA	2y	37	22/30	0.66	0.16	75,86,98,113	0
54	4SU	2w	8	20/21	0.69	0.14	93,96,104,114	0
54	PSU	1y	55	20/21	0.71	0.16	85,93,101,110	0
54	4SU	2y	8	20/21	0.71	0.13	89,94,101,109	0
54	5MU	1y	54	21/22	0.73	0.17	83,87,96,107	0
54	4SU	1y	8	20/21	0.77	0.12	88,90,99,100	0
54	PSU	2y	39	20/21	0.78	0.13	81,85,94,99	0
54	5MU	2w	54	21/22	0.79	0.13	74,84,90,94	0
54	PSU	2w	55	20/21	0.79	0.12	86,92,97,100	0
54	MIA	1y	37	22/30	0.80	0.13	72,79,86,96	0
32	2MG	2a	1207	24/25	0.82	0.14	81,88,93,96	0
54	PSU	2y	32	20/21	0.83	0.13	76,90,96,97	0
55	4SU	2x	8	20/21	0.83	0.13	79,85,89,89	0
55	5MU	2x	54	21/22	0.84	0.14	74,85,89,90	0
54	PSU	1w	55	20/21	0.84	0.12	63,83,88,89	0
54	PSU	1y	32	20/21	0.85	0.11	77,82,87,90	0
54	PSU	2w	32	20/21	0.85	0.16	85,89,97,102	0
55	PSU	2x	55	20/21	0.87	0.11	75,82,88,89	0
32	5MC	2a	967	21/22	0.87	0.16	68,74,83,87	0
54	PSU	1y	39	20/21	0.88	0.10	76,80,85,88	0
54	PSU	1w	32	20/21	0.88	0.13	63,71,83,85	0
54	4SU	1w	8	20/21	0.88	0.10	77,82,89,94	0
55	PSU	1x	55	20/21	0.89	0.12	62,67,77,81	0
1	5MU	2A	1915	21/22	0.89	0.14	67,74,76,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	1404	21/22	0.89	0.13	51,59,66,66	0
32	PSU	2a	516	20/21	0.89	0.12	73,77,81,83	0
32	G7M	2a	527	24/25	0.89	0.15	65,70,75,79	0
32	M2G	2a	966	25/26	0.89	0.17	66,73,85,86	0
32	4OC	2a	1402	22/23	0.90	0.13	50,68,76,76	0
1	PSU	2A	1917	20/21	0.90	0.11	63,70,78,81	0
54	MIA	2w	37	25/30	0.90	0.14	74,79,87,90	0
43	0TD	2l	92	10/11	0.90	0.12	67,71,75,87	0
32	5MC	2a	1400	21/22	0.91	0.15	72,75,78,82	0
55	5MU	1x	54	21/22	0.91	0.11	60,69,74,86	0
1	PSU	2A	1911	20/21	0.91	0.10	61,67,70,70	0
43	0TD	1l	92	10/11	0.91	0.12	48,54,57,75	0
32	2MG	1a	1207	24/25	0.92	0.11	71,74,78,79	0
54	PSU	2w	39	20/21	0.92	0.11	77,82,90,92	0
55	5MC	2x	32	21/22	0.92	0.14	66,75,81,82	0
32	UR3	2a	1498	21/22	0.93	0.12	59,64,65,70	0
55	4SU	1x	8	20/21	0.93	0.09	61,70,77,77	0
54	MIA	1w	37	29/30	0.93	0.13	55,63,68,76	0
54	PSU	1w	39	20/21	0.93	0.10	59,70,78,79	0
32	5MC	2a	1407	21/22	0.93	0.11	55,60,64,67	0
32	PSU	1a	516	20/21	0.94	0.09	57,63,68,68	0
1	5MU	1A	1915	21/22	0.94	0.10	50,59,61,63	0
55	5MC	1x	32	21/22	0.94	0.13	55,59,66,72	0
32	MA6	2a	1518	24/25	0.94	0.12	54,69,74,75	0
32	MA6	2a	1519	24/25	0.94	0.12	57,68,74,77	0
1	OMC	2A	1920	21/22	0.94	0.11	52,64,68,72	0
1	5MC	2A	1962	21/22	0.94	0.10	35,50,56,63	0
54	5MU	1w	54	21/22	0.94	0.09	61,75,81,81	0
32	G7M	1a	527	24/25	0.95	0.11	48,53,56,57	0
32	M2G	1a	966	25/26	0.95	0.11	48,55,62,63	0
32	5MC	1a	967	21/22	0.95	0.11	50,57,61,63	0
1	5MC	2A	1942	21/22	0.95	0.09	48,57,64,67	0
1	5MU	2A	1939	21/22	0.96	0.08	32,41,47,50	0
55	31H	1x	76	32/33	0.96	0.09	23,32,38,68	10
32	4OC	1a	1402	22/23	0.96	0.10	40,47,51,53	0
1	OMG	2A	2251	24/25	0.96	0.09	37,46,49,51	0
1	OMU	2A	2552	21/22	0.96	0.10	43,48,53,61	0
32	MA6	1a	1519	24/25	0.96	0.11	39,44,49,53	0
32	5MC	1a	1404	21/22	0.97	0.09	37,43,46,47	0
32	5MC	1a	1407	21/22	0.97	0.09	37,42,46,47	0
1	2MA	2A	2503	23/24	0.97	0.09	34,42,43,47	0
32	MA6	1a	1518	24/25	0.97	0.10	35,43,46,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	2A	2605	20/21	0.97	0.07	33,41,44,48	0
55	31H	2x	76	32/33	0.97	0.08	40,49,63,82	0
1	PSU	1A	1911	20/21	0.97	0.08	39,46,51,52	0
1	PSU	1A	1917	20/21	0.97	0.07	40,50,56,57	0
1	OMC	1A	1920	21/22	0.97	0.08	37,44,49,54	0
1	5MC	1A	1942	21/22	0.97	0.07	29,38,43,45	0
1	5MC	1A	1962	21/22	0.97	0.07	32,37,43,46	0
32	5MC	1a	1400	21/22	0.97	0.10	43,53,58,60	0
1	PSU	1A	2605	20/21	0.97	0.06	22,27,35,36	0
1	OMU	1A	2552	21/22	0.98	0.07	25,30,33,35	0
1	5MU	1A	1939	21/22	0.98	0.06	25,31,35,36	0
32	UR3	1a	1498	21/22	0.98	0.08	39,44,48,49	0
1	OMG	1A	2251	24/25	0.98	0.05	25,27,29,33	0
1	2MA	1A	2503	23/24	0.99	0.05	20,25,28,29	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	1A	3939	1/1	0.43	0.20	83,83,83,83	0
56	MG	2G	201	1/1	0.48	0.25	84,84,84,84	0
56	MG	2a	1777	1/1	0.55	0.24	76,76,76,76	0
56	MG	2A	3615	1/1	0.57	0.21	86,86,86,86	0
56	MG	1A	3924	1/1	0.62	0.20	64,64,64,64	0
56	MG	2A	3752	1/1	0.62	0.27	67,67,67,67	0
56	MG	1A	3391	1/1	0.63	0.49	63,63,63,63	0
56	MG	1B	232	1/1	0.63	0.22	82,82,82,82	0
56	MG	1A	3990	1/1	0.64	0.16	50,50,50,50	0
56	MG	1A	3768	1/1	0.64	0.17	67,67,67,67	0
56	MG	1A	3989	1/1	0.65	0.30	65,65,65,65	0
56	MG	1A	3758	1/1	0.65	0.25	95,95,95,95	0
56	MG	2A	3659	1/1	0.65	0.18	45,45,45,45	0
56	MG	1A	3979	1/1	0.66	0.13	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3918	1/1	0.66	0.21	52,52,52,52	0
56	MG	2a	1613	1/1	0.66	0.17	75,75,75,75	0
56	MG	2A	3665	1/1	0.66	0.24	56,56,56,56	0
56	MG	1a	1657	1/1	0.67	0.14	62,62,62,62	0
56	MG	2A	3765	1/1	0.68	0.19	79,79,79,79	0
56	MG	2a	1614	1/1	0.68	0.25	78,78,78,78	0
56	MG	2A	3091	1/1	0.68	0.26	69,69,69,69	0
56	MG	2A	3700	1/1	0.69	0.26	72,72,72,72	0
56	MG	2A	3100	1/1	0.70	0.23	71,71,71,71	0
56	MG	2a	1619	1/1	0.70	0.18	80,80,80,80	0
56	MG	2a	1698	1/1	0.70	0.29	75,75,75,75	0
56	MG	2A	3166	1/1	0.70	0.25	76,76,76,76	0
56	MG	2a	1620	1/1	0.71	0.36	77,77,77,77	0
56	MG	2A	3657	1/1	0.71	0.30	74,74,74,74	0
56	MG	1A	3800	1/1	0.71	0.22	69,69,69,69	0
56	MG	1B	225	1/1	0.72	0.21	66,66,66,66	0
56	MG	1a	1741	1/1	0.72	0.21	76,76,76,76	0
56	MG	2A	3185	1/1	0.72	0.25	67,67,67,67	0
56	MG	2A	3499	1/1	0.72	0.23	60,60,60,60	0
56	MG	1a	1782	1/1	0.72	0.29	72,72,72,72	0
56	MG	2a	1764	1/1	0.72	0.21	87,87,87,87	0
56	MG	1P	206	1/1	0.72	0.25	58,58,58,58	0
56	MG	2a	1787	1/1	0.72	0.20	80,80,80,80	0
56	MG	1a	1781	1/1	0.73	0.22	80,80,80,80	0
56	MG	2a	1602	1/1	0.73	0.19	74,74,74,74	0
56	MG	1A	3315	1/1	0.73	0.27	52,52,52,52	0
56	MG	2A	3651	1/1	0.73	0.22	74,74,74,74	0
56	MG	18	104	1/1	0.73	0.20	69,69,69,69	0
56	MG	1A	3867	1/1	0.73	0.13	57,57,57,57	0
56	MG	2a	1634	1/1	0.73	0.37	72,72,72,72	0
56	MG	1O	206	1/1	0.73	0.21	66,66,66,66	0
56	MG	1a	1743	1/1	0.73	0.17	74,74,74,74	0
56	MG	2A	3330	1/1	0.73	0.26	80,80,80,80	0
56	MG	2A	3434	1/1	0.73	0.19	67,67,67,67	0
56	MG	2A	3630	1/1	0.74	0.18	57,57,57,57	0
56	MG	2A	3264	1/1	0.74	0.25	74,74,74,74	0
56	MG	1A	3677	1/1	0.74	0.16	43,43,43,43	0
56	MG	2A	3368	1/1	0.74	0.32	82,82,82,82	0
56	MG	1A	3369	1/1	0.74	0.18	69,69,69,69	0
56	MG	1A	3404	1/1	0.74	0.20	62,62,62,62	0
56	MG	2A	3582	1/1	0.74	0.22	69,69,69,69	0
56	MG	2A	3595	1/1	0.74	0.19	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1767	1/1	0.74	0.20	76,76,76,76	0
56	MG	2D	303	1/1	0.74	0.23	70,70,70,70	0
56	MG	2A	3048	1/1	0.74	0.25	69,69,69,69	0
56	MG	2a	1606	1/1	0.75	0.38	79,79,79,79	0
56	MG	1a	1656	1/1	0.75	0.26	79,79,79,79	0
56	MG	2A	3579	1/1	0.75	0.14	72,72,72,72	0
56	MG	2A	3255	1/1	0.75	0.37	77,77,77,77	0
56	MG	1B	233	1/1	0.75	0.13	79,79,79,79	0
56	MG	2A	3612	1/1	0.75	0.19	70,70,70,70	0
56	MG	2a	1643	1/1	0.75	0.28	68,68,68,68	0
56	MG	1A	3386	1/1	0.75	0.59	82,82,82,82	0
56	MG	2a	1702	1/1	0.75	0.34	73,73,73,73	0
56	MG	1A	3492	1/1	0.75	0.17	83,83,83,83	0
56	MG	2D	308	1/1	0.75	0.21	69,69,69,69	0
56	MG	2A	3647	1/1	0.75	0.20	76,76,76,76	0
56	MG	2a	1780	1/1	0.75	0.17	78,78,78,78	0
56	MG	1A	3805	1/1	0.75	0.20	62,62,62,62	0
56	MG	2A	3777	1/1	0.76	0.20	67,67,67,67	0
56	MG	2A	3603	1/1	0.76	0.27	62,62,62,62	0
56	MG	2A	3387	1/1	0.76	0.29	76,76,76,76	0
56	MG	2A	3722	1/1	0.76	0.22	65,65,65,65	0
56	MG	2A	3331	1/1	0.76	0.23	75,75,75,75	0
56	MG	1A	3952	1/1	0.76	0.13	37,37,37,37	0
56	MG	2a	1689	1/1	0.76	0.24	70,70,70,70	0
56	MG	2l	202	1/1	0.76	0.21	67,67,67,67	0
56	MG	2A	3441	1/1	0.77	0.28	58,58,58,58	0
56	MG	1A	3557	1/1	0.77	0.25	47,47,47,47	0
56	MG	2A	3201	1/1	0.77	0.25	53,53,53,53	0
56	MG	2A	3207	1/1	0.77	0.27	66,66,66,66	0
56	MG	2A	3591	1/1	0.77	0.23	73,73,73,73	0
56	MG	2A	3242	1/1	0.77	0.23	62,62,62,62	0
56	MG	1A	3966	1/1	0.77	0.14	67,67,67,67	0
56	MG	1x	111	1/1	0.77	0.35	75,75,75,75	0
56	MG	1D	311	1/1	0.77	0.28	49,49,49,49	0
56	MG	2A	3090	1/1	0.77	0.21	75,75,75,75	0
56	MG	2T	204	1/1	0.77	0.26	83,83,83,83	0
56	MG	1A	3993	1/1	0.77	0.21	63,63,63,63	0
56	MG	1A	3547	1/1	0.77	0.16	65,65,65,65	0
56	MG	2a	1798	1/1	0.77	0.30	74,74,74,74	0
56	MG	1a	1759	1/1	0.77	0.19	57,57,57,57	0
56	MG	1b	301	1/1	0.78	0.18	81,81,81,81	0
56	MG	2A	3503	1/1	0.78	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	106	1/1	0.78	0.20	74,74,74,74	0
56	MG	1A	3959	1/1	0.78	0.16	31,31,31,31	0
56	MG	2a	1644	1/1	0.78	0.18	78,78,78,78	0
56	MG	1A	3850	1/1	0.78	0.20	35,35,35,35	0
56	MG	1E	313	1/1	0.78	0.16	60,60,60,60	0
56	MG	2A	3305	1/1	0.78	0.24	70,70,70,70	0
56	MG	2a	1729	1/1	0.78	0.25	75,75,75,75	0
56	MG	1F	312	1/1	0.78	0.20	66,66,66,66	0
56	MG	1A	4026	1/1	0.78	0.13	60,60,60,60	0
56	MG	2A	3343	1/1	0.78	0.18	59,59,59,59	0
56	MG	2A	3156	1/1	0.78	0.19	64,64,64,64	0
56	MG	1A	3475	1/1	0.78	0.18	64,64,64,64	0
56	MG	1A	3694	1/1	0.78	0.15	66,66,66,66	0
56	MG	2A	3195	1/1	0.78	0.30	52,52,52,52	0
56	MG	2A	3175	1/1	0.79	0.30	75,75,75,75	0
56	MG	1a	1666	1/1	0.79	0.23	78,78,78,78	0
56	MG	2a	1629	1/1	0.79	0.35	79,79,79,79	0
56	MG	1A	3965	1/1	0.79	0.17	81,81,81,81	0
56	MG	1A	3443	1/1	0.79	0.16	60,60,60,60	0
56	MG	2B	204	1/1	0.79	0.19	80,80,80,80	0
56	MG	2B	214	1/1	0.79	0.21	76,76,76,76	0
56	MG	2B	215	1/1	0.79	0.17	78,78,78,78	0
56	MG	1A	3238	1/1	0.79	0.30	75,75,75,75	0
56	MG	2a	1709	1/1	0.79	0.23	87,87,87,87	0
56	MG	1A	3163	1/1	0.79	0.14	48,48,48,48	0
56	MG	1A	3770	1/1	0.79	0.21	63,63,63,63	0
56	MG	2a	1766	1/1	0.79	0.26	75,75,75,75	0
56	MG	1A	3891	1/1	0.79	0.12	33,33,33,33	0
56	MG	2A	3286	1/1	0.79	0.19	78,78,78,78	0
56	MG	2A	3288	1/1	0.79	0.14	82,82,82,82	0
56	MG	2A	3580	1/1	0.79	0.18	75,75,75,75	0
56	MG	1x	105	1/1	0.79	0.23	79,79,79,79	0
56	MG	2a	1799	1/1	0.79	0.21	81,81,81,81	0
56	MG	2a	1617	1/1	0.79	0.24	79,79,79,79	0
56	MG	2A	3265	1/1	0.80	0.19	68,68,68,68	0
56	MG	1A	3983	1/1	0.80	0.10	65,65,65,65	0
56	MG	1W	206	1/1	0.80	0.26	50,50,50,50	0
56	MG	2A	3589	1/1	0.80	0.22	63,63,63,63	0
56	MG	2a	1662	1/1	0.80	0.23	69,69,69,69	0
56	MG	2A	3298	1/1	0.80	0.23	66,66,66,66	0
56	MG	1A	3801	1/1	0.80	0.18	71,71,71,71	0
56	MG	2A	3312	1/1	0.80	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1649	1/1	0.80	0.28	69,69,69,69	0
56	MG	1n	101	1/1	0.80	0.26	66,66,66,66	0
56	MG	2a	1752	1/1	0.80	0.24	73,73,73,73	0
56	MG	1A	3436	1/1	0.80	0.18	63,63,63,63	0
56	MG	2A	3643	1/1	0.80	0.20	75,75,75,75	0
56	MG	1A	3875	1/1	0.80	0.18	62,62,62,62	0
56	MG	2a	1776	1/1	0.80	0.18	78,78,78,78	0
56	MG	1A	3806	1/1	0.80	0.22	67,67,67,67	0
56	MG	1a	1679	1/1	0.80	0.17	57,57,57,57	0
56	MG	1A	4044	1/1	0.80	0.21	78,78,78,78	0
56	MG	2A	3258	1/1	0.80	0.34	69,69,69,69	0
56	MG	1B	216	1/1	0.80	0.19	73,73,73,73	0
56	MG	2A	3701	1/1	0.80	0.14	69,69,69,69	0
56	MG	2x	103	1/1	0.80	0.20	78,78,78,78	0
56	MG	2a	1607	1/1	0.81	0.27	75,75,75,75	0
56	MG	2A	3623	1/1	0.81	0.28	64,64,64,64	0
56	MG	2A	3250	1/1	0.81	0.14	62,62,62,62	0
56	MG	2A	3379	1/1	0.81	0.18	57,57,57,57	0
56	MG	1a	1726	1/1	0.81	0.29	81,81,81,81	0
56	MG	2A	3410	1/1	0.81	0.44	75,75,75,75	0
56	MG	2A	3423	1/1	0.81	0.23	68,68,68,68	0
56	MG	2A	3153	1/1	0.81	0.15	86,86,86,86	0
56	MG	2A	3261	1/1	0.81	0.31	59,59,59,59	0
56	MG	2A	3670	1/1	0.81	0.18	70,70,70,70	0
56	MG	1A	3388	1/1	0.81	0.29	70,70,70,70	0
56	MG	1A	3603	1/1	0.81	0.20	65,65,65,65	0
56	MG	2A	3703	1/1	0.81	0.18	67,67,67,67	0
56	MG	2a	1700	1/1	0.81	0.23	85,85,85,85	0
56	MG	2a	1701	1/1	0.81	0.32	67,67,67,67	0
56	MG	2A	3521	1/1	0.81	0.18	64,64,64,64	0
56	MG	2A	3748	1/1	0.81	0.13	56,56,56,56	0
56	MG	2A	3523	1/1	0.81	0.15	50,50,50,50	0
56	MG	2A	3525	1/1	0.81	0.18	71,71,71,71	0
56	MG	2A	3174	1/1	0.81	0.34	76,76,76,76	0
56	MG	1A	3821	1/1	0.81	0.15	67,67,67,67	0
56	MG	2A	3017	1/1	0.81	0.20	71,71,71,71	0
56	MG	2a	1774	1/1	0.81	0.18	74,74,74,74	0
56	MG	1A	3954	1/1	0.81	0.14	61,61,61,61	0
56	MG	2A	3054	1/1	0.81	0.20	81,81,81,81	0
56	MG	2A	3317	1/1	0.81	0.24	73,73,73,73	0
56	MG	2a	1784	1/1	0.81	0.10	75,75,75,75	0
56	MG	2a	1785	1/1	0.81	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3491	1/1	0.81	0.12	78,78,78,78	0
56	MG	2a	1789	1/1	0.81	0.20	79,79,79,79	0
56	MG	2A	3238	1/1	0.81	0.22	64,64,64,64	0
56	MG	25	105	1/1	0.81	0.16	67,67,67,67	0
56	MG	1a	1699	1/1	0.81	0.23	78,78,78,78	0
56	MG	2A	3622	1/1	0.81	0.28	63,63,63,63	0
56	MG	1F	314	1/1	0.82	0.28	55,55,55,55	0
56	MG	2A	3691	1/1	0.82	0.22	71,71,71,71	0
56	MG	2a	1621	1/1	0.82	0.39	78,78,78,78	0
56	MG	2a	1622	1/1	0.82	0.20	62,62,62,62	0
56	MG	2A	3697	1/1	0.82	0.17	59,59,59,59	0
56	MG	1A	3679	1/1	0.82	0.16	63,63,63,63	0
56	MG	1A	3403	1/1	0.82	0.17	75,75,75,75	0
56	MG	2A	3302	1/1	0.82	0.25	68,68,68,68	0
56	MG	2A	3707	1/1	0.82	0.22	64,64,64,64	0
56	MG	2A	3713	1/1	0.82	0.21	58,58,58,58	0
56	MG	2a	1697	1/1	0.82	0.18	79,79,79,79	0
56	MG	1A	4016	1/1	0.82	0.20	44,44,44,44	0
56	MG	1a	1740	1/1	0.82	0.16	72,72,72,72	0
56	MG	1A	3530	1/1	0.82	0.35	71,71,71,71	0
56	MG	2A	3587	1/1	0.82	0.18	78,78,78,78	0
56	MG	2A	3329	1/1	0.82	0.14	74,74,74,74	0
56	MG	2A	3219	1/1	0.82	0.25	77,77,77,77	0
56	MG	2a	1750	1/1	0.82	0.17	67,67,67,67	0
56	MG	2B	212	1/1	0.82	0.11	74,74,74,74	0
56	MG	2A	3229	1/1	0.82	0.15	75,75,75,75	0
56	MG	2a	1765	1/1	0.82	0.23	70,70,70,70	0
56	MG	2A	3234	1/1	0.82	0.23	73,73,73,73	0
56	MG	2A	3073	1/1	0.82	0.26	71,71,71,71	0
56	MG	2A	3080	1/1	0.82	0.22	70,70,70,70	0
56	MG	2E	307	1/1	0.82	0.17	65,65,65,65	0
56	MG	1a	1614	1/1	0.82	0.19	69,69,69,69	0
56	MG	1a	1623	1/1	0.82	0.20	76,76,76,76	0
56	MG	2Z	302	1/1	0.82	0.23	76,76,76,76	0
56	MG	1a	1629	1/1	0.82	0.28	73,73,73,73	0
56	MG	2A	3429	1/1	0.82	0.23	65,65,65,65	0
56	MG	1E	310	1/1	0.82	0.39	76,76,76,76	0
56	MG	1A	3619	1/1	0.82	0.11	65,65,65,65	0
56	MG	2A	3485	1/1	0.82	0.23	56,56,56,56	0
56	MG	2A	3496	1/1	0.82	0.16	76,76,76,76	0
56	MG	2q	202	1/1	0.82	0.20	76,76,76,76	0
56	MG	2w	103	1/1	0.82	0.30	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3434	1/1	0.82	0.34	64,64,64,64	0
56	MG	2a	1639	1/1	0.83	0.32	75,75,75,75	0
56	MG	1G	203	1/1	0.83	0.13	71,71,71,71	0
56	MG	1A	3199	1/1	0.83	0.19	69,69,69,69	0
56	MG	2a	1646	1/1	0.83	0.26	71,71,71,71	0
56	MG	2a	1652	1/1	0.83	0.30	68,68,68,68	0
56	MG	1a	1692	1/1	0.83	0.35	70,70,70,70	0
56	MG	2A	3756	1/1	0.83	0.19	61,61,61,61	0
56	MG	2A	3760	1/1	0.83	0.14	72,72,72,72	0
56	MG	1A	3776	1/1	0.83	0.15	59,59,59,59	0
56	MG	2A	3365	1/1	0.83	0.37	70,70,70,70	0
56	MG	2A	3055	1/1	0.83	0.17	79,79,79,79	0
56	MG	2A	3611	1/1	0.83	0.15	58,58,58,58	0
56	MG	1a	1721	1/1	0.83	0.28	71,71,71,71	0
56	MG	2A	3385	1/1	0.83	0.20	75,75,75,75	0
56	MG	2A	3244	1/1	0.83	0.24	76,76,76,76	0
56	MG	1V	206	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3571	1/1	0.83	0.14	43,43,43,43	0
56	MG	2A	3427	1/1	0.83	0.22	61,61,61,61	0
56	MG	2A	3645	1/1	0.83	0.18	69,69,69,69	0
56	MG	1A	3907	1/1	0.83	0.14	34,34,34,34	0
56	MG	1A	3483	1/1	0.83	0.15	66,66,66,66	0
56	MG	1A	3695	1/1	0.83	0.17	51,51,51,51	0
56	MG	1a	1780	1/1	0.83	0.35	82,82,82,82	0
56	MG	2A	3284	1/1	0.83	0.22	73,73,73,73	0
56	MG	1A	3708	1/1	0.83	0.13	56,56,56,56	0
56	MG	1a	1637	1/1	0.83	0.40	73,73,73,73	0
56	MG	2A	3518	1/1	0.83	0.18	73,73,73,73	0
56	MG	1A	3944	1/1	0.83	0.11	71,71,71,71	0
56	MG	1A	3609	1/1	0.83	0.17	55,55,55,55	0
56	MG	2A	3190	1/1	0.83	0.36	71,71,71,71	0
56	MG	1A	3027	1/1	0.83	0.17	82,82,82,82	0
56	MG	1a	1662	1/1	0.83	0.29	68,68,68,68	0
56	MG	2a	1632	1/1	0.83	0.16	79,79,79,79	0
56	MG	2A	3720	1/1	0.83	0.16	46,46,46,46	0
56	MG	1A	3747	1/1	0.84	0.14	45,45,45,45	0
56	MG	2A	3280	1/1	0.84	0.22	74,74,74,74	0
56	MG	2X	101	1/1	0.84	0.16	69,69,69,69	0
56	MG	2A	3086	1/1	0.84	0.17	75,75,75,75	0
56	MG	1A	3400	1/1	0.84	0.20	63,63,63,63	0
56	MG	1A	3318	1/1	0.84	0.16	53,53,53,53	0
56	MG	1A	3913	1/1	0.84	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3101	1/1	0.84	0.34	69,69,69,69	0
56	MG	2A	3124	1/1	0.84	0.13	63,63,63,63	0
56	MG	2A	3137	1/1	0.84	0.19	79,79,79,79	0
56	MG	2a	1615	1/1	0.84	0.26	66,66,66,66	0
56	MG	2A	3620	1/1	0.84	0.23	71,71,71,71	0
56	MG	1A	3999	1/1	0.84	0.17	50,50,50,50	0
56	MG	1A	3580	1/1	0.84	0.12	50,50,50,50	0
56	MG	1A	3188	1/1	0.84	0.24	61,61,61,61	0
56	MG	2A	3632	1/1	0.84	0.14	64,64,64,64	0
56	MG	2a	1623	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3637	1/1	0.84	0.18	68,68,68,68	0
56	MG	2A	3167	1/1	0.84	0.27	77,77,77,77	0
56	MG	2A	3173	1/1	0.84	0.22	66,66,66,66	0
56	MG	2A	3344	1/1	0.84	0.19	63,63,63,63	0
56	MG	10	105	1/1	0.84	0.18	65,65,65,65	0
56	MG	2A	3654	1/1	0.84	0.14	75,75,75,75	0
56	MG	2a	1645	1/1	0.84	0.36	80,80,80,80	0
56	MG	1a	1750	1/1	0.84	0.16	62,62,62,62	0
56	MG	1A	4034	1/1	0.84	0.12	59,59,59,59	0
56	MG	1A	3795	1/1	0.84	0.15	50,50,50,50	0
56	MG	1A	4046	1/1	0.84	0.19	66,66,66,66	0
56	MG	2a	1695	1/1	0.84	0.23	80,80,80,80	0
56	MG	1A	3246	1/1	0.84	0.13	69,69,69,69	0
56	MG	2A	3204	1/1	0.84	0.16	61,61,61,61	0
56	MG	1a	1793	1/1	0.84	0.17	68,68,68,68	0
56	MG	1a	1797	1/1	0.84	0.16	68,68,68,68	0
56	MG	1a	1631	1/1	0.84	0.34	69,69,69,69	0
56	MG	1A	3493	1/1	0.84	0.23	77,77,77,77	0
56	MG	2A	3456	1/1	0.84	0.35	77,77,77,77	0
56	MG	2a	1731	1/1	0.84	0.15	79,79,79,79	0
56	MG	2a	1748	1/1	0.84	0.14	80,80,80,80	0
56	MG	2A	3467	1/1	0.84	0.11	44,44,44,44	0
56	MG	2A	3236	1/1	0.84	0.21	72,72,72,72	0
56	MG	2a	1759	1/1	0.84	0.29	74,74,74,74	0
56	MG	2a	1762	1/1	0.84	0.24	77,77,77,77	0
56	MG	2A	3739	1/1	0.84	0.13	63,63,63,63	0
56	MG	1A	3494	1/1	0.84	0.10	69,69,69,69	0
56	MG	1a	1655	1/1	0.84	0.23	60,60,60,60	0
56	MG	1A	3505	1/1	0.84	0.28	55,55,55,55	0
56	MG	2A	3759	1/1	0.84	0.13	64,64,64,64	0
56	MG	2A	3247	1/1	0.84	0.14	74,74,74,74	0
56	MG	1A	3313	1/1	0.84	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1661	1/1	0.84	0.19	63,63,63,63	0
56	MG	2B	203	1/1	0.84	0.28	77,77,77,77	0
56	MG	1A	3053	1/1	0.84	0.13	56,56,56,56	0
56	MG	2B	208	1/1	0.84	0.33	73,73,73,73	0
56	MG	2a	1788	1/1	0.84	0.14	80,80,80,80	0
56	MG	2A	3529	1/1	0.84	0.19	66,66,66,66	0
56	MG	2a	1790	1/1	0.84	0.33	75,75,75,75	0
56	MG	2A	3556	1/1	0.84	0.21	47,47,47,47	0
56	MG	2A	3565	1/1	0.84	0.17	57,57,57,57	0
56	MG	2B	218	1/1	0.84	0.34	76,76,76,76	0
56	MG	2l	205	1/1	0.84	0.15	71,71,71,71	0
56	MG	2A	3569	1/1	0.84	0.24	70,70,70,70	0
56	MG	1A	3555	1/1	0.84	0.16	50,50,50,50	0
56	MG	1a	1673	1/1	0.84	0.29	57,57,57,57	0
56	MG	14	101	1/1	0.85	0.24	77,77,77,77	0
56	MG	1A	3833	1/1	0.85	0.11	30,30,30,30	0
56	MG	1a	1613	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3140	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3261	1/1	0.85	0.30	68,68,68,68	0
56	MG	2a	1605	1/1	0.85	0.28	67,67,67,67	0
56	MG	2A	3309	1/1	0.85	0.21	76,76,76,76	0
56	MG	1A	3766	1/1	0.85	0.13	45,45,45,45	0
56	MG	2A	3164	1/1	0.85	0.24	72,72,72,72	0
56	MG	2A	3326	1/1	0.85	0.10	68,68,68,68	0
56	MG	1A	3399	1/1	0.85	0.13	52,52,52,52	0
56	MG	1A	3309	1/1	0.85	0.18	57,57,57,57	0
56	MG	1A	3159	1/1	0.85	0.30	66,66,66,66	0
56	MG	1a	1638	1/1	0.85	0.24	66,66,66,66	0
56	MG	1a	1790	1/1	0.85	0.23	65,65,65,65	0
56	MG	2A	3350	1/1	0.85	0.39	65,65,65,65	0
56	MG	2A	3356	1/1	0.85	0.35	70,70,70,70	0
56	MG	2A	3644	1/1	0.85	0.17	62,62,62,62	0
56	MG	1A	3682	1/1	0.85	0.20	67,67,67,67	0
56	MG	1a	1652	1/1	0.85	0.26	65,65,65,65	0
56	MG	1A	3024	1/1	0.85	0.23	57,57,57,57	0
56	MG	2A	3652	1/1	0.85	0.21	62,62,62,62	0
56	MG	2A	3200	1/1	0.85	0.13	57,57,57,57	0
56	MG	1A	3578	1/1	0.85	0.12	49,49,49,49	0
56	MG	2A	3406	1/1	0.85	0.27	82,82,82,82	0
56	MG	2A	3661	1/1	0.85	0.15	60,60,60,60	0
56	MG	2a	1658	1/1	0.85	0.17	75,75,75,75	0
56	MG	2A	3408	1/1	0.85	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1686	1/1	0.85	0.39	77,77,77,77	0
56	MG	2a	1688	1/1	0.85	0.28	66,66,66,66	0
56	MG	2A	3409	1/1	0.85	0.14	67,67,67,67	0
56	MG	2a	1692	1/1	0.85	0.35	71,71,71,71	0
56	MG	2A	3682	1/1	0.85	0.20	69,69,69,69	0
56	MG	1A	4011	1/1	0.85	0.21	72,72,72,72	0
56	MG	2A	3206	1/1	0.85	0.11	71,71,71,71	0
56	MG	1A	3702	1/1	0.85	0.17	65,65,65,65	0
56	MG	1A	4019	1/1	0.85	0.11	55,55,55,55	0
56	MG	2A	3002	1/1	0.85	0.31	71,71,71,71	0
56	MG	2A	3706	1/1	0.85	0.13	65,65,65,65	0
56	MG	2A	3014	1/1	0.85	0.20	67,67,67,67	0
56	MG	2A	3710	1/1	0.85	0.13	60,60,60,60	0
56	MG	1A	4023	1/1	0.85	0.13	50,50,50,50	0
56	MG	2A	3023	1/1	0.85	0.22	70,70,70,70	0
56	MG	2A	3721	1/1	0.85	0.15	50,50,50,50	0
56	MG	2A	3025	1/1	0.85	0.11	52,52,52,52	0
56	MG	1Q	205	1/1	0.85	0.14	57,57,57,57	0
56	MG	2A	3245	1/1	0.85	0.16	76,76,76,76	0
56	MG	2A	3502	1/1	0.85	0.18	50,50,50,50	0
56	MG	1a	1675	1/1	0.85	0.39	68,68,68,68	0
56	MG	1A	3513	1/1	0.85	0.11	69,69,69,69	0
56	MG	2A	3057	1/1	0.85	0.27	57,57,57,57	0
56	MG	1a	1689	1/1	0.85	0.14	67,67,67,67	0
56	MG	2A	3768	1/1	0.85	0.13	66,66,66,66	0
56	MG	1A	3528	1/1	0.85	0.29	54,54,54,54	0
56	MG	2A	3778	1/1	0.85	0.30	69,69,69,69	0
56	MG	1Z	302	1/1	0.85	0.11	58,58,58,58	0
56	MG	2A	3534	1/1	0.85	0.12	68,68,68,68	0
56	MG	2A	3536	1/1	0.85	0.11	38,38,38,38	0
56	MG	2B	209	1/1	0.85	0.25	71,71,71,71	0
56	MG	2A	3549	1/1	0.85	0.16	65,65,65,65	0
56	MG	1a	1701	1/1	0.85	0.46	70,70,70,70	0
56	MG	2A	3563	1/1	0.85	0.17	47,47,47,47	0
56	MG	2A	3269	1/1	0.85	0.20	71,71,71,71	0
56	MG	2A	3273	1/1	0.85	0.13	72,72,72,72	0
56	MG	2A	3574	1/1	0.85	0.18	75,75,75,75	0
56	MG	1A	3831	1/1	0.85	0.13	47,47,47,47	0
56	MG	1a	1723	1/1	0.85	0.17	67,67,67,67	0
56	MG	2A	3181	1/1	0.86	0.14	60,60,60,60	0
56	MG	1B	224	1/1	0.86	0.14	66,66,66,66	0
56	MG	2a	1603	1/1	0.86	0.27	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1604	1/1	0.86	0.20	72,72,72,72	0
56	MG	2A	3189	1/1	0.86	0.17	58,58,58,58	0
56	MG	1A	3350	1/1	0.86	0.21	64,64,64,64	0
56	MG	2A	3364	1/1	0.86	0.21	64,64,64,64	0
56	MG	2A	3192	1/1	0.86	0.15	65,65,65,65	0
56	MG	1A	3402	1/1	0.86	0.29	69,69,69,69	0
56	MG	2A	3374	1/1	0.86	0.18	64,64,64,64	0
56	MG	2a	1616	1/1	0.86	0.18	67,67,67,67	0
56	MG	1A	3815	1/1	0.86	0.13	65,65,65,65	0
56	MG	1A	3451	1/1	0.86	0.27	55,55,55,55	0
56	MG	1A	3717	1/1	0.86	0.12	48,48,48,48	0
56	MG	2A	3205	1/1	0.86	0.17	66,66,66,66	0
56	MG	1x	107	1/1	0.86	0.18	74,74,74,74	0
56	MG	1x	109	1/1	0.86	0.24	68,68,68,68	0
56	MG	1a	1660	1/1	0.86	0.23	69,69,69,69	0
56	MG	2A	3422	1/1	0.86	0.26	61,61,61,61	0
56	MG	1A	3729	1/1	0.86	0.11	23,23,23,23	0
56	MG	1A	3985	1/1	0.86	0.12	79,79,79,79	0
56	MG	2a	1641	1/1	0.86	0.12	56,56,56,56	0
56	MG	1A	3834	1/1	0.86	0.18	54,54,54,54	0
56	MG	1A	3458	1/1	0.86	0.15	47,47,47,47	0
56	MG	2A	3435	1/1	0.86	0.17	38,38,38,38	0
56	MG	1A	3466	1/1	0.86	0.19	61,61,61,61	0
56	MG	2a	1647	1/1	0.86	0.13	75,75,75,75	0
56	MG	1A	3765	1/1	0.86	0.11	26,26,26,26	0
56	MG	1a	1681	1/1	0.86	0.26	67,67,67,67	0
56	MG	1A	3352	1/1	0.86	0.21	59,59,59,59	0
56	MG	2a	1668	1/1	0.86	0.20	68,68,68,68	0
56	MG	2a	1673	1/1	0.86	0.22	72,72,72,72	0
56	MG	1A	4012	1/1	0.86	0.08	19,19,19,19	0
56	MG	1a	1695	1/1	0.86	0.18	68,68,68,68	0
56	MG	1A	3642	1/1	0.86	0.07	21,21,21,21	0
56	MG	2a	1691	1/1	0.86	0.35	66,66,66,66	0
56	MG	1A	3353	1/1	0.86	0.18	54,54,54,54	0
56	MG	2A	3089	1/1	0.86	0.35	76,76,76,76	0
56	MG	1A	4020	1/1	0.86	0.11	34,34,34,34	0
56	MG	1A	3409	1/1	0.86	0.22	51,51,51,51	0
56	MG	2a	1699	1/1	0.86	0.18	72,72,72,72	0
56	MG	2A	3738	1/1	0.86	0.11	68,68,68,68	0
56	MG	2A	3270	1/1	0.86	0.16	61,61,61,61	0
56	MG	2A	3745	1/1	0.86	0.17	51,51,51,51	0
56	MG	2A	3099	1/1	0.86	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1710	1/1	0.86	0.28	76,76,76,76	0
56	MG	2a	1718	1/1	0.86	0.36	82,82,82,82	0
56	MG	2A	3277	1/1	0.86	0.16	70,70,70,70	0
56	MG	15	108	1/1	0.86	0.16	60,60,60,60	0
56	MG	1a	1731	1/1	0.86	0.27	78,78,78,78	0
56	MG	2A	3285	1/1	0.86	0.29	80,80,80,80	0
56	MG	2A	3763	1/1	0.86	0.20	62,62,62,62	0
56	MG	2A	3562	1/1	0.86	0.24	75,75,75,75	0
56	MG	2A	3767	1/1	0.86	0.18	58,58,58,58	0
56	MG	16	103	1/1	0.86	0.30	53,53,53,53	0
56	MG	1A	3781	1/1	0.86	0.14	61,61,61,61	0
56	MG	1a	1604	1/1	0.86	0.18	66,66,66,66	0
56	MG	2A	3571	1/1	0.86	0.34	75,75,75,75	0
56	MG	2a	1771	1/1	0.86	0.17	67,67,67,67	0
56	MG	2A	3151	1/1	0.86	0.12	80,80,80,80	0
56	MG	1A	3925	1/1	0.86	0.10	31,31,31,31	0
56	MG	2A	3308	1/1	0.86	0.22	46,46,46,46	0
56	MG	1A	3316	1/1	0.86	0.24	58,58,58,58	0
56	MG	1A	3693	1/1	0.86	0.18	59,59,59,59	0
56	MG	1B	203	1/1	0.86	0.29	64,64,64,64	0
56	MG	1B	212	1/1	0.86	0.15	61,61,61,61	0
56	MG	2A	3593	1/1	0.86	0.13	61,61,61,61	0
56	MG	2D	307	1/1	0.86	0.18	67,67,67,67	0
56	MG	2A	3328	1/1	0.86	0.17	79,79,79,79	0
56	MG	2A	3596	1/1	0.86	0.24	66,66,66,66	0
56	MG	2F	306	1/1	0.86	0.18	67,67,67,67	0
56	MG	1a	1783	1/1	0.86	0.20	68,68,68,68	0
56	MG	2O	202	1/1	0.86	0.16	56,56,56,56	0
56	MG	1a	1788	1/1	0.86	0.28	74,74,74,74	0
56	MG	2w	101	1/1	0.86	0.33	71,71,71,71	0
56	MG	1A	3562	1/1	0.86	0.31	69,69,69,69	0
56	MG	2A	3613	1/1	0.86	0.12	66,66,66,66	0
56	MG	2E	305	1/1	0.87	0.17	68,68,68,68	0
56	MG	1A	4051	1/1	0.87	0.19	51,51,51,51	0
56	MG	2A	3152	1/1	0.87	0.11	68,68,68,68	0
56	MG	2A	3578	1/1	0.87	0.17	71,71,71,71	0
56	MG	1a	1758	1/1	0.87	0.14	62,62,62,62	0
56	MG	1a	1627	1/1	0.87	0.23	70,70,70,70	0
56	MG	1a	1765	1/1	0.87	0.12	69,69,69,69	0
56	MG	1A	3336	1/1	0.87	0.13	65,65,65,65	0
56	MG	1A	3153	1/1	0.87	0.14	41,41,41,41	0
56	MG	2A	3169	1/1	0.87	0.32	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3319	1/1	0.87	0.22	76,76,76,76	0
56	MG	2A	3170	1/1	0.87	0.15	74,74,74,74	0
56	MG	1a	1635	1/1	0.87	0.23	58,58,58,58	0
56	MG	2A	3597	1/1	0.87	0.13	66,66,66,66	0
56	MG	2A	3599	1/1	0.87	0.16	64,64,64,64	0
56	MG	1B	214	1/1	0.87	0.15	59,59,59,59	0
56	MG	2A	3604	1/1	0.87	0.12	52,52,52,52	0
56	MG	2A	3608	1/1	0.87	0.14	62,62,62,62	0
56	MG	1a	1784	1/1	0.87	0.14	69,69,69,69	0
56	MG	1A	3312	1/1	0.87	0.29	66,66,66,66	0
56	MG	2a	1618	1/1	0.87	0.16	76,76,76,76	0
56	MG	2A	3334	1/1	0.87	0.12	71,71,71,71	0
56	MG	2A	3339	1/1	0.87	0.23	47,47,47,47	0
56	MG	2A	3616	1/1	0.87	0.18	68,68,68,68	0
56	MG	2A	3340	1/1	0.87	0.20	59,59,59,59	0
56	MG	1B	218	1/1	0.87	0.10	55,55,55,55	0
56	MG	1a	1650	1/1	0.87	0.14	58,58,58,58	0
56	MG	1A	3579	1/1	0.87	0.12	34,34,34,34	0
56	MG	2a	1633	1/1	0.87	0.24	67,67,67,67	0
56	MG	2A	3351	1/1	0.87	0.31	67,67,67,67	0
56	MG	2a	1636	1/1	0.87	0.48	81,81,81,81	0
56	MG	1a	1798	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3360	1/1	0.87	0.26	55,55,55,55	0
56	MG	2A	3362	1/1	0.87	0.17	58,58,58,58	0
56	MG	2A	3193	1/1	0.87	0.28	70,70,70,70	0
56	MG	1a	1653	1/1	0.87	0.16	65,65,65,65	0
56	MG	2A	3366	1/1	0.87	0.31	62,62,62,62	0
56	MG	2A	3198	1/1	0.87	0.11	56,56,56,56	0
56	MG	2a	1649	1/1	0.87	0.25	80,80,80,80	0
56	MG	2A	3369	1/1	0.87	0.29	62,62,62,62	0
56	MG	2a	1655	1/1	0.87	0.09	75,75,75,75	0
56	MG	1A	3968	1/1	0.87	0.09	27,27,27,27	0
56	MG	1u	101	1/1	0.87	0.23	70,70,70,70	0
56	MG	1A	3978	1/1	0.87	0.10	59,59,59,59	0
56	MG	1A	3251	1/1	0.87	0.16	56,56,56,56	0
56	MG	2a	1680	1/1	0.87	0.16	75,75,75,75	0
56	MG	2a	1685	1/1	0.87	0.19	72,72,72,72	0
56	MG	2A	3398	1/1	0.87	0.32	76,76,76,76	0
56	MG	1A	3595	1/1	0.87	0.20	59,59,59,59	0
56	MG	1A	3433	1/1	0.87	0.29	68,68,68,68	0
56	MG	2a	1690	1/1	0.87	0.12	77,77,77,77	0
56	MG	2A	3213	1/1	0.87	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3355	1/1	0.87	0.10	52,52,52,52	0
56	MG	2A	3224	1/1	0.87	0.24	65,65,65,65	0
56	MG	1A	3868	1/1	0.87	0.20	57,57,57,57	0
56	MG	2A	3704	1/1	0.87	0.15	68,68,68,68	0
56	MG	2A	3705	1/1	0.87	0.19	75,75,75,75	0
56	MG	1A	3097	1/1	0.87	0.13	68,68,68,68	0
56	MG	1a	1674	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3708	1/1	0.87	0.19	88,88,88,88	0
56	MG	1A	3634	1/1	0.87	0.12	32,32,32,32	0
56	MG	2A	3239	1/1	0.87	0.26	74,74,74,74	0
56	MG	2a	1712	1/1	0.87	0.23	65,65,65,65	0
56	MG	2A	3437	1/1	0.87	0.22	81,81,81,81	0
56	MG	2a	1727	1/1	0.87	0.23	61,61,61,61	0
56	MG	1A	4010	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3895	1/1	0.87	0.10	54,54,54,54	0
56	MG	2a	1736	1/1	0.87	0.12	68,68,68,68	0
56	MG	2A	3460	1/1	0.87	0.21	55,55,55,55	0
56	MG	1A	3265	1/1	0.87	0.11	53,53,53,53	0
56	MG	2a	1751	1/1	0.87	0.14	69,69,69,69	0
56	MG	2A	3472	1/1	0.87	0.14	50,50,50,50	0
56	MG	2A	3746	1/1	0.87	0.18	66,66,66,66	0
56	MG	2A	3479	1/1	0.87	0.13	69,69,69,69	0
56	MG	1a	1690	1/1	0.87	0.32	68,68,68,68	0
56	MG	1A	3674	1/1	0.87	0.14	30,30,30,30	0
56	MG	1A	3529	1/1	0.87	0.13	50,50,50,50	0
56	MG	1A	3317	1/1	0.87	0.14	54,54,54,54	0
56	MG	1A	3308	1/1	0.87	0.17	59,59,59,59	0
56	MG	2A	3506	1/1	0.87	0.12	63,63,63,63	0
56	MG	1a	1717	1/1	0.87	0.19	76,76,76,76	0
56	MG	1A	3938	1/1	0.87	0.14	80,80,80,80	0
56	MG	2a	1779	1/1	0.87	0.34	65,65,65,65	0
56	MG	1A	3319	1/1	0.87	0.24	66,66,66,66	0
56	MG	2a	1781	1/1	0.87	0.20	74,74,74,74	0
56	MG	1A	4043	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3779	1/1	0.87	0.20	71,71,71,71	0
56	MG	2A	3780	1/1	0.87	0.16	61,61,61,61	0
56	MG	2A	3527	1/1	0.87	0.16	65,65,65,65	0
56	MG	1A	3804	1/1	0.87	0.11	56,56,56,56	0
56	MG	2A	3274	1/1	0.87	0.32	77,77,77,77	0
56	MG	2a	1792	1/1	0.87	0.22	64,64,64,64	0
56	MG	2A	3276	1/1	0.87	0.19	57,57,57,57	0
56	MG	1a	1738	1/1	0.87	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3279	1/1	0.87	0.21	70,70,70,70	0
56	MG	1A	4045	1/1	0.87	0.16	68,68,68,68	0
56	MG	2A	3134	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3333	1/1	0.87	0.12	57,57,57,57	0
56	MG	2A	3568	1/1	0.87	0.14	57,57,57,57	0
56	MG	1A	4050	1/1	0.87	0.16	62,62,62,62	0
56	MG	1A	3802	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3803	1/1	0.88	0.11	40,40,40,40	0
56	MG	1A	3526	1/1	0.88	0.29	60,60,60,60	0
56	MG	2A	3291	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3442	1/1	0.88	0.20	68,68,68,68	0
56	MG	2Q	202	1/1	0.88	0.26	65,65,65,65	0
56	MG	2R	201	1/1	0.88	0.13	64,64,64,64	0
56	MG	1O	205	1/1	0.88	0.13	67,67,67,67	0
56	MG	2V	202	1/1	0.88	0.17	71,71,71,71	0
56	MG	1A	3026	1/1	0.88	0.13	58,58,58,58	0
56	MG	2A	3108	1/1	0.88	0.26	77,77,77,77	0
56	MG	25	104	1/1	0.88	0.13	63,63,63,63	0
56	MG	2A	3109	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3310	1/1	0.88	0.14	68,68,68,68	0
56	MG	1a	1706	1/1	0.88	0.21	68,68,68,68	0
56	MG	2A	3131	1/1	0.88	0.52	68,68,68,68	0
56	MG	1A	3259	1/1	0.88	0.17	62,62,62,62	0
56	MG	2A	3322	1/1	0.88	0.25	58,58,58,58	0
56	MG	1A	3820	1/1	0.88	0.16	46,46,46,46	0
56	MG	2a	1610	1/1	0.88	0.24	67,67,67,67	0
56	MG	1U	207	1/1	0.88	0.15	59,59,59,59	0
56	MG	1A	3684	1/1	0.88	0.14	59,59,59,59	0
56	MG	2A	3600	1/1	0.88	0.21	62,62,62,62	0
56	MG	1A	3996	1/1	0.88	0.15	58,58,58,58	0
56	MG	1a	1732	1/1	0.88	0.12	75,75,75,75	0
56	MG	1A	3827	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3335	1/1	0.88	0.17	67,67,67,67	0
56	MG	2A	3336	1/1	0.88	0.34	59,59,59,59	0
56	MG	2A	3158	1/1	0.88	0.18	63,63,63,63	0
56	MG	1A	3100	1/1	0.88	0.10	38,38,38,38	0
56	MG	1A	3460	1/1	0.88	0.15	53,53,53,53	0
56	MG	2a	1626	1/1	0.88	0.28	66,66,66,66	0
56	MG	2A	3617	1/1	0.88	0.10	68,68,68,68	0
56	MG	15	107	1/1	0.88	0.16	61,61,61,61	0
56	MG	2A	3347	1/1	0.88	0.27	68,68,68,68	0
56	MG	1A	3463	1/1	0.88	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1635	1/1	0.88	0.28	63,63,63,63	0
56	MG	1a	1755	1/1	0.88	0.17	51,51,51,51	0
56	MG	2A	3171	1/1	0.88	0.22	70,70,70,70	0
56	MG	2A	3635	1/1	0.88	0.10	63,63,63,63	0
56	MG	1A	4013	1/1	0.88	0.16	63,63,63,63	0
56	MG	1A	3843	1/1	0.88	0.16	45,45,45,45	0
56	MG	1A	3241	1/1	0.88	0.09	61,61,61,61	0
56	MG	1a	1772	1/1	0.88	0.24	71,71,71,71	0
56	MG	1a	1776	1/1	0.88	0.14	62,62,62,62	0
56	MG	2A	3648	1/1	0.88	0.10	59,59,59,59	0
56	MG	1a	1607	1/1	0.88	0.27	65,65,65,65	0
56	MG	1A	3706	1/1	0.88	0.10	53,53,53,53	0
56	MG	2A	3370	1/1	0.88	0.30	61,61,61,61	0
56	MG	1A	3566	1/1	0.88	0.31	70,70,70,70	0
56	MG	1A	3286	1/1	0.88	0.23	70,70,70,70	0
56	MG	2A	3660	1/1	0.88	0.14	62,62,62,62	0
56	MG	2a	1676	1/1	0.88	0.15	68,68,68,68	0
56	MG	1a	1625	1/1	0.88	0.25	61,61,61,61	0
56	MG	2a	1681	1/1	0.88	0.18	62,62,62,62	0
56	MG	1a	1787	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3667	1/1	0.88	0.28	65,65,65,65	0
56	MG	2A	3389	1/1	0.88	0.25	61,61,61,61	0
56	MG	1A	4033	1/1	0.88	0.12	53,53,53,53	0
56	MG	2A	3687	1/1	0.88	0.18	58,58,58,58	0
56	MG	1a	1789	1/1	0.88	0.20	64,64,64,64	0
56	MG	1A	3294	1/1	0.88	0.19	63,63,63,63	0
56	MG	2a	1694	1/1	0.88	0.24	76,76,76,76	0
56	MG	1A	4036	1/1	0.88	0.11	43,43,43,43	0
56	MG	2a	1696	1/1	0.88	0.17	67,67,67,67	0
56	MG	1a	1632	1/1	0.88	0.27	78,78,78,78	0
56	MG	1A	3296	1/1	0.88	0.27	58,58,58,58	0
56	MG	1A	3756	1/1	0.88	0.09	46,46,46,46	0
56	MG	2A	3218	1/1	0.88	0.26	67,67,67,67	0
56	MG	1l	202	1/1	0.88	0.15	60,60,60,60	0
56	MG	1A	3415	1/1	0.88	0.24	50,50,50,50	0
56	MG	2a	1703	1/1	0.88	0.22	68,68,68,68	0
56	MG	1a	1642	1/1	0.88	0.17	64,64,64,64	0
56	MG	1A	3764	1/1	0.88	0.11	28,28,28,28	0
56	MG	2A	3438	1/1	0.88	0.10	37,37,37,37	0
56	MG	2a	1714	1/1	0.88	0.24	69,69,69,69	0
56	MG	2A	3716	1/1	0.88	0.15	56,56,56,56	0
56	MG	2a	1719	1/1	0.88	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4049	1/1	0.88	0.29	52,52,52,52	0
56	MG	2A	3449	1/1	0.88	0.10	60,60,60,60	0
56	MG	1A	3431	1/1	0.88	0.23	47,47,47,47	0
56	MG	2A	3736	1/1	0.88	0.15	52,52,52,52	0
56	MG	2a	1742	1/1	0.88	0.16	74,74,74,74	0
56	MG	2A	3459	1/1	0.88	0.28	62,62,62,62	0
56	MG	1A	3076	1/1	0.88	0.10	29,29,29,29	0
56	MG	1a	1654	1/1	0.88	0.11	68,68,68,68	0
56	MG	1x	112	1/1	0.88	0.23	62,62,62,62	0
56	MG	1A	3495	1/1	0.88	0.14	76,76,76,76	0
56	MG	2A	3003	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3754	1/1	0.88	0.11	61,61,61,61	0
56	MG	2A	3489	1/1	0.88	0.14	59,59,59,59	0
56	MG	1A	3613	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3941	1/1	0.88	0.13	65,65,65,65	0
56	MG	2A	3257	1/1	0.88	0.16	63,63,63,63	0
56	MG	2a	1773	1/1	0.88	0.19	68,68,68,68	0
56	MG	1A	3387	1/1	0.88	0.20	63,63,63,63	0
56	MG	2a	1775	1/1	0.88	0.25	70,70,70,70	0
56	MG	2A	3504	1/1	0.88	0.19	78,78,78,78	0
56	MG	1A	3948	1/1	0.88	0.12	38,38,38,38	0
56	MG	2a	1778	1/1	0.88	0.19	68,68,68,68	0
56	MG	2A	3773	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3776	1/1	0.88	0.18	72,72,72,72	0
56	MG	2A	3512	1/1	0.88	0.20	70,70,70,70	0
56	MG	2A	3515	1/1	0.88	0.18	67,67,67,67	0
56	MG	2A	3033	1/1	0.88	0.32	74,74,74,74	0
56	MG	2A	3036	1/1	0.88	0.16	63,63,63,63	0
56	MG	1A	3631	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3329	1/1	0.88	0.18	53,53,53,53	0
56	MG	2B	205	1/1	0.88	0.19	65,65,65,65	0
56	MG	2A	3272	1/1	0.88	0.19	69,69,69,69	0
56	MG	1A	3955	1/1	0.88	0.11	54,54,54,54	0
56	MG	1A	3799	1/1	0.88	0.15	52,52,52,52	0
56	MG	2a	1800	1/1	0.88	0.28	60,60,60,60	0
56	MG	2a	1801	1/1	0.88	0.13	74,74,74,74	0
56	MG	2A	3058	1/1	0.88	0.30	69,69,69,69	0
56	MG	2A	3543	1/1	0.88	0.19	65,65,65,65	0
56	MG	2A	3070	1/1	0.88	0.18	55,55,55,55	0
56	MG	2r	101	1/1	0.88	0.14	79,79,79,79	0
56	MG	2v	101	1/1	0.88	0.31	65,65,65,65	0
56	MG	1A	3514	1/1	0.88	0.14	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1D	312	1/1	0.88	0.18	39,39,39,39	0
56	MG	1A	3664	1/1	0.88	0.13	47,47,47,47	0
56	MG	2x	104	1/1	0.88	0.18	70,70,70,70	0
56	MG	1A	3928	1/1	0.89	0.10	45,45,45,45	0
56	MG	2P	202	1/1	0.89	0.20	55,55,55,55	0
56	MG	2A	3325	1/1	0.89	0.24	64,64,64,64	0
56	MG	1A	3501	1/1	0.89	0.08	67,67,67,67	0
56	MG	2R	202	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3327	1/1	0.89	0.16	69,69,69,69	0
56	MG	2V	201	1/1	0.89	0.36	48,48,48,48	0
56	MG	1A	3446	1/1	0.89	0.17	57,57,57,57	0
56	MG	2W	201	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3159	1/1	0.89	0.20	57,57,57,57	0
56	MG	1A	3050	1/1	0.89	0.18	40,40,40,40	0
56	MG	20	101	1/1	0.89	0.16	72,72,72,72	0
56	MG	2A	3592	1/1	0.89	0.17	44,44,44,44	0
56	MG	1a	1626	1/1	0.89	0.14	62,62,62,62	0
56	MG	1A	3322	1/1	0.89	0.23	55,55,55,55	0
56	MG	1A	3704	1/1	0.89	0.11	54,54,54,54	0
56	MG	1B	201	1/1	0.89	0.09	49,49,49,49	0
56	MG	2A	3338	1/1	0.89	0.26	57,57,57,57	0
56	MG	1A	3357	1/1	0.89	0.11	50,50,50,50	0
56	MG	1a	1634	1/1	0.89	0.17	57,57,57,57	0
56	MG	2a	1609	1/1	0.89	0.45	76,76,76,76	0
56	MG	1a	1786	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3606	1/1	0.89	0.15	57,57,57,57	0
56	MG	1A	3527	1/1	0.89	0.23	56,56,56,56	0
56	MG	2A	3178	1/1	0.89	0.14	64,64,64,64	0
56	MG	1A	3817	1/1	0.89	0.11	55,55,55,55	0
56	MG	1B	215	1/1	0.89	0.25	71,71,71,71	0
56	MG	2A	3614	1/1	0.89	0.15	76,76,76,76	0
56	MG	1A	3140	1/1	0.89	0.20	47,47,47,47	0
56	MG	1A	3961	1/1	0.89	0.20	28,28,28,28	0
56	MG	1A	3372	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3619	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3363	1/1	0.89	0.15	50,50,50,50	0
56	MG	1A	3735	1/1	0.89	0.11	38,38,38,38	0
56	MG	2A	3194	1/1	0.89	0.20	69,69,69,69	0
56	MG	2A	3628	1/1	0.89	0.15	60,60,60,60	0
56	MG	1B	226	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3628	1/1	0.89	0.07	28,28,28,28	0
56	MG	1m	3002	1/1	0.89	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3976	1/1	0.89	0.12	55,55,55,55	0
56	MG	2a	1638	1/1	0.89	0.16	63,63,63,63	0
56	MG	2A	3642	1/1	0.89	0.18	60,60,60,60	0
56	MG	1A	3630	1/1	0.89	0.07	21,21,21,21	0
56	MG	1w	101	1/1	0.89	0.09	73,73,73,73	0
56	MG	1x	104	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3428	1/1	0.89	0.15	64,64,64,64	0
56	MG	1E	307	1/1	0.89	0.16	55,55,55,55	0
56	MG	2A	3394	1/1	0.89	0.15	66,66,66,66	0
56	MG	2A	3215	1/1	0.89	0.21	62,62,62,62	0
56	MG	2a	1651	1/1	0.89	0.09	66,66,66,66	0
56	MG	2A	3653	1/1	0.89	0.09	63,63,63,63	0
56	MG	2A	3399	1/1	0.89	0.29	63,63,63,63	0
56	MG	2A	3400	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3180	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3849	1/1	0.89	0.12	44,44,44,44	0
56	MG	2a	1672	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3221	1/1	0.89	0.24	73,73,73,73	0
56	MG	2a	1674	1/1	0.89	0.23	71,71,71,71	0
56	MG	2A	3662	1/1	0.89	0.10	41,41,41,41	0
56	MG	1x	110	1/1	0.89	0.10	62,62,62,62	0
56	MG	2A	3414	1/1	0.89	0.22	71,71,71,71	0
56	MG	2a	1682	1/1	0.89	0.34	65,65,65,65	0
56	MG	2a	1683	1/1	0.89	0.24	65,65,65,65	0
56	MG	1a	1663	1/1	0.89	0.32	72,72,72,72	0
56	MG	2A	3672	1/1	0.89	0.13	58,58,58,58	0
56	MG	2a	1687	1/1	0.89	0.21	60,60,60,60	0
56	MG	2A	3676	1/1	0.89	0.16	42,42,42,42	0
56	MG	2A	3230	1/1	0.89	0.19	60,60,60,60	0
56	MG	1F	304	1/1	0.89	0.18	69,69,69,69	0
56	MG	1A	3298	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3694	1/1	0.89	0.20	76,76,76,76	0
56	MG	2A	3696	1/1	0.89	0.14	78,78,78,78	0
56	MG	1A	3862	1/1	0.89	0.17	74,74,74,74	0
56	MG	1A	3339	1/1	0.89	0.17	72,72,72,72	0
56	MG	1a	1678	1/1	0.89	0.28	67,67,67,67	0
56	MG	1A	3670	1/1	0.89	0.08	27,27,27,27	0
56	MG	1A	3873	1/1	0.89	0.09	50,50,50,50	0
56	MG	1a	1683	1/1	0.89	0.26	60,60,60,60	0
56	MG	2A	3451	1/1	0.89	0.20	67,67,67,67	0
56	MG	2A	3249	1/1	0.89	0.34	64,64,64,64	0
56	MG	1A	3341	1/1	0.89	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1707	1/1	0.89	0.29	62,62,62,62	0
56	MG	2A	3251	1/1	0.89	0.19	62,62,62,62	0
56	MG	2A	3462	1/1	0.89	0.22	61,61,61,61	0
56	MG	1A	3072	1/1	0.89	0.26	63,63,63,63	0
56	MG	1R	203	1/1	0.89	0.24	44,44,44,44	0
56	MG	2a	1716	1/1	0.89	0.34	77,77,77,77	0
56	MG	2a	1717	1/1	0.89	0.15	71,71,71,71	0
56	MG	1A	3777	1/1	0.89	0.12	45,45,45,45	0
56	MG	2A	3259	1/1	0.89	0.27	73,73,73,73	0
56	MG	2a	1725	1/1	0.89	0.28	65,65,65,65	0
56	MG	1A	3897	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	4015	1/1	0.89	0.15	53,53,53,53	0
56	MG	1a	1702	1/1	0.89	0.35	62,62,62,62	0
56	MG	1A	3570	1/1	0.89	0.10	57,57,57,57	0
56	MG	2a	1737	1/1	0.89	0.26	74,74,74,74	0
56	MG	2a	1738	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1715	1/1	0.89	0.13	63,63,63,63	0
56	MG	2A	3083	1/1	0.89	0.15	51,51,51,51	0
56	MG	1A	3912	1/1	0.89	0.09	59,59,59,59	0
56	MG	2A	3507	1/1	0.89	0.25	63,63,63,63	0
56	MG	10	106	1/1	0.89	0.10	56,56,56,56	0
56	MG	2A	3514	1/1	0.89	0.09	66,66,66,66	0
56	MG	1a	1722	1/1	0.89	0.17	71,71,71,71	0
56	MG	2A	3761	1/1	0.89	0.13	66,66,66,66	0
56	MG	2A	3762	1/1	0.89	0.22	74,74,74,74	0
56	MG	10	107	1/1	0.89	0.09	71,71,71,71	0
56	MG	11	104	1/1	0.89	0.14	64,64,64,64	0
56	MG	2a	1770	1/1	0.89	0.17	68,68,68,68	0
56	MG	2A	3766	1/1	0.89	0.28	67,67,67,67	0
56	MG	1a	1730	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3794	1/1	0.89	0.09	44,44,44,44	0
56	MG	2A	3769	1/1	0.89	0.19	59,59,59,59	0
56	MG	2A	3526	1/1	0.89	0.24	74,74,74,74	0
56	MG	1A	3914	1/1	0.89	0.13	64,64,64,64	0
56	MG	2A	3528	1/1	0.89	0.19	73,73,73,73	0
56	MG	1A	3284	1/1	0.89	0.09	39,39,39,39	0
56	MG	2A	3532	1/1	0.89	0.12	60,60,60,60	0
56	MG	2A	3110	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3781	1/1	0.89	0.45	69,69,69,69	0
56	MG	2B	202	1/1	0.89	0.10	64,64,64,64	0
56	MG	2A	3535	1/1	0.89	0.09	39,39,39,39	0
56	MG	2A	3111	1/1	0.89	0.12	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3539	1/1	0.89	0.18	49,49,49,49	0
56	MG	2A	3293	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3544	1/1	0.89	0.20	71,71,71,71	0
56	MG	2B	210	1/1	0.89	0.12	74,74,74,74	0
56	MG	1a	1739	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3126	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3129	1/1	0.89	0.29	76,76,76,76	0
56	MG	2e	201	1/1	0.89	0.09	76,76,76,76	0
56	MG	2B	216	1/1	0.89	0.11	84,84,84,84	0
56	MG	2l	204	1/1	0.89	0.16	79,79,79,79	0
56	MG	1A	3919	1/1	0.89	0.11	58,58,58,58	0
56	MG	2A	3564	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3922	1/1	0.89	0.08	50,50,50,50	0
56	MG	1a	1603	1/1	0.89	0.12	59,59,59,59	0
56	MG	1a	1746	1/1	0.89	0.16	63,63,63,63	0
56	MG	2A	3570	1/1	0.89	0.19	46,46,46,46	0
56	MG	1A	3574	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3689	1/1	0.89	0.10	39,39,39,39	0
56	MG	2A	3321	1/1	0.90	0.19	63,63,63,63	0
56	MG	1Q	203	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3832	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3448	1/1	0.90	0.16	48,48,48,48	0
56	MG	1T	201	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3006	1/1	0.90	0.15	55,55,55,55	0
56	MG	28	102	1/1	0.90	0.27	52,52,52,52	0
56	MG	2a	1601	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	3835	1/1	0.90	0.10	49,49,49,49	0
56	MG	1A	3838	1/1	0.90	0.06	37,37,37,37	0
56	MG	2A	3605	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	3381	1/1	0.90	0.28	61,61,61,61	0
56	MG	1A	3703	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	3568	1/1	0.90	0.14	44,44,44,44	0
56	MG	2A	3146	1/1	0.90	0.14	46,46,46,46	0
56	MG	2A	3147	1/1	0.90	0.33	70,70,70,70	0
56	MG	2a	1612	1/1	0.90	0.20	60,60,60,60	0
56	MG	2A	3150	1/1	0.90	0.13	59,59,59,59	0
56	MG	1a	1736	1/1	0.90	0.28	65,65,65,65	0
56	MG	2A	3341	1/1	0.90	0.28	58,58,58,58	0
56	MG	1A	3382	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3461	1/1	0.90	0.21	56,56,56,56	0
56	MG	1A	3253	1/1	0.90	0.21	71,71,71,71	0
56	MG	2A	3349	1/1	0.90	0.17	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3870	1/1	0.90	0.13	39,39,39,39	0
56	MG	1A	3724	1/1	0.90	0.20	59,59,59,59	0
56	MG	2A	3163	1/1	0.90	0.23	62,62,62,62	0
56	MG	2A	3358	1/1	0.90	0.26	60,60,60,60	0
56	MG	2A	3634	1/1	0.90	0.16	50,50,50,50	0
56	MG	2a	1627	1/1	0.90	0.34	65,65,65,65	0
56	MG	2a	1628	1/1	0.90	0.11	88,88,88,88	0
56	MG	1A	3725	1/1	0.90	0.13	55,55,55,55	0
56	MG	1a	1748	1/1	0.90	0.11	64,64,64,64	0
56	MG	2A	3640	1/1	0.90	0.09	59,59,59,59	0
56	MG	1A	3881	1/1	0.90	0.11	25,25,25,25	0
56	MG	19	101	1/1	0.90	0.21	60,60,60,60	0
56	MG	1a	1601	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	4029	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3577	1/1	0.90	0.09	27,27,27,27	0
56	MG	1a	1771	1/1	0.90	0.07	84,84,84,84	0
56	MG	1A	3099	1/1	0.90	0.11	68,68,68,68	0
56	MG	2A	3177	1/1	0.90	0.22	63,63,63,63	0
56	MG	1a	1609	1/1	0.90	0.25	57,57,57,57	0
56	MG	1a	1778	1/1	0.90	0.25	63,63,63,63	0
56	MG	1A	3471	1/1	0.90	0.13	45,45,45,45	0
56	MG	1A	3472	1/1	0.90	0.12	46,46,46,46	0
56	MG	1a	1621	1/1	0.90	0.13	64,64,64,64	0
56	MG	1A	3049	1/1	0.90	0.24	42,42,42,42	0
56	MG	2a	1653	1/1	0.90	0.19	80,80,80,80	0
56	MG	1a	1624	1/1	0.90	0.25	60,60,60,60	0
56	MG	2a	1656	1/1	0.90	0.24	67,67,67,67	0
56	MG	1A	3194	1/1	0.90	0.09	43,43,43,43	0
56	MG	1A	3606	1/1	0.90	0.12	65,65,65,65	0
56	MG	2a	1667	1/1	0.90	0.25	74,74,74,74	0
56	MG	1A	3608	1/1	0.90	0.11	40,40,40,40	0
56	MG	1A	3020	1/1	0.90	0.14	48,48,48,48	0
56	MG	2A	3673	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3674	1/1	0.90	0.11	42,42,42,42	0
56	MG	1A	3204	1/1	0.90	0.08	47,47,47,47	0
56	MG	2A	3677	1/1	0.90	0.13	67,67,67,67	0
56	MG	2A	3678	1/1	0.90	0.27	70,70,70,70	0
56	MG	1A	3923	1/1	0.90	0.07	39,39,39,39	0
56	MG	1a	1633	1/1	0.90	0.12	51,51,51,51	0
56	MG	2a	1684	1/1	0.90	0.31	65,65,65,65	0
56	MG	2A	3689	1/1	0.90	0.09	42,42,42,42	0
56	MG	1A	3287	1/1	0.90	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	208	1/1	0.90	0.18	66,66,66,66	0
56	MG	1e	202	1/1	0.90	0.10	74,74,74,74	0
56	MG	2A	3430	1/1	0.90	0.19	73,73,73,73	0
56	MG	2A	3432	1/1	0.90	0.12	77,77,77,77	0
56	MG	1a	1636	1/1	0.90	0.21	56,56,56,56	0
56	MG	1A	3288	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3780	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3220	1/1	0.90	0.09	69,69,69,69	0
56	MG	1t	201	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3442	1/1	0.90	0.18	52,52,52,52	0
56	MG	1A	3930	1/1	0.90	0.14	43,43,43,43	0
56	MG	1a	1644	1/1	0.90	0.16	64,64,64,64	0
56	MG	2A	3452	1/1	0.90	0.09	40,40,40,40	0
56	MG	1w	103	1/1	0.90	0.15	67,67,67,67	0
56	MG	1a	1645	1/1	0.90	0.26	60,60,60,60	0
56	MG	1A	3937	1/1	0.90	0.09	64,64,64,64	0
56	MG	1B	217	1/1	0.90	0.11	62,62,62,62	0
56	MG	2A	3732	1/1	0.90	0.12	38,38,38,38	0
56	MG	1a	1651	1/1	0.90	0.20	57,57,57,57	0
56	MG	2a	1711	1/1	0.90	0.24	58,58,58,58	0
56	MG	1A	3234	1/1	0.90	0.33	46,46,46,46	0
56	MG	2A	3478	1/1	0.90	0.18	49,49,49,49	0
56	MG	1B	222	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3237	1/1	0.90	0.19	67,67,67,67	0
56	MG	2A	3488	1/1	0.90	0.10	38,38,38,38	0
56	MG	1A	3342	1/1	0.90	0.12	59,59,59,59	0
56	MG	2a	1720	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	3427	1/1	0.90	0.15	64,64,64,64	0
56	MG	1A	3654	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3004	1/1	0.90	0.10	51,51,51,51	0
56	MG	2a	1730	1/1	0.90	0.10	72,72,72,72	0
56	MG	2A	3011	1/1	0.90	0.22	77,77,77,77	0
56	MG	2a	1733	1/1	0.90	0.15	72,72,72,72	0
56	MG	1A	3659	1/1	0.90	0.11	26,26,26,26	0
56	MG	1B	235	1/1	0.90	0.09	55,55,55,55	0
56	MG	1B	237	1/1	0.90	0.11	65,65,65,65	0
56	MG	2a	1741	1/1	0.90	0.10	59,59,59,59	0
56	MG	2A	3260	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3344	1/1	0.90	0.24	56,56,56,56	0
56	MG	2A	3262	1/1	0.90	0.17	66,66,66,66	0
56	MG	1A	3665	1/1	0.90	0.10	32,32,32,32	0
56	MG	1a	1668	1/1	0.90	0.09	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1758	1/1	0.90	0.16	54,54,54,54	0
56	MG	2A	3266	1/1	0.90	0.15	71,71,71,71	0
56	MG	2A	3267	1/1	0.90	0.22	68,68,68,68	0
56	MG	2A	3040	1/1	0.90	0.16	37,37,37,37	0
56	MG	2A	3041	1/1	0.90	0.25	70,70,70,70	0
56	MG	1a	1671	1/1	0.90	0.08	63,63,63,63	0
56	MG	2A	3053	1/1	0.90	0.10	53,53,53,53	0
56	MG	1E	301	1/1	0.90	0.14	38,38,38,38	0
56	MG	2B	201	1/1	0.90	0.20	77,77,77,77	0
56	MG	2A	3275	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3525	1/1	0.90	0.14	39,39,39,39	0
56	MG	2A	3056	1/1	0.90	0.34	70,70,70,70	0
56	MG	2A	3278	1/1	0.90	0.10	55,55,55,55	0
56	MG	2B	206	1/1	0.90	0.21	74,74,74,74	0
56	MG	2A	3542	1/1	0.90	0.16	68,68,68,68	0
56	MG	1A	3085	1/1	0.90	0.16	38,38,38,38	0
56	MG	1a	1677	1/1	0.90	0.24	61,61,61,61	0
56	MG	2A	3547	1/1	0.90	0.19	62,62,62,62	0
56	MG	1E	311	1/1	0.90	0.12	26,26,26,26	0
56	MG	1A	3307	1/1	0.90	0.23	54,54,54,54	0
56	MG	1A	3091	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3287	1/1	0.90	0.21	82,82,82,82	0
56	MG	1A	3681	1/1	0.90	0.08	61,61,61,61	0
56	MG	1a	1685	1/1	0.90	0.13	60,60,60,60	0
56	MG	2a	1791	1/1	0.90	0.22	63,63,63,63	0
56	MG	1A	3243	1/1	0.90	0.10	67,67,67,67	0
56	MG	2a	1796	1/1	0.90	0.18	58,58,58,58	0
56	MG	2A	3296	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3162	1/1	0.90	0.10	40,40,40,40	0
56	MG	1N	206	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3304	1/1	0.90	0.29	72,72,72,72	0
56	MG	2N	201	1/1	0.90	0.07	57,57,57,57	0
56	MG	2A	3094	1/1	0.90	0.14	57,57,57,57	0
56	MG	2P	201	1/1	0.90	0.13	67,67,67,67	0
56	MG	1O	201	1/1	0.90	0.10	69,69,69,69	0
56	MG	1A	3825	1/1	0.90	0.11	61,61,61,61	0
56	MG	1A	3358	1/1	0.90	0.10	44,44,44,44	0
56	MG	2t	201	1/1	0.90	0.14	74,74,74,74	0
56	MG	2A	3311	1/1	0.90	0.25	63,63,63,63	0
56	MG	2T	203	1/1	0.90	0.30	65,65,65,65	0
56	MG	2A	3102	1/1	0.90	0.22	60,60,60,60	0
56	MG	2A	3104	1/1	0.90	0.26	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3247	1/1	0.90	0.12	76,76,76,76	0
56	MG	2A	3584	1/1	0.91	0.09	52,52,52,52	0
56	MG	1A	3496	1/1	0.91	0.07	53,53,53,53	0
56	MG	1A	3650	1/1	0.91	0.11	54,54,54,54	0
56	MG	1Y	201	1/1	0.91	0.16	67,67,67,67	0
56	MG	2A	3318	1/1	0.91	0.15	70,70,70,70	0
56	MG	1Y	202	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	3351	1/1	0.91	0.15	51,51,51,51	0
56	MG	1a	1737	1/1	0.91	0.10	66,66,66,66	0
56	MG	27	104	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3323	1/1	0.91	0.12	70,70,70,70	0
56	MG	10	101	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3143	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3602	1/1	0.91	0.17	74,74,74,74	0
56	MG	1A	3416	1/1	0.91	0.17	36,36,36,36	0
56	MG	1A	3661	1/1	0.91	0.12	75,75,75,75	0
56	MG	2A	3148	1/1	0.91	0.27	62,62,62,62	0
56	MG	2A	3149	1/1	0.91	0.17	51,51,51,51	0
56	MG	2A	3607	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	3997	1/1	0.91	0.09	49,49,49,49	0
56	MG	2A	3610	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3998	1/1	0.91	0.06	33,33,33,33	0
56	MG	11	105	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3507	1/1	0.91	0.29	59,59,59,59	0
56	MG	2A	3337	1/1	0.91	0.20	47,47,47,47	0
56	MG	1A	3508	1/1	0.91	0.26	54,54,54,54	0
56	MG	1a	1753	1/1	0.91	0.08	68,68,68,68	0
56	MG	1A	3666	1/1	0.91	0.12	37,37,37,37	0
56	MG	1A	3826	1/1	0.91	0.30	40,40,40,40	0
56	MG	17	104	1/1	0.91	0.16	55,55,55,55	0
56	MG	18	101	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	3016	1/1	0.91	0.27	54,54,54,54	0
56	MG	2A	3627	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	4014	1/1	0.91	0.15	47,47,47,47	0
56	MG	1A	3830	1/1	0.91	0.13	48,48,48,48	0
56	MG	2A	3631	1/1	0.91	0.15	62,62,62,62	0
56	MG	1a	1602	1/1	0.91	0.26	69,69,69,69	0
56	MG	1A	3120	1/1	0.91	0.21	54,54,54,54	0
56	MG	1A	3354	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3256	1/1	0.91	0.11	53,53,53,53	0
56	MG	2A	3639	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3197	1/1	0.91	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3198	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3180	1/1	0.91	0.10	67,67,67,67	0
56	MG	1a	1785	1/1	0.91	0.30	67,67,67,67	0
56	MG	2A	3184	1/1	0.91	0.31	75,75,75,75	0
56	MG	1A	4027	1/1	0.91	0.11	24,24,24,24	0
56	MG	2A	3187	1/1	0.91	0.24	52,52,52,52	0
56	MG	2A	3649	1/1	0.91	0.13	60,60,60,60	0
56	MG	1A	3440	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3371	1/1	0.91	0.11	49,49,49,49	0
56	MG	1a	1622	1/1	0.91	0.26	58,58,58,58	0
56	MG	1A	3367	1/1	0.91	0.32	31,31,31,31	0
56	MG	1A	3845	1/1	0.91	0.18	31,31,31,31	0
56	MG	1A	3846	1/1	0.91	0.13	65,65,65,65	0
56	MG	1A	3848	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3392	1/1	0.91	0.11	60,60,60,60	0
56	MG	2a	1664	1/1	0.91	0.20	55,55,55,55	0
56	MG	2A	3196	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3395	1/1	0.91	0.27	69,69,69,69	0
56	MG	2a	1669	1/1	0.91	0.23	62,62,62,62	0
56	MG	1A	3126	1/1	0.91	0.14	68,68,68,68	0
56	MG	2A	3668	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3669	1/1	0.91	0.15	67,67,67,67	0
56	MG	2a	1675	1/1	0.91	0.21	64,64,64,64	0
56	MG	1a	1628	1/1	0.91	0.36	66,66,66,66	0
56	MG	2a	1678	1/1	0.91	0.24	61,61,61,61	0
56	MG	1A	3134	1/1	0.91	0.12	42,42,42,42	0
56	MG	2A	3202	1/1	0.91	0.39	51,51,51,51	0
56	MG	1A	3380	1/1	0.91	0.10	41,41,41,41	0
56	MG	1A	4048	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3217	1/1	0.91	0.14	45,45,45,45	0
56	MG	2A	3413	1/1	0.91	0.21	61,61,61,61	0
56	MG	1A	3454	1/1	0.91	0.09	61,61,61,61	0
56	MG	2A	3418	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3421	1/1	0.91	0.31	68,68,68,68	0
56	MG	1A	3456	1/1	0.91	0.11	54,54,54,54	0
56	MG	2A	3214	1/1	0.91	0.13	72,72,72,72	0
56	MG	1A	3324	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3216	1/1	0.91	0.31	74,74,74,74	0
56	MG	2A	3699	1/1	0.91	0.14	49,49,49,49	0
56	MG	1w	102	1/1	0.91	0.13	71,71,71,71	0
56	MG	1A	3227	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3433	1/1	0.91	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	101	1/1	0.91	0.29	72,72,72,72	0
56	MG	1x	102	1/1	0.91	0.10	73,73,73,73	0
56	MG	1A	3711	1/1	0.91	0.13	38,38,38,38	0
56	MG	2A	3225	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3440	1/1	0.91	0.10	25,25,25,25	0
56	MG	2A	3709	1/1	0.91	0.12	61,61,61,61	0
56	MG	2a	1705	1/1	0.91	0.34	70,70,70,70	0
56	MG	2a	1706	1/1	0.91	0.21	60,60,60,60	0
56	MG	2A	3227	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3711	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3228	1/1	0.91	0.21	67,67,67,67	0
56	MG	2A	3448	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3714	1/1	0.91	0.26	65,65,65,65	0
56	MG	1A	3716	1/1	0.91	0.12	44,44,44,44	0
56	MG	2a	1715	1/1	0.91	0.24	63,63,63,63	0
56	MG	1A	3086	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3726	1/1	0.91	0.11	68,68,68,68	0
56	MG	1x	108	1/1	0.91	0.14	37,37,37,37	0
56	MG	1A	3040	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3465	1/1	0.91	0.18	48,48,48,48	0
56	MG	2a	1721	1/1	0.91	0.32	71,71,71,71	0
56	MG	1A	3727	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3744	1/1	0.91	0.10	64,64,64,64	0
56	MG	1A	3390	1/1	0.91	0.17	73,73,73,73	0
56	MG	1A	3917	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3246	1/1	0.91	0.18	68,68,68,68	0
56	MG	1A	3338	1/1	0.91	0.20	56,56,56,56	0
56	MG	2a	1734	1/1	0.91	0.15	74,74,74,74	0
56	MG	2A	3481	1/1	0.91	0.13	44,44,44,44	0
56	MG	2A	3482	1/1	0.91	0.17	43,43,43,43	0
56	MG	1A	3736	1/1	0.91	0.10	33,33,33,33	0
56	MG	1B	227	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3738	1/1	0.91	0.10	20,20,20,20	0
56	MG	2A	3252	1/1	0.91	0.37	73,73,73,73	0
56	MG	1A	3740	1/1	0.91	0.08	23,23,23,23	0
56	MG	1A	3586	1/1	0.91	0.11	18,18,18,18	0
56	MG	1A	3588	1/1	0.91	0.11	37,37,37,37	0
56	MG	1B	238	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3594	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3759	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3394	1/1	0.91	0.21	55,55,55,55	0
56	MG	2A	3042	1/1	0.91	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3045	1/1	0.91	0.22	65,65,65,65	0
56	MG	1A	3474	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3049	1/1	0.91	0.25	63,63,63,63	0
56	MG	1A	3092	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3478	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3769	1/1	0.91	0.08	47,47,47,47	0
56	MG	1F	302	1/1	0.91	0.28	38,38,38,38	0
56	MG	1A	3479	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3610	1/1	0.91	0.08	25,25,25,25	0
56	MG	2A	3530	1/1	0.91	0.22	55,55,55,55	0
56	MG	2A	3065	1/1	0.91	0.14	72,72,72,72	0
56	MG	1a	1682	1/1	0.91	0.31	67,67,67,67	0
56	MG	1A	3611	1/1	0.91	0.08	20,20,20,20	0
56	MG	1A	3160	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3956	1/1	0.91	0.17	43,43,43,43	0
56	MG	2B	213	1/1	0.91	0.19	60,60,60,60	0
56	MG	2A	3283	1/1	0.91	0.16	79,79,79,79	0
56	MG	2A	3085	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3616	1/1	0.91	0.08	28,28,28,28	0
56	MG	1O	203	1/1	0.91	0.22	66,66,66,66	0
56	MG	1A	3783	1/1	0.91	0.11	33,33,33,33	0
56	MG	2a	1794	1/1	0.91	0.20	65,65,65,65	0
56	MG	2D	305	1/1	0.91	0.39	45,45,45,45	0
56	MG	2a	1797	1/1	0.91	0.23	70,70,70,70	0
56	MG	1A	3093	1/1	0.91	0.18	38,38,38,38	0
56	MG	1A	3624	1/1	0.91	0.12	47,47,47,47	0
56	MG	2E	302	1/1	0.91	0.12	67,67,67,67	0
56	MG	1A	3625	1/1	0.91	0.10	50,50,50,50	0
56	MG	2d	301	1/1	0.91	0.10	65,65,65,65	0
56	MG	1A	3052	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3297	1/1	0.91	0.14	64,64,64,64	0
56	MG	1a	1708	1/1	0.91	0.11	66,66,66,66	0
56	MG	2A	3299	1/1	0.91	0.37	70,70,70,70	0
56	MG	1A	3349	1/1	0.91	0.17	47,47,47,47	0
56	MG	2A	3303	1/1	0.91	0.12	66,66,66,66	0
56	MG	2r	102	1/1	0.91	0.09	81,81,81,81	0
56	MG	1S	202	1/1	0.91	0.15	53,53,53,53	0
56	MG	2t	202	1/1	0.91	0.18	52,52,52,52	0
56	MG	1S	203	1/1	0.91	0.07	62,62,62,62	0
56	MG	1A	3408	1/1	0.91	0.24	58,58,58,58	0
56	MG	1A	3080	1/1	0.91	0.28	38,38,38,38	0
56	MG	2x	102	1/1	0.91	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3581	1/1	0.91	0.15	68,68,68,68	0
56	MG	1a	1724	1/1	0.91	0.10	56,56,56,56	0
56	MG	2T	205	1/1	0.92	0.10	65,65,65,65	0
56	MG	2A	3320	1/1	0.92	0.16	66,66,66,66	0
56	MG	1A	3161	1/1	0.92	0.17	38,38,38,38	0
56	MG	1A	3058	1/1	0.92	0.08	50,50,50,50	0
56	MG	1A	3828	1/1	0.92	0.12	46,46,46,46	0
56	MG	2Z	301	1/1	0.92	0.24	67,67,67,67	0
56	MG	1A	3249	1/1	0.92	0.07	39,39,39,39	0
56	MG	1A	3297	1/1	0.92	0.13	44,44,44,44	0
56	MG	2I	101	1/1	0.92	0.23	56,56,56,56	0
56	MG	1A	3477	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	3707	1/1	0.92	0.10	49,49,49,49	0
56	MG	27	103	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	4000	1/1	0.92	0.08	57,57,57,57	0
56	MG	10	104	1/1	0.92	0.31	71,71,71,71	0
56	MG	1A	4003	1/1	0.92	0.09	36,36,36,36	0
56	MG	2A	3154	1/1	0.92	0.13	59,59,59,59	0
56	MG	2A	3155	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	4004	1/1	0.92	0.10	34,34,34,34	0
56	MG	1A	3401	1/1	0.92	0.13	52,52,52,52	0
56	MG	1a	1754	1/1	0.92	0.15	67,67,67,67	0
56	MG	1I	103	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3250	1/1	0.92	0.08	41,41,41,41	0
56	MG	1A	3343	1/1	0.92	0.12	56,56,56,56	0
56	MG	2A	3342	1/1	0.92	0.18	39,39,39,39	0
56	MG	1A	3300	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3168	1/1	0.92	0.09	63,63,63,63	0
56	MG	2A	3346	1/1	0.92	0.41	71,71,71,71	0
56	MG	2A	3618	1/1	0.92	0.17	57,57,57,57	0
56	MG	1a	1766	1/1	0.92	0.12	49,49,49,49	0
56	MG	1A	3345	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3346	1/1	0.92	0.23	55,55,55,55	0
56	MG	1A	3303	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3354	1/1	0.92	0.19	55,55,55,55	0
56	MG	1a	1777	1/1	0.92	0.07	56,56,56,56	0
56	MG	1A	3726	1/1	0.92	0.09	24,24,24,24	0
56	MG	1A	3306	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	4021	1/1	0.92	0.15	63,63,63,63	0
56	MG	2A	3179	1/1	0.92	0.19	72,72,72,72	0
56	MG	1A	3852	1/1	0.92	0.13	35,35,35,35	0
56	MG	1A	3853	1/1	0.92	0.13	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3182	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3367	1/1	0.92	0.27	64,64,64,64	0
56	MG	2A	3641	1/1	0.92	0.10	37,37,37,37	0
56	MG	2A	3183	1/1	0.92	0.17	68,68,68,68	0
56	MG	2a	1637	1/1	0.92	0.21	70,70,70,70	0
56	MG	1A	3859	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	4028	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3186	1/1	0.92	0.12	67,67,67,67	0
56	MG	1A	3861	1/1	0.92	0.09	26,26,26,26	0
56	MG	1A	4031	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3612	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3386	1/1	0.92	0.21	62,62,62,62	0
56	MG	1A	3863	1/1	0.92	0.08	43,43,43,43	0
56	MG	1A	4035	1/1	0.92	0.14	24,24,24,24	0
56	MG	2a	1650	1/1	0.92	0.25	65,65,65,65	0
56	MG	1a	1618	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3655	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3422	1/1	0.92	0.10	61,61,61,61	0
56	MG	1A	3425	1/1	0.92	0.16	58,58,58,58	0
56	MG	1A	3502	1/1	0.92	0.24	46,46,46,46	0
56	MG	1A	3131	1/1	0.92	0.14	46,46,46,46	0
56	MG	2a	1661	1/1	0.92	0.23	62,62,62,62	0
56	MG	1A	3224	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3663	1/1	0.92	0.11	55,55,55,55	0
56	MG	2a	1665	1/1	0.92	0.24	60,60,60,60	0
56	MG	1A	4047	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3666	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3878	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3753	1/1	0.92	0.08	35,35,35,35	0
56	MG	1A	3882	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3883	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3211	1/1	0.92	0.17	58,58,58,58	0
56	MG	1A	3885	1/1	0.92	0.09	34,34,34,34	0
56	MG	1A	3255	1/1	0.92	0.08	47,47,47,47	0
56	MG	2a	1679	1/1	0.92	0.32	72,72,72,72	0
56	MG	1w	104	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3893	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3425	1/1	0.92	0.23	62,62,62,62	0
56	MG	1A	3432	1/1	0.92	0.09	53,53,53,53	0
56	MG	2A	3686	1/1	0.92	0.20	63,63,63,63	0
56	MG	1B	213	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3225	1/1	0.92	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3515	1/1	0.92	0.20	58,58,58,58	0
56	MG	1a	1639	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3034	1/1	0.92	0.27	41,41,41,41	0
56	MG	1A	3647	1/1	0.92	0.22	48,48,48,48	0
56	MG	2A	3436	1/1	0.92	0.23	65,65,65,65	0
56	MG	1A	3649	1/1	0.92	0.08	35,35,35,35	0
56	MG	1B	221	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3702	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3314	1/1	0.92	0.31	63,63,63,63	0
56	MG	2A	3231	1/1	0.92	0.37	75,75,75,75	0
56	MG	2A	3233	1/1	0.92	0.24	74,74,74,74	0
56	MG	2A	3445	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	3652	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	3771	1/1	0.92	0.06	25,25,25,25	0
56	MG	1A	3182	1/1	0.92	0.13	34,34,34,34	0
56	MG	1A	3362	1/1	0.92	0.11	42,42,42,42	0
56	MG	2A	3453	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3454	1/1	0.92	0.08	44,44,44,44	0
56	MG	1B	229	1/1	0.92	0.12	55,55,55,55	0
56	MG	2a	1708	1/1	0.92	0.23	59,59,59,59	0
56	MG	1A	3263	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3018	1/1	0.92	0.24	70,70,70,70	0
56	MG	1A	3088	1/1	0.92	0.20	53,53,53,53	0
56	MG	2A	3723	1/1	0.92	0.10	57,57,57,57	0
56	MG	1a	1658	1/1	0.92	0.21	69,69,69,69	0
56	MG	2A	3248	1/1	0.92	0.36	69,69,69,69	0
56	MG	2A	3733	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3735	1/1	0.92	0.09	65,65,65,65	0
56	MG	2A	3030	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3267	1/1	0.92	0.09	49,49,49,49	0
56	MG	1B	236	1/1	0.92	0.10	68,68,68,68	0
56	MG	2A	3038	1/1	0.92	0.24	63,63,63,63	0
56	MG	2A	3253	1/1	0.92	0.17	64,64,64,64	0
56	MG	2A	3486	1/1	0.92	0.17	62,62,62,62	0
56	MG	2A	3747	1/1	0.92	0.08	44,44,44,44	0
56	MG	2A	3487	1/1	0.92	0.19	59,59,59,59	0
56	MG	2A	3751	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3254	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3753	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3786	1/1	0.92	0.07	40,40,40,40	0
56	MG	2A	3256	1/1	0.92	0.12	58,58,58,58	0
56	MG	2A	3757	1/1	0.92	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3498	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3788	1/1	0.92	0.07	27,27,27,27	0
56	MG	2a	1744	1/1	0.92	0.25	70,70,70,70	0
56	MG	2a	1745	1/1	0.92	0.10	52,52,52,52	0
56	MG	1a	1665	1/1	0.92	0.34	60,60,60,60	0
56	MG	2a	1749	1/1	0.92	0.20	70,70,70,70	0
56	MG	1D	301	1/1	0.92	0.15	55,55,55,55	0
56	MG	2A	3047	1/1	0.92	0.18	63,63,63,63	0
56	MG	1D	302	1/1	0.92	0.16	43,43,43,43	0
56	MG	1A	3554	1/1	0.92	0.22	46,46,46,46	0
56	MG	1A	3377	1/1	0.92	0.16	43,43,43,43	0
56	MG	2a	1760	1/1	0.92	0.21	77,77,77,77	0
56	MG	1A	3797	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	3672	1/1	0.92	0.13	55,55,55,55	0
56	MG	2A	3771	1/1	0.92	0.17	59,59,59,59	0
56	MG	1E	309	1/1	0.92	0.15	49,49,49,49	0
56	MG	2A	3520	1/1	0.92	0.12	55,55,55,55	0
56	MG	2a	1769	1/1	0.92	0.23	71,71,71,71	0
56	MG	1A	3945	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3556	1/1	0.92	0.07	38,38,38,38	0
56	MG	2a	1772	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3281	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3953	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	3678	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3079	1/1	0.92	0.15	65,65,65,65	0
56	MG	1F	305	1/1	0.92	0.15	39,39,39,39	0
56	MG	2A	3082	1/1	0.92	0.28	53,53,53,53	0
56	MG	1a	1687	1/1	0.92	0.17	53,53,53,53	0
56	MG	1F	307	1/1	0.92	0.16	31,31,31,31	0
56	MG	1A	3320	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3282	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3537	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3045	1/1	0.92	0.08	35,35,35,35	0
56	MG	2B	211	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3383	1/1	0.92	0.15	57,57,57,57	0
56	MG	1N	201	1/1	0.92	0.30	53,53,53,53	0
56	MG	1a	1700	1/1	0.92	0.27	66,66,66,66	0
56	MG	2A	3097	1/1	0.92	0.35	70,70,70,70	0
56	MG	1N	204	1/1	0.92	0.30	48,48,48,48	0
56	MG	1A	3285	1/1	0.92	0.23	51,51,51,51	0
56	MG	1A	3807	1/1	0.92	0.12	57,57,57,57	0
56	MG	1A	3811	1/1	0.92	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3103	1/1	0.92	0.15	55,55,55,55	0
56	MG	1a	1709	1/1	0.92	0.09	52,52,52,52	0
56	MG	2E	301	1/1	0.92	0.22	64,64,64,64	0
56	MG	1A	3814	1/1	0.92	0.09	49,49,49,49	0
56	MG	1a	1716	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3970	1/1	0.92	0.13	40,40,40,40	0
56	MG	1A	3325	1/1	0.92	0.24	57,57,57,57	0
56	MG	2A	3113	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3114	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3691	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3692	1/1	0.92	0.15	50,50,50,50	0
56	MG	1Q	206	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3117	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3054	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3986	1/1	0.92	0.11	48,48,48,48	0
56	MG	2w	102	1/1	0.92	0.08	79,79,79,79	0
56	MG	2T	201	1/1	0.92	0.12	62,62,62,62	0
56	MG	2T	202	1/1	0.92	0.21	62,62,62,62	0
56	MG	2A	3138	1/1	0.92	0.14	67,67,67,67	0
56	MG	2A	3590	1/1	0.92	0.12	58,58,58,58	0
56	MG	2x	105	1/1	0.92	0.21	56,56,56,56	0
56	MG	2A	3294	1/1	0.93	0.35	75,75,75,75	0
56	MG	2A	3561	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3295	1/1	0.93	0.15	62,62,62,62	0
56	MG	2A	3107	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3064	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	4001	1/1	0.93	0.10	48,48,48,48	0
56	MG	1U	204	1/1	0.93	0.25	38,38,38,38	0
56	MG	1a	1725	1/1	0.93	0.08	63,63,63,63	0
56	MG	1A	3509	1/1	0.93	0.09	55,55,55,55	0
56	MG	1a	1729	1/1	0.93	0.18	66,66,66,66	0
56	MG	2A	3573	1/1	0.93	0.09	67,67,67,67	0
56	MG	2A	3121	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3577	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3306	1/1	0.93	0.11	63,63,63,63	0
56	MG	1A	3851	1/1	0.93	0.08	28,28,28,28	0
56	MG	1W	205	1/1	0.93	0.11	31,31,31,31	0
56	MG	1A	4007	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3130	1/1	0.93	0.16	65,65,65,65	0
56	MG	1a	1735	1/1	0.93	0.13	60,60,60,60	0
56	MG	2A	3314	1/1	0.93	0.21	63,63,63,63	0
56	MG	2A	3315	1/1	0.93	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3316	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3622	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3135	1/1	0.93	0.21	54,54,54,54	0
56	MG	2A	3136	1/1	0.93	0.23	56,56,56,56	0
56	MG	2A	3594	1/1	0.93	0.12	72,72,72,72	0
56	MG	1A	3139	1/1	0.93	0.12	46,46,46,46	0
56	MG	1Z	301	1/1	0.93	0.15	69,69,69,69	0
56	MG	2A	3139	1/1	0.93	0.16	59,59,59,59	0
56	MG	1A	3019	1/1	0.93	0.15	44,44,44,44	0
56	MG	2a	1608	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3324	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3601	1/1	0.93	0.22	66,66,66,66	0
56	MG	2a	1611	1/1	0.93	0.23	68,68,68,68	0
56	MG	1A	3732	1/1	0.93	0.08	35,35,35,35	0
56	MG	2A	3144	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3389	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3629	1/1	0.93	0.07	24,24,24,24	0
56	MG	1a	1744	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3521	1/1	0.93	0.15	42,42,42,42	0
56	MG	1a	1747	1/1	0.93	0.07	72,72,72,72	0
56	MG	2A	3332	1/1	0.93	0.15	67,67,67,67	0
56	MG	2A	3333	1/1	0.93	0.14	59,59,59,59	0
56	MG	1A	3522	1/1	0.93	0.27	48,48,48,48	0
56	MG	1a	1749	1/1	0.93	0.15	72,72,72,72	0
56	MG	1A	3632	1/1	0.93	0.08	44,44,44,44	0
56	MG	2a	1625	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3750	1/1	0.93	0.10	25,25,25,25	0
56	MG	1A	3144	1/1	0.93	0.29	42,42,42,42	0
56	MG	1A	3877	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3638	1/1	0.93	0.08	44,44,44,44	0
56	MG	1A	3242	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3643	1/1	0.93	0.12	26,26,26,26	0
56	MG	1A	3002	1/1	0.93	0.10	53,53,53,53	0
56	MG	17	105	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3624	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3455	1/1	0.93	0.13	65,65,65,65	0
56	MG	1a	1774	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3889	1/1	0.93	0.07	57,57,57,57	0
56	MG	2a	1640	1/1	0.93	0.14	68,68,68,68	0
56	MG	1A	3244	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3892	1/1	0.93	0.07	44,44,44,44	0
56	MG	2A	3352	1/1	0.93	0.36	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3353	1/1	0.93	0.28	61,61,61,61	0
56	MG	1A	4041	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3118	1/1	0.93	0.35	51,51,51,51	0
56	MG	1A	3077	1/1	0.93	0.12	54,54,54,54	0
56	MG	2A	3359	1/1	0.93	0.14	71,71,71,71	0
56	MG	1A	3657	1/1	0.93	0.11	40,40,40,40	0
56	MG	2A	3361	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3902	1/1	0.93	0.09	37,37,37,37	0
56	MG	1A	3658	1/1	0.93	0.16	30,30,30,30	0
56	MG	1A	3908	1/1	0.93	0.09	62,62,62,62	0
56	MG	2a	1657	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	3910	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3550	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3321	1/1	0.93	0.10	39,39,39,39	0
56	MG	1A	4054	1/1	0.93	0.09	59,59,59,59	0
56	MG	1a	1792	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	4058	1/1	0.93	0.32	59,59,59,59	0
56	MG	1a	1794	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3188	1/1	0.93	0.19	51,51,51,51	0
56	MG	2a	1670	1/1	0.93	0.12	71,71,71,71	0
56	MG	2A	3377	1/1	0.93	0.15	44,44,44,44	0
56	MG	1a	1795	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3295	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3915	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3122	1/1	0.93	0.26	37,37,37,37	0
56	MG	2A	3664	1/1	0.93	0.25	44,44,44,44	0
56	MG	1B	209	1/1	0.93	0.18	67,67,67,67	0
56	MG	2A	3390	1/1	0.93	0.17	53,53,53,53	0
56	MG	2A	3391	1/1	0.93	0.16	64,64,64,64	0
56	MG	1B	211	1/1	0.93	0.14	51,51,51,51	0
56	MG	2A	3393	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3782	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3671	1/1	0.93	0.13	63,63,63,63	0
56	MG	2A	3197	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3405	1/1	0.93	0.09	51,51,51,51	0
56	MG	1n	102	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3920	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3667	1/1	0.93	0.06	22,22,22,22	0
56	MG	1A	3668	1/1	0.93	0.23	64,64,64,64	0
56	MG	2A	3681	1/1	0.93	0.09	50,50,50,50	0
56	MG	2a	1693	1/1	0.93	0.07	76,76,76,76	0
56	MG	1A	3669	1/1	0.93	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3467	1/1	0.93	0.13	68,68,68,68	0
56	MG	2A	3412	1/1	0.93	0.34	69,69,69,69	0
56	MG	1A	3206	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3210	1/1	0.93	0.09	53,53,53,53	0
56	MG	2A	3417	1/1	0.93	0.24	57,57,57,57	0
56	MG	2A	3695	1/1	0.93	0.19	54,54,54,54	0
56	MG	1A	3929	1/1	0.93	0.10	22,22,22,22	0
56	MG	1A	3326	1/1	0.93	0.18	53,53,53,53	0
56	MG	1a	1643	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3932	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3933	1/1	0.93	0.12	58,58,58,58	0
56	MG	2A	3217	1/1	0.93	0.29	74,74,74,74	0
56	MG	1A	3934	1/1	0.93	0.15	62,62,62,62	0
56	MG	1A	3936	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3473	1/1	0.93	0.08	61,61,61,61	0
56	MG	1A	3410	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3222	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3223	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3364	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3680	1/1	0.93	0.13	49,49,49,49	0
56	MG	2A	3226	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3712	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3327	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	3420	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3421	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3686	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3446	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3808	1/1	0.93	0.06	36,36,36,36	0
56	MG	1A	3481	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3728	1/1	0.93	0.09	63,63,63,63	0
56	MG	2a	1732	1/1	0.93	0.08	76,76,76,76	0
56	MG	2A	3731	1/1	0.93	0.22	69,69,69,69	0
56	MG	2A	3450	1/1	0.93	0.14	35,35,35,35	0
56	MG	1A	3581	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3209	1/1	0.93	0.07	46,46,46,46	0
56	MG	2A	3237	1/1	0.93	0.11	63,63,63,63	0
56	MG	2a	1739	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3958	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3026	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3741	1/1	0.93	0.12	66,66,66,66	0
56	MG	2A	3458	1/1	0.93	0.13	77,77,77,77	0
56	MG	2a	1747	1/1	0.93	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3027	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3028	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3461	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3029	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3463	1/1	0.93	0.12	56,56,56,56	0
56	MG	2a	1753	1/1	0.93	0.20	61,61,61,61	0
56	MG	2a	1755	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3465	1/1	0.93	0.12	61,61,61,61	0
56	MG	1A	3489	1/1	0.93	0.18	60,60,60,60	0
56	MG	2A	3469	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3471	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3370	1/1	0.93	0.59	48,48,48,48	0
56	MG	2A	3758	1/1	0.93	0.11	66,66,66,66	0
56	MG	2A	3035	1/1	0.93	0.17	73,73,73,73	0
56	MG	1A	3216	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3698	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3599	1/1	0.93	0.07	34,34,34,34	0
56	MG	1A	3373	1/1	0.93	0.08	53,53,53,53	0
56	MG	1a	1676	1/1	0.93	0.33	58,58,58,58	0
56	MG	1A	3974	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3429	1/1	0.93	0.21	50,50,50,50	0
56	MG	1A	3607	1/1	0.93	0.11	56,56,56,56	0
56	MG	2A	3492	1/1	0.93	0.10	37,37,37,37	0
56	MG	2A	3494	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1680	1/1	0.93	0.38	75,75,75,75	0
56	MG	2A	3497	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3056	1/1	0.93	0.10	43,43,43,43	0
56	MG	1I	201	1/1	0.93	0.09	64,64,64,64	0
56	MG	2a	1783	1/1	0.93	0.30	70,70,70,70	0
56	MG	1A	3980	1/1	0.93	0.10	51,51,51,51	0
56	MG	1N	202	1/1	0.93	0.08	50,50,50,50	0
56	MG	2a	1786	1/1	0.93	0.12	71,71,71,71	0
56	MG	1a	1686	1/1	0.93	0.12	67,67,67,67	0
56	MG	2A	3263	1/1	0.93	0.09	58,58,58,58	0
56	MG	1A	3022	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3063	1/1	0.93	0.08	55,55,55,55	0
56	MG	1a	1688	1/1	0.93	0.23	63,63,63,63	0
56	MG	1A	3984	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3710	1/1	0.93	0.10	24,24,24,24	0
56	MG	2A	3075	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3165	1/1	0.93	0.09	48,48,48,48	0
56	MG	1O	204	1/1	0.93	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1697	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3987	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3713	1/1	0.93	0.06	20,20,20,20	0
56	MG	1P	205	1/1	0.93	0.08	46,46,46,46	0
56	MG	1A	3166	1/1	0.93	0.29	42,42,42,42	0
56	MG	1a	1703	1/1	0.93	0.15	61,61,61,61	0
56	MG	1A	3841	1/1	0.93	0.28	34,34,34,34	0
56	MG	2A	3093	1/1	0.93	0.16	62,62,62,62	0
56	MG	1A	3435	1/1	0.93	0.13	34,34,34,34	0
56	MG	1A	3230	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	1713	1/1	0.93	0.13	55,55,55,55	0
56	MG	2A	3538	1/1	0.93	0.09	52,52,52,52	0
56	MG	1R	202	1/1	0.93	0.25	51,51,51,51	0
56	MG	2E	303	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3720	1/1	0.93	0.11	36,36,36,36	0
56	MG	1S	201	1/1	0.93	0.29	51,51,51,51	0
56	MG	2F	303	1/1	0.93	0.12	64,64,64,64	0
56	MG	1a	1718	1/1	0.93	0.15	59,59,59,59	0
56	MG	2A	3292	1/1	0.93	0.21	63,63,63,63	0
56	MG	1A	3722	1/1	0.93	0.08	42,42,42,42	0
56	MG	2A	3550	1/1	0.93	0.13	46,46,46,46	0
56	MG	2x	106	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3778	1/1	0.94	0.06	33,33,33,33	0
56	MG	2A	3290	1/1	0.94	0.10	64,64,64,64	0
56	MG	2E	308	1/1	0.94	0.11	43,43,43,43	0
56	MG	2F	302	1/1	0.94	0.07	43,43,43,43	0
56	MG	1D	305	1/1	0.94	0.07	37,37,37,37	0
56	MG	1a	1684	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3260	1/1	0.94	0.29	53,53,53,53	0
56	MG	2A	3087	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3552	1/1	0.94	0.10	38,38,38,38	0
56	MG	2A	3088	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3558	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3218	1/1	0.94	0.09	56,56,56,56	0
56	MG	1A	3223	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3174	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3175	1/1	0.94	0.13	63,63,63,63	0
56	MG	1A	3940	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3567	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3095	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3096	1/1	0.94	0.16	48,48,48,48	0
56	MG	2U	201	1/1	0.94	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3272	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3098	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3572	1/1	0.94	0.27	56,56,56,56	0
56	MG	2A	3307	1/1	0.94	0.19	57,57,57,57	0
56	MG	2Y	201	1/1	0.94	0.30	62,62,62,62	0
56	MG	1a	1693	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3576	1/1	0.94	0.12	59,59,59,59	0
56	MG	1a	1694	1/1	0.94	0.23	51,51,51,51	0
56	MG	1E	312	1/1	0.94	0.12	27,27,27,27	0
56	MG	25	103	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3789	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3790	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	3947	1/1	0.94	0.09	23,23,23,23	0
56	MG	1A	3275	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3950	1/1	0.94	0.12	28,28,28,28	0
56	MG	2A	3585	1/1	0.94	0.08	57,57,57,57	0
56	MG	2A	3586	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3441	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3796	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3660	1/1	0.94	0.07	26,26,26,26	0
56	MG	1G	204	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3378	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3116	1/1	0.94	0.08	60,60,60,60	0
56	MG	2A	3117	1/1	0.94	0.17	74,74,74,74	0
56	MG	1a	1714	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3663	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3379	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3445	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3960	1/1	0.94	0.09	19,19,19,19	0
56	MG	1A	3534	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3132	1/1	0.94	0.23	39,39,39,39	0
56	MG	1O	202	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3964	1/1	0.94	0.13	70,70,70,70	0
56	MG	1A	3539	1/1	0.94	0.26	38,38,38,38	0
56	MG	1A	3542	1/1	0.94	0.61	42,42,42,42	0
56	MG	1A	3543	1/1	0.94	0.09	44,44,44,44	0
56	MG	1a	1728	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3278	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3972	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3447	1/1	0.94	0.23	63,63,63,63	0
56	MG	1Q	204	1/1	0.94	0.11	53,53,53,53	0
56	MG	1A	3673	1/1	0.94	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3813	1/1	0.94	0.17	58,58,58,58	0
56	MG	2a	1630	1/1	0.94	0.23	55,55,55,55	0
56	MG	2a	1631	1/1	0.94	0.27	56,56,56,56	0
56	MG	1A	3553	1/1	0.94	0.19	54,54,54,54	0
56	MG	1A	3676	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3345	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3816	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3323	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3621	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3348	1/1	0.94	0.27	61,61,61,61	0
56	MG	1A	3279	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3176	1/1	0.94	0.10	70,70,70,70	0
56	MG	1A	3385	1/1	0.94	0.32	64,64,64,64	0
56	MG	1A	3559	1/1	0.94	0.34	61,61,61,61	0
56	MG	1A	3561	1/1	0.94	0.28	59,59,59,59	0
56	MG	1A	3177	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3160	1/1	0.94	0.13	52,52,52,52	0
56	MG	2A	3357	1/1	0.94	0.28	58,58,58,58	0
56	MG	2a	1648	1/1	0.94	0.10	68,68,68,68	0
56	MG	2A	3162	1/1	0.94	0.30	64,64,64,64	0
56	MG	2A	3636	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3994	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3995	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3829	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3116	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3688	1/1	0.94	0.10	59,59,59,59	0
56	MG	1a	1756	1/1	0.94	0.09	62,62,62,62	0
56	MG	1Z	303	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3181	1/1	0.94	0.19	41,41,41,41	0
56	MG	1a	1762	1/1	0.94	0.11	54,54,54,54	0
56	MG	2a	1663	1/1	0.94	0.20	65,65,65,65	0
56	MG	10	103	1/1	0.94	0.24	47,47,47,47	0
56	MG	1A	3332	1/1	0.94	0.25	64,64,64,64	0
56	MG	2A	3650	1/1	0.94	0.18	57,57,57,57	0
56	MG	2A	3176	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3142	1/1	0.94	0.26	35,35,35,35	0
56	MG	1A	3573	1/1	0.94	0.09	34,34,34,34	0
56	MG	2a	1671	1/1	0.94	0.10	65,65,65,65	0
56	MG	2A	3375	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3837	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	4006	1/1	0.94	0.13	51,51,51,51	0
56	MG	2A	3658	1/1	0.94	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3384	1/1	0.94	0.13	69,69,69,69	0
56	MG	2a	1677	1/1	0.94	0.17	70,70,70,70	0
56	MG	1A	3335	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	4008	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3393	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3239	1/1	0.94	0.25	53,53,53,53	0
56	MG	1A	3844	1/1	0.94	0.19	37,37,37,37	0
56	MG	16	102	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3396	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3291	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3184	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3705	1/1	0.94	0.06	54,54,54,54	0
56	MG	2A	3397	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3191	1/1	0.94	0.27	62,62,62,62	0
56	MG	18	103	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3584	1/1	0.94	0.08	25,25,25,25	0
56	MG	2A	3404	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3585	1/1	0.94	0.06	35,35,35,35	0
56	MG	1A	3001	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3148	1/1	0.94	0.18	44,44,44,44	0
56	MG	2A	3679	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3593	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3411	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3683	1/1	0.94	0.12	76,76,76,76	0
56	MG	1A	3476	1/1	0.94	0.11	62,62,62,62	0
56	MG	2A	3199	1/1	0.94	0.09	47,47,47,47	0
56	MG	1a	1605	1/1	0.94	0.08	63,63,63,63	0
56	MG	2A	3416	1/1	0.94	0.12	63,63,63,63	0
56	MG	2A	3692	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3693	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3004	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	3096	1/1	0.94	0.11	48,48,48,48	0
56	MG	1d	301	1/1	0.94	0.32	64,64,64,64	0
56	MG	1a	1612	1/1	0.94	0.08	72,72,72,72	0
56	MG	1f	3102	1/1	0.94	0.22	68,68,68,68	0
56	MG	1A	3865	1/1	0.94	0.09	55,55,55,55	0
56	MG	2a	1713	1/1	0.94	0.10	70,70,70,70	0
56	MG	2A	3209	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3600	1/1	0.94	0.06	22,22,22,22	0
56	MG	1a	1615	1/1	0.94	0.14	61,61,61,61	0
56	MG	2A	3212	1/1	0.94	0.29	56,56,56,56	0
56	MG	1A	3718	1/1	0.94	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3602	1/1	0.94	0.08	25,25,25,25	0
56	MG	1A	3299	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	4038	1/1	0.94	0.13	49,49,49,49	0
56	MG	2a	1724	1/1	0.94	0.31	58,58,58,58	0
56	MG	1A	4039	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3406	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3439	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3482	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	3087	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3714	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3485	1/1	0.94	0.18	39,39,39,39	0
56	MG	2A	3719	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3301	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	3730	1/1	0.94	0.06	37,37,37,37	0
56	MG	1A	3884	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3731	1/1	0.94	0.06	27,27,27,27	0
56	MG	2A	3724	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3490	1/1	0.94	0.13	42,42,42,42	0
56	MG	2a	1743	1/1	0.94	0.09	69,69,69,69	0
56	MG	1A	3890	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3730	1/1	0.94	0.07	75,75,75,75	0
56	MG	1A	3733	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	4055	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	4057	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3124	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3457	1/1	0.94	0.06	33,33,33,33	0
56	MG	2A	3232	1/1	0.94	0.16	53,53,53,53	0
56	MG	1a	1640	1/1	0.94	0.17	64,64,64,64	0
56	MG	1a	1641	1/1	0.94	0.10	57,57,57,57	0
56	MG	2a	1757	1/1	0.94	0.14	60,60,60,60	0
56	MG	2A	3743	1/1	0.94	0.08	71,71,71,71	0
56	MG	2A	3007	1/1	0.94	0.15	61,61,61,61	0
56	MG	1A	3413	1/1	0.94	0.22	43,43,43,43	0
56	MG	1B	202	1/1	0.94	0.22	54,54,54,54	0
56	MG	1A	3737	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3240	1/1	0.94	0.15	58,58,58,58	0
56	MG	1B	205	1/1	0.94	0.19	55,55,55,55	0
56	MG	2A	3019	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3020	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3475	1/1	0.94	0.12	49,49,49,49	0
56	MG	1a	1647	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3205	1/1	0.94	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3029	1/1	0.94	0.10	35,35,35,35	0
56	MG	1B	210	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3906	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	3743	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3048	1/1	0.94	0.06	19,19,19,19	0
56	MG	1A	3909	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3034	1/1	0.94	0.28	64,64,64,64	0
56	MG	1A	3749	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3254	1/1	0.94	0.37	69,69,69,69	0
56	MG	2a	1782	1/1	0.94	0.28	58,58,58,58	0
56	MG	1A	3499	1/1	0.94	0.27	37,37,37,37	0
56	MG	1a	1659	1/1	0.94	0.13	62,62,62,62	0
56	MG	1A	3627	1/1	0.94	0.06	31,31,31,31	0
56	MG	1A	3310	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3774	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3044	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	3424	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	3760	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3504	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3215	1/1	0.94	0.13	47,47,47,47	0
56	MG	2A	3509	1/1	0.94	0.15	59,59,59,59	0
56	MG	2a	1795	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3510	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3050	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3101	1/1	0.94	0.20	40,40,40,40	0
56	MG	1a	1669	1/1	0.94	0.25	57,57,57,57	0
56	MG	1a	1670	1/1	0.94	0.19	65,65,65,65	0
56	MG	2A	3271	1/1	0.94	0.07	49,49,49,49	0
56	MG	2a	1802	1/1	0.94	0.26	66,66,66,66	0
56	MG	2B	207	1/1	0.94	0.13	63,63,63,63	0
56	MG	1B	228	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3361	1/1	0.94	0.27	40,40,40,40	0
56	MG	2A	3524	1/1	0.94	0.25	64,64,64,64	0
56	MG	1A	3635	1/1	0.94	0.06	35,35,35,35	0
56	MG	2A	3059	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3062	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	3637	1/1	0.94	0.08	31,31,31,31	0
56	MG	1B	234	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3105	1/1	0.94	0.34	39,39,39,39	0
56	MG	2A	3071	1/1	0.94	0.26	60,60,60,60	0
56	MG	2A	3533	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3072	1/1	0.94	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2D	306	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3772	1/1	0.94	0.07	26,26,26,26	0
56	MG	1A	3510	1/1	0.94	0.24	60,60,60,60	0
56	MG	2A	3078	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3931	1/1	0.94	0.09	34,34,34,34	0
56	MG	1A	3512	1/1	0.94	0.10	62,62,62,62	0
56	MG	2x	107	1/1	0.94	0.07	59,59,59,59	0
60	K	2x	101	1/1	0.94	0.14	79,79,79,79	0
56	MG	1A	3283	1/1	0.95	0.19	34,34,34,34	0
56	MG	1A	3337	1/1	0.95	0.11	61,61,61,61	0
56	MG	27	102	1/1	0.95	0.21	59,59,59,59	0
56	MG	2A	3001	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3942	1/1	0.95	0.08	66,66,66,66	0
56	MG	2A	3380	1/1	0.95	0.19	66,66,66,66	0
56	MG	2A	3382	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3582	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3017	1/1	0.95	0.13	70,70,70,70	0
56	MG	1A	3809	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3226	1/1	0.95	0.27	45,45,45,45	0
56	MG	2A	3388	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3949	1/1	0.95	0.14	37,37,37,37	0
56	MG	2A	3626	1/1	0.95	0.15	35,35,35,35	0
56	MG	2A	3016	1/1	0.95	0.14	50,50,50,50	0
56	MG	2A	3208	1/1	0.95	0.14	57,57,57,57	0
56	MG	2A	3629	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3812	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3055	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3228	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3591	1/1	0.95	0.08	29,29,29,29	0
56	MG	2A	3022	1/1	0.95	0.21	50,50,50,50	0
56	MG	1a	1664	1/1	0.95	0.19	58,58,58,58	0
56	MG	1E	303	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3486	1/1	0.95	0.31	36,36,36,36	0
56	MG	2A	3402	1/1	0.95	0.13	44,44,44,44	0
56	MG	2A	3403	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3701	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3405	1/1	0.95	0.35	59,59,59,59	0
56	MG	2a	1624	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3818	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3819	1/1	0.95	0.07	21,21,21,21	0
56	MG	2A	3646	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3487	1/1	0.95	0.31	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3123	1/1	0.95	0.18	32,32,32,32	0
56	MG	1E	315	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3962	1/1	0.95	0.09	24,24,24,24	0
56	MG	1A	3822	1/1	0.95	0.14	23,23,23,23	0
56	MG	1A	3824	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3041	1/1	0.95	0.11	37,37,37,37	0
56	MG	1F	309	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3018	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3419	1/1	0.95	0.33	66,66,66,66	0
56	MG	2A	3043	1/1	0.95	0.18	67,67,67,67	0
56	MG	1A	3128	1/1	0.95	0.09	46,46,46,46	0
56	MG	1G	202	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3424	1/1	0.95	0.13	54,54,54,54	0
56	MG	2a	1642	1/1	0.95	0.07	81,81,81,81	0
56	MG	1A	3414	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3605	1/1	0.95	0.09	29,29,29,29	0
56	MG	1A	3348	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3235	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3431	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3059	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3051	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3417	1/1	0.95	0.21	44,44,44,44	0
56	MG	1A	3240	1/1	0.95	0.16	43,43,43,43	0
56	MG	1N	205	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3981	1/1	0.95	0.08	44,44,44,44	0
56	MG	2a	1654	1/1	0.95	0.26	64,64,64,64	0
56	MG	1A	3062	1/1	0.95	0.40	60,60,60,60	0
56	MG	1A	3135	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3836	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3503	1/1	0.95	0.18	48,48,48,48	0
56	MG	2a	1660	1/1	0.95	0.40	72,72,72,72	0
56	MG	1A	3187	1/1	0.95	0.23	39,39,39,39	0
56	MG	2A	3444	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3064	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3839	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3067	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3684	1/1	0.95	0.06	55,55,55,55	0
56	MG	1A	3614	1/1	0.95	0.11	24,24,24,24	0
56	MG	1A	3992	1/1	0.95	0.06	52,52,52,52	0
56	MG	2A	3688	1/1	0.95	0.07	71,71,71,71	0
56	MG	1A	3842	1/1	0.95	0.20	38,38,38,38	0
56	MG	2A	3690	1/1	0.95	0.10	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3615	1/1	0.95	0.08	32,32,32,32	0
56	MG	2A	3074	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3046	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3077	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3302	1/1	0.95	0.19	32,32,32,32	0
56	MG	1Q	207	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3620	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	3847	1/1	0.95	0.05	35,35,35,35	0
56	MG	1A	3621	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3084	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3245	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3305	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3189	1/1	0.95	0.07	44,44,44,44	0
56	MG	1T	202	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3190	1/1	0.95	0.27	40,40,40,40	0
56	MG	1U	205	1/1	0.95	0.19	34,34,34,34	0
56	MG	1A	3191	1/1	0.95	0.18	45,45,45,45	0
56	MG	1V	202	1/1	0.95	0.36	35,35,35,35	0
56	MG	1A	3365	1/1	0.95	0.14	43,43,43,43	0
56	MG	1W	201	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3860	1/1	0.95	0.06	28,28,28,28	0
56	MG	2A	3484	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3067	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3520	1/1	0.95	0.15	37,37,37,37	0
56	MG	2A	3718	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3368	1/1	0.95	0.16	30,30,30,30	0
56	MG	1A	3864	1/1	0.95	0.12	38,38,38,38	0
56	MG	2A	3281	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3741	1/1	0.95	0.07	27,27,27,27	0
56	MG	1A	3866	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3439	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	3744	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3106	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3069	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3872	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3289	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	4022	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3748	1/1	0.95	0.07	52,52,52,52	0
56	MG	1a	1745	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3508	1/1	0.95	0.13	64,64,64,64	0
56	MG	11	102	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3740	1/1	0.95	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4024	1/1	0.95	0.09	18,18,18,18	0
56	MG	2A	3115	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3636	1/1	0.95	0.05	24,24,24,24	0
56	MG	1A	3311	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3118	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3119	1/1	0.95	0.21	49,49,49,49	0
56	MG	2a	1722	1/1	0.95	0.28	66,66,66,66	0
56	MG	2a	1723	1/1	0.95	0.32	60,60,60,60	0
56	MG	2A	3300	1/1	0.95	0.17	68,68,68,68	0
56	MG	2A	3750	1/1	0.95	0.19	54,54,54,54	0
56	MG	2A	3522	1/1	0.95	0.13	55,55,55,55	0
56	MG	2a	1728	1/1	0.95	0.11	61,61,61,61	0
56	MG	2A	3301	1/1	0.95	0.25	66,66,66,66	0
56	MG	2A	3120	1/1	0.95	0.06	51,51,51,51	0
56	MG	12	101	1/1	0.95	0.10	55,55,55,55	0
56	MG	13	102	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3751	1/1	0.95	0.06	74,74,74,74	0
56	MG	2A	3127	1/1	0.95	0.12	42,42,42,42	0
56	MG	15	102	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3371	1/1	0.95	0.25	36,36,36,36	0
56	MG	1A	3015	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3444	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3645	1/1	0.95	0.05	24,24,24,24	0
56	MG	17	101	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3032	1/1	0.95	0.20	24,24,24,24	0
56	MG	1a	1767	1/1	0.95	0.14	69,69,69,69	0
56	MG	1A	3761	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3762	1/1	0.95	0.05	23,23,23,23	0
56	MG	2A	3540	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3541	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3200	1/1	0.95	0.06	54,54,54,54	0
56	MG	2A	3775	1/1	0.95	0.11	73,73,73,73	0
56	MG	2A	3141	1/1	0.95	0.18	43,43,43,43	0
56	MG	1a	1775	1/1	0.95	0.07	57,57,57,57	0
56	MG	2A	3545	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3546	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3149	1/1	0.95	0.06	39,39,39,39	0
56	MG	2A	3145	1/1	0.95	0.13	60,60,60,60	0
56	MG	2A	3782	1/1	0.95	0.32	64,64,64,64	0
56	MG	2a	1761	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	4042	1/1	0.95	0.11	45,45,45,45	0
56	MG	2a	1763	1/1	0.95	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3551	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3540	1/1	0.95	0.20	43,43,43,43	0
56	MG	2A	3554	1/1	0.95	0.14	68,68,68,68	0
56	MG	1a	1779	1/1	0.95	0.27	66,66,66,66	0
56	MG	2A	3557	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3767	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3257	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3899	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3900	1/1	0.95	0.07	36,36,36,36	0
56	MG	1A	3655	1/1	0.95	0.07	24,24,24,24	0
56	MG	1A	3450	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3566	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3025	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3548	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	4052	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3154	1/1	0.95	0.08	51,51,51,51	0
56	MG	2D	302	1/1	0.95	0.33	59,59,59,59	0
56	MG	1a	1617	1/1	0.95	0.09	60,60,60,60	0
56	MG	1a	1791	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3109	1/1	0.95	0.23	34,34,34,34	0
56	MG	1A	3262	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3210	1/1	0.95	0.15	34,34,34,34	0
56	MG	1A	3112	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3114	1/1	0.95	0.18	34,34,34,34	0
56	MG	1A	3271	1/1	0.95	0.44	47,47,47,47	0
56	MG	1B	204	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3785	1/1	0.95	0.23	29,29,29,29	0
56	MG	2A	3172	1/1	0.95	0.28	60,60,60,60	0
56	MG	2a	1793	1/1	0.95	0.27	69,69,69,69	0
56	MG	2E	309	1/1	0.95	0.10	70,70,70,70	0
56	MG	1e	201	1/1	0.95	0.33	67,67,67,67	0
56	MG	1B	206	1/1	0.95	0.11	45,45,45,45	0
56	MG	2F	304	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3035	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3787	1/1	0.95	0.07	45,45,45,45	0
56	MG	1m	3001	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3921	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3274	1/1	0.95	0.26	31,31,31,31	0
56	MG	1A	3563	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3355	1/1	0.95	0.20	60,60,60,60	0
56	MG	2k	201	1/1	0.95	0.17	61,61,61,61	0
56	MG	1A	3084	1/1	0.95	0.28	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2l	203	1/1	0.95	0.11	67,67,67,67	0
56	MG	1A	3793	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3926	1/1	0.95	0.11	69,69,69,69	0
56	MG	2q	201	1/1	0.95	0.07	73,73,73,73	0
56	MG	1A	3468	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3598	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3328	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3276	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3395	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3798	1/1	0.95	0.16	56,56,56,56	0
56	MG	1x	103	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3220	1/1	0.95	0.18	28,28,28,28	0
56	MG	1A	3575	1/1	0.95	0.10	30,30,30,30	0
56	MG	1A	3935	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3576	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3398	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3164	1/1	0.95	0.23	59,59,59,59	0
56	MG	1A	3036	1/1	0.95	0.12	40,40,40,40	0
56	MG	25	101	1/1	0.95	0.27	59,59,59,59	0
58	ZN	24	501	1/1	0.95	0.17	126,126,126,126	0
56	MG	2A	3373	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3590	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3051	1/1	0.96	0.13	31,31,31,31	0
56	MG	1A	3592	1/1	0.96	0.10	25,25,25,25	0
56	MG	1l	101	1/1	0.96	0.38	40,40,40,40	0
56	MG	1A	3155	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3426	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3498	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3927	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3268	1/1	0.96	0.34	71,71,71,71	0
56	MG	2A	3455	1/1	0.96	0.14	66,66,66,66	0
56	MG	1A	3208	1/1	0.96	0.33	42,42,42,42	0
56	MG	12	102	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	4056	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3258	1/1	0.96	0.16	46,46,46,46	0
56	MG	15	101	1/1	0.96	0.26	29,29,29,29	0
56	MG	1A	3042	1/1	0.96	0.15	32,32,32,32	0
56	MG	2A	3675	1/1	0.96	0.11	40,40,40,40	0
56	MG	15	103	1/1	0.96	0.19	35,35,35,35	0
56	MG	1A	4059	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3090	1/1	0.96	0.12	31,31,31,31	0
56	MG	16	101	1/1	0.96	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3680	1/1	0.96	0.13	70,70,70,70	0
56	MG	2A	3468	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3211	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3043	1/1	0.96	0.29	35,35,35,35	0
56	MG	2A	3105	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3473	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3506	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3119	1/1	0.96	0.20	40,40,40,40	0
56	MG	1a	1757	1/1	0.96	0.05	71,71,71,71	0
56	MG	1A	3712	1/1	0.96	0.06	47,47,47,47	0
56	MG	1B	207	1/1	0.96	0.12	50,50,50,50	0
56	MG	1a	1760	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3112	1/1	0.96	0.24	61,61,61,61	0
56	MG	18	102	1/1	0.96	0.08	43,43,43,43	0
56	MG	1a	1763	1/1	0.96	0.10	58,58,58,58	0
56	MG	1a	1764	1/1	0.96	0.12	58,58,58,58	0
56	MG	1A	3008	1/1	0.96	0.11	26,26,26,26	0
56	MG	2A	3698	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3374	1/1	0.96	0.16	34,34,34,34	0
56	MG	2A	3493	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3438	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3495	1/1	0.96	0.24	58,58,58,58	0
56	MG	1a	1768	1/1	0.96	0.08	77,77,77,77	0
56	MG	1A	3511	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3266	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3123	1/1	0.96	0.17	44,44,44,44	0
56	MG	2A	3500	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3501	1/1	0.96	0.15	42,42,42,42	0
56	MG	1a	1773	1/1	0.96	0.07	67,67,67,67	0
56	MG	2A	3125	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3823	1/1	0.96	0.14	26,26,26,26	0
56	MG	1A	3075	1/1	0.96	0.15	36,36,36,36	0
56	MG	2A	3128	1/1	0.96	0.22	55,55,55,55	0
56	MG	1A	3269	1/1	0.96	0.07	23,23,23,23	0
56	MG	1a	1606	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3946	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3723	1/1	0.96	0.10	61,61,61,61	0
56	MG	1a	1611	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3270	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3517	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3519	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3518	1/1	0.96	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3094	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3222	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3623	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3028	1/1	0.96	0.27	38,38,38,38	0
56	MG	2A	3142	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3523	1/1	0.96	0.16	38,38,38,38	0
56	MG	1A	3384	1/1	0.96	0.10	40,40,40,40	0
56	MG	1B	231	1/1	0.96	0.05	35,35,35,35	0
56	MG	1A	3734	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3167	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3172	1/1	0.96	0.06	18,18,18,18	0
56	MG	1A	3125	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3047	1/1	0.96	0.18	34,34,34,34	0
56	MG	1a	1796	1/1	0.96	0.29	64,64,64,64	0
56	MG	1a	1630	1/1	0.96	0.16	26,26,26,26	0
56	MG	1A	3739	1/1	0.96	0.07	59,59,59,59	0
56	MG	1A	3452	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3280	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3969	1/1	0.96	0.04	29,29,29,29	0
56	MG	1D	303	1/1	0.96	0.09	33,33,33,33	0
56	MG	2a	1704	1/1	0.96	0.18	63,63,63,63	0
56	MG	1f	3101	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3535	1/1	0.96	0.22	51,51,51,51	0
56	MG	2A	3161	1/1	0.96	0.09	46,46,46,46	0
56	MG	1D	306	1/1	0.96	0.10	33,33,33,33	0
56	MG	1D	307	1/1	0.96	0.11	43,43,43,43	0
56	MG	1D	308	1/1	0.96	0.09	52,52,52,52	0
56	MG	2A	3548	1/1	0.96	0.06	45,45,45,45	0
56	MG	1D	309	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3127	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3745	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3334	1/1	0.96	0.13	68,68,68,68	0
56	MG	1A	3282	1/1	0.96	0.07	50,50,50,50	0
56	MG	1E	306	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	3459	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3544	1/1	0.96	0.09	36,36,36,36	0
56	MG	2A	3559	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3770	1/1	0.96	0.22	53,53,53,53	0
56	MG	2A	3560	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3098	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3982	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3232	1/1	0.96	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1726	1/1	0.96	0.20	64,64,64,64	0
56	MG	1A	3856	1/1	0.96	0.07	37,37,37,37	0
56	MG	1E	314	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3857	1/1	0.96	0.07	26,26,26,26	0
56	MG	1E	316	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3754	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3755	1/1	0.96	0.04	35,35,35,35	0
56	MG	1A	3011	1/1	0.96	0.06	37,37,37,37	0
56	MG	1F	306	1/1	0.96	0.06	41,41,41,41	0
56	MG	2a	1735	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3552	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3464	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3235	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3575	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3340	1/1	0.96	0.09	54,54,54,54	0
56	MG	1G	201	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3006	1/1	0.96	0.17	61,61,61,61	0
56	MG	1A	3132	1/1	0.96	0.17	33,33,33,33	0
56	MG	2A	3008	1/1	0.96	0.05	44,44,44,44	0
56	MG	1a	1667	1/1	0.96	0.13	66,66,66,66	0
56	MG	2A	3012	1/1	0.96	0.15	44,44,44,44	0
56	MG	2A	3013	1/1	0.96	0.05	35,35,35,35	0
56	MG	1A	3081	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3470	1/1	0.96	0.14	36,36,36,36	0
56	MG	1A	3869	1/1	0.96	0.07	39,39,39,39	0
56	MG	2B	217	1/1	0.96	0.18	75,75,75,75	0
56	MG	2A	3588	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3372	1/1	0.96	0.08	64,64,64,64	0
56	MG	1A	3560	1/1	0.96	0.26	47,47,47,47	0
56	MG	2D	304	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3871	1/1	0.96	0.19	24,24,24,24	0
56	MG	1A	3083	1/1	0.96	0.21	30,30,30,30	0
56	MG	2A	3021	1/1	0.96	0.05	43,43,43,43	0
56	MG	2A	3203	1/1	0.96	0.25	51,51,51,51	0
56	MG	1A	3136	1/1	0.96	0.11	33,33,33,33	0
56	MG	2A	3381	1/1	0.96	0.24	48,48,48,48	0
56	MG	1A	3102	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3024	1/1	0.96	0.19	49,49,49,49	0
56	MG	2a	1768	1/1	0.96	0.09	70,70,70,70	0
56	MG	2E	306	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	4005	1/1	0.96	0.05	43,43,43,43	0
56	MG	1A	3876	1/1	0.96	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3564	1/1	0.96	0.24	57,57,57,57	0
56	MG	2F	301	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3030	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3567	1/1	0.96	0.21	48,48,48,48	0
56	MG	1A	3775	1/1	0.96	0.33	29,29,29,29	0
56	MG	2A	3032	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3107	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3407	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3143	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3886	1/1	0.96	0.07	68,68,68,68	0
56	MG	1A	3779	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	4018	1/1	0.96	0.05	22,22,22,22	0
56	MG	1A	3192	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3193	1/1	0.96	0.07	29,29,29,29	0
56	MG	2A	3401	1/1	0.96	0.09	71,71,71,71	0
56	MG	1A	3480	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	3675	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3784	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3411	1/1	0.96	0.07	56,56,56,56	0
56	MG	1a	1696	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3061	1/1	0.96	0.33	59,59,59,59	0
56	MG	1A	3248	1/1	0.96	0.20	31,31,31,31	0
56	MG	1U	201	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3901	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3146	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3110	1/1	0.96	0.11	30,30,30,30	0
56	MG	1a	1704	1/1	0.96	0.20	66,66,66,66	0
56	MG	2A	3415	1/1	0.96	0.11	34,34,34,34	0
56	MG	1a	1705	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3356	1/1	0.96	0.15	42,42,42,42	0
56	MG	1V	205	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3791	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3420	1/1	0.96	0.20	47,47,47,47	0
56	MG	2f	201	1/1	0.96	0.05	46,46,46,46	0
56	MG	2j	201	1/1	0.96	0.17	69,69,69,69	0
56	MG	1a	1711	1/1	0.96	0.15	44,44,44,44	0
56	MG	2l	201	1/1	0.96	0.10	73,73,73,73	0
56	MG	1a	1712	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3638	1/1	0.96	0.07	39,39,39,39	0
56	MG	28	101	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3792	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3241	1/1	0.96	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3419	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3068	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3069	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3583	1/1	0.96	0.09	57,57,57,57	0
56	MG	1X	101	1/1	0.96	0.35	43,43,43,43	0
56	MG	1X	106	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	3685	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	4040	1/1	0.96	0.14	50,50,50,50	0
56	MG	1Y	203	1/1	0.96	0.21	43,43,43,43	0
56	MG	2A	3076	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3007	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3687	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3151	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3113	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3081	1/1	0.96	0.11	39,39,39,39	0
57	A1A1L	2A	3783	36/36	0.96	0.09	33,42,49,58	0
58	ZN	14	102	1/1	0.96	0.12	118,118,118,118	0
56	MG	1A	3587	1/1	0.96	0.06	34,34,34,34	0
58	ZN	2n	501	1/1	0.96	0.07	89,89,89,89	0
56	MG	1A	3423	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3376	1/1	0.97	0.40	53,53,53,53	0
56	MG	1A	3277	1/1	0.97	0.14	49,49,49,49	0
56	MG	2A	3378	1/1	0.97	0.09	21,21,21,21	0
56	MG	1A	3911	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3359	1/1	0.97	0.04	42,42,42,42	0
56	MG	1a	1616	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3553	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	3202	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3555	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3383	1/1	0.97	0.09	54,54,54,54	0
56	MG	2A	3734	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3104	1/1	0.97	0.16	37,37,37,37	0
56	MG	1a	1619	1/1	0.97	0.06	50,50,50,50	0
56	MG	1a	1620	1/1	0.97	0.32	63,63,63,63	0
56	MG	1A	3141	1/1	0.97	0.14	25,25,25,25	0
56	MG	1F	301	1/1	0.97	0.15	38,38,38,38	0
56	MG	2a	1666	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	4017	1/1	0.97	0.04	42,42,42,42	0
56	MG	2A	3742	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3916	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3071	1/1	0.97	0.08	16,16,16,16	0
56	MG	1A	3366	1/1	0.97	0.41	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3412	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3662	1/1	0.97	0.08	29,29,29,29	0
56	MG	1F	310	1/1	0.97	0.06	47,47,47,47	0
56	MG	2A	3396	1/1	0.97	0.07	52,52,52,52	0
56	MG	1F	311	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3173	1/1	0.97	0.06	33,33,33,33	0
56	MG	1F	313	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3746	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	4025	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3033	1/1	0.97	0.25	31,31,31,31	0
56	MG	1A	3108	1/1	0.97	0.17	33,33,33,33	0
56	MG	1A	3145	1/1	0.97	0.17	28,28,28,28	0
56	MG	1A	3212	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3469	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	4032	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3213	1/1	0.97	0.10	50,50,50,50	0
56	MG	2A	3764	1/1	0.97	0.15	43,43,43,43	0
56	MG	1A	3524	1/1	0.97	0.15	44,44,44,44	0
56	MG	2A	3583	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3073	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3330	1/1	0.97	0.18	29,29,29,29	0
56	MG	1A	3757	1/1	0.97	0.08	20,20,20,20	0
56	MG	1a	1646	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3376	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3331	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3840	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3596	1/1	0.97	0.06	21,21,21,21	0
56	MG	1P	202	1/1	0.97	0.19	34,34,34,34	0
56	MG	1P	203	1/1	0.97	0.20	30,30,30,30	0
56	MG	1A	3598	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3122	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3290	1/1	0.97	0.14	37,37,37,37	0
56	MG	1Q	202	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	3763	1/1	0.97	0.05	25,25,25,25	0
56	MG	2A	3426	1/1	0.97	0.06	72,72,72,72	0
56	MG	1A	3252	1/1	0.97	0.07	50,50,50,50	0
56	MG	2A	3428	1/1	0.97	0.07	68,68,68,68	0
56	MG	1A	3531	1/1	0.97	0.15	35,35,35,35	0
56	MG	1l	201	1/1	0.97	0.04	74,74,74,74	0
56	MG	1A	3532	1/1	0.97	0.06	25,25,25,25	0
56	MG	1A	3604	1/1	0.97	0.11	28,28,28,28	0
56	MG	1R	201	1/1	0.97	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3683	1/1	0.97	0.04	15,15,15,15	0
56	MG	2A	3133	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3533	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3147	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3074	1/1	0.97	0.31	48,48,48,48	0
56	MG	1A	3536	1/1	0.97	0.27	41,41,41,41	0
56	MG	1A	3854	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3855	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3538	1/1	0.97	0.20	40,40,40,40	0
56	MG	2A	3443	1/1	0.97	0.10	43,43,43,43	0
56	MG	2D	301	1/1	0.97	0.11	42,42,42,42	0
56	MG	1U	202	1/1	0.97	0.25	38,38,38,38	0
56	MG	1a	1672	1/1	0.97	0.16	48,48,48,48	0
56	MG	1U	203	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3447	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3111	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3858	1/1	0.97	0.05	29,29,29,29	0
56	MG	1A	3150	1/1	0.97	0.07	34,34,34,34	0
56	MG	1V	201	1/1	0.97	0.24	28,28,28,28	0
56	MG	1A	3957	1/1	0.97	0.05	40,40,40,40	0
56	MG	1V	204	1/1	0.97	0.17	53,53,53,53	0
56	MG	2E	304	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3430	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3185	1/1	0.97	0.26	36,36,36,36	0
56	MG	1A	3066	1/1	0.97	0.07	32,32,32,32	0
56	MG	1W	202	1/1	0.97	0.18	48,48,48,48	0
56	MG	2a	1740	1/1	0.97	0.24	55,55,55,55	0
56	MG	1W	203	1/1	0.97	0.22	38,38,38,38	0
56	MG	1A	3546	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3697	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3005	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3129	1/1	0.97	0.05	45,45,45,45	0
56	MG	2F	305	1/1	0.97	0.16	48,48,48,48	0
56	MG	1X	102	1/1	0.97	0.07	39,39,39,39	0
56	MG	2A	3464	1/1	0.97	0.06	47,47,47,47	0
56	MG	1X	103	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3466	1/1	0.97	0.07	56,56,56,56	0
56	MG	1X	104	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3618	1/1	0.97	0.04	26,26,26,26	0
56	MG	2Q	201	1/1	0.97	0.12	64,64,64,64	0
56	MG	2a	1756	1/1	0.97	0.20	54,54,54,54	0
56	MG	1A	3130	1/1	0.97	0.06	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3470	1/1	0.97	0.06	48,48,48,48	0
56	MG	2A	3165	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3021	1/1	0.97	0.09	25,25,25,25	0
56	MG	1A	3488	1/1	0.97	0.09	33,33,33,33	0
56	MG	2A	3474	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3157	1/1	0.97	0.12	28,28,28,28	0
56	MG	2A	3476	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3063	1/1	0.97	0.10	34,34,34,34	0
56	MG	1a	1698	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3480	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3656	1/1	0.97	0.26	48,48,48,48	0
56	MG	1A	3973	1/1	0.97	0.05	35,35,35,35	0
56	MG	2X	102	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3089	1/1	0.97	0.15	56,56,56,56	0
56	MG	2A	3483	1/1	0.97	0.10	52,52,52,52	0
56	MG	10	102	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3392	1/1	0.97	0.25	56,56,56,56	0
56	MG	1B	219	1/1	0.97	0.05	55,55,55,55	0
56	MG	23	101	1/1	0.97	0.06	54,54,54,54	0
56	MG	1B	220	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3977	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3709	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3490	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3491	1/1	0.97	0.10	39,39,39,39	0
56	MG	1B	223	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3626	1/1	0.97	0.10	36,36,36,36	0
56	MG	1a	1710	1/1	0.97	0.05	39,39,39,39	0
56	MG	2A	3031	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3231	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3079	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3268	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3195	1/1	0.97	0.11	25,25,25,25	0
56	MG	1A	3715	1/1	0.97	0.07	52,52,52,52	0
56	MG	2A	3037	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	3497	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3196	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3236	1/1	0.97	0.07	45,45,45,45	0
56	MG	1a	1720	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3887	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3888	1/1	0.97	0.05	38,38,38,38	0
56	MG	15	105	1/1	0.97	0.26	35,35,35,35	0
56	MG	2A	3685	1/1	0.97	0.05	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	15	106	1/1	0.97	0.08	34,34,34,34	0
56	MG	1A	3719	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3565	1/1	0.97	0.23	37,37,37,37	0
56	MG	1a	1727	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3500	1/1	0.97	0.29	39,39,39,39	0
56	MG	2A	3052	1/1	0.97	0.05	53,53,53,53	0
56	MG	1B	239	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3070	1/1	0.97	0.26	33,33,33,33	0
56	MG	1A	3273	1/1	0.97	0.24	31,31,31,31	0
56	MG	1A	3640	1/1	0.97	0.05	20,20,20,20	0
56	MG	1a	1734	1/1	0.97	0.05	56,56,56,56	0
56	MG	1A	3569	1/1	0.97	0.19	30,30,30,30	0
56	MG	1A	3137	1/1	0.97	0.05	18,18,18,18	0
56	MG	2A	3061	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3810	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3138	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	4002	1/1	0.97	0.10	26,26,26,26	0
56	MG	2A	3531	1/1	0.97	0.08	45,45,45,45	0
56	MG	1D	310	1/1	0.97	0.14	26,26,26,26	0
56	MG	2A	3066	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3646	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3903	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3904	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3572	1/1	0.97	0.05	25,25,25,25	0
56	MG	1E	305	1/1	0.97	0.16	28,28,28,28	0
56	MG	1A	3648	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3103	1/1	0.97	0.07	30,30,30,30	0
56	MG	1a	1608	1/1	0.97	0.06	55,55,55,55	0
56	MG	1E	308	1/1	0.97	0.12	35,35,35,35	0
57	A1A1L	1A	4060	36/36	0.97	0.08	19,28,35,44	0
56	MG	2A	3715	1/1	0.97	0.04	39,39,39,39	0
56	MG	1a	1751	1/1	0.97	0.08	62,62,62,62	0
56	MG	1a	1610	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	4009	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3453	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3003	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3178	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3541	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3203	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3690	1/1	0.98	0.07	26,26,26,26	0
56	MG	2A	3313	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3046	1/1	0.98	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3179	1/1	0.98	0.06	40,40,40,40	0
56	MG	2A	3407	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3589	1/1	0.98	0.08	54,54,54,54	0
56	MG	1A	3233	1/1	0.98	0.26	35,35,35,35	0
56	MG	1a	1707	1/1	0.98	0.11	57,57,57,57	0
56	MG	1A	3752	1/1	0.98	0.08	51,51,51,51	0
56	MG	2A	3505	1/1	0.98	0.05	32,32,32,32	0
56	MG	1X	105	1/1	0.98	0.05	47,47,47,47	0
56	MG	2a	1746	1/1	0.98	0.11	80,80,80,80	0
56	MG	1A	3639	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3545	1/1	0.98	0.18	32,32,32,32	0
56	MG	1A	3696	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3289	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3158	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	3700	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3106	1/1	0.98	0.23	30,30,30,30	0
56	MG	2a	1754	1/1	0.98	0.08	59,59,59,59	0
56	MG	2A	3060	1/1	0.98	0.11	34,34,34,34	0
56	MG	1A	3292	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	3207	1/1	0.98	0.23	39,39,39,39	0
56	MG	1a	1719	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3597	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3264	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3243	1/1	0.98	0.18	51,51,51,51	0
56	MG	1A	3013	1/1	0.98	0.16	29,29,29,29	0
56	MG	2a	1659	1/1	0.98	0.06	60,60,60,60	0
56	MG	2A	3717	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3651	1/1	0.98	0.07	24,24,24,24	0
56	MG	1A	3943	1/1	0.98	0.09	53,53,53,53	0
56	MG	2A	3157	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3360	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3601	1/1	0.98	0.04	26,26,26,26	0
56	MG	1a	1648	1/1	0.98	0.09	47,47,47,47	0
56	MG	2O	201	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3183	1/1	0.98	0.16	39,39,39,39	0
56	MG	2A	3725	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3656	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3397	1/1	0.98	0.16	39,39,39,39	0
56	MG	2A	3729	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3558	1/1	0.98	0.15	33,33,33,33	0
56	MG	1N	203	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3031	1/1	0.98	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3951	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3363	1/1	0.98	0.10	49,49,49,49	0
56	MG	1A	3133	1/1	0.98	0.28	35,35,35,35	0
56	MG	1A	3516	1/1	0.98	0.28	34,34,34,34	0
56	MG	15	104	1/1	0.98	0.19	27,27,27,27	0
56	MG	1A	3121	1/1	0.98	0.16	34,34,34,34	0
56	MG	1A	3894	1/1	0.98	0.05	44,44,44,44	0
56	MG	1a	1742	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3010	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3214	1/1	0.98	0.16	42,42,42,42	0
56	MG	1P	201	1/1	0.98	0.28	33,33,33,33	0
56	MG	1A	3068	1/1	0.98	0.10	19,19,19,19	0
56	MG	1B	230	1/1	0.98	0.06	41,41,41,41	0
56	MG	1P	204	1/1	0.98	0.25	33,33,33,33	0
56	MG	2A	3092	1/1	0.98	0.05	28,28,28,28	0
56	MG	17	102	1/1	0.98	0.08	31,31,31,31	0
56	MG	17	103	1/1	0.98	0.10	35,35,35,35	0
56	MG	25	102	1/1	0.98	0.20	47,47,47,47	0
56	MG	1A	3304	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3044	1/1	0.98	0.08	36,36,36,36	0
56	MG	2A	3009	1/1	0.98	0.07	46,46,46,46	0
56	MG	27	101	1/1	0.98	0.10	39,39,39,39	0
56	MG	2A	3755	1/1	0.98	0.04	54,54,54,54	0
56	MG	2A	3010	1/1	0.98	0.06	43,43,43,43	0
56	MG	1Q	201	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3484	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	3060	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3671	1/1	0.98	0.03	16,16,16,16	0
56	MG	2A	3015	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	4030	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3617	1/1	0.98	0.03	27,27,27,27	0
56	MG	1A	3967	1/1	0.98	0.07	32,32,32,32	0
56	MG	1a	1761	1/1	0.98	0.06	68,68,68,68	0
56	MG	1A	3168	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3219	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	3169	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3971	1/1	0.98	0.06	23,23,23,23	0
56	MG	1D	304	1/1	0.98	0.09	22,22,22,22	0
56	MG	1A	4037	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3375	1/1	0.98	0.07	30,30,30,30	0
56	MG	2A	3477	1/1	0.98	0.11	35,35,35,35	0
56	MG	1A	3170	1/1	0.98	0.06	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3152	1/1	0.98	0.21	30,30,30,30	0
56	MG	1A	3037	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3082	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3038	1/1	0.98	0.17	36,36,36,36	0
56	MG	1a	1691	1/1	0.98	0.15	47,47,47,47	0
56	MG	1A	3156	1/1	0.98	0.16	35,35,35,35	0
56	MG	1A	3457	1/1	0.98	0.15	40,40,40,40	0
56	MG	1E	302	1/1	0.98	0.22	35,35,35,35	0
56	MG	1A	3537	1/1	0.98	0.12	41,41,41,41	0
56	MG	1E	304	1/1	0.98	0.09	33,33,33,33	0
58	ZN	2Y	202	1/1	0.98	0.04	91,91,91,91	0
56	MG	1A	3742	1/1	0.98	0.03	44,44,44,44	0
58	ZN	29	501	1/1	0.98	0.05	74,74,74,74	0
56	MG	2A	3039	1/1	0.98	0.12	50,50,50,50	0
56	MG	1A	3347	1/1	0.98	0.09	42,42,42,42	0
56	MG	2A	3517	1/1	0.99	0.03	41,41,41,41	0
56	MG	2A	3625	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3551	1/1	0.99	0.05	36,36,36,36	0
56	MG	1A	3012	1/1	0.99	0.03	30,30,30,30	0
56	MG	1F	303	1/1	0.99	0.16	33,33,33,33	0
56	MG	1A	3115	1/1	0.99	0.07	36,36,36,36	0
56	MG	1A	3653	1/1	0.99	0.06	30,30,30,30	0
56	MG	1A	3171	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3773	1/1	0.99	0.03	46,46,46,46	0
56	MG	2A	3633	1/1	0.99	0.05	60,60,60,60	0
56	MG	1F	308	1/1	0.99	0.17	30,30,30,30	0
56	MG	2A	3749	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	4053	1/1	0.99	0.03	37,37,37,37	0
56	MG	1A	3975	1/1	0.99	0.06	34,34,34,34	0
56	MG	13	101	1/1	0.99	0.07	33,33,33,33	0
56	MG	1A	3095	1/1	0.99	0.11	24,24,24,24	0
56	MG	1A	3905	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3005	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3186	1/1	0.99	0.24	26,26,26,26	0
56	MG	1A	3449	1/1	0.99	0.07	36,36,36,36	0
56	MG	1a	1770	1/1	0.99	0.04	52,52,52,52	0
56	MG	1U	206	1/1	0.99	0.28	35,35,35,35	0
56	MG	1A	3293	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3229	1/1	0.99	0.17	32,32,32,32	0
56	MG	1A	3633	1/1	0.99	0.04	37,37,37,37	0
56	MG	1V	203	1/1	0.99	0.15	29,29,29,29	0
56	MG	1A	3078	1/1	0.99	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3201	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3721	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3879	1/1	0.99	0.03	24,24,24,24	0
56	MG	1A	3988	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3880	1/1	0.99	0.03	27,27,27,27	0
56	MG	1W	204	1/1	0.99	0.09	40,40,40,40	0
56	MG	1a	1733	1/1	0.99	0.09	59,59,59,59	0
56	MG	2A	3772	1/1	0.99	0.06	57,57,57,57	0
56	MG	1A	3014	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	3991	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3023	1/1	0.99	0.08	19,19,19,19	0
56	MG	1A	3519	1/1	0.99	0.09	27,27,27,27	0
56	MG	1A	3418	1/1	0.99	0.20	39,39,39,39	0
56	MG	1A	3437	1/1	0.99	0.23	37,37,37,37	0
56	MG	1A	3641	1/1	0.99	0.06	24,24,24,24	0
56	MG	1A	3057	1/1	0.99	0.07	25,25,25,25	0
56	MG	2A	3609	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3699	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3065	1/1	0.99	0.12	30,30,30,30	0
56	MG	1A	3644	1/1	0.99	0.04	24,24,24,24	0
56	MG	1A	3039	1/1	0.99	0.27	35,35,35,35	0
56	MG	1A	3963	1/1	0.99	0.03	35,35,35,35	0
56	MG	2A	3727	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	3221	1/1	0.99	0.14	33,33,33,33	0
56	MG	1A	3462	1/1	0.99	0.08	37,37,37,37	0
56	MG	1A	3549	1/1	0.99	0.10	39,39,39,39	0
56	MG	2A	3511	1/1	0.99	0.08	43,43,43,43	0
58	ZN	1Y	204	1/1	0.99	0.03	65,65,65,65	0
56	MG	1A	3009	1/1	0.99	0.03	23,23,23,23	0
58	ZN	15	109	1/1	0.99	0.08	49,49,49,49	0
58	ZN	1n	103	1/1	0.99	0.03	66,66,66,66	0
56	MG	2A	3513	1/1	0.99	0.07	66,66,66,66	0
56	MG	1A	3896	1/1	0.99	0.02	14,14,14,14	0
58	ZN	25	106	1/1	0.99	0.04	54,54,54,54	0
58	ZN	26	501	1/1	0.99	0.05	66,66,66,66	0
56	MG	1a	1752	1/1	0.99	0.09	56,56,56,56	0
56	MG	2A	3516	1/1	0.99	0.07	41,41,41,41	0
59	SF4	1d	302	8/8	0.99	0.05	62,68,71,74	0
59	SF4	2d	302	8/8	0.99	0.05	62,71,81,82	0
56	MG	2A	3737	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3728	1/1	1.00	0.08	37,37,37,37	0
56	MG	1A	3898	1/1	1.00	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	16	104	1/1	1.00	0.04	46,46,46,46	0
58	ZN	19	102	1/1	1.00	0.06	47,47,47,47	0
56	MG	1A	3874	1/1	1.00	0.07	39,39,39,39	0
56	MG	1a	1769	1/1	1.00	0.04	49,49,49,49	0
56	MG	1A	3774	1/1	1.00	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.