



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 12:53 AM UTC

PDB ID : 9O3L / pdb_00009o3l
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with macrolide erythromycin, mRNA, deacylated A-site tRNA^{phe}, P-site fMRC-peptidyl-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.75Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Kruglov, A.A.; Paranjpe, M.N.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2025-04-07
Resolution : 2.75 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

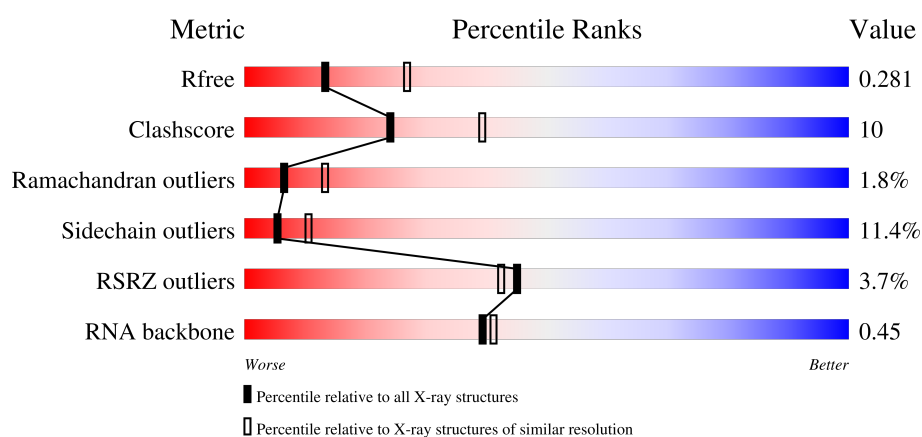
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



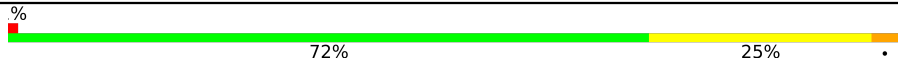
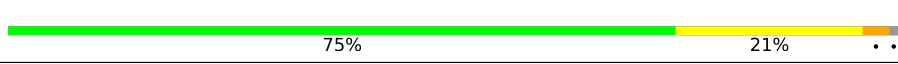
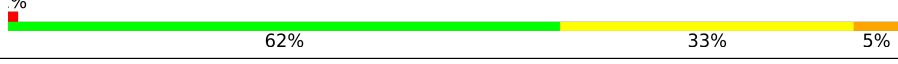
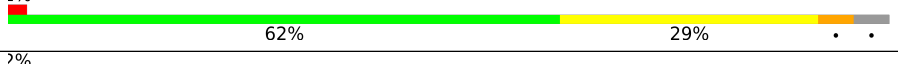
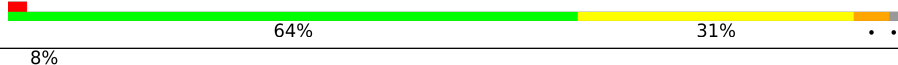
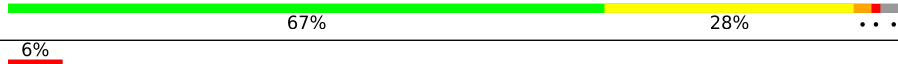
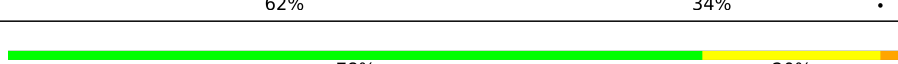
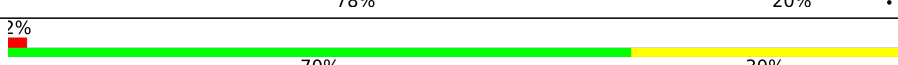
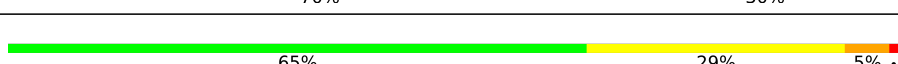
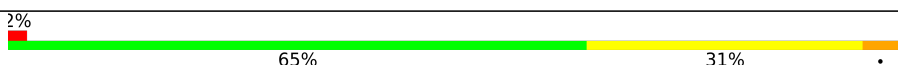
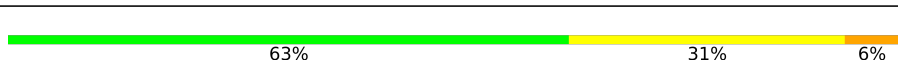
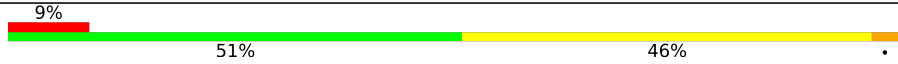
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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	2% 59% 33% 7%
1	2A	2915	% 53% 35% 8%
2	1B	121	60% 38%
2	2B	121	% 43% 47% 9%

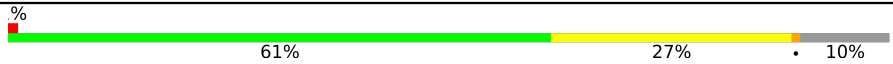
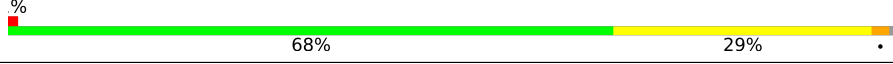
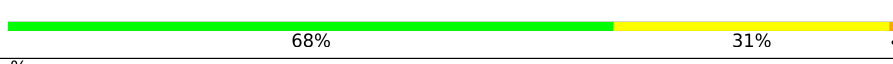
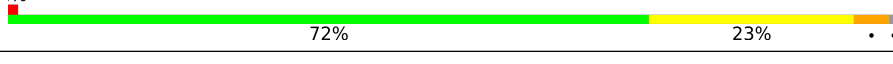
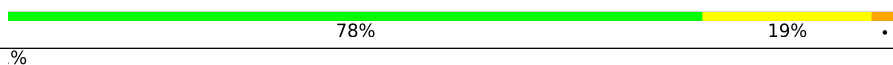
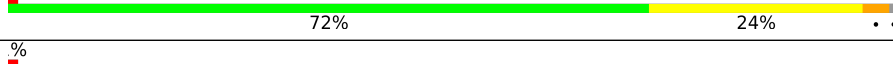
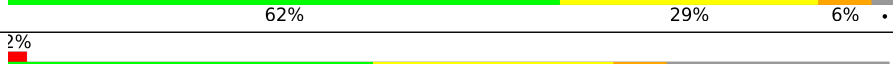
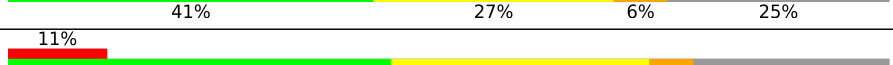
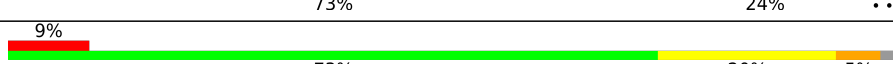
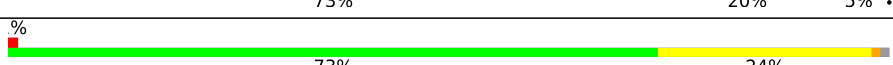
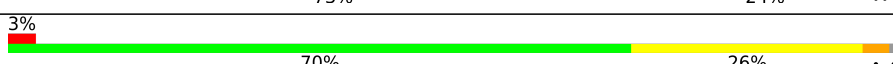
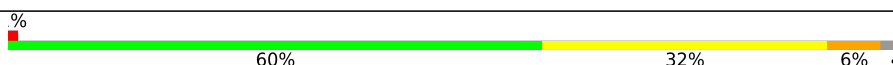
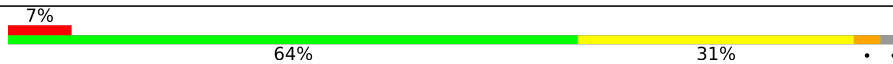
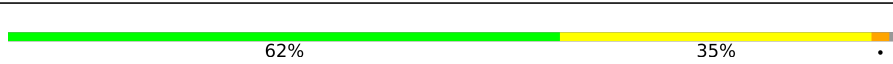
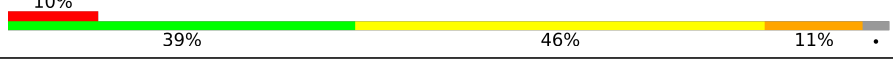
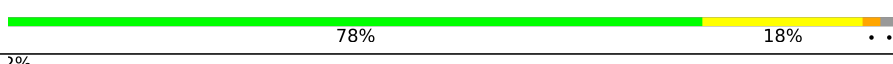
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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118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

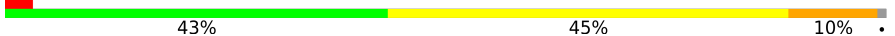
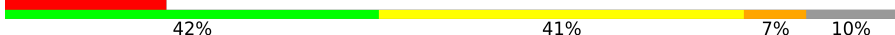
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

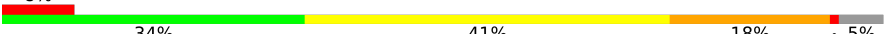
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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	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	
56	1z	3	
56	2z	3	

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
57	MG	2a	1695	-	-	-	X
61	SF4	2d	303	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299368 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	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

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

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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 MET-PHE-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 tRNAphe.

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

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMRC-tRNAcys RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			27	15	6	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			27	15	6	4	2			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1085	Total	Mg	0	0
			1085	1085		
57	1B	38	Total	Mg	0	0
			38	38		
57	1D	12	Total	Mg	0	0
			12	12		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1E	13	Total 13	Mg 13	0	0
57	1F	13	Total 13	Mg 13	0	0
57	1G	4	Total 4	Mg 4	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	4	Total 4	Mg 4	0	0
57	1P	6	Total 6	Mg 6	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	6	Total 6	Mg 6	0	0
57	1S	2	Total 2	Mg 2	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	11	Total 11	Mg 11	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	7	Total 7	Mg 7	0	0
57	1X	7	Total 7	Mg 7	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	10	Total 10	Mg 10	0	0
57	11	3	Total 3	Mg 3	0	0
57	12	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	9	Total 9	Mg 9	0	0
57	16	2	Total 2	Mg 2	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	7	Total 7	Mg 7	0	0
57	1a	211	Total 211	Mg 211	0	0
57	1b	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	1	Total 1	Mg 1	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1j	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	3	Total 3	Mg 3	0	0
57	1p	1	Total 1	Mg 1	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1w	6	Total 6	Mg 6	0	0
57	1x	12	Total 12	Mg 12	0	0
57	2A	855	Total 855	Mg 855	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2B	20	Total 20	Mg 20	0	0
57	2D	6	Total 6	Mg 6	0	0
57	2E	9	Total 9	Mg 9	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	2	Total 2	Mg 2	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	1	Total 1	Mg 1	0	0
57	2R	4	Total 4	Mg 4	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	1	Total 1	Mg 1	0	0
57	2W	2	Total 2	Mg 2	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	3	Total 3	Mg 3	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	1	Total 1	Mg 1	0	0
57	26	1	Total 1	Mg 1	0	0

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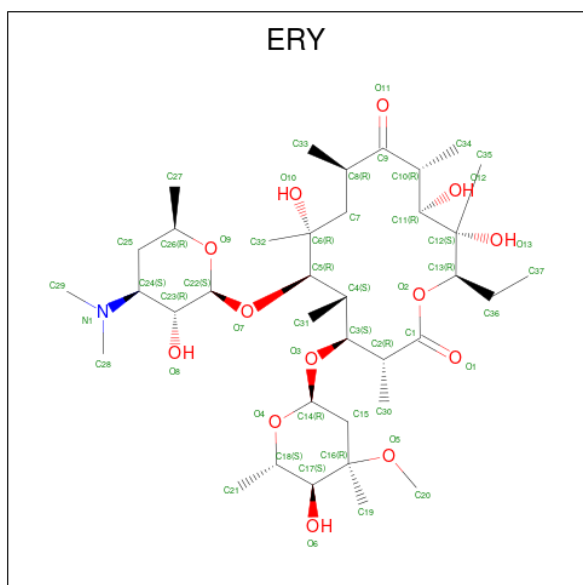
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	27	4	Total 4	Mg 4	0	0
57	28	3	Total 3	Mg 3	0	0
57	2a	225	Total 225	Mg 225	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	4	Total 4	Mg 4	0	0
57	2o	1	Total 1	Mg 1	0	0
57	2q	3	Total 3	Mg 3	0	0
57	2r	1	Total 1	Mg 1	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2w	5	Total 5	Mg 5	0	0
57	2x	6	Total 6	Mg 6	0	0
57	2z	1	Total 1	Mg 1	0	0
57	2y	1	Total 1	Mg 1	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2A	1	Total K 1 1	0	0

- Molecule 59 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total C N O 51 37 1 13	0	0
59	2A	1	Total C N O 51 37 1 13	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

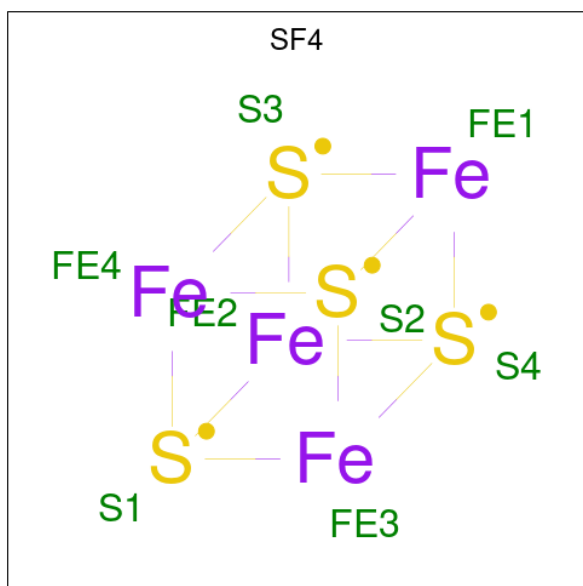
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0

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

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1680	Total 1680	O 1680	0	0
62	1B	54	Total 54	O 54	0	0
62	1D	32	Total 32	O 32	0	0
62	1E	23	Total 23	O 23	0	0
62	1F	17	Total 17	O 17	0	0
62	1G	1	Total 1	O 1	0	0
62	1H	1	Total 1	O 1	0	0
62	1N	4	Total 4	O 4	0	0
62	1O	3	Total 3	O 3	0	0
62	1P	15	Total 15	O 15	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	12	Total 12	O 12	0	0
62	1S	3	Total 3	O 3	0	0
62	1T	6	Total 6	O 6	0	0
62	1U	8	Total 8	O 8	0	0
62	1V	9	Total 9	O 9	0	0
62	1W	9	Total 9	O 9	0	0
62	1X	6	Total 6	O 6	0	0
62	1Y	1	Total 1	O 1	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	8	Total 8	O 8	0	0
62	11	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	12	3	Total 3	O 3	0	0
62	13	4	Total 4	O 4	0	0
62	14	1	Total 1	O 1	0	0
62	15	6	Total 6	O 6	0	0
62	16	3	Total 3	O 3	0	0
62	17	10	Total 10	O 10	0	0
62	18	8	Total 8	O 8	0	0
62	1a	252	Total 252	O 252	0	0
62	1b	1	Total 1	O 1	0	0
62	1d	1	Total 1	O 1	0	0
62	1f	1	Total 1	O 1	0	0
62	1l	3	Total 3	O 3	0	0
62	1m	2	Total 2	O 2	0	0
62	1o	1	Total 1	O 1	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	3	Total 3	O 3	0	0
62	1w	8	Total 8	O 8	0	0
62	1x	7	Total 7	O 7	0	0
62	1z	1	Total 1	O 1	0	0

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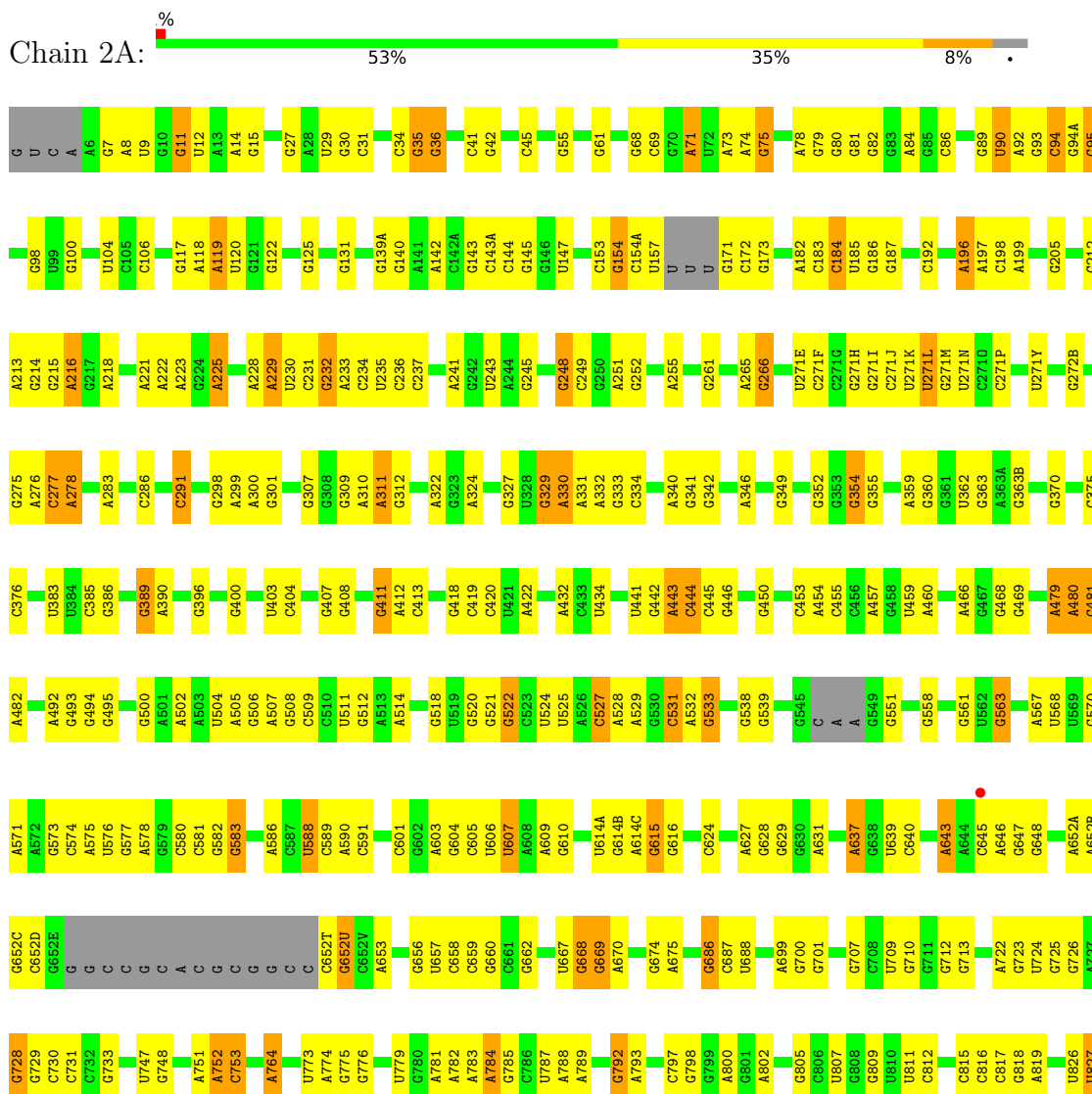
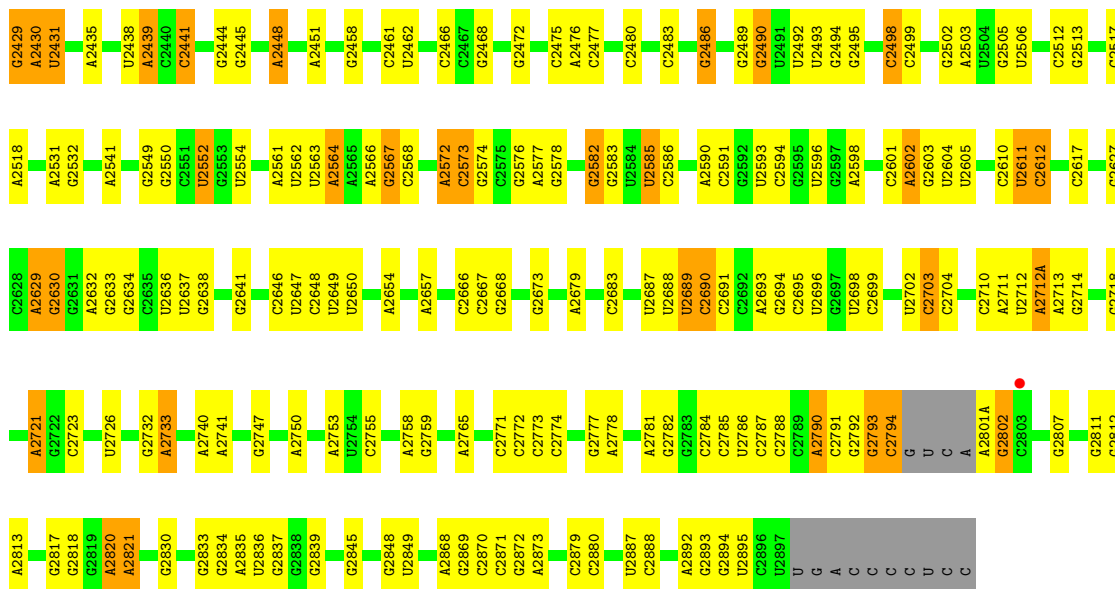
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1y	1	Total 1	O 1	0	0
62	2A	952	Total 952	O 952	0	0
62	2B	21	Total 21	O 21	0	0
62	2D	15	Total 15	O 15	0	0
62	2E	5	Total 5	O 5	0	0
62	2F	13	Total 13	O 13	0	0
62	2O	3	Total 3	O 3	0	0
62	2P	6	Total 6	O 6	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	4	Total 4	O 4	0	0
62	2T	2	Total 2	O 2	0	0
62	2U	2	Total 2	O 2	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	1	Total 1	O 1	0	0
62	2X	5	Total 5	O 5	0	0
62	20	2	Total 2	O 2	0	0
62	21	6	Total 6	O 6	0	0
62	23	1	Total 1	O 1	0	0
62	25	2	Total 2	O 2	0	0
62	27	2	Total 2	O 2	0	0
62	28	3	Total 3	O 3	0	0

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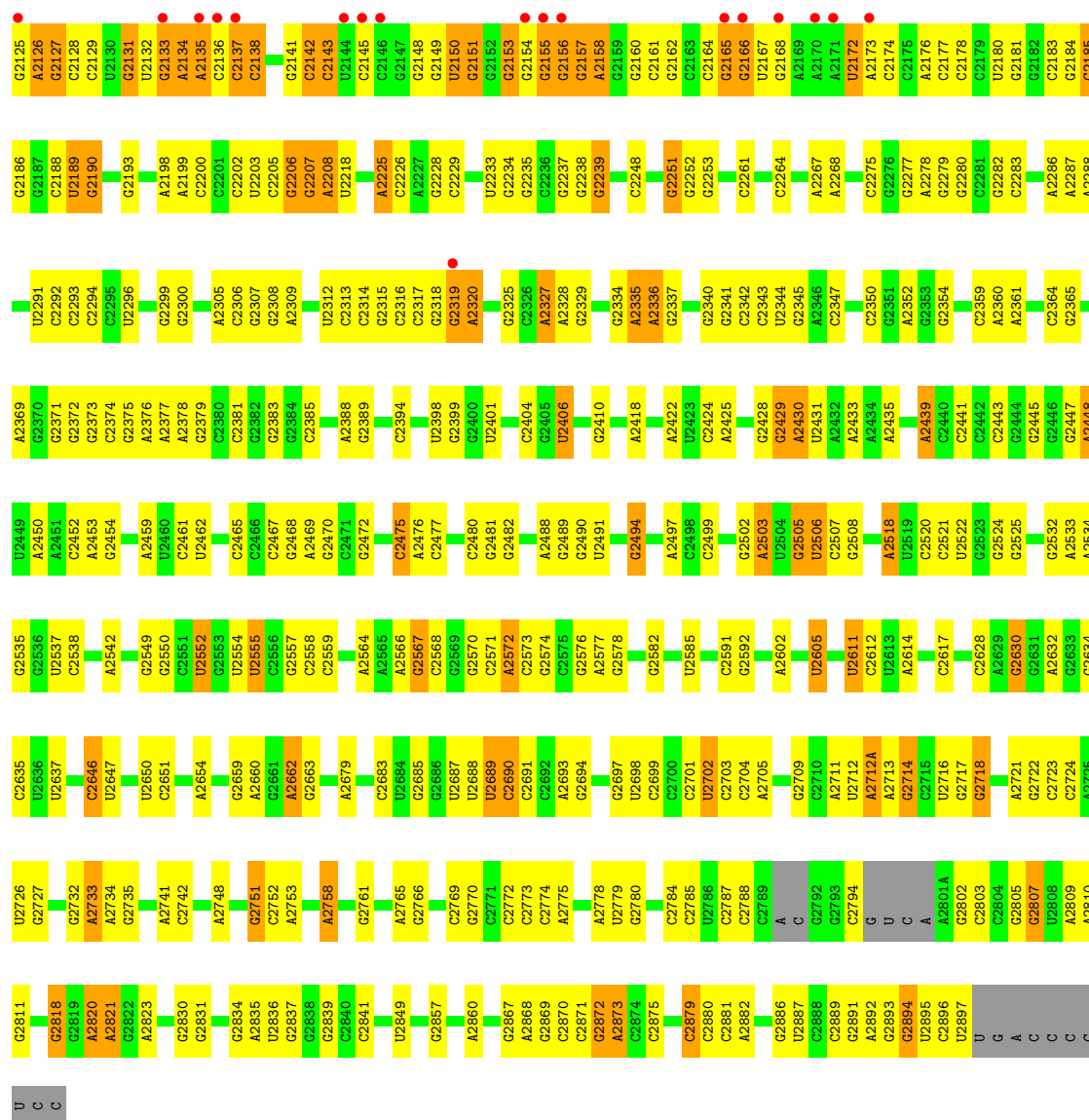
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	29	1	Total 1	O 1	0	0
62	2a	150	Total 150	O 150	0	0
62	2e	1	Total 1	O 1	0	0
62	2j	1	Total 1	O 1	0	0
62	2l	4	Total 4	O 4	0	0
62	2q	1	Total 1	O 1	0	0
62	2v	3	Total 3	O 3	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	4	Total 4	O 4	0	0
62	2z	1	Total 1	O 1	0	0

G2331	G2334	G2335	G2336	G2337	G2341	G2342	G2343	G2344	G2356	G2357	A2361	G2364	G2365	G2371	G2372	G2375	A2376	A2377	A2378	G2379	G2383	G2384	G2385	U2390	A2393	G2396	G2404	G2405	U2406	G2407	G2417	A2418	U2419	A2422	U2423	G2326	A2425	A2426	G2329	G2330	G2332																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
C2231	G2238	G2239	U2243	U2245	U2246	G2247	G2248	G2251	G2257	G2258	G2259	G2260	G2262	G2263	G2264	G2266	G2267	G2268	A2269	G2280	G2281	G2282	G2283	A2286	A2287	U2291	G2292	U2296	A2305	G2306	G2307	G2308	A2309	G2313	G2314	G2315	G2316	G2319	A2320	G2325	G2326	G2327	G2328																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	G2159	G2160	G2162	G2163	G2164	G2165	G2166	G2167	G2168	A2169	U2170	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	A2181	G2182	G2183	G2184	G2187	C2188	U2189	G2190	C2191	G2192	G2193	A2198	G2206	G2207	A2208	U2218	G2219	G2222	G2223	G2224	A2225	A2226	A2328	A2329	G2330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C2065	C2066	G2069	G2070	A2071	G2072	C2073	U2074	U2075	U2096	C2097	U2098	U2099	G2100	G2101	U2102	C2103	G2106	C2107	C2108	A2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	U2119	G2120	G2121	U2122	A2126	G2127	C2128	C2129	U2130	G2131	U2132	G2133	A2134	G2135	G2207	C2136	G2316	G2319	G2320	G2321	G2322	G2323	G2324	A2327	A2328	G2329	G2330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A1970	A1971	A1972	G1975	U1976	G1977	A1978	A1979	G1980	G1989	A1990	G1991	G1992	U1993	C1996	A1997	A1998	G1999	G2000	A2001	G2002	U1911	C1914	U1915	A1916	U1917	A1918	A1919	C1920	G1929	U1931	A1932	G1933	A1937	A1938	U1939	C1942	U1943	G1949	G1950	A2042	C2043	U2049	G2050	A2051	G2052	G2053	C2140	G2141	C2142	G2143	U2144	A2225	A2327	A2328	G2329	G2330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G1772	A1773	U1778	U1779	A1780	C1781	G1782	A1783	A1784	A1785	C1881	A1889	A1890	A1900	G1906	U1911	C1914	U1915	A1916	U1917	A1918	A1919	C1920	G1929	U1931	A1932	G1933	A1937	A1938	U1939	C1942	U1943	G1949	G1950	A2042	C2043	U2049	G2050	A2051	G2052	G2053	C2140	G2141	C2142	G2143	U2144	A2225	A2327	A2328	G2329	G2330																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G1647	C1648	A1655	C1656	C1662	C1663	A1664	A1665	A1669	C1670	U1671	C1672	G1674	U1680	C1683	C1684	C1685	C1686	G1687	U1688	C1691	U1692	U1693	C1694	C1695	G1696	A1700	A1701	G1702	G1703	U1713	G1714	U1720	G1721	A1722	U1739	G1740	A1741	G1746	G1756	A1762	G1763	G1764	G1769	C1770	C1771																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U	A	C	G1537	U1540	G1541	A1542	C1543	A1554	C1557	A1558	G1559	A1566	A1569	U1578	A1579	A1580	G1581	C1584	A1586	A1587	C1588	C1589	G1594	G1595	U1602	A1603	C1604	C1607	A1608	A1610	A1614	C1617	G1618	G1619	G1627	G1633	A1634	G1635	C1636	A1637	G1643	C1644																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1141	U1142	G1144	C1145	G1149	C1153	A1156	G1164	U1165	C1166	U1167	G1170	G1171	G1172	G1173	U1089	U1090	G1091	A1020	G1092	G1093	U1094	A1095	A1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	G1114	C1115	C1116	G1125	U1130	U1133	C1135	G1136	G1137	G1138	G1139	C1140	U1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C2040	C2043	G2049	C2050	A2051	C2052	C2055	G2056	A2057	A2060	G2061	A2062	C2063	C2064	C2065	G2066	G2067	C2068	G2069	G2070	A2071	U2074	U2075	C2078	U2079	G2093	G2094	U2098	U2099	G2100	G2101	G2104	C2105	G2106	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123					
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G1826	G1828	A1829	C1837	A1847	A1848	A1853	A1854	G1855	G1856	G1857	G1858	C1866	A1876	A1877	G1878	C1882	G1883	C1886	A1889	A1890	G1899	A1900	G1906	G1907	C1908	U1911	A1912	A1913	C1914	U1915	U1916	U1917	A1918	A1919	C1920	C1924	G1929	G1930	G1935	A1936	A1937	A1938	U1939	U1940									
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U1130	G1131	A1132	U1133	G1135	G1136	G1139	C1140	U1141	U1142	A1142A	G1149	C1150	G1151	C1152	C1153	A1156	G1157	C1158	U1159	G1160	G1164	U1165	C1166	U1167	G1168	G1169	G1170	G1171	G	A	U	U	A	C1178	C1179	C1180	C1181	A1182	G1183	G1184	C1185	G1186	G1187	U1188	G1191	G1192	G1193	A1194	G1195	U1199	C1200	G1201	C1202
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A	G	A	A	C	A	G	C	U	C	C	U	U	U	A	A	G	G	A	U	G	C	G	A	A	U	C	U	C	A	C	A	C	A	G	G1112	U1113	G1114	G1115	C1116	G1117	G1120	A984	C985	A986	A987	A988	A989	A990	A991	C992	C993	A994	C995



• Molecule 2: 5S Ribosomal RNA

Chain 1B: 60% 38% ..



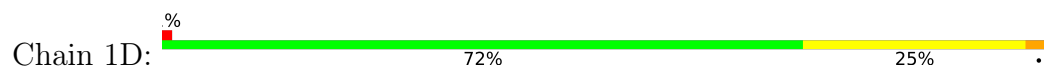
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 43% 47% 9% .

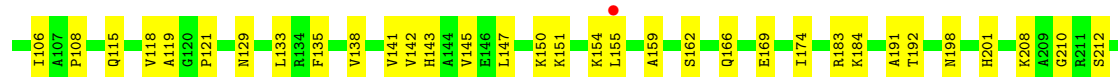
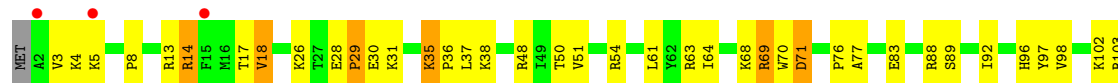




• Molecule 3: 50S ribosomal protein L2



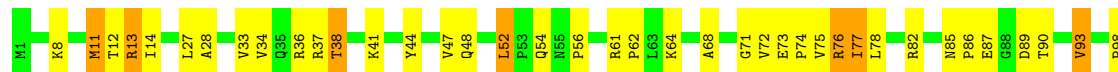
• Molecule 3: 50S ribosomal protein L2

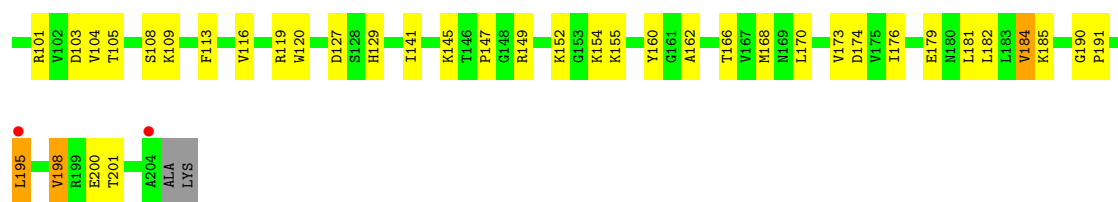


• Molecule 4: 50S ribosomal protein L3



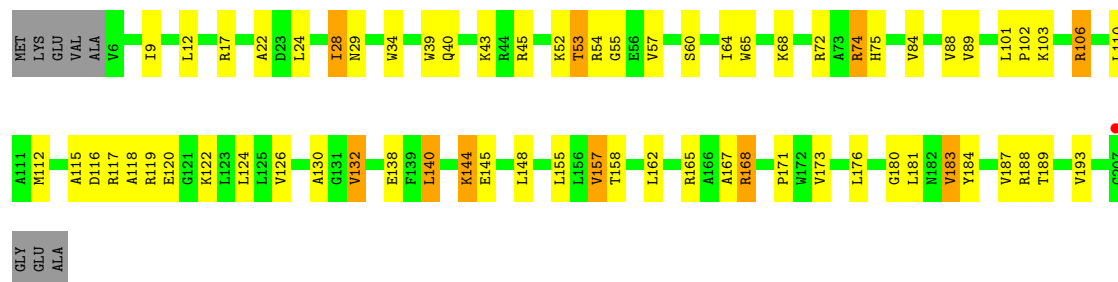
• Molecule 4: 50S ribosomal protein L3





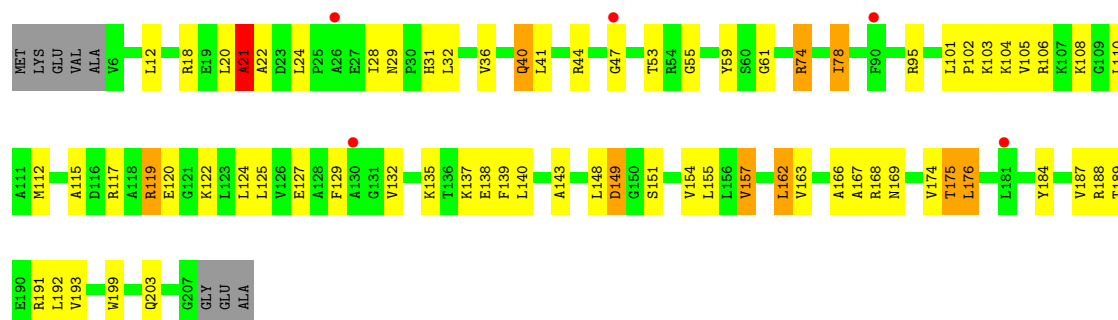
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 64% 27% 5%



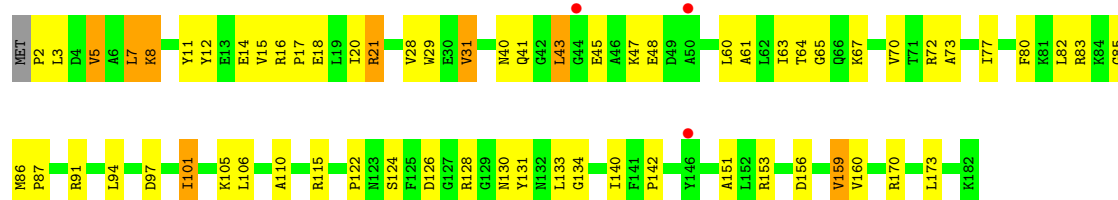
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 2% 62% 29%



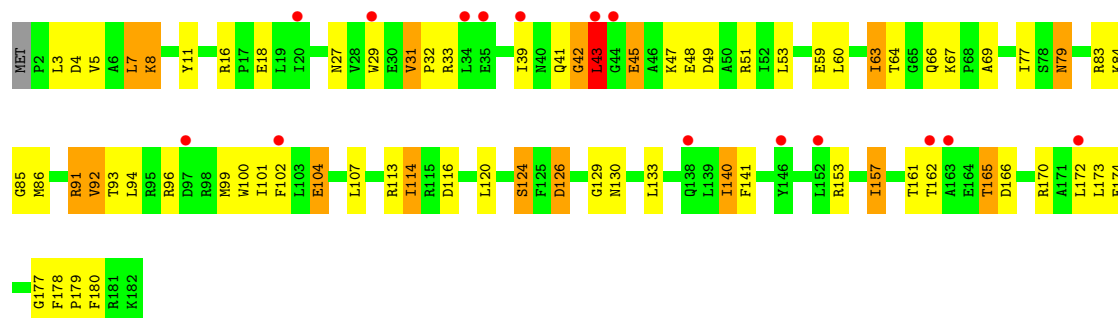
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 2% 64% 31%



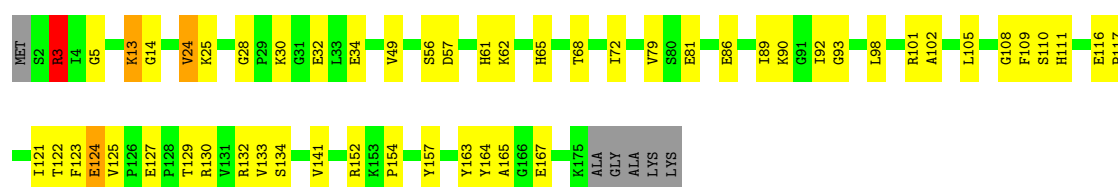
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 8% 60% 30%



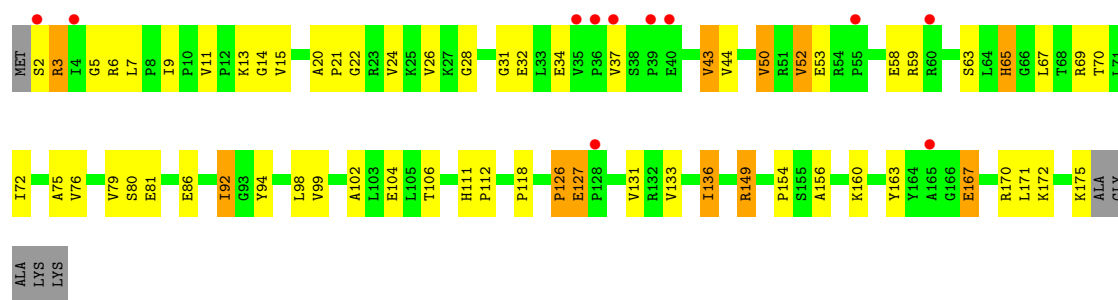
• Molecule 7: 50S ribosomal protein L6

Chain 1H: 67% 28% . . .



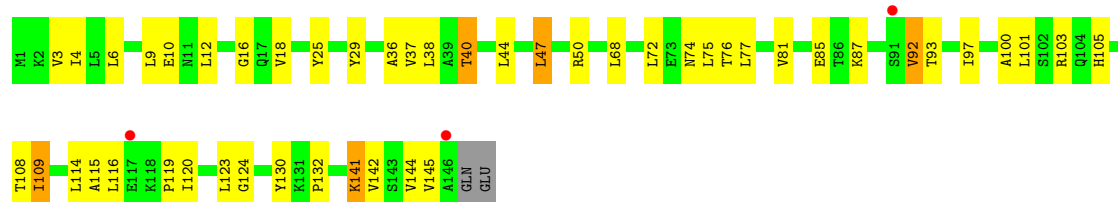
• Molecule 7: 50S ribosomal protein L6

Chain 2H: 6% 61% 29% 6% .



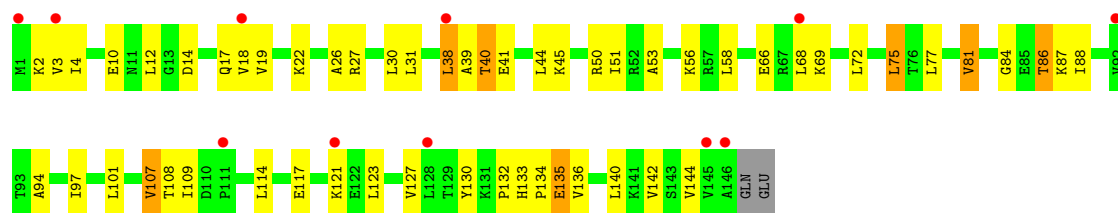
• Molecule 8: 50S ribosomal protein L9

Chain 1I: 2% 66% 29% . .

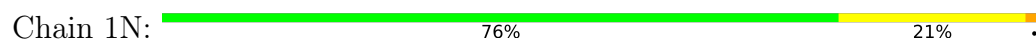


• Molecule 8: 50S ribosomal protein L9

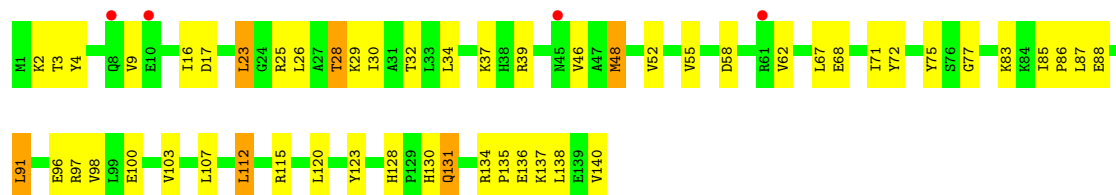
Chain 2I: 7% 61% 33% 5% .



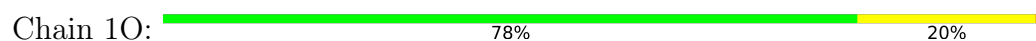
• Molecule 9: 50S ribosomal protein L13



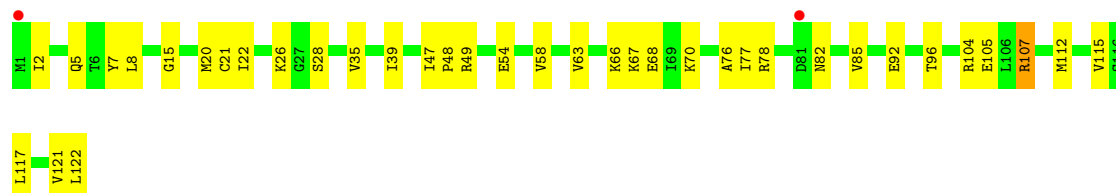
• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L14



• Molecule 11: 50S ribosomal protein L15





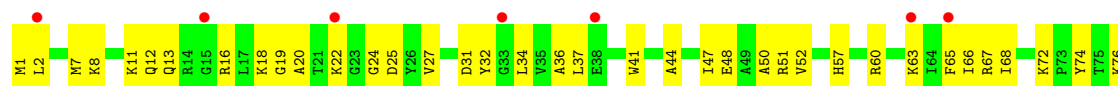
- Molecule 11: 50S ribosomal protein L15



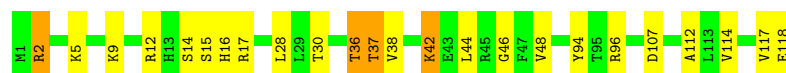
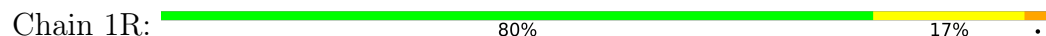
- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



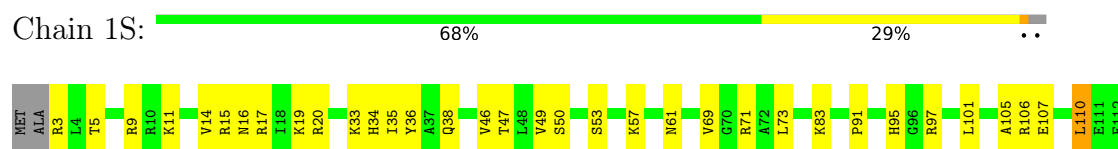
- Molecule 13: 50S ribosomal protein L17



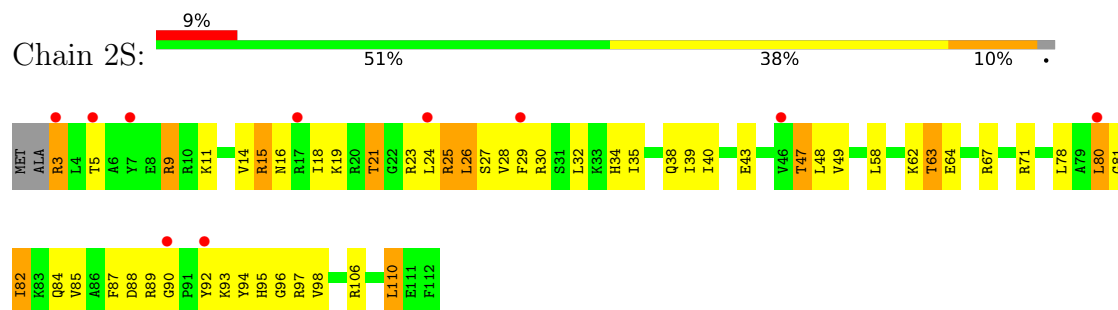
- Molecule 13: 50S ribosomal protein L17



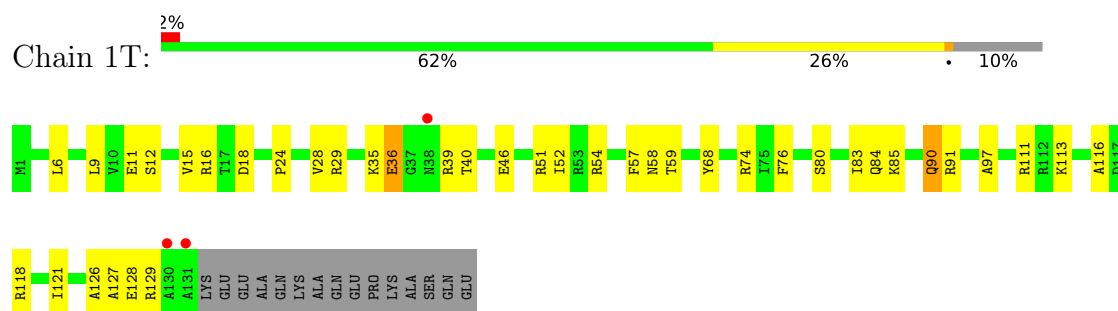
• Molecule 14: 50S ribosomal protein L18



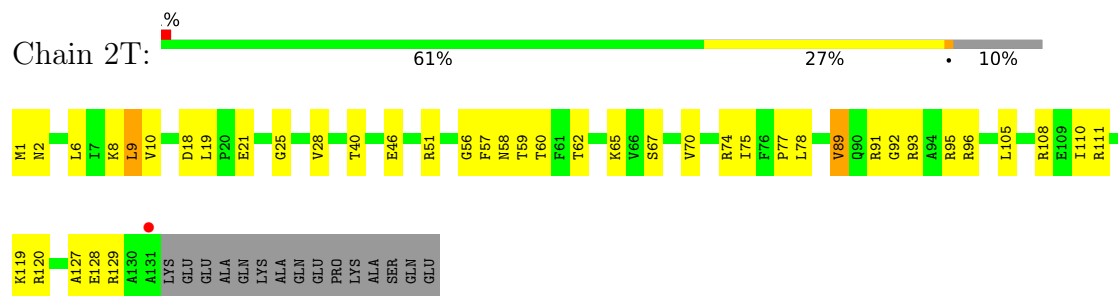
• Molecule 14: 50S ribosomal protein L18



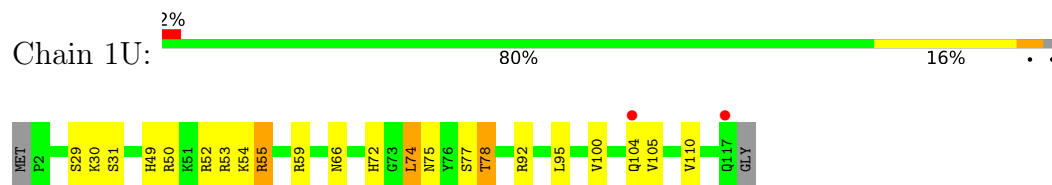
• Molecule 15: 50S ribosomal protein L19



• Molecule 15: 50S ribosomal protein L19

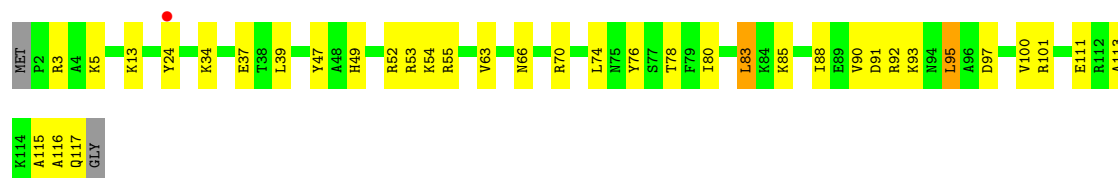


• Molecule 16: 50S ribosomal protein L20



• Molecule 16: 50S ribosomal protein L20

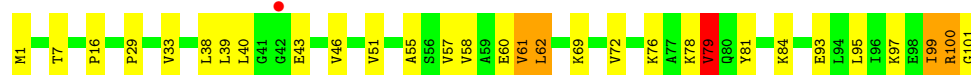




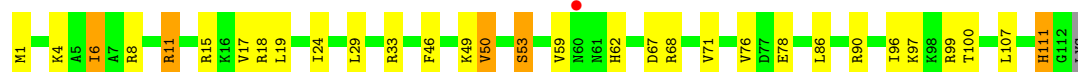
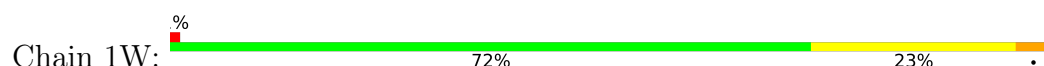
- Molecule 17: 50S ribosomal protein L21



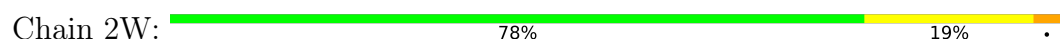
- Molecule 17: 50S ribosomal protein L21



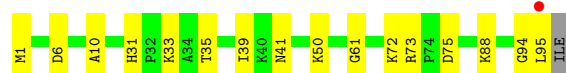
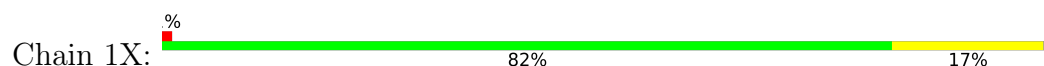
- Molecule 18: 50S ribosomal protein L22



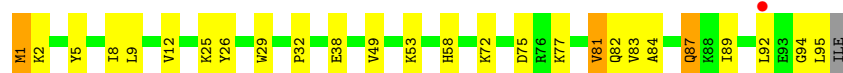
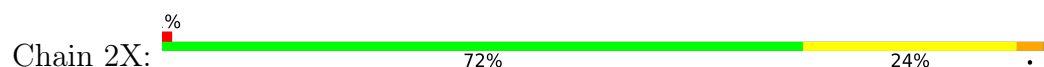
- Molecule 18: 50S ribosomal protein L22



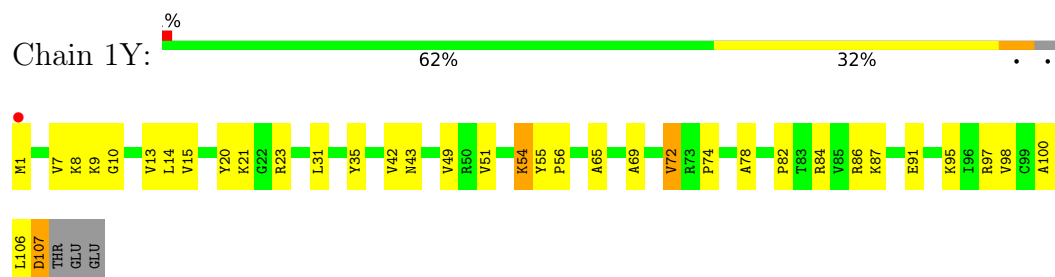
- Molecule 19: 50S ribosomal protein L23



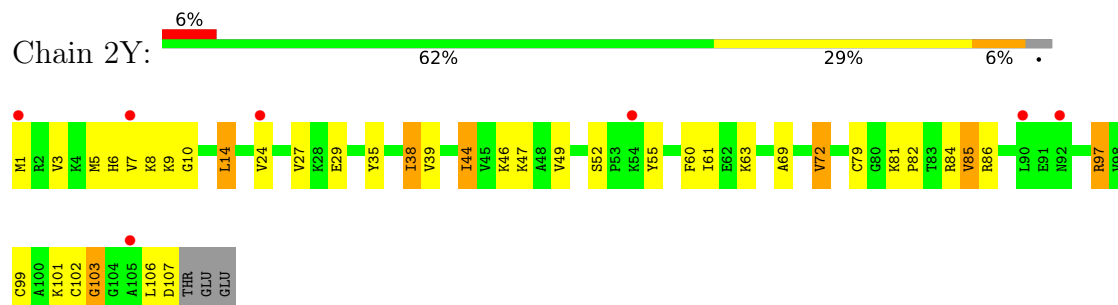
- Molecule 19: 50S ribosomal protein L23



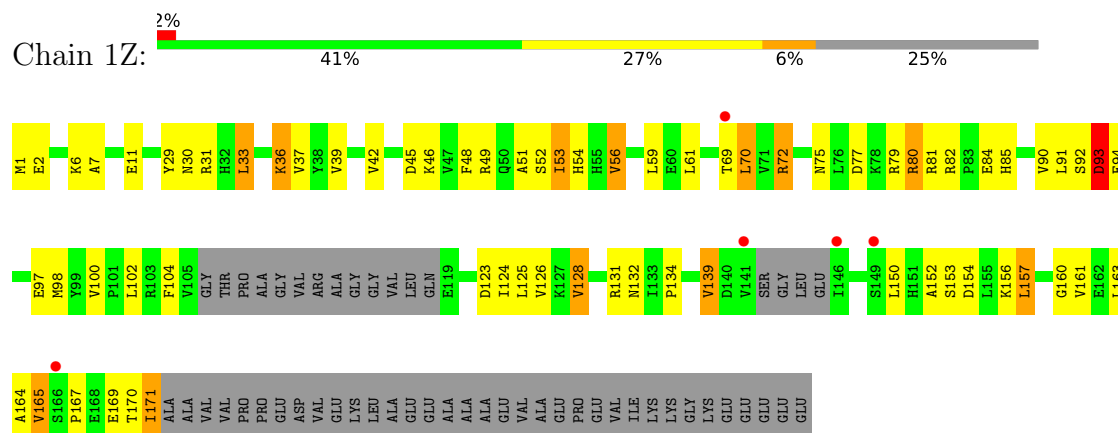
- Molecule 20: 50S ribosomal protein L24



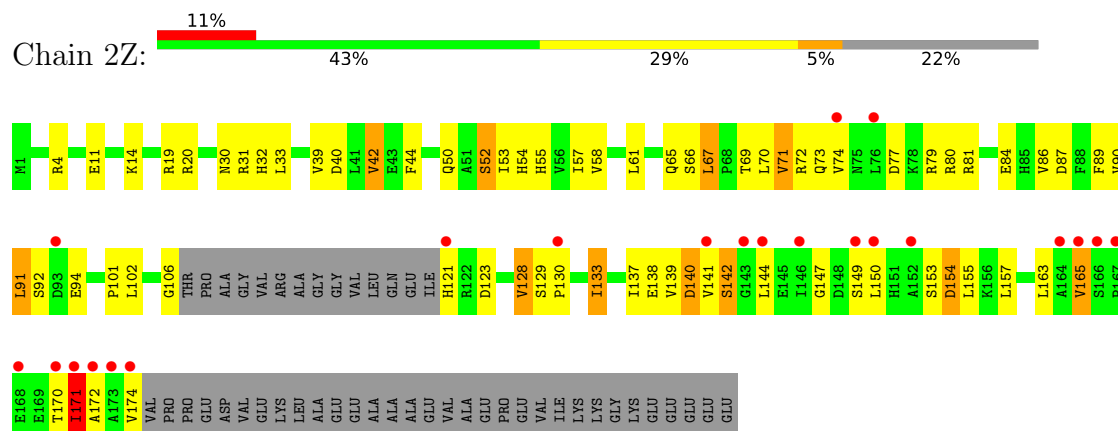
- Molecule 20: 50S ribosomal protein L24



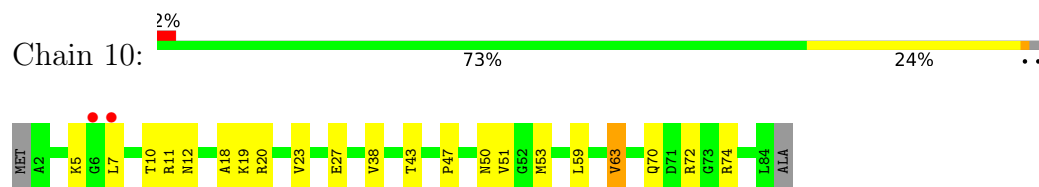
- Molecule 21: 50S ribosomal protein L25



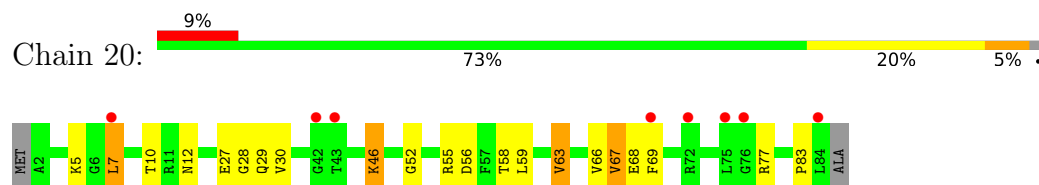
- Molecule 21: 50S ribosomal protein L25



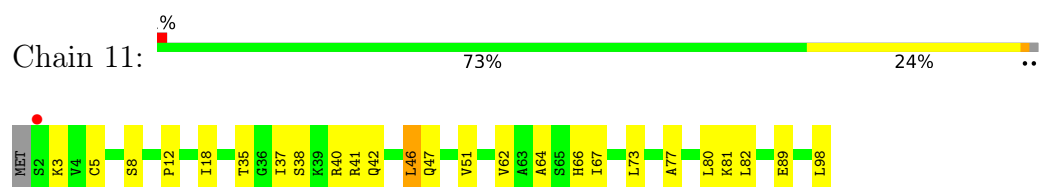
- Molecule 22: 50S ribosomal protein L27



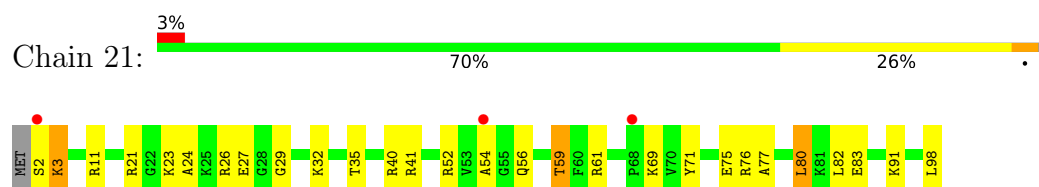
- Molecule 22: 50S ribosomal protein L27



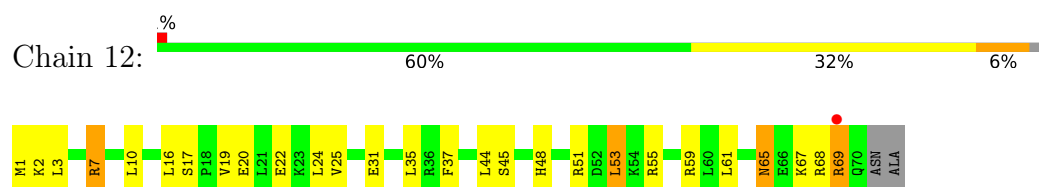
- Molecule 23: 50S ribosomal protein L28



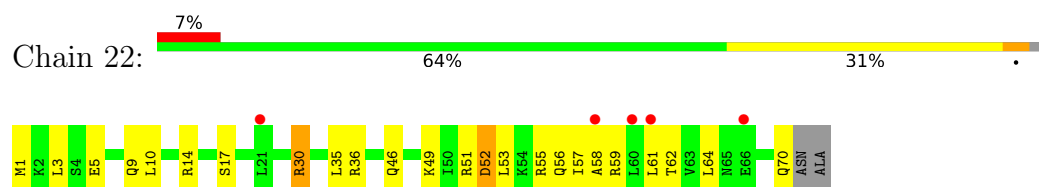
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

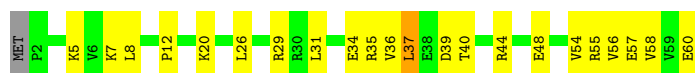


- Molecule 24: 50S ribosomal protein L29

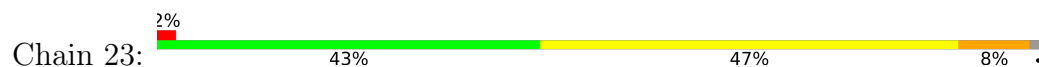


- Molecule 25: 50S ribosomal protein L30

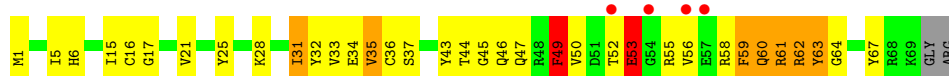




- Molecule 25: 50S ribosomal protein L30



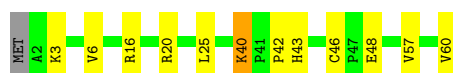
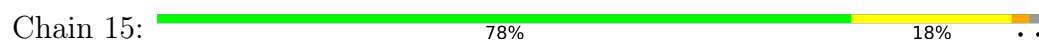
- Molecule 26: 50S ribosomal protein L31



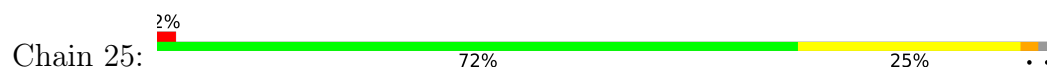
- Molecule 26: 50S ribosomal protein L31



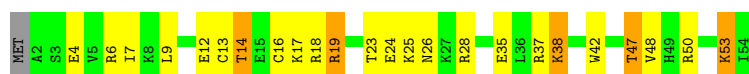
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33





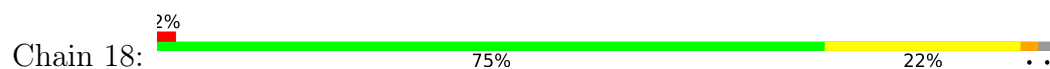
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



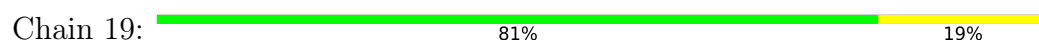
- Molecule 30: 50S ribosomal protein L35



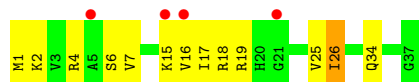
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



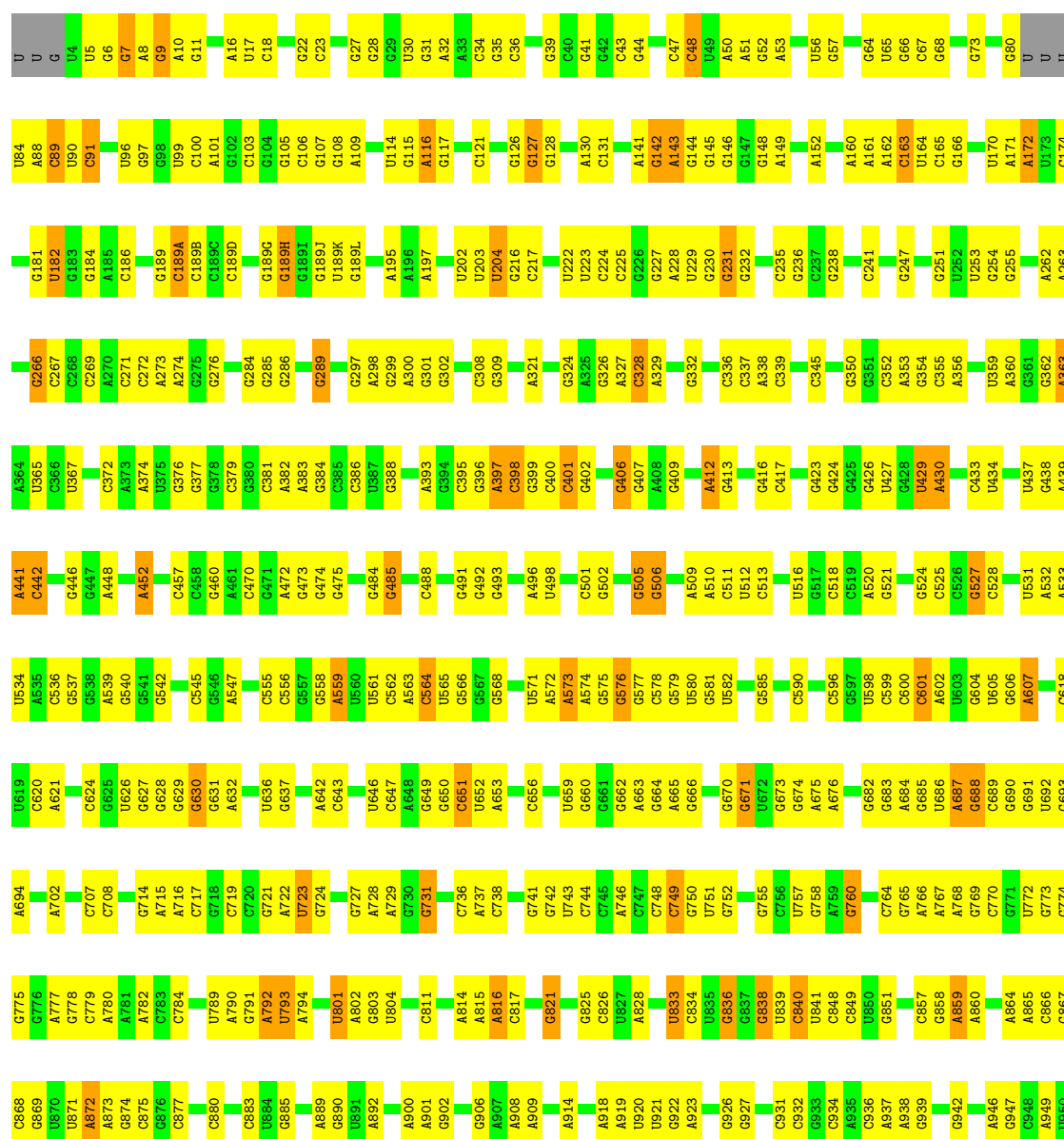
- Molecule 31: 50S ribosomal protein L36



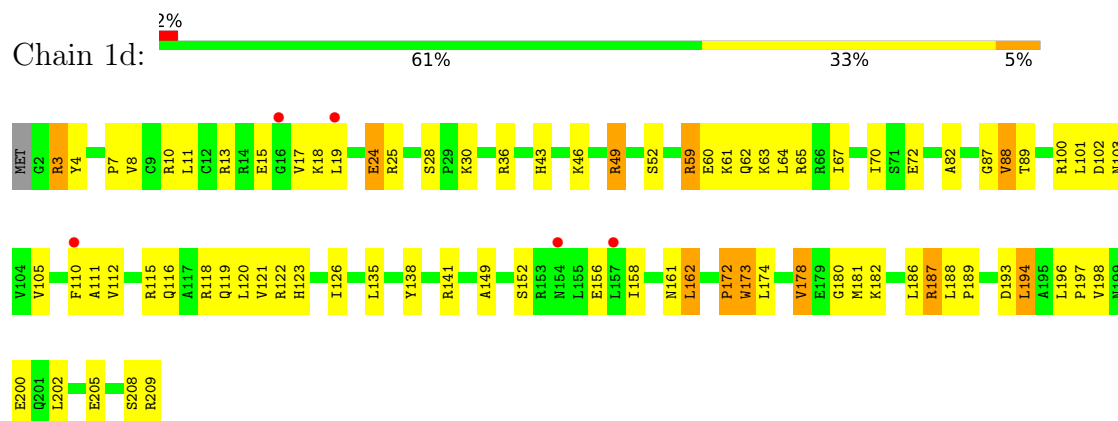
- Molecule 32: 16S Ribosomal RNA



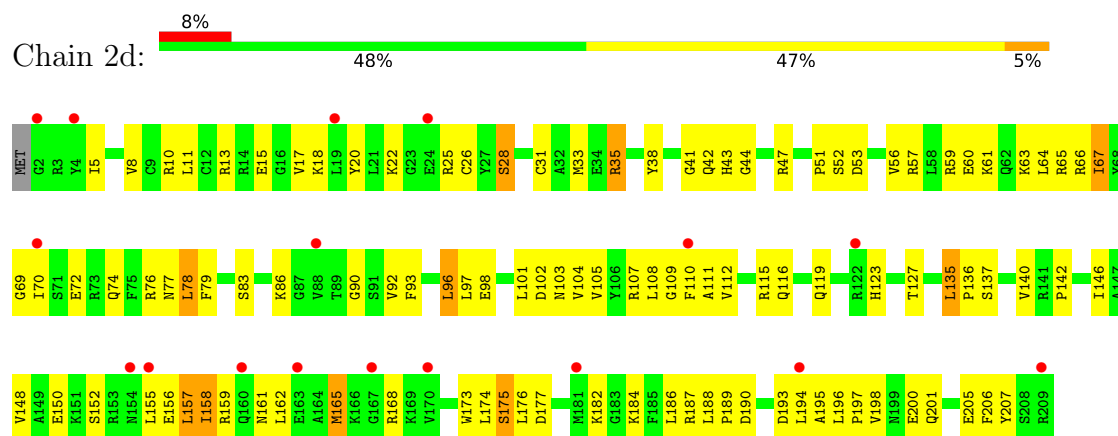
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U	U90	C175	U256	U344	U437	G540	G638	C738	A859	A965	A1030D	A1123	G1207	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
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C18	C106	C187	G266	U368		A553	G662	G755	C875	A975	C1039	C1132	G1224	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C19	G107	C189B	C267	U368	C455	A553	G662	G756	C876	G976	A1040	C1134	A1225	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
U20	C108	C189C	G268	C372	C455	G557	G663	U757	C877	A977	G1042	U1135	A1227	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C21	A109	A373	A270	A374	C458	G558	G664	G758	C880	C978	G1043	U1136	C1228	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C22	G110	U189E	C271	U375	G476	A559	G665	A759	C881	C979	G1044	C1137	A1229	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C23	G111	U189F	C271	U376	G476	U560			C882	U982	C1045	G1138	A1236	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
A26	G112		G276	G376	C470	U561	G671	A766	C882	U983	C1054	G1139	A1236	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G31	G113	G189J	C277	G380	G474	C564	U672	A767	C889	U984	A1055	C1140	A1238	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
A32	A116	U189K	G278	G381	G475	C564	G673	A768	A909	G987	U1056	G1142	A1239	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
A33	A120	G192	C280	A382	G475	C564	G674	G769	C910	G987	U1057	G1143	A1240	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
	C121	C194		A383	G476		A675		C911	U992	G1058	C1144	G1241	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C36	G128	A195		C385	C479	A572	U677	C784	A914	U997	C1063	C1145	G1241	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G39	A130	A196	G293	G388	G484	A573	G682	U789	A918	U997	C1068	A1151	A1252	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
	C131	A197	G297	A389	C484	A574	G683	A790	A918	U997	C1068	A1151	A1252	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G44	C132		A298	C390	G485	G577	A687	A792	G922	U1000	C1069	C1152	G1255	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
U45	C136	U202	G299	A397	U498	G584	G688	U793	A923	U1001	C1070	C1153	G1256	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G46		G301	A300	C398	A499	G585	G689	A794	G925	A1001	C1071	U1159	U1257	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C47	G145	U204	G309	C399	G500	G585	G691	C806	G926	G1001A	U1073	G1160	G1258	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
U48		G216	C400	C400	C501	G593	U692	A807	G927	G1003	C1074	G1166	C1259	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
A50	G148		G310	C401	G502	G594	G693	A814	G933	A1004	G1081	G1166	C1259	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
A51	A149	C219	A313	G402	C504	G595	A694	A815	G934	A1005	G1081	G1167	A1260	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G52	C150		A314	C401	C504	C596	A695	A816	G935	A1006	G1082	A1168	A1260	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
U56	A151	U222	A315	U405	A509	U598	A706	C817	A936	C936	G1084	G1174	A1275	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G57	C152	C224	G316	G407	A510	C599	C707	G818	A937	C937	U1086	G1174	A1275	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C58		C225		G407	C511			A819	A938	G1011		A1179	G1276	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
	G156		G319	G410	U516	A608	G713	U820	G942	A1015	G1094	A1179	G1276	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G61		C233	C320	A411	G517	G610	C717	G821	G942	A1016	U1095	A1180	G1278	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
G66	A160	C235	A321	A412	C518		G718	C824	A946	G1017	G1099	A1181	G1278	U1219	C1260	U1260	A1275	G1276	C1277	U1278	A1279	U1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	U1291	U1292	C1298	U1299
C67	A161	G236		G413	C519	C618	C719		A947	U1020	C1100	A1182	G1282	U1219	C1260	U1260	A1275</																	



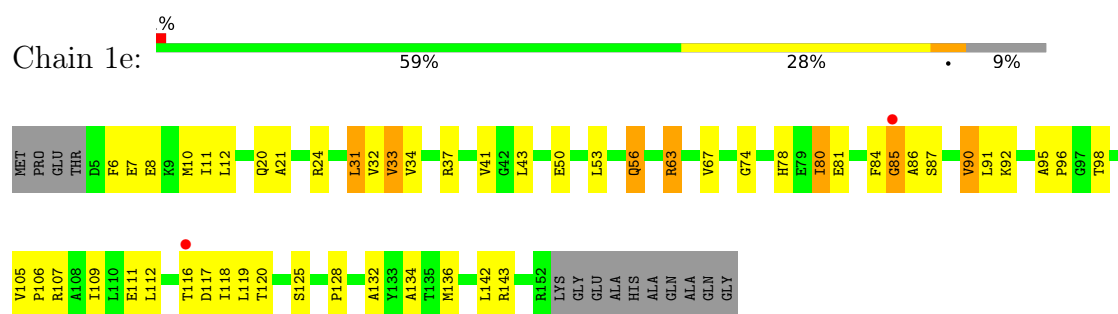
- Molecule 35: 30S ribosomal protein S4



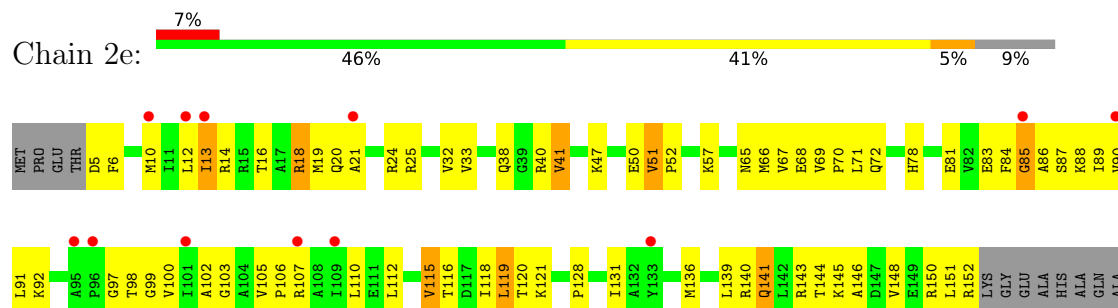
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5

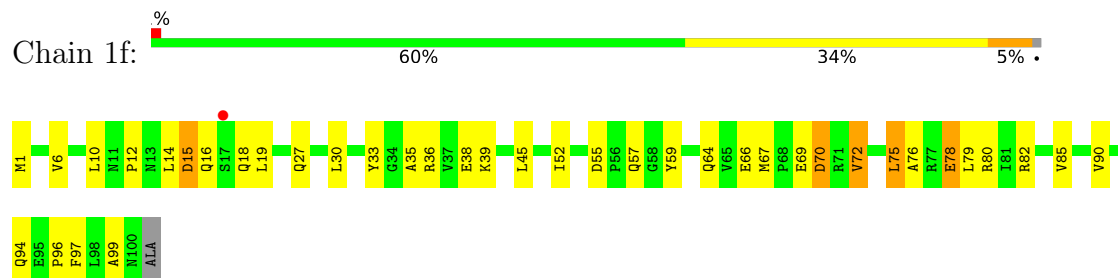


- Molecule 36: 30S ribosomal protein S5

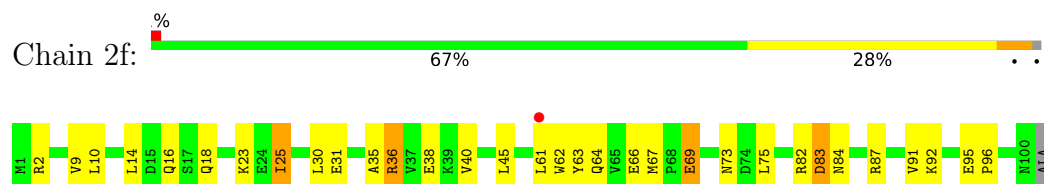


GLN
GLY

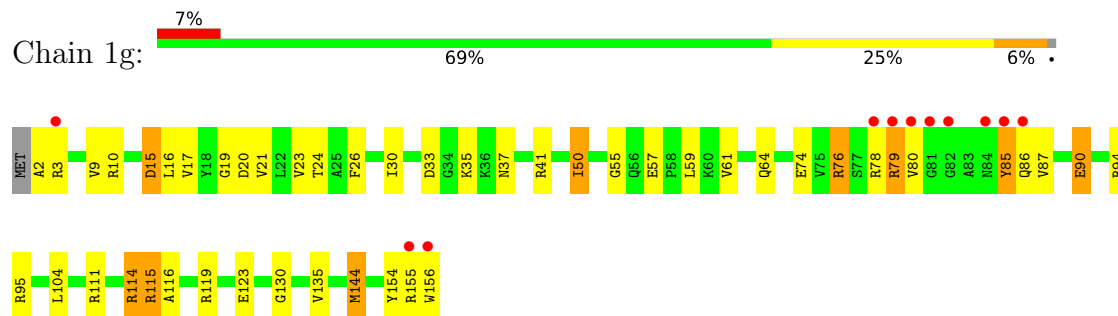
- Molecule 37: 30S ribosomal protein S6



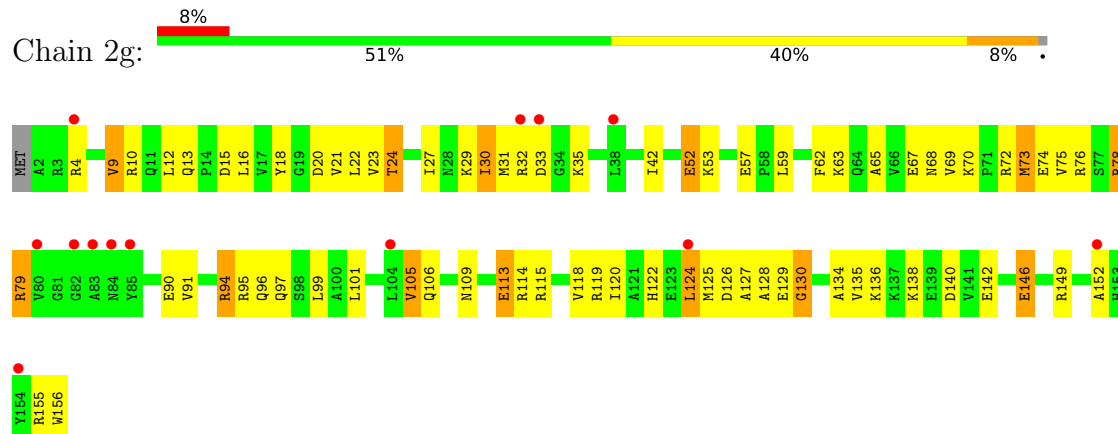
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

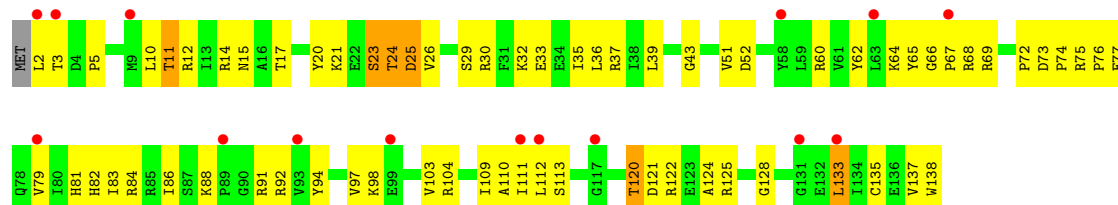


- Molecule 39: 30S ribosomal protein S8

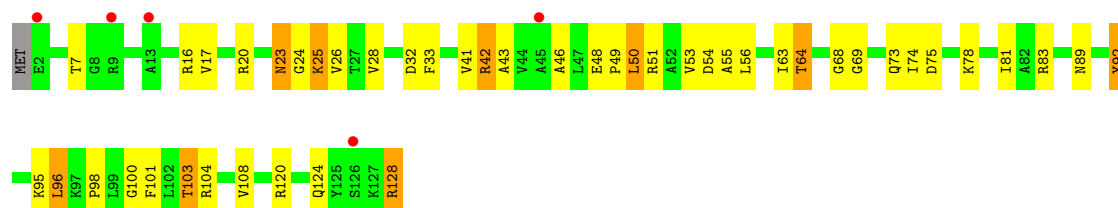




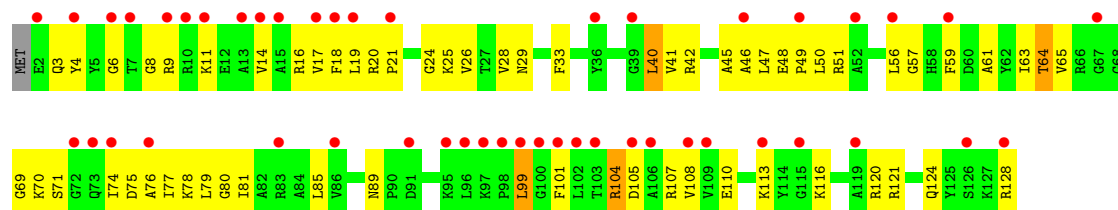
• Molecule 39: 30S ribosomal protein S8



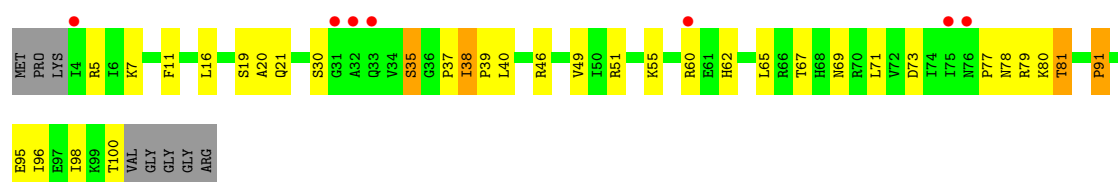
• Molecule 40: 30S ribosomal protein S9



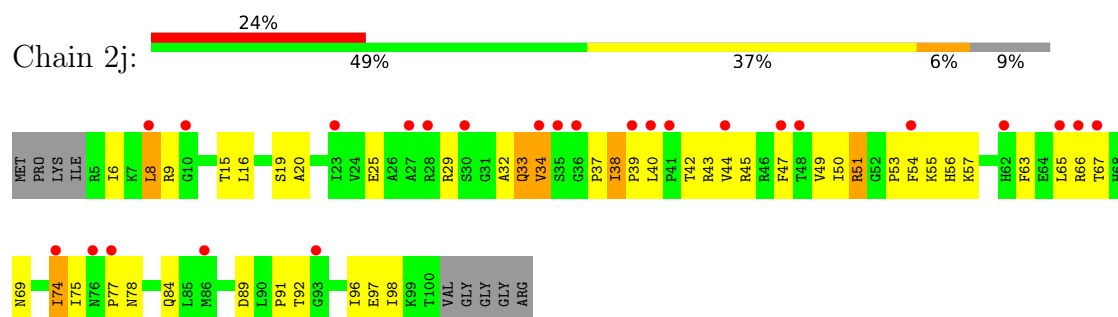
• Molecule 40: 30S ribosomal protein S9



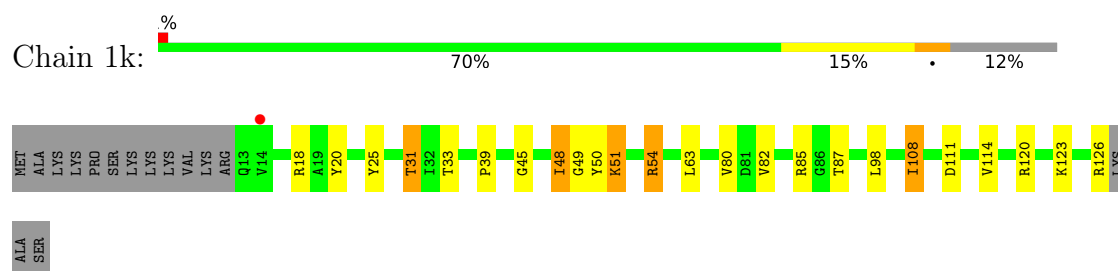
• Molecule 41: 30S ribosomal protein S10



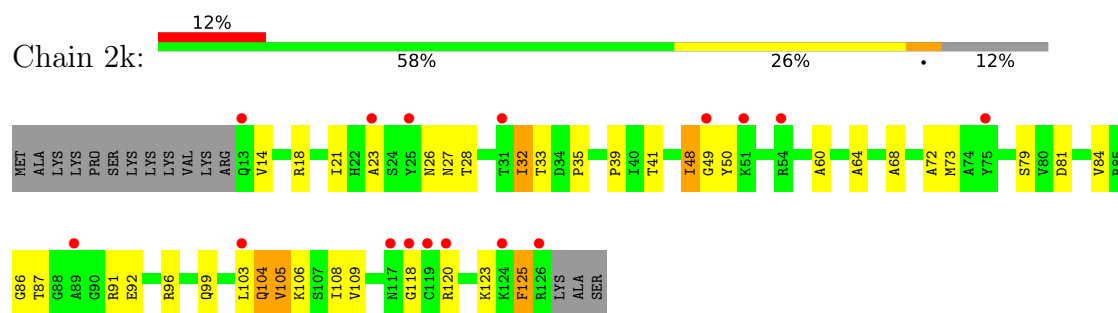
• Molecule 41: 30S ribosomal protein S10



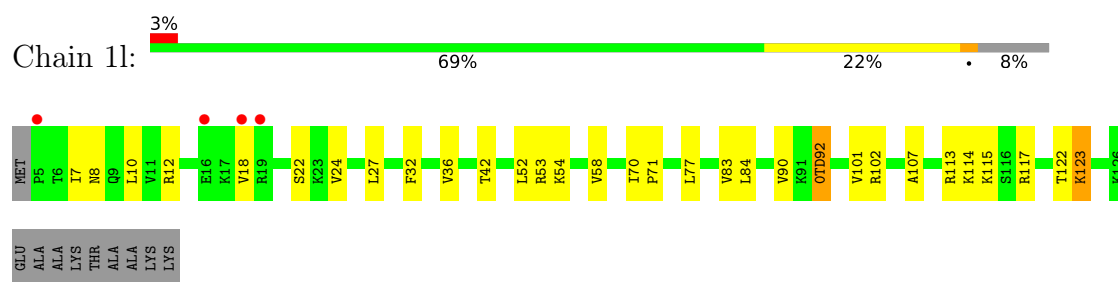
• Molecule 42: 30S ribosomal protein S11



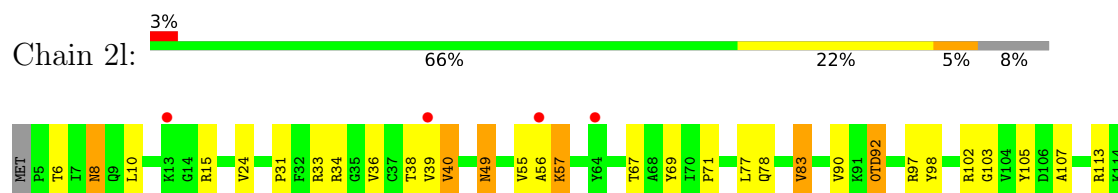
• Molecule 42: 30S ribosomal protein S11

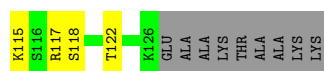


• Molecule 43: 30S ribosomal protein S12



• Molecule 43: 30S ribosomal protein S12





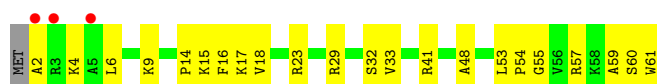
- Molecule 44: 30S ribosomal protein S13



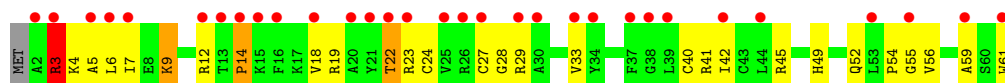
- Molecule 44: 30S ribosomal protein S13



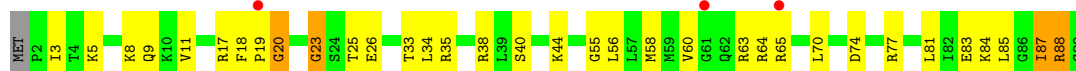
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

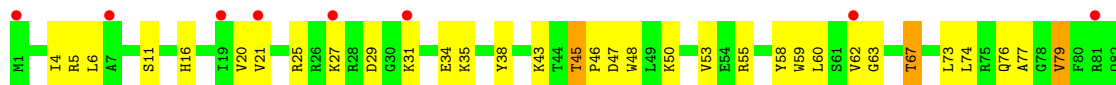


- Molecule 46: 30S ribosomal protein S15



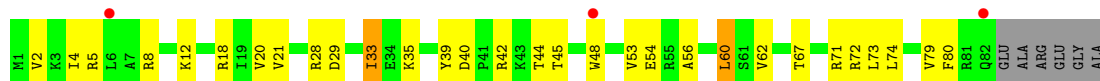


- Molecule 47: 30S ribosomal protein S16

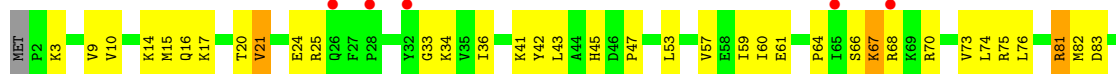


GLU
ALA
ARG
GLU
GLY
ALA

- Molecule 47: 30S ribosomal protein S16

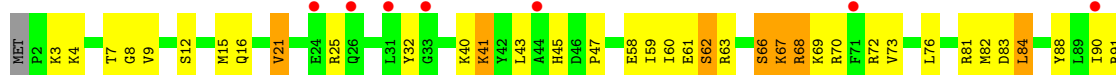


- Molecule 48: 30S ribosomal protein S17



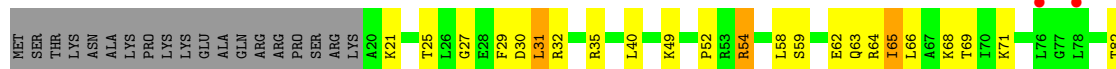
Y88
L89
R90
R91
R92
R93
R94
R95
R96
R97
R98
R99
K100
ARG
GLY
GLY
LYS
ALA

- Molecule 48: 30S ribosomal protein S17



S97
L98
S99
K100
ARG
GLY
GLY
LYS
ALA

- Molecule 49: 30S ribosomal protein S18





- Molecule 49: 30S ribosomal protein S18

Chain 2r: 48% 23% 7% 23%



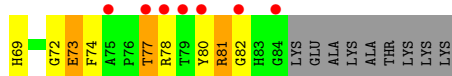
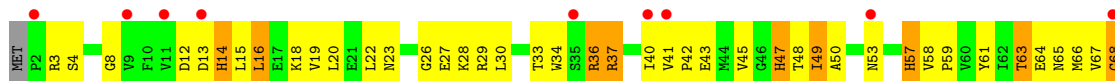
- Molecule 50: 30S ribosomal protein S19

Chain 1s: 59% 28% 11%



- Molecule 50: 30S ribosomal protein S19

Chain 2s: 17% 34% 42% 13% 11%



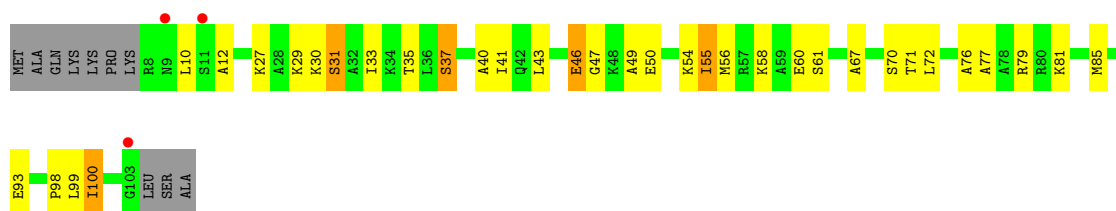
- Molecule 51: 30S ribosomal protein S20

Chain 1t: 7% 61% 22% 6% 9%



- Molecule 51: 30S ribosomal protein S20

Chain 2t: 3% 58% 28% 5% 9%



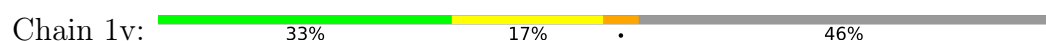
- Molecule 52: 30S ribosomal protein Thx



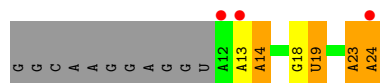
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: MET-PHE-mRNA



- Molecule 53: MET-PHE-mRNA

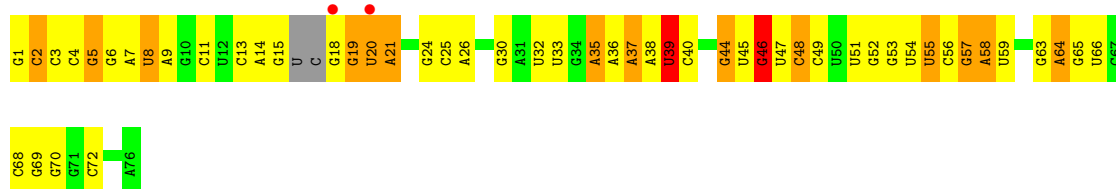


- Molecule 54: A-site and E-site Deacylated tRNAphe

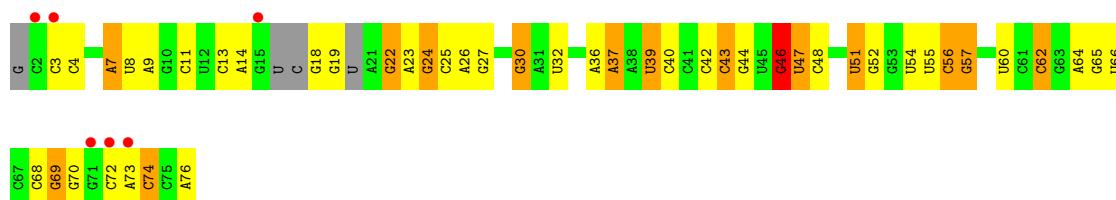


- Molecule 54: A-site and E-site Deacylated tRNAphe

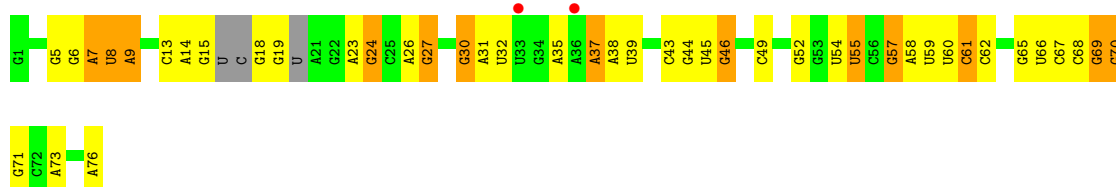




- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



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



- Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA^{cys} RNA-part



- Molecule 55: P-site Peptidyl-tRNA fMRC-tRNA^{cys} RNA-part



- Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA^{cys} Peptide-part



- Molecule 56: P-site Peptidyl-tRNA fMRC-tRNA^{cys} Peptide-part



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.76Å 447.07Å 617.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.56 – 2.75 122.56 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (122.56-2.75) 99.8 (122.56-2.75)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.228 , 0.282 0.230 , 0.281	Depositor DCC
R_{free} test set	73954 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299368	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: PSU, G7M, 2MA, 4SU, FME, UR3, MIA, 8AN, M2G, MG, MA6, ERY, 5MC, 4OC, OMC, OMG, K, 2MG, OMU, 0TD, 5MU, ZN, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	1/69011 (0.0%)	0.45	1/107720 (0.0%)
1	2A	0.22	0/67295	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.20	0/2879	0.37	0/4487
3	1D	0.28	0/2186	0.50	0/2944
3	2D	0.23	0/2186	0.51	3/2944 (0.1%)
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.23	0/1592	0.46	0/2149
5	1F	0.27	0/1618	0.50	0/2191
5	2F	0.21	0/1614	0.46	2/2186 (0.1%)
6	1G	0.23	0/1448	0.46	0/1957
6	2G	0.20	0/1453	0.46	0/1963
7	1H	0.22	0/1356	0.41	0/1834
7	2H	0.21	0/1356	0.40	0/1834
8	1I	0.20	0/1112	0.46	0/1514
8	2I	0.22	0/1079	0.45	0/1475
9	1N	0.24	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.43	0/1543
10	1O	0.27	0/943	0.46	0/1269
10	2O	0.21	0/943	0.45	0/1269
11	1P	0.28	0/1152	0.49	0/1533
11	2P	0.22	0/1152	0.51	0/1533
12	1Q	0.27	0/1143	0.48	0/1527
12	2Q	0.21	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.46	0/1312
13	2R	0.22	0/982	0.45	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.23	0/880	0.47	0/1172
15	1T	0.24	0/1105	0.48	0/1477
15	2T	0.23	0/1097	0.45	0/1468
16	1U	0.26	0/977	0.42	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.42	0/1301
17	1V	0.23	0/782	0.43	0/1049
17	2V	0.19	0/782	0.41	0/1049
18	1W	0.26	0/897	0.44	0/1205
18	2W	0.22	0/897	0.41	0/1205
19	1X	0.28	0/764	0.51	0/1025
19	2X	0.22	0/764	0.48	0/1025
20	1Y	0.23	0/819	0.48	0/1095
20	2Y	0.20	0/819	0.45	0/1095
21	1Z	0.22	0/1267	0.48	0/1717
21	2Z	0.22	0/1299	0.43	0/1763
22	10	0.24	0/662	0.51	0/881
22	20	0.22	0/662	0.45	0/881
23	11	0.26	0/762	0.42	0/1014
23	21	0.22	0/762	0.43	0/1014
24	12	0.25	0/590	0.46	0/781
24	22	0.22	0/590	0.40	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.19	0/469	0.42	0/630
26	14	0.24	0/565	0.55	0/761
26	24	0.26	0/545	0.51	0/737
27	15	0.24	0/469	0.47	0/635
27	25	0.26	0/469	0.50	0/635
28	16	0.25	0/460	0.50	0/613
28	26	0.21	0/456	0.41	0/608
29	17	0.31	0/426	0.58	0/561
29	27	0.25	0/426	0.53	0/561
30	18	0.28	0/525	0.50	0/691
30	28	0.22	0/525	0.44	0/691
31	19	0.28	0/310	0.58	0/407
31	29	0.20	0/310	0.43	0/407
32	1a	0.21	0/35795	0.39	2/55864 (0.0%)
32	2a	0.20	1/35886 (0.0%)	0.38	3/56005 (0.0%)
33	1b	0.22	0/1881	0.53	0/2542
33	2b	0.24	0/1860	0.50	0/2518
34	1c	0.20	0/1572	0.41	0/2126
34	2c	0.25	0/1566	0.49	0/2119
35	1d	0.21	0/1685	0.45	0/2262
35	2d	0.21	0/1704	0.47	0/2284
36	1e	0.21	0/1145	0.46	0/1543
36	2e	0.21	0/1149	0.50	0/1548
37	1f	0.20	0/823	0.39	0/1115
37	2f	0.21	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.21	0/1250	0.43	0/1679
38	2g	0.20	0/1254	0.46	0/1683
39	1h	0.20	0/1108	0.41	0/1494
39	2h	0.19	0/1108	0.41	0/1494
40	1i	0.22	0/1002	0.47	0/1346
40	2i	0.21	0/997	0.49	0/1343
41	1j	0.20	0/722	0.44	0/982
41	2j	0.21	0/727	0.44	0/988
42	1k	0.20	0/844	0.40	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.23	0/937	0.43	0/1260
43	2l	0.21	0/937	0.44	0/1260
44	1m	0.20	0/969	0.45	0/1302
44	2m	0.21	0/961	0.46	0/1291
45	1n	0.22	0/501	0.52	0/664
45	2n	0.21	0/501	0.45	0/664
46	1o	0.20	0/739	0.42	0/985
46	2o	0.19	0/739	0.41	0/985
47	1p	0.22	0/697	0.49	0/939
47	2p	0.19	0/693	0.42	0/935
48	1q	0.19	0/836	0.43	0/1117
48	2q	0.20	0/836	0.48	0/1117
49	1r	0.22	0/560	0.50	0/746
49	2r	0.21	0/560	0.45	0/746
50	1s	0.21	0/667	0.49	0/900
50	2s	0.28	0/661	0.58	0/893
51	1t	0.23	0/730	0.53	0/965
51	2t	0.22	0/729	0.50	0/965
52	1u	0.19	0/203	0.44	0/266
52	2u	0.20	0/203	0.52	0/266
53	1v	0.23	0/310	0.35	0/480
53	2v	0.21	0/310	0.40	0/480
54	1w	0.30	2/1606 (0.1%)	0.42	0/2497
54	1y	0.28	1/1606 (0.1%)	0.43	0/2497
54	2w	0.30	1/1556 (0.1%)	0.43	0/2418
54	2y	0.28	1/1583 (0.1%)	0.39	0/2459
55	1x	0.27	0/1723	0.42	0/2684
55	2x	0.24	0/1723	0.40	0/2684
56	1z	0.34	0/16	0.38	0/19
56	2z	0.34	0/16	0.64	0/19
All	All	0.23	7/316716 (0.0%)	0.43	12/474153 (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
33	1b	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	G7M	O3'-P	5.71	1.61	1.56
54	1w	8	4SU	O3'-P	5.36	1.61	1.56
54	1y	8	4SU	O3'-P	5.13	1.61	1.56
1	1A	2552	OMU	O3'-P	5.12	1.61	1.56
32	2a	527	G7M	O3'-P	5.08	1.61	1.56

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	5.93	118.40	109.50
5	2F	21	ALA	CA-C-N	5.85	132.22	121.70
5	2F	21	ALA	C-N-CA	5.85	132.22	121.70
1	2A	1992	G	C2'-C3'-O3'	5.64	117.97	109.50
32	1a	266	G	C2'-C3'-O3'	5.61	117.91	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide
33	1b	20	GLU	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	31192	706	0
1	2A	60322	0	30425	775	0
2	1B	2577	0	1305	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2B	2575	0	1303	49	0
3	1D	2136	0	2218	54	0
3	2D	2136	0	2218	50	0
4	1E	1559	0	1618	29	0
4	2E	1559	0	1618	46	0
5	1F	1583	0	1625	46	0
5	2F	1579	0	1619	52	0
6	1G	1423	0	1436	47	0
6	2G	1428	0	1438	60	0
7	1H	1330	0	1407	29	0
7	2H	1330	0	1407	35	0
8	1I	1097	0	1140	25	0
8	2I	1064	0	1082	35	0
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	30	0
10	1O	933	0	996	19	0
10	2O	933	0	996	21	0
11	1P	1135	0	1212	38	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1179	44	0
12	2Q	1122	0	1179	47	0
13	1R	968	0	1033	18	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	20	0
14	2S	870	0	923	41	0
15	1T	1091	0	1151	28	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1018	16	0
16	2U	959	0	1019	24	0
17	1V	771	0	828	13	0
17	2V	771	0	830	17	0
18	1W	886	0	940	19	0
18	2W	886	0	940	14	0
19	1X	750	0	814	11	0
19	2X	750	0	813	14	0
20	1Y	806	0	881	20	0
20	2Y	806	0	881	20	0
21	1Z	1240	0	1240	39	0
21	2Z	1271	0	1273	44	0
22	10	653	0	674	19	0
22	20	653	0	674	12	0
23	11	755	0	826	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	21	755	0	826	21	0
24	12	588	0	643	16	0
24	22	588	0	643	14	0
25	13	469	0	518	10	0
25	23	464	0	514	20	0
26	14	552	0	533	27	0
26	24	532	0	503	30	0
27	15	455	0	465	9	0
27	25	455	0	465	9	0
28	16	453	0	473	15	0
28	26	449	0	469	16	0
29	17	418	0	467	8	0
29	27	418	0	467	13	0
30	18	517	0	582	14	0
30	28	517	0	582	20	0
31	19	307	0	335	4	0
31	29	307	0	335	8	0
32	1a	32246	0	16293	438	0
32	2a	32327	0	16337	585	0
33	1b	1846	0	1867	61	0
33	2b	1825	0	1828	81	0
34	1c	1548	0	1535	40	0
34	2c	1542	0	1517	68	0
35	1d	1655	0	1672	64	0
35	2d	1674	0	1714	76	0
36	1e	1129	0	1185	38	0
36	2e	1133	0	1191	50	0
37	1f	810	0	804	23	0
37	2f	816	0	808	19	0
38	1g	1231	0	1238	36	0
38	2g	1235	0	1249	48	0
39	1h	1088	0	1126	26	0
39	2h	1088	0	1126	45	0
40	1i	983	0	986	36	0
40	2i	978	0	966	45	0
41	1j	709	0	650	23	0
41	2j	714	0	672	30	0
42	1k	829	0	825	18	0
42	2k	833	0	834	23	0
43	1l	932	0	981	18	0
43	2l	932	0	980	23	0
44	1m	958	0	1002	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	2m	950	0	988	48	0
45	1n	492	0	529	17	0
45	2n	492	0	529	27	0
46	1o	728	0	760	18	0
46	2o	728	0	760	18	0
47	1p	681	0	697	19	0
47	2p	677	0	686	19	0
48	1q	823	0	891	31	0
48	2q	823	0	891	24	0
49	1r	555	0	618	19	0
49	2r	555	0	618	17	0
50	1s	652	0	662	22	0
50	2s	646	0	644	51	0
51	1t	728	0	798	23	0
51	2t	727	0	796	24	0
52	1u	199	0	208	2	0
52	2u	199	0	208	12	0
53	1v	277	0	140	3	0
53	2v	277	0	139	8	0
54	1w	1592	0	818	27	0
54	1y	1585	0	803	29	0
54	2w	1544	0	786	28	0
54	2y	1565	0	793	23	0
55	1x	1646	0	839	22	0
55	2x	1646	0	838	24	0
56	1z	27	0	28	1	0
56	2z	27	0	28	1	0
57	10	10	0	0	0	0
57	11	3	0	0	0	0
57	12	2	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	9	0	0	0	0
57	16	2	0	0	0	0
57	17	6	0	0	0	0
57	18	7	0	0	0	0
57	1A	1085	0	0	0	0
57	1B	38	0	0	0	0
57	1D	12	0	0	0	0
57	1E	13	0	0	0	0
57	1F	13	0	0	0	0
57	1G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	4	0	0	0	0
57	1O	4	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	6	0	0	0	0
57	1S	2	0	0	0	0
57	1T	3	0	0	0	0
57	1U	11	0	0	0	0
57	1V	7	0	0	0	0
57	1W	7	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	211	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	1	0	0	0	0
57	1f	1	0	0	0	0
57	1j	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	3	0	0	0	0
57	1p	1	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1w	6	0	0	0	0
57	1x	12	0	0	0	0
57	20	3	0	0	0	0
57	21	1	0	0	0	0
57	23	2	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	27	4	0	0	0	0
57	28	3	0	0	0	0
57	2A	855	0	0	0	0
57	2B	20	0	0	0	0
57	2D	6	0	0	0	0
57	2E	9	0	0	0	0
57	2F	6	0	0	0	0
57	2N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2O	2	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	1	0	0	0	0
57	2R	4	0	0	0	0
57	2T	3	0	0	0	0
57	2U	2	0	0	0	0
57	2V	1	0	0	0	0
57	2W	2	0	0	0	0
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	225	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	1	0	0	0	0
57	2l	4	0	0	0	0
57	2o	1	0	0	0	0
57	2q	3	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	5	0	0	0	0
57	2x	6	0	0	0	0
57	2y	1	0	0	0	0
57	2z	1	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	51	0	67	9	0
59	2A	51	0	67	4	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	1	0
61	2d	8	0	0	2	0
62	10	8	0	0	1	0
62	11	7	0	0	0	0
62	12	3	0	0	0	0
62	13	4	0	0	0	0
62	14	1	0	0	0	0
62	15	6	0	0	0	0
62	16	3	0	0	0	0
62	17	10	0	0	1	0
62	18	8	0	0	0	0
62	1A	1680	0	0	117	0
62	1B	54	0	0	3	0
62	1D	32	0	0	3	0
62	1E	23	0	0	1	0
62	1F	17	0	0	2	0
62	1G	1	0	0	0	0
62	1H	1	0	0	0	0
62	1N	4	0	0	0	0
62	1O	3	0	0	0	0
62	1P	15	0	0	3	0
62	1Q	8	0	0	1	0
62	1R	12	0	0	1	0
62	1S	3	0	0	0	0
62	1T	6	0	0	0	0
62	1U	8	0	0	0	0
62	1V	9	0	0	0	0
62	1W	9	0	0	0	0
62	1X	6	0	0	1	0
62	1Y	1	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	252	0	0	20	0
62	1b	1	0	0	0	0
62	1d	1	0	0	0	0
62	1f	1	0	0	0	0
62	1l	3	0	0	0	0
62	1m	2	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1u	1	0	0	0	0
62	1v	3	0	0	0	0
62	1w	8	0	0	0	0
62	1x	7	0	0	1	0
62	1y	1	0	0	0	0
62	1z	1	0	0	0	0
62	20	2	0	0	0	0
62	21	6	0	0	1	0
62	23	1	0	0	0	0
62	25	2	0	0	0	0
62	27	2	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	952	0	0	89	0
62	2B	21	0	0	2	0
62	2D	15	0	0	0	0
62	2E	5	0	0	1	0
62	2F	13	0	0	1	0
62	2O	3	0	0	0	0
62	2P	6	0	0	0	0
62	2Q	1	0	0	0	0
62	2R	4	0	0	0	0
62	2T	2	0	0	0	0
62	2U	2	0	0	0	0
62	2V	1	0	0	0	0
62	2W	1	0	0	0	0
62	2X	5	0	0	0	0
62	2a	150	0	0	13	0
62	2e	1	0	0	0	0
62	2j	1	0	0	1	0
62	2l	4	0	0	0	0
62	2q	1	0	0	0	0
62	2v	3	0	0	0	0
62	2w	3	0	0	0	0
62	2x	4	0	0	1	0
62	2z	1	0	0	0	0
All	All	299368	0	196882	4775	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4775 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
22:20:10:THR:HG22	22:20:12:ASN:H	1.28	0.97
1:1A:1082:U:N3	1:1A:1086:A:N6	2.06	0.96
1:1A:1603:A:OP1	62:1A:4102:HOH:O	1.84	0.94
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.15	0.93

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%)	250 (92%)	22 (8%)	1 (0%)	30	50
3	2D	273/276 (99%)	245 (90%)	25 (9%)	3 (1%)	11	22
4	1E	202/206 (98%)	182 (90%)	19 (9%)	1 (0%)	24	43
4	2E	202/206 (98%)	181 (90%)	20 (10%)	1 (0%)	24	43
5	1F	200/210 (95%)	187 (94%)	11 (6%)	2 (1%)	12	24
5	2F	200/210 (95%)	179 (90%)	18 (9%)	3 (2%)	8	15
6	1G	179/182 (98%)	154 (86%)	25 (14%)	0	100	100
6	2G	179/182 (98%)	141 (79%)	28 (16%)	10 (6%)	1	2
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	38
7	2H	172/180 (96%)	142 (83%)	27 (16%)	3 (2%)	7	14
8	1I	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
8	2I	144/148 (97%)	107 (74%)	32 (22%)	5 (4%)	3	5
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	9	17
10	1O	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	14
10	2O	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	4	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	130 (88%)	11 (8%)	6 (4%)	2	3
11	2P	147/150 (98%)	129 (88%)	14 (10%)	4 (3%)	4	7
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	121 (87%)	17 (12%)	1 (1%)	18	34
13	1R	116/118 (98%)	110 (95%)	4 (3%)	2 (2%)	7	14
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	96 (89%)	9 (8%)	3 (3%)	4	6
15	1T	129/146 (88%)	114 (88%)	14 (11%)	1 (1%)	16	30
15	2T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	16	30
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	3	6
17	2V	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	6	11
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	102 (93%)	8 (7%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
19	2X	93/96 (97%)	81 (87%)	11 (12%)	1 (1%)	11	22
20	1Y	105/110 (96%)	94 (90%)	8 (8%)	3 (3%)	3	6
20	2Y	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	6	12
21	1Z	148/206 (72%)	126 (85%)	18 (12%)	4 (3%)	4	7
21	2Z	156/206 (76%)	123 (79%)	24 (15%)	9 (6%)	1	2
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	20
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	22
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	22
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	3	5
26	14	67/71 (94%)	46 (69%)	15 (22%)	6 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	47 (70%)	15 (22%)	5 (8%)	1	1
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
31	19	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
31	29	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
33	1b	229/256 (90%)	184 (80%)	31 (14%)	14 (6%)	1	1
33	2b	229/256 (90%)	170 (74%)	51 (22%)	8 (4%)	3	5
34	1c	204/239 (85%)	185 (91%)	16 (8%)	3 (2%)	8	15
34	2c	204/239 (85%)	153 (75%)	48 (24%)	3 (2%)	8	15
35	1d	206/209 (99%)	191 (93%)	12 (6%)	3 (2%)	8	15
35	2d	206/209 (99%)	173 (84%)	27 (13%)	6 (3%)	3	6
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	17
36	2e	146/162 (90%)	116 (80%)	23 (16%)	7 (5%)	2	2
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
38	1g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	6	11
38	2g	153/156 (98%)	129 (84%)	21 (14%)	3 (2%)	6	11
39	1h	135/138 (98%)	120 (89%)	13 (10%)	2 (2%)	8	15
39	2h	135/138 (98%)	122 (90%)	11 (8%)	2 (2%)	8	15
40	1i	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	4	9
40	2i	125/128 (98%)	105 (84%)	16 (13%)	4 (3%)	3	5
41	1j	95/105 (90%)	80 (84%)	11 (12%)	4 (4%)	2	3
41	2j	94/105 (90%)	72 (77%)	17 (18%)	5 (5%)	1	2
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	28
42	2k	112/129 (87%)	96 (86%)	13 (12%)	3 (3%)	4	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	108 (91%)	10 (8%)	1 (1%)	16	30
43	2l	119/132 (90%)	108 (91%)	9 (8%)	2 (2%)	7	14
44	1m	121/126 (96%)	102 (84%)	16 (13%)	3 (2%)	4	8
44	2m	120/126 (95%)	99 (82%)	17 (14%)	4 (3%)	3	5
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	5
46	1o	86/89 (97%)	74 (86%)	8 (9%)	4 (5%)	2	2
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	9	18
47	2p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	18
48	1q	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
48	2q	97/105 (92%)	78 (80%)	16 (16%)	3 (3%)	3	6
49	1r	66/88 (75%)	57 (86%)	8 (12%)	1 (2%)	8	15
49	2r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
50	1s	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	4	8
51	1t	94/106 (89%)	81 (86%)	8 (8%)	5 (5%)	1	2
51	2t	94/106 (89%)	82 (87%)	11 (12%)	1 (1%)	11	22
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	13 (62%)	6 (29%)	2 (10%)	0	0
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11370/12134 (94%)	10019 (88%)	1148 (10%)	203 (2%)	6	13

5 of 203 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	38	GLN
21	1Z	53	ILE
21	1Z	93	ASP
26	14	46	GLN

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	32
3	2D	215/218 (99%)	197 (92%)	18 (8%)	10	19
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9	17
4	2E	164/166 (99%)	145 (88%)	19 (12%)	5	10
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	11
5	2F	159/166 (96%)	145 (91%)	14 (9%)	9	18
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7	15
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	8
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	23
7	2H	144/148 (97%)	124 (86%)	20 (14%)	3	6
8	1I	113/124 (91%)	99 (88%)	14 (12%)	4	8
8	2I	105/124 (85%)	93 (89%)	12 (11%)	5	10
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	23
9	2N	118/119 (99%)	104 (88%)	14 (12%)	5	8
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	50
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	20
11	1P	115/116 (99%)	99 (86%)	16 (14%)	3	6
11	2P	115/116 (99%)	102 (89%)	13 (11%)	5	11
12	1Q	111/111 (100%)	97 (87%)	14 (13%)	4	8
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	15
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22	42
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	60
14	1S	86/88 (98%)	73 (85%)	13 (15%)	3	4
14	2S	85/88 (97%)	65 (76%)	20 (24%)	1	1
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	31
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	24
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	24
17	1V	80/82 (98%)	71 (89%)	9 (11%)	5	11
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	6
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9	17
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	21
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	63
19	2X	77/78 (99%)	69 (90%)	8 (10%)	7	13
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	13
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	3	4
21	1Z	135/179 (75%)	109 (81%)	26 (19%)	1	2
21	2Z	137/179 (76%)	114 (83%)	23 (17%)	2	3
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	59
22	20	65/67 (97%)	60 (92%)	5 (8%)	12	22
23	11	80/83 (96%)	71 (89%)	9 (11%)	5	11
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	24
24	12	65/67 (97%)	57 (88%)	8 (12%)	4	8
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	12
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	6
25	23	50/52 (96%)	43 (86%)	7 (14%)	3	6
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	3
26	24	53/63 (84%)	41 (77%)	12 (23%)	1	1
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	32
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	32
28	16	51/52 (98%)	42 (82%)	9 (18%)	2	3
28	26	50/52 (96%)	41 (82%)	9 (18%)	2	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	24
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	8
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	54
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	24
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	29 (85%)	5 (15%)	3	5
33	1b	192/220 (87%)	164 (85%)	28 (15%)	3	5
33	2b	187/220 (85%)	148 (79%)	39 (21%)	1	2
34	1c	142/188 (76%)	128 (90%)	14 (10%)	7	15
34	2c	140/188 (74%)	121 (86%)	19 (14%)	3	6
35	1d	169/181 (93%)	151 (89%)	18 (11%)	6	12
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4	8
36	1e	113/123 (92%)	100 (88%)	13 (12%)	5	10
36	2e	114/123 (93%)	95 (83%)	19 (17%)	2	3
37	1f	84/90 (93%)	74 (88%)	10 (12%)	5	8
37	2f	85/90 (94%)	74 (87%)	11 (13%)	4	7
38	1g	119/127 (94%)	103 (87%)	16 (13%)	4	7
38	2g	120/127 (94%)	97 (81%)	23 (19%)	1	2
39	1h	114/119 (96%)	100 (88%)	14 (12%)	4	8
39	2h	114/119 (96%)	102 (90%)	12 (10%)	6	13
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	8
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	11
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	4
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	5
42	1k	82/99 (83%)	70 (85%)	12 (15%)	3	5
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	15
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	30
43	2l	96/108 (89%)	84 (88%)	12 (12%)	4	8
44	1m	93/101 (92%)	84 (90%)	9 (10%)	8	15
44	2m	92/101 (91%)	77 (84%)	15 (16%)	2	3
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	20
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	14
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	29
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	52
47	1p	69/74 (93%)	56 (81%)	13 (19%)	1	3
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	84 (89%)	10 (11%)	6	13
48	2q	94/97 (97%)	82 (87%)	12 (13%)	4	7
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	14
49	2r	59/77 (77%)	49 (83%)	10 (17%)	2	3
50	1s	69/80 (86%)	62 (90%)	7 (10%)	7	14
50	2s	67/80 (84%)	51 (76%)	16 (24%)	1	1
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	7
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	10
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	11
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	11
56	1z	2/2 (100%)	1 (50%)	1 (50%)	0	0
56	2z	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	9307/10068 (92%)	8242 (89%)	1065 (11%)	5	10

5 of 1065 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	2g	113	GLU
40	2i	108	VAL
38	2g	106	GLN
50	2s	27	GLU
40	1i	64	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
36	2e	127	ASN
38	2g	97	GLN
46	2o	13	GLN
38	1g	86	GLN
38	1g	28	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	505 (17%)	24 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2791/2915 (95%)	520 (18%)	23 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	30 (25%)	0
32	1a	1497/1521 (98%)	277 (18%)	0
32	2a	1501/1521 (98%)	347 (23%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	5 (41%)	0
54	1w	72/76 (94%)	24 (33%)	0
54	1y	72/76 (94%)	26 (36%)	0
54	2w	69/76 (90%)	24 (34%)	0
54	2y	70/76 (92%)	25 (35%)	0
55	1x	75/77 (97%)	16 (21%)	0
55	2x	75/77 (97%)	13 (17%)	0
All	All	9347/9620 (97%)	1821 (19%)	47 (0%)

5 of 1821 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	27	G

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	277	C
1	2A	1210	A
1	2A	479	A
1	2A	752	A
1	2A	1420	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	4SU	2x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.77	5 (20%)
54	MIA	1w	37	54	28,31,32	2.25	7 (25%)	38,44,47	2.48	13 (34%)
43	0TD	2l	92	43	8,9,10	4.51	1 (12%)	6,11,13	4.08	1 (16%)
32	5MC	1a	1400	32	19,22,23	1.54	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.43	3 (16%)	21,30,33	2.11	5 (23%)
54	5MU	2w	54	54	19,22,23	1.46	4 (21%)	27,32,35	1.62	5 (18%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.88	3 (14%)
1	5MC	2A	1962	57,1	19,22,23	1.56	3 (15%)	26,32,35	1.21	2 (7%)
55	5MU	1x	54	55	19,22,23	1.38	5 (26%)	27,32,35	1.91	7 (25%)
55	5MC	2x	32	55	19,22,23	1.55	3 (15%)	26,32,35	1.14	3 (11%)
54	PSU	2y	55	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	4 (19%)
1	OMU	2A	2552	57,1	19,22,23	1.20	3 (15%)	25,31,34	1.74	5 (20%)
32	5MC	1a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.12	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.56	2 (10%)	26,32,35	1.17	3 (11%)
54	PSU	1w	32	54	18,21,22	1.32	2 (11%)	21,30,33	1.93	3 (14%)
32	4OC	2a	1402	57,32	20,23,24	0.78	0	25,32,35	1.00	1 (4%)
54	G7M	1y	46	54	23,26,27	1.53	3 (13%)	34,39,42	1.82	5 (14%)
1	OMU	1A	2552	57,1	19,22,23	1.18	3 (15%)	25,31,34	1.85	5 (20%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.98	1 (4%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	1.12	2 (8%)
1	PSU	2A	1917	1	18,21,22	1.42	3 (16%)	21,30,33	2.09	4 (19%)
32	PSU	1a	516	57,32	18,21,22	1.34	2 (11%)	21,30,33	2.12	4 (19%)
55	8AN	1x	76	57,55	21,24,25	1.44	3 (14%)	26,35,38	2.30	10 (38%)
54	5MU	1w	54	54	19,22,23	1.40	4 (21%)	27,32,35	1.95	7 (25%)
1	5MC	1A	1962	57,1	19,22,23	1.69	3 (15%)	26,32,35	0.99	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.92	1 (4%)
54	MIA	2y	37	54	21,24,32	1.63	4 (19%)	30,35,47	2.02	7 (23%)
1	5MC	2A	1942	1	19,22,23	1.70	2 (10%)	26,32,35	1.14	2 (7%)
55	5MC	1x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.17	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	2.04	9 (27%)
32	5MC	2a	967	32	19,22,23	1.72	3 (15%)	26,32,35	1.14	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.10	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.85	4 (19%)
32	UR3	2a	1498	57,32	19,22,23	1.11	2 (10%)	26,32,35	1.76	4 (15%)
54	PSU	2y	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.73	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.18	2 (7%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
1	5MU	1A	1939	57,1	19,22,23	1.56	6 (31%)	27,32,35	2.24	5 (18%)
1	PSU	1A	1911	1	18,21,22	1.44	4 (22%)	21,30,33	2.15	3 (14%)
32	G7M	2a	527	32	23,26,27	1.49	3 (13%)	34,39,42	1.71	5 (14%)
54	PSU	1w	39	54	18,21,22	1.26	2 (11%)	21,30,33	2.06	4 (19%)
54	5MU	1y	54	54	19,22,23	1.45	4 (21%)	27,32,35	1.94	6 (22%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.09	9 (27%)
54	MIA	2w	37	54,53	24,27,32	2.25	4 (16%)	32,39,47	3.06	10 (31%)
55	5MU	2x	54	55	19,22,23	1.43	5 (26%)	27,32,35	2.08	6 (22%)
54	G7M	2y	46	54	23,26,27	1.63	3 (13%)	34,39,42	1.69	3 (8%)
1	PSU	1A	1917	1	18,21,22	1.46	3 (16%)	21,30,33	2.12	5 (23%)
1	5MU	2A	1915	57,1	19,22,23	1.45	5 (26%)	27,32,35	2.05	5 (18%)
54	4SU	2w	8	54	18,21,22	1.81	5 (27%)	25,30,33	2.11	5 (20%)
32	UR3	1a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.76	4 (15%)
1	PSU	1A	2605	57,1	18,21,22	1.35	3 (16%)	21,30,33	2.02	3 (14%)
32	G7M	1a	527	57,32	23,26,27	1.55	3 (13%)	34,39,42	1.83	5 (14%)
54	G7M	2w	46	54	23,26,27	1.46	3 (13%)	34,39,42	1.74	6 (17%)
56	FME	2z	1	56	8,9,10	0.98	0	8,9,11	1.05	0
54	4SU	1w	8	54	18,21,22	1.90	5 (27%)	25,30,33	1.74	5 (20%)
54	PSU	2y	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.97	4 (19%)
1	OMG	2A	2251	57,1,55	23,26,27	1.27	3 (13%)	32,38,41	2.02	7 (21%)
55	PSU	2x	55	55	18,21,22	1.38	3 (16%)	21,30,33	1.94	3 (14%)
1	OMG	1A	2251	57,1,55	23,26,27	1.24	3 (13%)	32,38,41	2.03	5 (15%)
55	8AN	2x	76	57,58,55	21,24,25	1.39	3 (14%)	26,35,38	2.76	11 (42%)
54	4SU	2y	8	54	18,21,22	1.61	3 (16%)	25,30,33	2.26	5 (20%)
32	2MG	1a	1207	32	23,26,27	1.25	2 (8%)	33,38,41	2.33	10 (30%)
54	PSU	1y	55	54	18,21,22	1.35	2 (11%)	21,30,33	2.06	3 (14%)
54	MIA	1y	37	54	21,24,32	1.63	4 (19%)	30,35,47	2.03	7 (23%)
32	PSU	2a	516	57,32	18,21,22	1.35	2 (11%)	21,30,33	2.01	5 (23%)
1	2MA	2A	2503	57,1	22,25,26	1.47	5 (22%)	32,37,40	2.27	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	1x	8	55	18,21,22	2.19	5 (27%)	25,30,33	1.78	6 (24%)
32	M2G	2a	966	32	24,27,28	1.33	3 (12%)	33,40,43	1.85	5 (15%)
56	FME	1z	1	56	8,9,10	0.99	0	8,9,11	0.70	0
54	G7M	1w	46	54	23,26,27	1.48	3 (13%)	34,39,42	1.75	5 (14%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	1.94	3 (14%)
1	2MA	1A	2503	57,1	22,25,26	1.40	4 (18%)	32,37,40	2.29	11 (34%)
54	PSU	2w	55	54	18,21,22	1.41	2 (11%)	21,30,33	2.05	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.64	3 (15%)	26,32,35	1.20	3 (11%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.57	3 (14%)
1	5MU	2A	1939	1	19,22,23	1.46	6 (31%)	27,32,35	2.25	6 (22%)
32	2MG	2a	1207	57,32	23,26,27	1.23	2 (8%)	33,38,41	2.25	8 (24%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.16	10 (30%)
54	4SU	1y	8	54	18,21,22	1.77	6 (33%)	25,30,33	2.08	4 (16%)
32	M2G	1a	966	32	24,27,28	1.31	3 (12%)	33,40,43	1.92	5 (15%)
43	0TD	1l	92	43	8,9,10	4.46	1 (12%)	6,11,13	4.45	2 (33%)
1	5MU	1A	1915	1	19,22,23	1.41	6 (31%)	27,32,35	2.08	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.19	3 (11%)
1	5MC	1A	1942	1	19,22,23	1.67	3 (15%)	26,32,35	1.14	3 (11%)
54	5MU	2y	54	54	19,22,23	1.51	5 (26%)	27,32,35	1.77	7 (25%)

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
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	55	54	-	5/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	57,32	-	1/9/29/30	0/2/2/2
54	G7M	1y	46	54	-	2/7/25/26	0/3/3/3
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	OMC	1A	1920	1	-	2/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,55	-	3/7/25/26	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	57,32	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
54	MIA	2w	37	54,53	-	4/11/29/34	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	2/7/25/26	0/3/3/3
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
56	FME	2z	1	56	-	1/7/9/11	-
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	57,1,55	-	0/9/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/9/27/28	0/3/3/3
55	8AN	2x	76	57,58,55	-	3/7/25/26	0/3/3/3
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
56	FME	1z	1	56	-	4/7/9/11	-
54	G7M	1w	46	54	-	2/7/25/26	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	57,32	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	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	-12.35	1.69	1.82
43	1l	92	0TD	CB-SB	-12.14	1.70	1.82
54	2w	37	MIA	C2-S10	-7.90	1.69	1.75
54	1w	37	MIA	C13-C14	7.07	1.53	1.32
32	2a	1404	5MC	C5-C4	6.38	1.48	1.44

The worst 5 of 416 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	37	MIA	C11-S10-C2	-10.36	94.48	102.25
43	1l	92	0TD	CSB-SB-CB	10.24	120.77	102.36
43	2l	92	0TD	CSB-SB-CB	-9.64	85.04	102.36
54	2w	37	MIA	C5-C4-N3	-8.88	117.83	127.18
32	1a	1207	2MG	C2-N3-C4	7.36	121.21	112.00

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12

There are no ring outliers.

45 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	37	MIA	2	0
43	2l	92	0TD	1	0
32	1a	1400	5MC	1	0
1	2A	2605	PSU	1	0
54	2y	55	PSU	6	0
1	2A	2552	OMU	1	0
32	1a	967	5MC	1	0
32	2a	1402	4OC	4	0
54	1y	46	G7M	1	0
1	1A	2552	OMU	2	0
1	2A	1920	OMC	1	0
55	1x	76	8AN	2	0
32	1a	1402	4OC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	37	MIA	1	0
32	1a	1518	MA6	2	0
32	2a	967	5MC	3	0
32	2a	1519	MA6	3	0
54	1y	39	PSU	2	0
32	2a	1400	5MC	2	0
1	1A	1939	5MU	1	0
32	1a	1519	MA6	2	0
54	2w	37	MIA	2	0
54	2y	46	G7M	1	0
1	1A	1917	PSU	1	0
1	2A	1915	5MU	1	0
54	2w	46	G7M	1	0
54	1w	8	4SU	1	0
1	2A	2251	OMG	1	0
55	2x	55	PSU	2	0
55	2x	76	8AN	2	0
54	1y	55	PSU	1	0
54	1y	37	MIA	1	0
1	2A	2503	2MA	1	0
55	1x	8	4SU	2	0
32	2a	966	M2G	2	0
54	1w	46	G7M	1	0
54	2w	39	PSU	1	0
1	2A	1939	5MU	1	0
32	2a	1518	MA6	1	0
54	1y	8	4SU	2	0
32	1a	966	M2G	1	0
43	1l	92	0TD	1	0
1	1A	1915	5MU	1	0
32	2a	1404	5MC	1	0
1	1A	1942	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2731 ligands modelled in this entry, 2727 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	ERY	2A	3857	-	53,53,53	0.93	1 (1%)	82,82,82	1.49	15 (18%)
61	SF4	2d	303	35	0,12,12	-	-	-	-	-
59	ERY	1A	4087	-	53,53,53	0.95	1 (1%)	82,82,82	1.72	17 (20%)
61	SF4	1d	302	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ERY	2A	3857	-	-	19/72/107/107	0/3/3/3
61	SF4	2d	303	35	-	-	0/6/5/5
59	ERY	1A	4087	-	-	15/72/107/107	0/3/3/3
61	SF4	1d	302	35	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4087	ERY	O2-C1	5.17	1.46	1.34
59	2A	3857	ERY	O2-C1	4.97	1.45	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	4087	ERY	C15-C16-C17	4.64	115.58	107.64
59	1A	4087	ERY	O5-C16-C15	-4.23	106.44	112.95
59	1A	4087	ERY	O7-C5-C4	-4.20	105.50	111.58
59	1A	4087	ERY	C6-C5-C4	-4.19	107.81	113.89
59	2A	3857	ERY	O5-C16-C15	-3.98	106.83	112.95

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4087	ERY	C17-C16-O5-C20
59	1A	4087	ERY	C19-C16-O5-C20
59	2A	3857	ERY	C9-C10-C11-C12
59	2A	3857	ERY	C9-C10-C11-O12
59	2A	3857	ERY	C34-C10-C11-C12

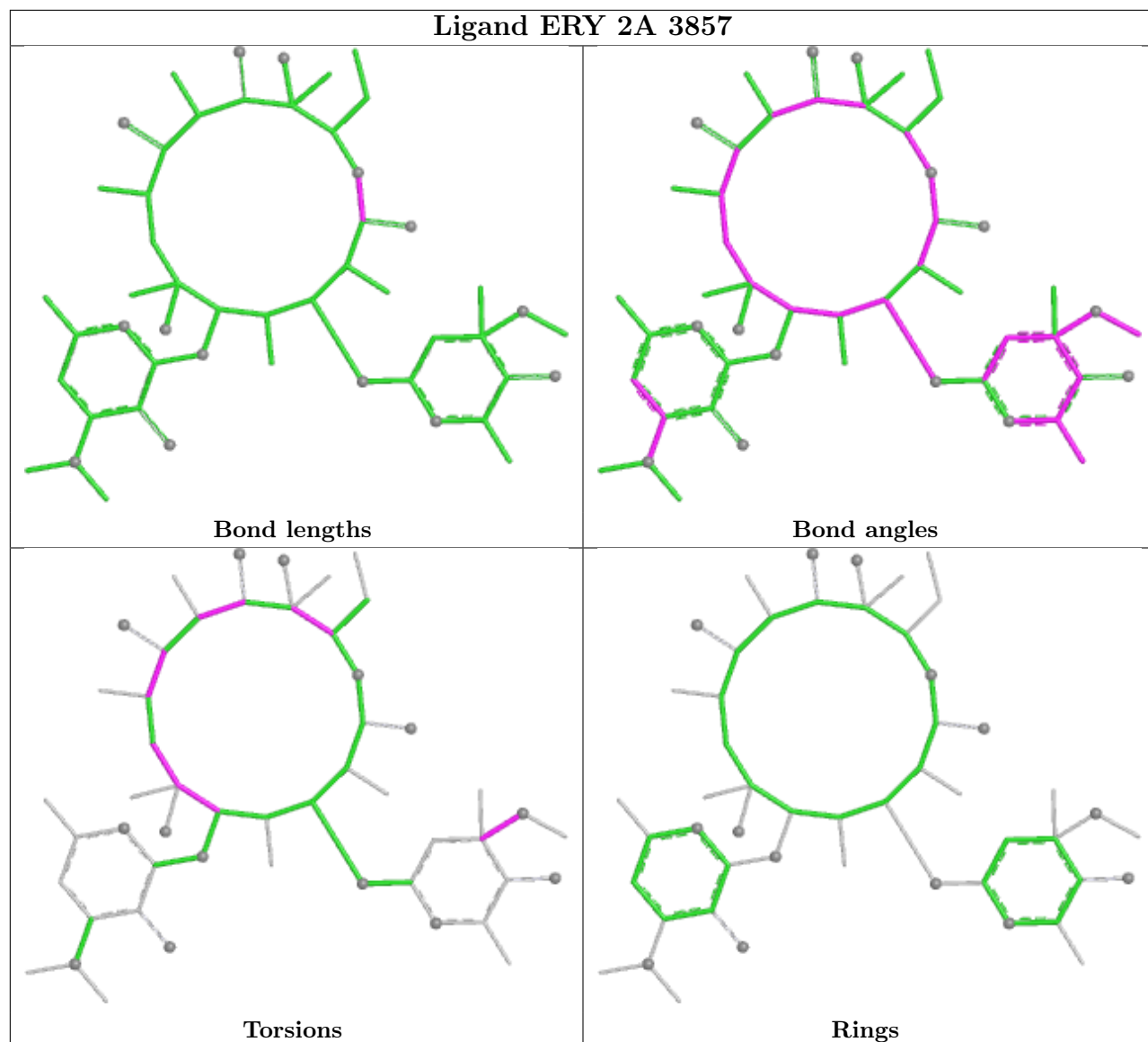
There are no ring outliers.

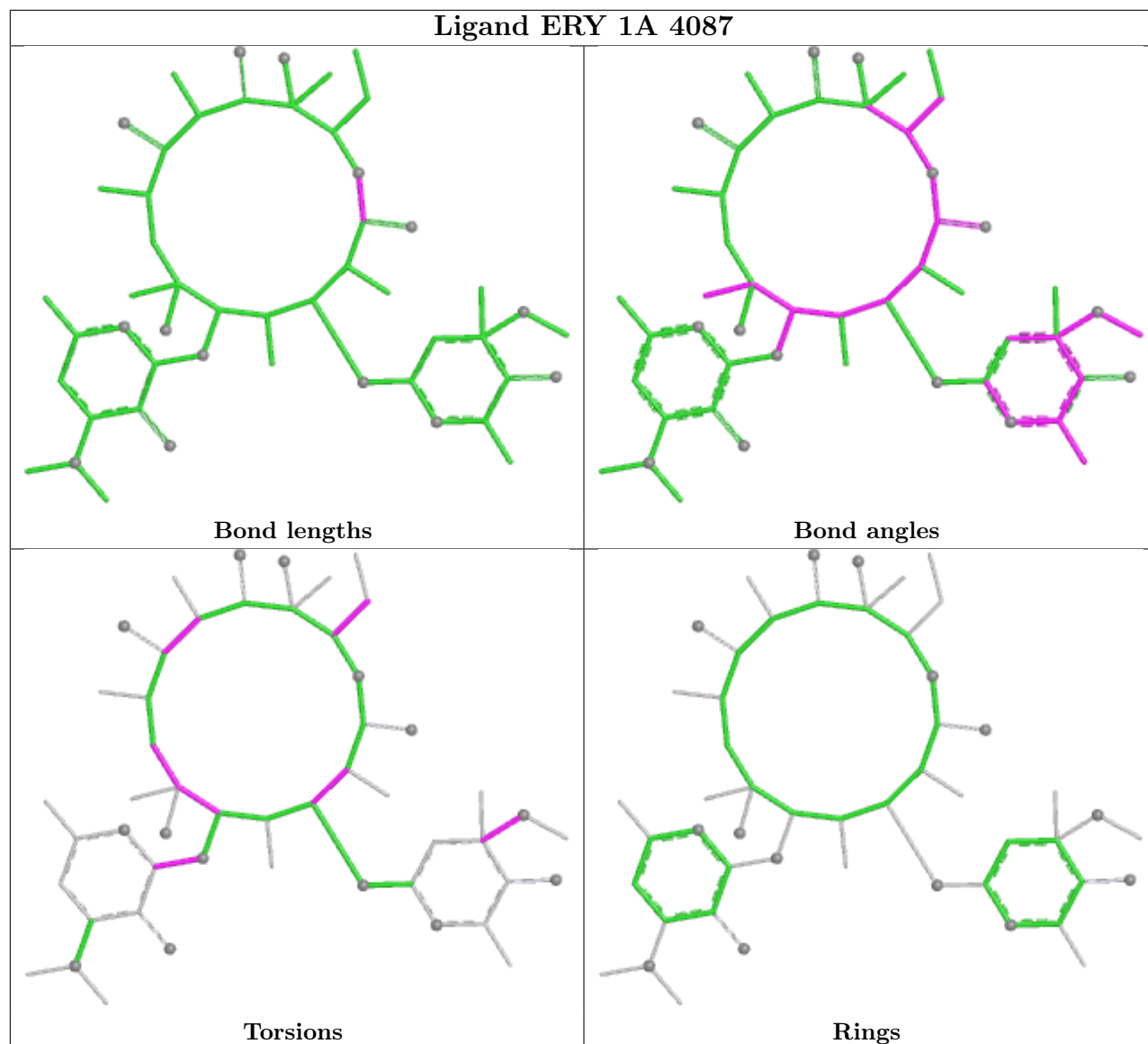
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2A	3857	ERY	4	0
61	2d	303	SF4	2	0
59	1A	4087	ERY	9	0
61	1d	302	SF4	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.

Ligand ERY 2A 3857





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%)	-0.59	44 (1%) 72 71	19, 37, 92, 108	0
1	2A	2789/2915 (95%)	-0.19	39 (1%) 73 73	32, 56, 91, 105	0
2	1B	120/121 (99%)	-0.53	0 100 100	31, 50, 64, 83	0
2	2B	120/121 (99%)	0.48	1 (0%) 82 82	57, 77, 86, 91	0
3	1D	275/276 (99%)	-0.15	2 (0%) 84 84	19, 36, 51, 71	0
3	2D	275/276 (99%)	0.26	7 (2%) 58 56	29, 50, 62, 75	0
4	1E	204/206 (99%)	-0.00	1 (0%) 87 87	20, 44, 63, 79	0
4	2E	204/206 (99%)	0.21	2 (0%) 79 79	29, 56, 69, 81	0
5	1F	202/210 (96%)	-0.13	1 (0%) 87 87	19, 43, 65, 84	0
5	2F	202/210 (96%)	0.35	5 (2%) 58 56	34, 67, 80, 85	0
6	1G	181/182 (99%)	0.34	3 (1%) 69 67	39, 57, 74, 88	0
6	2G	181/182 (99%)	1.05	15 (8%) 17 18	66, 78, 86, 89	0
7	1H	174/180 (96%)	0.17	0 100 100	39, 54, 67, 75	0
7	2H	174/180 (96%)	0.92	11 (6%) 26 26	62, 80, 87, 95	0
8	1I	146/148 (98%)	0.48	3 (2%) 63 61	39, 70, 80, 84	0
8	2I	146/148 (98%)	0.93	11 (7%) 20 20	57, 74, 84, 87	0
9	1N	140/140 (100%)	0.01	0 100 100	28, 45, 61, 79	0
9	2N	140/140 (100%)	0.63	4 (2%) 53 52	44, 63, 75, 83	0
10	1O	122/122 (100%)	-0.11	0 100 100	28, 42, 60, 67	0
10	2O	122/122 (100%)	0.36	2 (1%) 70 69	37, 55, 68, 72	0
11	1P	149/150 (99%)	0.08	0 100 100	21, 43, 67, 75	0
11	2P	149/150 (99%)	0.42	3 (2%) 65 63	36, 66, 82, 87	0
12	1Q	141/141 (100%)	-0.06	0 100 100	27, 42, 55, 73	0
12	2Q	141/141 (100%)	0.79	12 (8%) 16 17	46, 64, 74, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.11	0 100 100	29, 38, 51, 60	0
13	2R	118/118 (100%)	0.11	0 100 100	37, 50, 60, 69	0
14	1S	110/112 (98%)	0.14	0 100 100	38, 49, 60, 65	0
14	2S	110/112 (98%)	1.00	10 (9%) 15 14	60, 70, 78, 82	0
15	1T	131/146 (89%)	0.16	3 (2%) 61 59	35, 49, 71, 80	0
15	2T	131/146 (89%)	0.41	1 (0%) 82 82	45, 57, 73, 83	0
16	1U	116/118 (98%)	-0.07	2 (1%) 69 67	24, 37, 55, 73	0
16	2U	116/118 (98%)	0.31	1 (0%) 81 81	43, 58, 73, 78	0
17	1V	101/101 (100%)	0.01	0 100 100	23, 48, 62, 72	0
17	2V	101/101 (100%)	0.59	1 (0%) 79 79	46, 70, 78, 82	0
18	1W	112/113 (99%)	-0.21	1 (0%) 81 81	27, 38, 56, 76	0
18	2W	112/113 (99%)	0.34	0 100 100	38, 50, 67, 93	0
19	1X	95/96 (98%)	-0.15	1 (1%) 78 77	28, 38, 55, 71	0
19	2X	95/96 (98%)	0.51	1 (1%) 78 77	41, 58, 71, 76	0
20	1Y	107/110 (97%)	0.27	1 (0%) 81 81	35, 50, 68, 75	0
20	2Y	107/110 (97%)	0.91	7 (6%) 25 24	60, 72, 80, 86	0
21	1Z	154/206 (74%)	0.29	5 (3%) 50 48	42, 63, 82, 90	0
21	2Z	160/206 (77%)	1.09	22 (13%) 6 5	67, 79, 89, 99	0
22	10	83/85 (97%)	-0.00	2 (2%) 59 57	28, 37, 56, 64	0
22	20	83/85 (97%)	0.98	8 (9%) 13 13	47, 61, 70, 81	0
23	11	97/98 (98%)	0.14	1 (1%) 79 79	23, 43, 65, 70	0
23	21	97/98 (98%)	0.60	3 (3%) 51 49	38, 56, 73, 76	0
24	12	70/72 (97%)	0.15	1 (1%) 73 73	34, 47, 57, 71	0
24	22	70/72 (97%)	0.79	5 (7%) 22 22	58, 68, 75, 77	0
25	13	59/60 (98%)	-0.10	0 100 100	29, 41, 65, 78	0
25	23	59/60 (98%)	0.38	1 (1%) 69 67	52, 65, 78, 83	0
26	14	69/71 (97%)	0.55	4 (5%) 29 29	50, 73, 87, 93	0
26	24	69/71 (97%)	0.93	7 (10%) 12 11	75, 85, 93, 96	0
27	15	59/60 (98%)	-0.22	0 100 100	21, 42, 64, 74	0
27	25	59/60 (98%)	0.17	1 (1%) 69 67	34, 51, 70, 80	0
28	16	53/54 (98%)	-0.02	0 100 100	31, 40, 53, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.61	0 100 100	49, 59, 66, 73	0
29	17	48/49 (97%)	-0.42	0 100 100	21, 27, 46, 54	0
29	27	48/49 (97%)	0.05	1 (2%) 63 61	32, 41, 60, 67	0
30	18	64/65 (98%)	-0.09	1 (1%) 70 69	28, 33, 42, 55	0
30	28	64/65 (98%)	0.50	1 (1%) 70 69	42, 54, 64, 71	0
31	19	37/37 (100%)	0.15	0 100 100	34, 42, 55, 64	0
31	29	37/37 (100%)	1.04	4 (10%) 11 9	57, 66, 76, 78	0
32	1a	1488/1521 (97%)	-0.05	14 (0%) 81 81	34, 63, 90, 107	0
32	2a	1491/1521 (98%)	0.34	42 (2%) 55 53	51, 76, 94, 109	0
33	1b	231/256 (90%)	0.96	28 (12%) 8 7	61, 76, 84, 94	0
33	2b	231/256 (90%)	1.30	45 (19%) 3 2	72, 84, 90, 93	0
34	1c	206/239 (86%)	0.54	5 (2%) 59 57	54, 66, 77, 87	0
34	2c	206/239 (86%)	1.24	38 (18%) 3 2	68, 83, 88, 93	0
35	1d	208/209 (99%)	0.46	5 (2%) 59 57	51, 64, 75, 81	0
35	2d	208/209 (99%)	0.93	17 (8%) 17 18	63, 72, 81, 86	0
36	1e	148/162 (91%)	0.37	2 (1%) 73 73	47, 61, 73, 86	0
36	2e	148/162 (91%)	0.95	12 (8%) 18 18	64, 77, 83, 87	0
37	1f	100/101 (99%)	0.43	1 (1%) 79 79	47, 60, 75, 77	0
37	2f	100/101 (99%)	0.45	1 (1%) 79 79	60, 69, 78, 86	0
38	1g	155/156 (99%)	0.58	11 (7%) 22 22	54, 67, 79, 86	0
38	2g	155/156 (99%)	0.88	13 (8%) 17 17	69, 79, 87, 94	0
39	1h	137/138 (99%)	0.45	4 (2%) 53 52	56, 65, 73, 78	0
39	2h	137/138 (99%)	1.06	15 (10%) 10 9	67, 77, 84, 89	0
40	1i	127/128 (99%)	0.80	5 (3%) 43 40	52, 72, 81, 87	0
40	2i	127/128 (99%)	1.79	47 (37%) 1 0	70, 83, 90, 93	0
41	1j	97/105 (92%)	0.82	7 (7%) 21 21	51, 73, 84, 91	0
41	2j	96/105 (91%)	1.43	25 (26%) 1 1	72, 83, 89, 93	0
42	1k	114/129 (88%)	0.29	1 (0%) 81 81	40, 63, 74, 82	0
42	2k	114/129 (88%)	1.09	16 (14%) 6 5	63, 74, 80, 85	0
43	1l	121/132 (91%)	0.16	4 (3%) 49 47	40, 51, 64, 71	0
43	2l	121/132 (91%)	0.55	4 (3%) 49 47	46, 65, 74, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.53	7 (5%) 29 29	49, 65, 76, 93	0
44	2m	122/126 (96%)	1.22	20 (16%) 4 4	72, 81, 88, 91	0
45	1n	60/61 (98%)	0.66	3 (5%) 34 34	52, 61, 68, 69	0
45	2n	60/61 (98%)	2.08	31 (51%) 0 0	74, 82, 88, 89	0
46	1o	88/89 (98%)	0.59	3 (3%) 48 46	47, 60, 71, 76	0
46	2o	88/89 (98%)	0.79	3 (3%) 48 46	60, 72, 80, 83	0
47	1p	82/88 (93%)	0.93	8 (9%) 13 12	57, 66, 74, 79	0
47	2p	82/88 (93%)	0.87	3 (3%) 45 42	56, 65, 75, 77	0
48	1q	99/105 (94%)	0.98	7 (7%) 22 22	53, 66, 76, 81	0
48	2q	99/105 (94%)	0.94	7 (7%) 22 22	64, 72, 80, 86	0
49	1r	68/88 (77%)	0.38	2 (2%) 53 52	49, 63, 75, 77	0
49	2r	68/88 (77%)	0.51	0 100 100	63, 74, 83, 85	0
50	1s	83/93 (89%)	0.31	1 (1%) 76 76	54, 66, 76, 81	0
50	2s	83/93 (89%)	1.41	16 (19%) 3 2	75, 83, 90, 93	0
51	1t	96/106 (90%)	0.75	7 (7%) 21 21	55, 66, 78, 89	0
51	2t	96/106 (90%)	0.73	3 (3%) 51 49	54, 65, 82, 85	0
52	1u	23/27 (85%)	0.85	1 (4%) 40 38	57, 64, 71, 72	0
52	2u	23/27 (85%)	1.83	10 (43%) 0 0	75, 78, 83, 87	0
53	1v	13/24 (54%)	0.18	0 100 100	42, 57, 82, 91	0
53	2v	13/24 (54%)	1.43	3 (23%) 2 1	72, 79, 92, 94	0
54	1w	67/76 (88%)	0.62	5 (7%) 20 20	34, 90, 98, 109	0
54	1y	67/76 (88%)	0.39	2 (2%) 52 50	38, 90, 98, 102	0
54	2w	65/76 (85%)	0.74	6 (9%) 14 14	52, 92, 100, 103	0
54	2y	66/76 (86%)	0.69	2 (3%) 52 50	50, 96, 101, 104	0
55	1x	72/77 (93%)	-0.02	0 100 100	29, 61, 79, 84	0
55	2x	72/77 (93%)	0.35	0 100 100	44, 78, 88, 91	0
56	1z	2/3 (66%)	0.14	0 100 100	35, 35, 35, 38	0
56	2z	2/3 (66%)	0.58	0 100 100	48, 48, 48, 52	0
All	All	20877/21754 (95%)	0.22	774 (3%) 45 42	19, 62, 88, 109	0

The worst 5 of 774 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	7.5
44	2m	124	PRO	7.3
44	2m	123	ALA	6.8
23	21	2	SER	6.7
44	2m	122	LYS	6.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	G7M	2y	46	24/25	0.57	0.15	90,98,107,119	0
54	G7M	1w	46	24/25	0.63	0.12	83,92,104,119	0
54	PSU	1y	55	20/21	0.66	0.13	87,97,107,116	0
54	PSU	2y	55	20/21	0.66	0.14	84,95,107,111	0
54	G7M	1y	46	24/25	0.67	0.12	87,93,102,111	0
54	G7M	2w	46	24/25	0.69	0.12	83,93,106,120	0
54	PSU	2w	55	20/21	0.72	0.11	79,89,96,103	0
54	4SU	2y	8	20/21	0.73	0.13	90,99,108,111	0
54	MIA	2y	37	22/30	0.75	0.15	87,92,98,108	0
54	4SU	2w	8	20/21	0.75	0.11	89,95,108,109	0
54	5MU	2y	54	21/22	0.75	0.15	85,90,102,117	0
54	5MU	1y	54	21/22	0.75	0.14	82,93,102,114	0
54	4SU	1w	8	20/21	0.76	0.10	87,93,101,103	0
54	5MU	2w	54	21/22	0.76	0.12	73,81,85,96	0
54	MIA	1y	37	22/30	0.78	0.11	69,83,100,110	0
54	PSU	2y	32	20/21	0.79	0.14	86,90,97,103	0
54	PSU	2y	39	20/21	0.81	0.14	84,90,98,102	0
54	4SU	1y	8	20/21	0.81	0.09	88,94,103,104	0
32	2MG	2a	1207	24/25	0.83	0.13	81,89,99,109	0
54	PSU	1w	55	20/21	0.83	0.10	76,85,92,94	0
55	4SU	2x	8	20/21	0.86	0.10	74,78,81,86	0
55	PSU	2x	55	20/21	0.87	0.10	70,77,88,94	0
54	PSU	1w	32	20/21	0.87	0.13	61,74,77,78	0
54	PSU	1y	32	20/21	0.88	0.09	74,80,91,97	0
32	M2G	2a	966	25/26	0.88	0.16	63,74,87,94	0
54	PSU	2w	39	20/21	0.88	0.12	73,83,91,93	0
32	PSU	2a	516	20/21	0.89	0.09	63,73,85,88	0
54	PSU	1y	39	20/21	0.89	0.08	74,81,85,87	0
54	PSU	2w	32	20/21	0.89	0.12	73,83,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	967	21/22	0.89	0.13	70,77,82,88	0
55	5MU	2x	54	21/22	0.90	0.10	79,82,86,93	0
54	5MU	1w	54	21/22	0.90	0.09	63,74,83,85	0
55	5MU	1x	54	21/22	0.90	0.10	59,67,72,75	0
54	MIA	1w	37	29/30	0.91	0.15	49,63,78,88	0
1	5MU	2A	1915	21/22	0.91	0.09	66,71,76,82	0
55	5MC	2x	32	21/22	0.92	0.12	69,74,79,80	0
32	G7M	2a	527	24/25	0.92	0.11	58,63,69,74	0
32	5MC	2a	1400	21/22	0.92	0.15	68,74,79,81	0
54	MIA	2w	37	25/30	0.92	0.10	64,76,84,92	0
43	0TD	2l	92	10/11	0.92	0.12	61,63,71,79	0
1	PSU	2A	1917	20/21	0.93	0.08	58,64,72,74	0
55	PSU	1x	55	20/21	0.93	0.08	56,59,70,71	0
32	5MC	2a	1407	21/22	0.94	0.10	50,62,65,68	0
32	UR3	2a	1498	21/22	0.94	0.11	51,59,66,71	0
32	MA6	2a	1519	24/25	0.94	0.13	60,67,74,77	0
55	4SU	1x	8	20/21	0.94	0.09	51,57,64,77	0
32	PSU	1a	516	20/21	0.94	0.10	52,57,61,63	0
1	PSU	2A	1911	20/21	0.94	0.09	42,59,66,66	0
1	5MU	1A	1915	21/22	0.94	0.08	43,51,55,59	0
54	PSU	1w	39	20/21	0.94	0.08	67,71,74,87	0
1	5MC	2A	1962	21/22	0.94	0.11	44,54,58,73	0
32	4OC	2a	1402	22/23	0.94	0.10	59,70,73,73	0
32	5MC	2a	1404	21/22	0.94	0.10	52,64,70,74	0
56	FME	1z	1	10/11	0.94	0.15	37,49,52,63	0
1	OMC	2A	1920	21/22	0.95	0.08	54,60,62,63	0
32	2MG	1a	1207	24/25	0.95	0.09	57,65,68,77	0
55	5MC	1x	32	21/22	0.95	0.09	38,45,52,57	0
56	FME	2z	1	10/11	0.95	0.14	52,55,58,58	0
32	4OC	1a	1402	22/23	0.96	0.09	43,48,52,58	0
43	0TD	1l	92	10/11	0.96	0.08	34,44,50,51	0
1	PSU	1A	1917	20/21	0.96	0.08	36,47,51,52	0
1	5MC	2A	1942	21/22	0.96	0.09	42,58,62,69	0
32	M2G	1a	966	25/26	0.96	0.10	46,51,56,57	0
1	OMU	2A	2552	21/22	0.96	0.09	35,39,48,49	0
32	5MC	1a	967	21/22	0.96	0.09	44,55,61,68	0
32	MA6	2a	1518	24/25	0.96	0.09	57,65,70,73	0
1	5MC	1A	1942	21/22	0.96	0.08	33,39,43,54	0
32	5MC	1a	1400	21/22	0.96	0.10	37,42,49,56	0
32	5MC	1a	1407	21/22	0.97	0.08	26,40,45,48	0
55	8AN	1x	76	22/23	0.97	0.08	25,33,41,43	0
55	8AN	2x	76	22/23	0.97	0.09	40,44,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	1a	1518	24/25	0.97	0.09	32,41,45,48	0
32	MA6	1a	1519	24/25	0.97	0.08	36,43,48,56	0
32	G7M	1a	527	24/25	0.97	0.07	38,44,50,56	0
1	5MU	2A	1939	21/22	0.97	0.07	34,38,44,45	0
1	5MC	1A	1962	21/22	0.97	0.07	27,34,40,46	0
1	OMC	1A	1920	21/22	0.97	0.07	34,40,46,50	0
1	OMG	2A	2251	24/25	0.97	0.07	33,39,44,46	0
32	5MC	1a	1404	21/22	0.97	0.09	28,40,43,51	0
1	PSU	2A	2605	20/21	0.97	0.07	30,38,46,47	0
1	PSU	1A	1911	20/21	0.98	0.06	38,42,46,50	0
1	5MU	1A	1939	21/22	0.98	0.06	23,26,32,35	0
1	OMG	1A	2251	24/25	0.98	0.07	17,26,28,30	0
1	2MA	1A	2503	23/24	0.98	0.05	20,22,26,26	0
32	UR3	1a	1498	21/22	0.98	0.07	36,41,46,51	0
1	2MA	2A	2503	23/24	0.98	0.06	28,34,36,39	0
1	OMU	1A	2552	21/22	0.98	0.06	24,28,32,40	0
1	PSU	1A	2605	20/21	0.99	0.06	18,27,31,34	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1720	1/1	0.51	0.38	82,82,82,82	0
57	MG	1B	232	1/1	0.55	0.16	76,76,76,76	0
57	MG	2A	3772	1/1	0.56	0.15	71,71,71,71	0
57	MG	2A	3710	1/1	0.58	0.17	79,79,79,79	0
57	MG	2A	3434	1/1	0.58	0.21	78,78,78,78	0
57	MG	2A	3576	1/1	0.64	0.18	67,67,67,67	0
57	MG	1A	3589	1/1	0.66	0.27	71,71,71,71	0
57	MG	2A	3273	1/1	0.66	0.22	78,78,78,78	0
57	MG	2a	1738	1/1	0.66	0.25	79,79,79,79	0
57	MG	2a	1800	1/1	0.67	0.25	79,79,79,79	0
57	MG	2A	3678	1/1	0.68	0.23	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3203	1/1	0.69	0.27	68,68,68,68	0
57	MG	2a	1647	1/1	0.70	0.21	64,64,64,64	0
57	MG	1w	104	1/1	0.70	0.23	81,81,81,81	0
57	MG	2A	3236	1/1	0.70	0.18	67,67,67,67	0
57	MG	18	105	1/1	0.71	0.20	65,65,65,65	0
57	MG	2A	3643	1/1	0.71	0.34	83,83,83,83	0
57	MG	2A	3655	1/1	0.71	0.18	70,70,70,70	0
57	MG	2A	3569	1/1	0.72	0.19	79,79,79,79	0
57	MG	2A	3107	1/1	0.72	0.17	70,70,70,70	0
57	MG	2A	3199	1/1	0.72	0.24	71,71,71,71	0
57	MG	2A	3340	1/1	0.72	0.18	70,70,70,70	0
57	MG	1A	3749	1/1	0.72	0.21	60,60,60,60	0
57	MG	2A	3200	1/1	0.73	0.25	68,68,68,68	0
57	MG	1A	4070	1/1	0.73	0.36	89,89,89,89	0
57	MG	2y	101	1/1	0.73	0.29	79,79,79,79	0
57	MG	2A	3321	1/1	0.74	0.16	84,84,84,84	0
57	MG	2A	3326	1/1	0.74	0.25	77,77,77,77	0
57	MG	2A	3305	1/1	0.74	0.18	62,62,62,62	0
57	MG	2A	3103	1/1	0.75	0.17	76,76,76,76	0
57	MG	2a	1695	1/1	0.75	0.48	81,81,81,81	0
57	MG	2A	3276	1/1	0.75	0.13	70,70,70,70	0
57	MG	2B	204	1/1	0.75	0.15	77,77,77,77	0
57	MG	2w	101	1/1	0.75	0.28	83,83,83,83	0
57	MG	2B	215	1/1	0.75	0.23	69,69,69,69	0
57	MG	2A	3278	1/1	0.76	0.17	72,72,72,72	0
57	MG	1A	4001	1/1	0.76	0.11	76,76,76,76	0
57	MG	2A	3212	1/1	0.76	0.15	58,58,58,58	0
57	MG	1A	3894	1/1	0.76	0.16	62,62,62,62	0
57	MG	1A	3939	1/1	0.76	0.18	79,79,79,79	0
57	MG	2a	1784	1/1	0.76	0.21	73,73,73,73	0
57	MG	2A	3097	1/1	0.76	0.32	80,80,80,80	0
57	MG	2A	3741	1/1	0.76	0.12	50,50,50,50	0
57	MG	2A	3469	1/1	0.76	0.19	65,65,65,65	0
57	MG	2a	1605	1/1	0.77	0.36	73,73,73,73	0
57	MG	1a	1804	1/1	0.77	0.25	74,74,74,74	0
57	MG	2a	1671	1/1	0.77	0.25	69,69,69,69	0
57	MG	1A	3256	1/1	0.77	0.26	63,63,63,63	0
57	MG	2a	1721	1/1	0.77	0.15	50,50,50,50	0
57	MG	2A	3734	1/1	0.77	0.17	80,80,80,80	0
57	MG	2A	3089	1/1	0.77	0.10	64,64,64,64	0
57	MG	1A	3873	1/1	0.77	0.15	67,67,67,67	0
57	MG	2v	102	1/1	0.77	0.30	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3955	1/1	0.77	0.22	39,39,39,39	0
57	MG	1A	3877	1/1	0.77	0.12	22,22,22,22	0
57	MG	1A	3543	1/1	0.78	0.14	40,40,40,40	0
57	MG	2A	3649	1/1	0.78	0.20	74,74,74,74	0
57	MG	1A	3505	1/1	0.78	0.12	61,61,61,61	0
57	MG	2A	3671	1/1	0.78	0.18	63,63,63,63	0
57	MG	2a	1713	1/1	0.78	0.12	64,64,64,64	0
57	MG	2A	3253	1/1	0.78	0.16	74,74,74,74	0
57	MG	2a	1728	1/1	0.78	0.35	80,80,80,80	0
57	MG	1A	3725	1/1	0.78	0.20	73,73,73,73	0
57	MG	2A	3384	1/1	0.78	0.13	73,73,73,73	0
57	MG	2a	1785	1/1	0.78	0.17	85,85,85,85	0
57	MG	1A	3968	1/1	0.78	0.13	61,61,61,61	0
57	MG	2a	1809	1/1	0.78	0.29	65,65,65,65	0
57	MG	1a	1607	1/1	0.78	0.31	73,73,73,73	0
57	MG	2A	3294	1/1	0.78	0.12	66,66,66,66	0
57	MG	2A	3302	1/1	0.78	0.15	66,66,66,66	0
57	MG	2A	3184	1/1	0.79	0.29	66,66,66,66	0
57	MG	2A	3785	1/1	0.79	0.13	55,55,55,55	0
57	MG	2A	3065	1/1	0.79	0.12	57,57,57,57	0
57	MG	2A	3383	1/1	0.79	0.09	63,63,63,63	0
57	MG	1B	236	1/1	0.79	0.18	76,76,76,76	0
57	MG	2a	1786	1/1	0.79	0.15	66,66,66,66	0
57	MG	1A	3833	1/1	0.79	0.17	70,70,70,70	0
57	MG	1A	3228	1/1	0.79	0.20	66,66,66,66	0
57	MG	2A	3052	1/1	0.79	0.16	73,73,73,73	0
57	MG	2A	3168	1/1	0.79	0.26	77,77,77,77	0
57	MG	2a	1720	1/1	0.79	0.26	55,55,55,55	0
57	MG	2a	1639	1/1	0.80	0.21	76,76,76,76	0
57	MG	2A	3600	1/1	0.80	0.10	74,74,74,74	0
57	MG	1a	1736	1/1	0.80	0.20	65,65,65,65	0
57	MG	1a	1738	1/1	0.80	0.14	74,74,74,74	0
57	MG	2a	1705	1/1	0.80	0.26	78,78,78,78	0
57	MG	1a	1765	1/1	0.80	0.11	58,58,58,58	0
57	MG	1A	3809	1/1	0.80	0.14	48,48,48,48	0
57	MG	1w	101	1/1	0.80	0.17	66,66,66,66	0
57	MG	1A	4074	1/1	0.80	0.18	49,49,49,49	0
57	MG	2A	3382	1/1	0.80	0.12	74,74,74,74	0
57	MG	2a	1783	1/1	0.80	0.15	71,71,71,71	0
57	MG	1A	3347	1/1	0.80	0.19	43,43,43,43	0
57	MG	2A	3754	1/1	0.80	0.12	59,59,59,59	0
57	MG	1A	3947	1/1	0.80	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1788	1/1	0.80	0.21	72,72,72,72	0
57	MG	1A	3687	1/1	0.80	0.12	57,57,57,57	0
57	MG	2A	3827	1/1	0.80	0.13	45,45,45,45	0
57	MG	2A	3093	1/1	0.80	0.15	58,58,58,58	0
57	MG	1A	3874	1/1	0.80	0.13	46,46,46,46	0
57	MG	1A	3774	1/1	0.80	0.10	20,20,20,20	0
57	MG	2A	3242	1/1	0.81	0.14	57,57,57,57	0
57	MG	2a	1736	1/1	0.81	0.20	69,69,69,69	0
57	MG	1a	1713	1/1	0.81	0.16	50,50,50,50	0
57	MG	2a	1771	1/1	0.81	0.32	77,77,77,77	0
57	MG	1A	3206	1/1	0.81	0.13	67,67,67,67	0
57	MG	2a	1618	1/1	0.81	0.14	61,61,61,61	0
57	MG	2A	3690	1/1	0.81	0.23	77,77,77,77	0
57	MG	2A	3021	1/1	0.81	0.24	72,72,72,72	0
57	MG	2A	3531	1/1	0.81	0.29	65,65,65,65	0
57	MG	1A	3555	1/1	0.81	0.14	46,46,46,46	0
57	MG	2a	1808	1/1	0.81	0.14	64,64,64,64	0
57	MG	2A	3355	1/1	0.81	0.24	73,73,73,73	0
57	MG	2A	3366	1/1	0.81	0.16	74,74,74,74	0
57	MG	2A	3375	1/1	0.81	0.38	66,66,66,66	0
57	MG	2x	102	1/1	0.81	0.10	71,71,71,71	0
57	MG	2A	3188	1/1	0.81	0.11	62,62,62,62	0
57	MG	1A	3860	1/1	0.82	0.09	45,45,45,45	0
57	MG	2a	1744	1/1	0.82	0.29	69,69,69,69	0
57	MG	2B	219	1/1	0.82	0.22	67,67,67,67	0
57	MG	2A	3252	1/1	0.82	0.18	71,71,71,71	0
57	MG	1w	102	1/1	0.82	0.09	69,69,69,69	0
57	MG	1a	1678	1/1	0.82	0.16	59,59,59,59	0
57	MG	2A	3737	1/1	0.82	0.17	49,49,49,49	0
57	MG	1A	3322	1/1	0.82	0.14	53,53,53,53	0
57	MG	1a	1795	1/1	0.82	0.09	75,75,75,75	0
57	MG	2A	3159	1/1	0.82	0.15	70,70,70,70	0
57	MG	2A	3301	1/1	0.82	0.16	71,71,71,71	0
57	MG	1A	4080	1/1	0.82	0.27	57,57,57,57	0
57	MG	2A	3837	1/1	0.82	0.12	74,74,74,74	0
57	MG	2A	3842	1/1	0.82	0.13	54,54,54,54	0
57	MG	2A	3303	1/1	0.82	0.23	60,60,60,60	0
57	MG	2a	1637	1/1	0.83	0.19	65,65,65,65	0
57	MG	2a	1638	1/1	0.83	0.28	70,70,70,70	0
57	MG	2A	3654	1/1	0.83	0.11	82,82,82,82	0
57	MG	1w	103	1/1	0.83	0.18	72,72,72,72	0
57	MG	2a	1654	1/1	0.83	0.20	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1663	1/1	0.83	0.27	63,63,63,63	0
57	MG	1a	1656	1/1	0.83	0.12	64,64,64,64	0
57	MG	1A	3865	1/1	0.83	0.23	45,45,45,45	0
57	MG	1a	1694	1/1	0.83	0.20	78,78,78,78	0
57	MG	2A	3692	1/1	0.83	0.11	69,69,69,69	0
57	MG	2a	1715	1/1	0.83	0.23	61,61,61,61	0
57	MG	1A	3944	1/1	0.83	0.13	60,60,60,60	0
57	MG	2A	3718	1/1	0.83	0.28	63,63,63,63	0
57	MG	2a	1727	1/1	0.83	0.08	60,60,60,60	0
57	MG	1A	3101	1/1	0.83	0.08	50,50,50,50	0
57	MG	1A	3717	1/1	0.83	0.08	62,62,62,62	0
57	MG	1A	3579	1/1	0.83	0.25	65,65,65,65	0
57	MG	2A	3257	1/1	0.83	0.22	63,63,63,63	0
57	MG	2a	1745	1/1	0.83	0.24	73,73,73,73	0
57	MG	2A	3389	1/1	0.83	0.13	46,46,46,46	0
57	MG	2A	3101	1/1	0.83	0.26	58,58,58,58	0
57	MG	2A	3444	1/1	0.83	0.17	68,68,68,68	0
57	MG	1D	311	1/1	0.83	0.15	33,33,33,33	0
57	MG	1a	1778	1/1	0.83	0.17	53,53,53,53	0
57	MG	2A	3850	1/1	0.83	0.23	58,58,58,58	0
57	MG	2A	3134	1/1	0.83	0.25	65,65,65,65	0
57	MG	2a	1803	1/1	0.83	0.21	72,72,72,72	0
57	MG	2B	214	1/1	0.83	0.17	75,75,75,75	0
57	MG	1G	203	1/1	0.83	0.10	54,54,54,54	0
57	MG	2a	1818	1/1	0.83	0.21	74,74,74,74	0
57	MG	2d	302	1/1	0.83	0.20	76,76,76,76	0
57	MG	1Q	204	1/1	0.83	0.10	52,52,52,52	0
57	MG	1A	3987	1/1	0.83	0.24	62,62,62,62	0
57	MG	1A	3027	1/1	0.83	0.21	54,54,54,54	0
57	MG	2x	103	1/1	0.83	0.24	74,74,74,74	0
57	MG	2a	1635	1/1	0.83	0.25	63,63,63,63	0
57	MG	2A	3255	1/1	0.84	0.20	58,58,58,58	0
57	MG	1a	1660	1/1	0.84	0.19	63,63,63,63	0
57	MG	1A	3830	1/1	0.84	0.13	67,67,67,67	0
57	MG	2A	3789	1/1	0.84	0.11	55,55,55,55	0
57	MG	2A	3137	1/1	0.84	0.20	63,63,63,63	0
57	MG	1F	301	1/1	0.84	0.22	36,36,36,36	0
57	MG	2A	3289	1/1	0.84	0.15	51,51,51,51	0
57	MG	1A	3161	1/1	0.84	0.21	51,51,51,51	0
57	MG	2B	203	1/1	0.84	0.17	54,54,54,54	0
57	MG	2A	3173	1/1	0.84	0.17	49,49,49,49	0
57	MG	2a	1750	1/1	0.84	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1764	1/1	0.84	0.16	73,73,73,73	0
57	MG	2A	3174	1/1	0.84	0.12	66,66,66,66	0
57	MG	1x	109	1/1	0.84	0.13	70,70,70,70	0
57	MG	1B	216	1/1	0.84	0.11	61,61,61,61	0
57	MG	1A	3250	1/1	0.84	0.21	74,74,74,74	0
57	MG	1B	233	1/1	0.84	0.15	61,61,61,61	0
57	MG	2a	1633	1/1	0.84	0.32	73,73,73,73	0
57	MG	2A	3676	1/1	0.84	0.15	66,66,66,66	0
57	MG	2A	3086	1/1	0.84	0.18	50,50,50,50	0
57	MG	2A	3684	1/1	0.84	0.09	69,69,69,69	0
57	MG	1a	1622	1/1	0.84	0.19	62,62,62,62	0
57	MG	2a	1812	1/1	0.84	0.28	69,69,69,69	0
57	MG	1a	1768	1/1	0.84	0.12	71,71,71,71	0
57	MG	2A	3367	1/1	0.84	0.16	75,75,75,75	0
57	MG	2j	201	1/1	0.84	0.20	63,63,63,63	0
57	MG	2q	202	1/1	0.84	0.13	77,77,77,77	0
57	MG	2a	1659	1/1	0.84	0.12	73,73,73,73	0
57	MG	2A	3237	1/1	0.84	0.13	60,60,60,60	0
57	MG	2x	101	1/1	0.84	0.20	72,72,72,72	0
57	MG	1a	1655	1/1	0.84	0.19	63,63,63,63	0
57	MG	1A	3642	1/1	0.84	0.11	43,43,43,43	0
57	MG	1a	1659	1/1	0.84	0.28	74,74,74,74	0
57	MG	2A	3339	1/1	0.85	0.08	56,56,56,56	0
57	MG	1a	1709	1/1	0.85	0.28	46,46,46,46	0
57	MG	2a	1677	1/1	0.85	0.13	61,61,61,61	0
57	MG	2A	3343	1/1	0.85	0.13	53,53,53,53	0
57	MG	2a	1703	1/1	0.85	0.18	66,66,66,66	0
57	MG	2A	3099	1/1	0.85	0.16	52,52,52,52	0
57	MG	1a	1806	1/1	0.85	0.21	74,74,74,74	0
57	MG	1A	3647	1/1	0.85	0.14	65,65,65,65	0
57	MG	1a	1719	1/1	0.85	0.16	64,64,64,64	0
57	MG	1a	1630	1/1	0.85	0.23	73,73,73,73	0
57	MG	1A	3935	1/1	0.85	0.24	64,64,64,64	0
57	MG	1A	3128	1/1	0.85	0.13	59,59,59,59	0
57	MG	2a	1732	1/1	0.85	0.14	58,58,58,58	0
57	MG	2A	3258	1/1	0.85	0.11	82,82,82,82	0
57	MG	2A	3410	1/1	0.85	0.13	51,51,51,51	0
57	MG	2A	3260	1/1	0.85	0.10	65,65,65,65	0
57	MG	2A	3261	1/1	0.85	0.12	63,63,63,63	0
57	MG	2A	3457	1/1	0.85	0.12	50,50,50,50	0
57	MG	2A	3852	1/1	0.85	0.14	45,45,45,45	0
57	MG	2A	3264	1/1	0.85	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3165	1/1	0.85	0.08	60,60,60,60	0
57	MG	1A	4082	1/1	0.85	0.18	69,69,69,69	0
57	MG	1A	4007	1/1	0.85	0.17	53,53,53,53	0
57	MG	2A	3057	1/1	0.85	0.21	62,62,62,62	0
57	MG	2W	202	1/1	0.85	0.14	57,57,57,57	0
57	MG	2a	1797	1/1	0.85	0.14	79,79,79,79	0
57	MG	2a	1604	1/1	0.85	0.09	54,54,54,54	0
57	MG	2A	3637	1/1	0.85	0.13	40,40,40,40	0
57	MG	2a	1614	1/1	0.85	0.26	68,68,68,68	0
57	MG	2A	3064	1/1	0.85	0.20	41,41,41,41	0
57	MG	2a	1624	1/1	0.85	0.15	65,65,65,65	0
57	MG	1A	4021	1/1	0.85	0.10	35,35,35,35	0
57	MG	2a	1822	1/1	0.85	0.18	67,67,67,67	0
57	MG	2A	3195	1/1	0.85	0.10	61,61,61,61	0
57	MG	1a	1789	1/1	0.85	0.16	77,77,77,77	0
57	MG	2A	3664	1/1	0.85	0.14	48,48,48,48	0
57	MG	2v	101	1/1	0.85	0.21	68,68,68,68	0
57	MG	1A	4025	1/1	0.85	0.12	35,35,35,35	0
57	MG	2a	1642	1/1	0.85	0.13	78,78,78,78	0
57	MG	2w	105	1/1	0.85	0.13	64,64,64,64	0
57	MG	1a	1798	1/1	0.85	0.22	63,63,63,63	0
57	MG	2A	3206	1/1	0.85	0.13	53,53,53,53	0
57	MG	2A	3334	1/1	0.85	0.22	53,53,53,53	0
57	MG	2a	1661	1/1	0.85	0.22	60,60,60,60	0
57	MG	1A	3423	1/1	0.86	0.13	42,42,42,42	0
57	MG	2A	3784	1/1	0.86	0.08	67,67,67,67	0
57	MG	1A	3458	1/1	0.86	0.15	70,70,70,70	0
57	MG	1a	1799	1/1	0.86	0.23	62,62,62,62	0
57	MG	2A	3826	1/1	0.86	0.15	54,54,54,54	0
57	MG	2a	1719	1/1	0.86	0.18	60,60,60,60	0
57	MG	2A	3495	1/1	0.86	0.12	61,61,61,61	0
57	MG	1A	4023	1/1	0.86	0.12	57,57,57,57	0
57	MG	2A	3315	1/1	0.86	0.15	62,62,62,62	0
57	MG	2A	3575	1/1	0.86	0.17	62,62,62,62	0
57	MG	1A	3471	1/1	0.86	0.10	64,64,64,64	0
57	MG	2a	1733	1/1	0.86	0.10	67,67,67,67	0
57	MG	2A	3584	1/1	0.86	0.10	68,68,68,68	0
57	MG	2a	1737	1/1	0.86	0.18	64,64,64,64	0
57	MG	2A	3599	1/1	0.86	0.18	50,50,50,50	0
57	MG	1A	4069	1/1	0.86	0.11	75,75,75,75	0
57	MG	2A	3614	1/1	0.86	0.22	59,59,59,59	0
57	MG	2A	3327	1/1	0.86	0.14	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1760	1/1	0.86	0.20	70,70,70,70	0
57	MG	2B	220	1/1	0.86	0.16	65,65,65,65	0
57	MG	2E	309	1/1	0.86	0.08	41,41,41,41	0
57	MG	1A	3301	1/1	0.86	0.11	51,51,51,51	0
57	MG	1A	3254	1/1	0.86	0.17	52,52,52,52	0
57	MG	2A	3155	1/1	0.86	0.10	58,58,58,58	0
57	MG	1A	3959	1/1	0.86	0.10	66,66,66,66	0
57	MG	2a	1787	1/1	0.86	0.28	72,72,72,72	0
57	MG	1a	1723	1/1	0.86	0.24	59,59,59,59	0
57	MG	2a	1621	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3356	1/1	0.86	0.21	68,68,68,68	0
57	MG	2a	1801	1/1	0.86	0.22	64,64,64,64	0
57	MG	2a	1626	1/1	0.86	0.08	88,88,88,88	0
57	MG	2a	1805	1/1	0.86	0.21	66,66,66,66	0
57	MG	2A	3358	1/1	0.86	0.18	64,64,64,64	0
57	MG	2a	1634	1/1	0.86	0.35	68,68,68,68	0
57	MG	1A	3050	1/1	0.86	0.13	33,33,33,33	0
57	MG	1B	214	1/1	0.86	0.10	40,40,40,40	0
57	MG	1a	1763	1/1	0.86	0.12	60,60,60,60	0
57	MG	2A	3691	1/1	0.86	0.12	70,70,70,70	0
57	MG	1a	1647	1/1	0.86	0.15	63,63,63,63	0
57	MG	2A	3699	1/1	0.86	0.23	64,64,64,64	0
57	MG	1a	1652	1/1	0.86	0.18	51,51,51,51	0
57	MG	2A	3071	1/1	0.86	0.11	57,57,57,57	0
57	MG	1A	3910	1/1	0.86	0.18	49,49,49,49	0
57	MG	1A	3916	1/1	0.86	0.10	46,46,46,46	0
57	MG	2A	3424	1/1	0.86	0.10	56,56,56,56	0
57	MG	2A	3299	1/1	0.86	0.18	72,72,72,72	0
57	MG	2a	1678	1/1	0.86	0.15	70,70,70,70	0
57	MG	2a	1682	1/1	0.86	0.28	56,56,56,56	0
57	MG	1B	210	1/1	0.87	0.09	51,51,51,51	0
57	MG	1A	3812	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	3566	1/1	0.87	0.21	56,56,56,56	0
57	MG	1a	1676	1/1	0.87	0.17	62,62,62,62	0
57	MG	2a	1676	1/1	0.87	0.19	64,64,64,64	0
57	MG	1B	226	1/1	0.87	0.13	41,41,41,41	0
57	MG	2A	3717	1/1	0.87	0.21	70,70,70,70	0
57	MG	2A	3232	1/1	0.87	0.17	57,57,57,57	0
57	MG	1a	1688	1/1	0.87	0.27	50,50,50,50	0
57	MG	1A	3065	1/1	0.87	0.13	53,53,53,53	0
57	MG	2A	3239	1/1	0.87	0.15	64,64,64,64	0
57	MG	2a	1707	1/1	0.87	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1709	1/1	0.87	0.18	75,75,75,75	0
57	MG	2A	3747	1/1	0.87	0.12	56,56,56,56	0
57	MG	1A	3845	1/1	0.87	0.10	51,51,51,51	0
57	MG	2a	1717	1/1	0.87	0.16	62,62,62,62	0
57	MG	2A	3755	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3767	1/1	0.87	0.10	66,66,66,66	0
57	MG	2A	3386	1/1	0.87	0.10	52,52,52,52	0
57	MG	2a	1726	1/1	0.87	0.30	75,75,75,75	0
57	MG	1A	3371	1/1	0.87	0.09	62,62,62,62	0
57	MG	1a	1716	1/1	0.87	0.15	49,49,49,49	0
57	MG	2A	3423	1/1	0.87	0.18	62,62,62,62	0
57	MG	2A	3794	1/1	0.87	0.07	72,72,72,72	0
57	MG	1A	3989	1/1	0.87	0.13	51,51,51,51	0
57	MG	1A	3130	1/1	0.87	0.06	70,70,70,70	0
57	MG	1F	311	1/1	0.87	0.14	56,56,56,56	0
57	MG	2A	3838	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3094	1/1	0.87	0.21	68,68,68,68	0
57	MG	2A	3466	1/1	0.87	0.08	70,70,70,70	0
57	MG	2a	1756	1/1	0.87	0.06	87,87,87,87	0
57	MG	1A	3066	1/1	0.87	0.13	44,44,44,44	0
57	MG	2A	3487	1/1	0.87	0.20	75,75,75,75	0
57	MG	1a	1737	1/1	0.87	0.12	54,54,54,54	0
57	MG	2B	208	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3654	1/1	0.87	0.12	58,58,58,58	0
57	MG	1Q	207	1/1	0.87	0.10	37,37,37,37	0
57	MG	1R	203	1/1	0.87	0.16	49,49,49,49	0
57	MG	2A	3112	1/1	0.87	0.24	63,63,63,63	0
57	MG	1T	201	1/1	0.87	0.12	50,50,50,50	0
57	MG	2P	202	1/1	0.87	0.26	51,51,51,51	0
57	MG	2A	3597	1/1	0.87	0.14	50,50,50,50	0
57	MG	2Z	301	1/1	0.87	0.20	72,72,72,72	0
57	MG	1A	3180	1/1	0.87	0.16	51,51,51,51	0
57	MG	1A	3704	1/1	0.87	0.07	34,34,34,34	0
57	MG	2a	1606	1/1	0.87	0.16	70,70,70,70	0
57	MG	2a	1613	1/1	0.87	0.18	57,57,57,57	0
57	MG	2A	3601	1/1	0.87	0.16	53,53,53,53	0
57	MG	2a	1814	1/1	0.87	0.16	75,75,75,75	0
57	MG	1a	1621	1/1	0.87	0.38	73,73,73,73	0
57	MG	2A	3620	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3492	1/1	0.87	0.08	29,29,29,29	0
57	MG	1A	3200	1/1	0.87	0.11	47,47,47,47	0
57	MG	2k	201	1/1	0.87	0.16	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3170	1/1	0.87	0.12	55,55,55,55	0
57	MG	2A	3318	1/1	0.87	0.16	54,54,54,54	0
57	MG	1a	1800	1/1	0.87	0.10	41,41,41,41	0
57	MG	1A	3513	1/1	0.87	0.09	55,55,55,55	0
57	MG	2A	3180	1/1	0.87	0.15	62,62,62,62	0
57	MG	2A	3672	1/1	0.87	0.11	53,53,53,53	0
57	MG	1A	3302	1/1	0.87	0.17	53,53,53,53	0
57	MG	1a	1807	1/1	0.87	0.13	52,52,52,52	0
57	MG	1A	3053	1/1	0.87	0.18	55,55,55,55	0
57	MG	2a	1646	1/1	0.88	0.18	57,57,57,57	0
57	MG	2A	3329	1/1	0.88	0.22	68,68,68,68	0
57	MG	2a	1648	1/1	0.88	0.13	73,73,73,73	0
57	MG	2A	3194	1/1	0.88	0.11	54,54,54,54	0
57	MG	2a	1656	1/1	0.88	0.16	65,65,65,65	0
57	MG	1a	1708	1/1	0.88	0.17	46,46,46,46	0
57	MG	2A	3018	1/1	0.88	0.09	59,59,59,59	0
57	MG	1A	3246	1/1	0.88	0.07	47,47,47,47	0
57	MG	2A	3044	1/1	0.88	0.08	78,78,78,78	0
57	MG	1A	3718	1/1	0.88	0.10	48,48,48,48	0
57	MG	1O	201	1/1	0.88	0.08	61,61,61,61	0
57	MG	2A	3365	1/1	0.88	0.34	66,66,66,66	0
57	MG	2A	3215	1/1	0.88	0.19	64,64,64,64	0
57	MG	2A	3222	1/1	0.88	0.19	43,43,43,43	0
57	MG	2a	1697	1/1	0.88	0.11	68,68,68,68	0
57	MG	2A	3372	1/1	0.88	0.09	40,40,40,40	0
57	MG	1a	1717	1/1	0.88	0.13	51,51,51,51	0
57	MG	2A	3376	1/1	0.88	0.10	56,56,56,56	0
57	MG	2A	3378	1/1	0.88	0.10	49,49,49,49	0
57	MG	2A	3379	1/1	0.88	0.25	66,66,66,66	0
57	MG	1A	3875	1/1	0.88	0.13	67,67,67,67	0
57	MG	1A	3414	1/1	0.88	0.12	47,47,47,47	0
57	MG	1A	3884	1/1	0.88	0.13	25,25,25,25	0
57	MG	2A	3241	1/1	0.88	0.44	76,76,76,76	0
57	MG	1A	3494	1/1	0.88	0.13	57,57,57,57	0
57	MG	2A	3786	1/1	0.88	0.13	59,59,59,59	0
57	MG	2A	3246	1/1	0.88	0.14	57,57,57,57	0
57	MG	2A	3419	1/1	0.88	0.18	58,58,58,58	0
57	MG	2A	3821	1/1	0.88	0.10	58,58,58,58	0
57	MG	1A	3900	1/1	0.88	0.10	45,45,45,45	0
57	MG	1A	3599	1/1	0.88	0.35	60,60,60,60	0
57	MG	1A	3641	1/1	0.88	0.13	27,27,27,27	0
57	MG	1A	4081	1/1	0.88	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1743	1/1	0.88	0.21	66,66,66,66	0
57	MG	2A	3454	1/1	0.88	0.15	51,51,51,51	0
57	MG	1a	1628	1/1	0.88	0.17	52,52,52,52	0
57	MG	1A	3917	1/1	0.88	0.09	27,27,27,27	0
57	MG	2A	3468	1/1	0.88	0.23	64,64,64,64	0
57	MG	2a	1758	1/1	0.88	0.19	67,67,67,67	0
57	MG	2a	1759	1/1	0.88	0.18	72,72,72,72	0
57	MG	1a	1780	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3262	1/1	0.88	0.17	61,61,61,61	0
57	MG	2A	3493	1/1	0.88	0.18	48,48,48,48	0
57	MG	2a	1777	1/1	0.88	0.22	59,59,59,59	0
57	MG	1B	203	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3499	1/1	0.88	0.16	64,64,64,64	0
57	MG	2A	3119	1/1	0.88	0.13	69,69,69,69	0
57	MG	2A	3544	1/1	0.88	0.10	41,41,41,41	0
57	MG	2F	302	1/1	0.88	0.10	48,48,48,48	0
57	MG	1a	1648	1/1	0.88	0.21	55,55,55,55	0
57	MG	2A	3571	1/1	0.88	0.17	51,51,51,51	0
57	MG	1A	3340	1/1	0.88	0.09	57,57,57,57	0
57	MG	20	101	1/1	0.88	0.20	66,66,66,66	0
57	MG	2A	3279	1/1	0.88	0.24	69,69,69,69	0
57	MG	2A	3149	1/1	0.88	0.27	64,64,64,64	0
57	MG	1A	3427	1/1	0.88	0.19	65,65,65,65	0
57	MG	2A	3158	1/1	0.88	0.13	50,50,50,50	0
57	MG	1A	3526	1/1	0.88	0.23	62,62,62,62	0
57	MG	1A	3841	1/1	0.88	0.15	56,56,56,56	0
57	MG	1A	3441	1/1	0.88	0.10	56,56,56,56	0
57	MG	2a	1821	1/1	0.88	0.16	65,65,65,65	0
57	MG	1a	1665	1/1	0.88	0.15	57,57,57,57	0
57	MG	2A	3309	1/1	0.88	0.18	63,63,63,63	0
57	MG	2a	1627	1/1	0.88	0.21	67,67,67,67	0
57	MG	2a	1628	1/1	0.88	0.30	69,69,69,69	0
57	MG	2A	3641	1/1	0.88	0.13	59,59,59,59	0
57	MG	1A	3846	1/1	0.88	0.15	43,43,43,43	0
57	MG	1A	3694	1/1	0.88	0.09	25,25,25,25	0
57	MG	2a	1636	1/1	0.88	0.37	71,71,71,71	0
57	MG	1A	3096	1/1	0.88	0.12	61,61,61,61	0
57	MG	2A	3324	1/1	0.88	0.11	63,63,63,63	0
57	MG	1A	3870	1/1	0.88	0.17	50,50,50,50	0
57	MG	1x	105	1/1	0.88	0.24	58,58,58,58	0
57	MG	2a	1645	1/1	0.88	0.23	58,58,58,58	0
57	MG	2a	1625	1/1	0.89	0.28	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	231	1/1	0.89	0.08	46,46,46,46	0
57	MG	1a	1700	1/1	0.89	0.20	63,63,63,63	0
57	MG	1A	3837	1/1	0.89	0.09	51,51,51,51	0
57	MG	2A	3292	1/1	0.89	0.10	53,53,53,53	0
57	MG	1A	3403	1/1	0.89	0.08	52,52,52,52	0
57	MG	2A	3602	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3612	1/1	0.89	0.13	43,43,43,43	0
57	MG	1B	234	1/1	0.89	0.15	65,65,65,65	0
57	MG	1A	3949	1/1	0.89	0.09	48,48,48,48	0
57	MG	1A	3844	1/1	0.89	0.19	50,50,50,50	0
57	MG	2A	3110	1/1	0.89	0.17	58,58,58,58	0
57	MG	1A	3502	1/1	0.89	0.14	46,46,46,46	0
57	MG	2A	3306	1/1	0.89	0.15	56,56,56,56	0
57	MG	1A	3967	1/1	0.89	0.12	54,54,54,54	0
57	MG	1a	1721	1/1	0.89	0.22	65,65,65,65	0
57	MG	1A	3325	1/1	0.89	0.21	61,61,61,61	0
57	MG	1A	3657	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3669	1/1	0.89	0.10	44,44,44,44	0
57	MG	2a	1660	1/1	0.89	0.08	56,56,56,56	0
57	MG	2A	3673	1/1	0.89	0.12	48,48,48,48	0
57	MG	2A	3325	1/1	0.89	0.25	64,64,64,64	0
57	MG	2a	1666	1/1	0.89	0.12	68,68,68,68	0
57	MG	1A	3992	1/1	0.89	0.09	26,26,26,26	0
57	MG	2a	1673	1/1	0.89	0.15	55,55,55,55	0
57	MG	2A	3680	1/1	0.89	0.11	60,60,60,60	0
57	MG	2A	3682	1/1	0.89	0.09	51,51,51,51	0
57	MG	1A	3507	1/1	0.89	0.09	52,52,52,52	0
57	MG	1A	3332	1/1	0.89	0.21	59,59,59,59	0
57	MG	2a	1684	1/1	0.89	0.28	64,64,64,64	0
57	MG	2a	1688	1/1	0.89	0.12	65,65,65,65	0
57	MG	2A	3333	1/1	0.89	0.08	49,49,49,49	0
57	MG	2a	1696	1/1	0.89	0.18	62,62,62,62	0
57	MG	1Y	202	1/1	0.89	0.10	57,57,57,57	0
57	MG	1a	1769	1/1	0.89	0.12	64,64,64,64	0
57	MG	1a	1772	1/1	0.89	0.14	63,63,63,63	0
57	MG	2a	1706	1/1	0.89	0.18	68,68,68,68	0
57	MG	2A	3713	1/1	0.89	0.14	56,56,56,56	0
57	MG	13	105	1/1	0.89	0.10	51,51,51,51	0
57	MG	2a	1711	1/1	0.89	0.27	55,55,55,55	0
57	MG	2A	3346	1/1	0.89	0.14	61,61,61,61	0
57	MG	2A	3720	1/1	0.89	0.21	55,55,55,55	0
57	MG	2A	3722	1/1	0.89	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	14	101	1/1	0.89	0.19	75,75,75,75	0
57	MG	2A	3735	1/1	0.89	0.19	69,69,69,69	0
57	MG	2A	3181	1/1	0.89	0.14	55,55,55,55	0
57	MG	2a	1723	1/1	0.89	0.25	51,51,51,51	0
57	MG	1a	1784	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3187	1/1	0.89	0.32	63,63,63,63	0
57	MG	16	101	1/1	0.89	0.11	44,44,44,44	0
57	MG	2A	3189	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	3333	1/1	0.89	0.08	55,55,55,55	0
57	MG	2A	3770	1/1	0.89	0.09	72,72,72,72	0
57	MG	1A	3533	1/1	0.89	0.23	47,47,47,47	0
57	MG	2A	3775	1/1	0.89	0.15	50,50,50,50	0
57	MG	1a	1617	1/1	0.89	0.16	56,56,56,56	0
57	MG	1A	3088	1/1	0.89	0.27	42,42,42,42	0
57	MG	2A	3201	1/1	0.89	0.09	48,48,48,48	0
57	MG	1A	4027	1/1	0.89	0.07	29,29,29,29	0
57	MG	2a	1754	1/1	0.89	0.12	71,71,71,71	0
57	MG	1a	1623	1/1	0.89	0.23	59,59,59,59	0
57	MG	1a	1627	1/1	0.89	0.17	54,54,54,54	0
57	MG	1p	101	1/1	0.89	0.10	51,51,51,51	0
57	MG	1A	3722	1/1	0.89	0.12	54,54,54,54	0
57	MG	2A	3830	1/1	0.89	0.13	61,61,61,61	0
57	MG	2a	1767	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3836	1/1	0.89	0.13	67,67,67,67	0
57	MG	1A	3885	1/1	0.89	0.11	36,36,36,36	0
57	MG	2A	3417	1/1	0.89	0.18	67,67,67,67	0
57	MG	2A	3840	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3233	1/1	0.89	0.08	45,45,45,45	0
57	MG	2A	3848	1/1	0.89	0.16	50,50,50,50	0
57	MG	1a	1638	1/1	0.89	0.14	51,51,51,51	0
57	MG	1A	3454	1/1	0.89	0.21	58,58,58,58	0
57	MG	2a	1795	1/1	0.89	0.21	72,72,72,72	0
57	MG	2a	1796	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3430	1/1	0.89	0.21	53,53,53,53	0
57	MG	2A	3238	1/1	0.89	0.25	60,60,60,60	0
57	MG	1A	3257	1/1	0.89	0.10	63,63,63,63	0
57	MG	2A	3240	1/1	0.89	0.19	61,61,61,61	0
57	MG	1A	3467	1/1	0.89	0.07	56,56,56,56	0
57	MG	2B	217	1/1	0.89	0.12	66,66,66,66	0
57	MG	1A	3585	1/1	0.89	0.08	49,49,49,49	0
57	MG	1A	3300	1/1	0.89	0.17	47,47,47,47	0
57	MG	2A	3041	1/1	0.89	0.28	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3486	1/1	0.89	0.18	55,55,55,55	0
57	MG	1B	209	1/1	0.89	0.13	48,48,48,48	0
57	MG	2Q	201	1/1	0.89	0.12	68,68,68,68	0
57	MG	2T	202	1/1	0.89	0.19	55,55,55,55	0
57	MG	1A	3933	1/1	0.89	0.10	31,31,31,31	0
57	MG	2A	3054	1/1	0.89	0.17	66,66,66,66	0
57	MG	1B	211	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3511	1/1	0.89	0.10	24,24,24,24	0
57	MG	2A	3062	1/1	0.89	0.19	66,66,66,66	0
57	MG	1a	1672	1/1	0.89	0.12	64,64,64,64	0
57	MG	2A	3566	1/1	0.89	0.20	51,51,51,51	0
57	MG	1A	3489	1/1	0.89	0.12	45,45,45,45	0
57	MG	1A	3391	1/1	0.89	0.20	45,45,45,45	0
57	MG	1a	1682	1/1	0.89	0.18	63,63,63,63	0
57	MG	1A	3941	1/1	0.89	0.11	46,46,46,46	0
57	MG	2A	3438	1/1	0.90	0.18	51,51,51,51	0
57	MG	1A	3243	1/1	0.90	0.14	57,57,57,57	0
57	MG	1A	3193	1/1	0.90	0.17	32,32,32,32	0
57	MG	1a	1775	1/1	0.90	0.09	56,56,56,56	0
57	MG	2A	3460	1/1	0.90	0.26	45,45,45,45	0
57	MG	1a	1777	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3195	1/1	0.90	0.16	40,40,40,40	0
57	MG	1A	3730	1/1	0.90	0.13	71,71,71,71	0
57	MG	2a	1610	1/1	0.90	0.12	48,48,48,48	0
57	MG	2a	1612	1/1	0.90	0.12	68,68,68,68	0
57	MG	2A	3470	1/1	0.90	0.16	64,64,64,64	0
57	MG	2A	3472	1/1	0.90	0.06	63,63,63,63	0
57	MG	2A	3483	1/1	0.90	0.14	42,42,42,42	0
57	MG	1A	3739	1/1	0.90	0.10	57,57,57,57	0
57	MG	2a	1622	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3957	1/1	0.90	0.15	61,61,61,61	0
57	MG	1A	3199	1/1	0.90	0.39	47,47,47,47	0
57	MG	2A	3226	1/1	0.90	0.21	71,71,71,71	0
57	MG	2A	3227	1/1	0.90	0.15	66,66,66,66	0
57	MG	2A	3231	1/1	0.90	0.10	34,34,34,34	0
57	MG	2a	1632	1/1	0.90	0.05	78,78,78,78	0
57	MG	2A	3527	1/1	0.90	0.08	40,40,40,40	0
57	MG	1a	1796	1/1	0.90	0.19	57,57,57,57	0
57	MG	2A	3543	1/1	0.90	0.09	44,44,44,44	0
57	MG	1a	1797	1/1	0.90	0.07	66,66,66,66	0
57	MG	2A	3556	1/1	0.90	0.13	50,50,50,50	0
57	MG	15	106	1/1	0.90	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	15	109	1/1	0.90	0.10	62,62,62,62	0
57	MG	1A	3962	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3255	1/1	0.90	0.28	72,72,72,72	0
57	MG	1a	1602	1/1	0.90	0.15	57,57,57,57	0
57	MG	1A	3793	1/1	0.90	0.18	70,70,70,70	0
57	MG	2A	3586	1/1	0.90	0.16	58,58,58,58	0
57	MG	1f	201	1/1	0.90	0.12	54,54,54,54	0
57	MG	1l	201	1/1	0.90	0.07	57,57,57,57	0
57	MG	1A	3058	1/1	0.90	0.13	41,41,41,41	0
57	MG	1t	201	1/1	0.90	0.17	59,59,59,59	0
57	MG	1A	3988	1/1	0.90	0.15	65,65,65,65	0
57	MG	1A	3810	1/1	0.90	0.14	47,47,47,47	0
57	MG	1A	3379	1/1	0.90	0.23	56,56,56,56	0
57	MG	1A	3814	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	3519	1/1	0.90	0.17	40,40,40,40	0
57	MG	2a	1674	1/1	0.90	0.27	69,69,69,69	0
57	MG	2a	1675	1/1	0.90	0.21	61,61,61,61	0
57	MG	1a	1629	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3001	1/1	0.90	0.19	37,37,37,37	0
57	MG	2A	3646	1/1	0.90	0.16	59,59,59,59	0
57	MG	1A	3171	1/1	0.90	0.13	45,45,45,45	0
57	MG	1A	3400	1/1	0.90	0.09	49,49,49,49	0
57	MG	2A	3028	1/1	0.90	0.15	54,54,54,54	0
57	MG	2a	1690	1/1	0.90	0.18	63,63,63,63	0
57	MG	2A	3658	1/1	0.90	0.08	37,37,37,37	0
57	MG	2A	3031	1/1	0.90	0.14	51,51,51,51	0
57	MG	2A	3670	1/1	0.90	0.20	55,55,55,55	0
57	MG	2A	3035	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3264	1/1	0.90	0.16	44,44,44,44	0
57	MG	1A	3404	1/1	0.90	0.16	47,47,47,47	0
57	MG	2A	3296	1/1	0.90	0.13	62,62,62,62	0
57	MG	2a	1708	1/1	0.90	0.33	69,69,69,69	0
57	MG	2A	3045	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	4067	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3277	1/1	0.90	0.17	46,46,46,46	0
57	MG	1A	3422	1/1	0.90	0.20	37,37,37,37	0
57	MG	1A	4072	1/1	0.90	0.09	49,49,49,49	0
57	MG	1A	3582	1/1	0.90	0.30	55,55,55,55	0
57	MG	1A	3584	1/1	0.90	0.14	61,61,61,61	0
57	MG	1a	1668	1/1	0.90	0.07	58,58,58,58	0
57	MG	2A	3083	1/1	0.90	0.10	52,52,52,52	0
57	MG	1a	1670	1/1	0.90	0.31	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3087	1/1	0.90	0.08	45,45,45,45	0
57	MG	1A	3286	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	3223	1/1	0.90	0.11	48,48,48,48	0
57	MG	1a	1677	1/1	0.90	0.19	51,51,51,51	0
57	MG	2A	3726	1/1	0.90	0.11	43,43,43,43	0
57	MG	2A	3095	1/1	0.90	0.09	51,51,51,51	0
57	MG	1B	201	1/1	0.90	0.07	44,44,44,44	0
57	MG	2A	3098	1/1	0.90	0.26	67,67,67,67	0
57	MG	2A	3335	1/1	0.90	0.11	52,52,52,52	0
57	MG	1A	3598	1/1	0.90	0.12	41,41,41,41	0
57	MG	1a	1684	1/1	0.90	0.07	50,50,50,50	0
57	MG	1B	208	1/1	0.90	0.08	57,57,57,57	0
57	MG	1A	3435	1/1	0.90	0.11	48,48,48,48	0
57	MG	1a	1698	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3876	1/1	0.90	0.17	47,47,47,47	0
57	MG	2A	3357	1/1	0.90	0.26	63,63,63,63	0
57	MG	2A	3776	1/1	0.90	0.20	65,65,65,65	0
57	MG	2A	3116	1/1	0.90	0.16	49,49,49,49	0
57	MG	1A	3600	1/1	0.90	0.21	43,43,43,43	0
57	MG	2a	1775	1/1	0.90	0.18	58,58,58,58	0
57	MG	1A	3438	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3149	1/1	0.90	0.13	43,43,43,43	0
57	MG	2A	3791	1/1	0.90	0.08	39,39,39,39	0
57	MG	1A	3446	1/1	0.90	0.08	41,41,41,41	0
57	MG	2A	3801	1/1	0.90	0.11	40,40,40,40	0
57	MG	2A	3373	1/1	0.90	0.12	48,48,48,48	0
57	MG	1A	3232	1/1	0.90	0.36	34,34,34,34	0
57	MG	1A	3304	1/1	0.90	0.22	51,51,51,51	0
57	MG	1A	3459	1/1	0.90	0.20	55,55,55,55	0
57	MG	2A	3833	1/1	0.90	0.08	47,47,47,47	0
57	MG	2A	3164	1/1	0.90	0.18	60,60,60,60	0
57	MG	1A	3463	1/1	0.90	0.32	45,45,45,45	0
57	MG	1A	3927	1/1	0.90	0.21	48,48,48,48	0
57	MG	1a	1725	1/1	0.90	0.17	61,61,61,61	0
57	MG	1A	3932	1/1	0.90	0.10	23,23,23,23	0
57	MG	2A	3846	1/1	0.90	0.07	60,60,60,60	0
57	MG	2a	1811	1/1	0.90	0.21	73,73,73,73	0
57	MG	2A	3388	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	3241	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3396	1/1	0.90	0.17	47,47,47,47	0
57	MG	2A	3403	1/1	0.90	0.24	53,53,53,53	0
57	MG	1A	3934	1/1	0.90	0.15	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1742	1/1	0.90	0.23	68,68,68,68	0
57	MG	2g	201	1/1	0.90	0.10	67,67,67,67	0
57	MG	2B	211	1/1	0.90	0.22	64,64,64,64	0
57	MG	2B	212	1/1	0.90	0.24	61,61,61,61	0
57	MG	2l	204	1/1	0.90	0.05	51,51,51,51	0
57	MG	2B	213	1/1	0.90	0.14	56,56,56,56	0
57	MG	1a	1747	1/1	0.90	0.09	59,59,59,59	0
57	MG	1a	1757	1/1	0.90	0.15	54,54,54,54	0
57	MG	1F	312	1/1	0.90	0.08	53,53,53,53	0
57	MG	2w	102	1/1	0.90	0.23	52,52,52,52	0
57	MG	2A	3429	1/1	0.90	0.23	51,51,51,51	0
57	MG	1A	3324	1/1	0.90	0.07	42,42,42,42	0
57	MG	1A	3479	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3435	1/1	0.90	0.25	46,46,46,46	0
57	MG	2A	3436	1/1	0.90	0.11	49,49,49,49	0
57	MG	1A	3940	1/1	0.91	0.10	55,55,55,55	0
57	MG	1a	1735	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3303	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	3202	1/1	0.91	0.08	26,26,26,26	0
57	MG	1O	202	1/1	0.91	0.20	52,52,52,52	0
57	MG	2A	3854	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3166	1/1	0.91	0.15	67,67,67,67	0
57	MG	1A	3406	1/1	0.91	0.16	55,55,55,55	0
57	MG	2B	205	1/1	0.91	0.06	55,55,55,55	0
57	MG	2B	206	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3319	1/1	0.91	0.06	39,39,39,39	0
57	MG	2A	3421	1/1	0.91	0.20	43,43,43,43	0
57	MG	1A	3520	1/1	0.91	0.26	57,57,57,57	0
57	MG	1S	201	1/1	0.91	0.08	44,44,44,44	0
57	MG	2A	3177	1/1	0.91	0.22	53,53,53,53	0
57	MG	1A	3762	1/1	0.91	0.08	24,24,24,24	0
57	MG	1A	3770	1/1	0.91	0.12	31,31,31,31	0
57	MG	10	107	1/1	0.91	0.09	50,50,50,50	0
57	MG	10	108	1/1	0.91	0.13	53,53,53,53	0
57	MG	1a	1774	1/1	0.91	0.10	36,36,36,36	0
57	MG	2A	3442	1/1	0.91	0.07	60,60,60,60	0
57	MG	2N	201	1/1	0.91	0.23	65,65,65,65	0
57	MG	10	110	1/1	0.91	0.21	66,66,66,66	0
57	MG	2A	3449	1/1	0.91	0.14	50,50,50,50	0
57	MG	2A	3452	1/1	0.91	0.44	57,57,57,57	0
57	MG	11	103	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3455	1/1	0.91	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3415	1/1	0.91	0.12	56,56,56,56	0
57	MG	23	101	1/1	0.91	0.15	56,56,56,56	0
57	MG	28	101	1/1	0.91	0.12	62,62,62,62	0
57	MG	2a	1602	1/1	0.91	0.17	55,55,55,55	0
57	MG	2a	1603	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3459	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	3964	1/1	0.91	0.08	54,54,54,54	0
57	MG	1A	3531	1/1	0.91	0.09	68,68,68,68	0
57	MG	1A	3801	1/1	0.91	0.13	44,44,44,44	0
57	MG	1a	1794	1/1	0.91	0.08	77,77,77,77	0
57	MG	1A	3532	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3208	1/1	0.91	0.17	52,52,52,52	0
57	MG	2A	3479	1/1	0.91	0.24	48,48,48,48	0
57	MG	2a	1619	1/1	0.91	0.19	64,64,64,64	0
57	MG	1A	3114	1/1	0.91	0.09	41,41,41,41	0
57	MG	18	106	1/1	0.91	0.26	47,47,47,47	0
57	MG	2A	3216	1/1	0.91	0.12	51,51,51,51	0
57	MG	2A	3488	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3115	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3223	1/1	0.91	0.29	52,52,52,52	0
57	MG	1A	3424	1/1	0.91	0.09	52,52,52,52	0
57	MG	2a	1630	1/1	0.91	0.20	64,64,64,64	0
57	MG	2a	1631	1/1	0.91	0.10	46,46,46,46	0
57	MG	2A	3504	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3505	1/1	0.91	0.18	53,53,53,53	0
57	MG	1A	3996	1/1	0.91	0.08	50,50,50,50	0
57	MG	2A	3516	1/1	0.91	0.20	65,65,65,65	0
57	MG	2A	3520	1/1	0.91	0.11	62,62,62,62	0
57	MG	1a	1802	1/1	0.91	0.10	54,54,54,54	0
57	MG	2A	3529	1/1	0.91	0.11	62,62,62,62	0
57	MG	1A	3999	1/1	0.91	0.10	44,44,44,44	0
57	MG	2a	1640	1/1	0.91	0.16	58,58,58,58	0
57	MG	2a	1641	1/1	0.91	0.08	59,59,59,59	0
57	MG	2A	3534	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3536	1/1	0.91	0.08	44,44,44,44	0
57	MG	1A	3004	1/1	0.91	0.08	31,31,31,31	0
57	MG	2A	3234	1/1	0.91	0.16	57,57,57,57	0
57	MG	1A	3575	1/1	0.91	0.10	37,37,37,37	0
57	MG	2a	1651	1/1	0.91	0.20	67,67,67,67	0
57	MG	2a	1652	1/1	0.91	0.06	70,70,70,70	0
57	MG	2A	3563	1/1	0.91	0.09	38,38,38,38	0
57	MG	2a	1655	1/1	0.91	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3565	1/1	0.91	0.08	37,37,37,37	0
57	MG	2a	1658	1/1	0.91	0.17	50,50,50,50	0
57	MG	1a	1809	1/1	0.91	0.08	65,65,65,65	0
57	MG	1A	4016	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3329	1/1	0.91	0.12	56,56,56,56	0
57	MG	1n	102	1/1	0.91	0.17	46,46,46,46	0
57	MG	1A	3261	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3578	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3030	1/1	0.91	0.30	64,64,64,64	0
57	MG	1a	1633	1/1	0.91	0.13	35,35,35,35	0
57	MG	2A	3595	1/1	0.91	0.13	57,57,57,57	0
57	MG	2A	3247	1/1	0.91	0.12	48,48,48,48	0
57	MG	1a	1636	1/1	0.91	0.10	40,40,40,40	0
57	MG	1a	1637	1/1	0.91	0.22	55,55,55,55	0
57	MG	2a	1680	1/1	0.91	0.24	70,70,70,70	0
57	MG	1A	3267	1/1	0.91	0.06	53,53,53,53	0
57	MG	1x	102	1/1	0.91	0.15	58,58,58,58	0
57	MG	2A	3609	1/1	0.91	0.11	50,50,50,50	0
57	MG	1a	1644	1/1	0.91	0.12	43,43,43,43	0
57	MG	2a	1694	1/1	0.91	0.12	66,66,66,66	0
57	MG	1A	4039	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	4044	1/1	0.91	0.11	58,58,58,58	0
57	MG	2A	3623	1/1	0.91	0.10	36,36,36,36	0
57	MG	2a	1702	1/1	0.91	0.20	68,68,68,68	0
57	MG	1A	4058	1/1	0.91	0.12	42,42,42,42	0
57	MG	1A	3448	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	3147	1/1	0.91	0.14	46,46,46,46	0
57	MG	2A	3029	1/1	0.91	0.10	37,37,37,37	0
57	MG	2A	3030	1/1	0.91	0.09	47,47,47,47	0
57	MG	1A	3353	1/1	0.91	0.22	35,35,35,35	0
57	MG	2a	1710	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3361	1/1	0.91	0.18	52,52,52,52	0
57	MG	2A	3290	1/1	0.91	0.08	51,51,51,51	0
57	MG	2A	3038	1/1	0.91	0.24	66,66,66,66	0
57	MG	1A	3631	1/1	0.91	0.15	54,54,54,54	0
57	MG	1a	1666	1/1	0.91	0.22	63,63,63,63	0
57	MG	1a	1667	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3300	1/1	0.91	0.21	64,64,64,64	0
57	MG	2A	3675	1/1	0.91	0.20	52,52,52,52	0
57	MG	2A	3047	1/1	0.91	0.10	49,49,49,49	0
57	MG	2A	3050	1/1	0.91	0.21	58,58,58,58	0
57	MG	1A	3634	1/1	0.91	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3681	1/1	0.91	0.20	59,59,59,59	0
57	MG	2A	3304	1/1	0.91	0.17	60,60,60,60	0
57	MG	2a	1734	1/1	0.91	0.34	72,72,72,72	0
57	MG	1A	3639	1/1	0.91	0.18	56,56,56,56	0
57	MG	1A	3461	1/1	0.91	0.14	40,40,40,40	0
57	MG	2A	3059	1/1	0.91	0.16	56,56,56,56	0
57	MG	2a	1741	1/1	0.91	0.32	60,60,60,60	0
57	MG	2a	1742	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3314	1/1	0.91	0.14	41,41,41,41	0
57	MG	2A	3693	1/1	0.91	0.07	58,58,58,58	0
57	MG	1A	3370	1/1	0.91	0.15	43,43,43,43	0
57	MG	2a	1748	1/1	0.91	0.26	68,68,68,68	0
57	MG	2A	3700	1/1	0.91	0.11	61,61,61,61	0
57	MG	2A	3316	1/1	0.91	0.09	40,40,40,40	0
57	MG	1A	3148	1/1	0.91	0.33	37,37,37,37	0
57	MG	1A	3470	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3070	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	3890	1/1	0.91	0.12	43,43,43,43	0
57	MG	2A	3079	1/1	0.91	0.10	49,49,49,49	0
57	MG	2a	1765	1/1	0.91	0.14	58,58,58,58	0
57	MG	2a	1766	1/1	0.91	0.13	60,60,60,60	0
57	MG	1A	3055	1/1	0.91	0.09	38,38,38,38	0
57	MG	2a	1769	1/1	0.91	0.24	71,71,71,71	0
57	MG	2A	3727	1/1	0.91	0.22	51,51,51,51	0
57	MG	2A	3730	1/1	0.91	0.16	68,68,68,68	0
57	MG	1a	1686	1/1	0.91	0.18	35,35,35,35	0
57	MG	2a	1782	1/1	0.91	0.13	51,51,51,51	0
57	MG	1A	3898	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3088	1/1	0.91	0.23	63,63,63,63	0
57	MG	1a	1689	1/1	0.91	0.20	47,47,47,47	0
57	MG	1A	3665	1/1	0.91	0.09	35,35,35,35	0
57	MG	2A	3749	1/1	0.91	0.11	53,53,53,53	0
57	MG	1a	1695	1/1	0.91	0.23	59,59,59,59	0
57	MG	2a	1791	1/1	0.91	0.22	60,60,60,60	0
57	MG	2a	1794	1/1	0.91	0.24	69,69,69,69	0
57	MG	1A	3380	1/1	0.91	0.23	38,38,38,38	0
57	MG	1B	218	1/1	0.91	0.12	49,49,49,49	0
57	MG	2A	3351	1/1	0.91	0.18	55,55,55,55	0
57	MG	2a	1798	1/1	0.91	0.16	58,58,58,58	0
57	MG	2A	3353	1/1	0.91	0.07	63,63,63,63	0
57	MG	1a	1705	1/1	0.91	0.14	50,50,50,50	0
57	MG	1A	3480	1/1	0.91	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1804	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3779	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3782	1/1	0.91	0.20	54,54,54,54	0
57	MG	1A	3690	1/1	0.91	0.06	45,45,45,45	0
57	MG	1a	1710	1/1	0.91	0.23	41,41,41,41	0
57	MG	2A	3361	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3364	1/1	0.91	0.20	51,51,51,51	0
57	MG	2a	1817	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3923	1/1	0.91	0.09	42,42,42,42	0
57	MG	2A	3793	1/1	0.91	0.10	54,54,54,54	0
57	MG	2A	3108	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3798	1/1	0.91	0.17	43,43,43,43	0
57	MG	2e	201	1/1	0.91	0.07	82,82,82,82	0
57	MG	2A	3800	1/1	0.91	0.11	63,63,63,63	0
57	MG	1a	1714	1/1	0.91	0.12	48,48,48,48	0
57	MG	2A	3802	1/1	0.91	0.07	28,28,28,28	0
57	MG	2l	201	1/1	0.91	0.11	58,58,58,58	0
57	MG	2A	3817	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3383	1/1	0.91	0.22	66,66,66,66	0
57	MG	2A	3113	1/1	0.91	0.16	47,47,47,47	0
57	MG	2A	3115	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3388	1/1	0.91	0.20	42,42,42,42	0
57	MG	1A	3706	1/1	0.91	0.15	25,25,25,25	0
57	MG	2w	104	1/1	0.91	0.09	89,89,89,89	0
57	MG	2A	3122	1/1	0.91	0.25	46,46,46,46	0
57	MG	1A	3708	1/1	0.91	0.08	40,40,40,40	0
57	MG	1A	3248	1/1	0.91	0.14	47,47,47,47	0
57	MG	1A	3201	1/1	0.91	0.07	32,32,32,32	0
57	MG	2x	104	1/1	0.91	0.28	65,65,65,65	0
57	MG	2x	105	1/1	0.91	0.17	60,60,60,60	0
57	MG	2A	3841	1/1	0.91	0.13	65,65,65,65	0
58	K	1A	3546	1/1	0.91	0.20	73,73,73,73	0
58	K	2A	3445	1/1	0.91	0.08	64,64,64,64	0
57	MG	2B	202	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3399	1/1	0.92	0.15	45,45,45,45	0
57	MG	1B	206	1/1	0.92	0.07	56,56,56,56	0
57	MG	1A	3565	1/1	0.92	0.14	42,42,42,42	0
57	MG	2A	3414	1/1	0.92	0.25	53,53,53,53	0
57	MG	2B	207	1/1	0.92	0.15	68,68,68,68	0
57	MG	1A	3338	1/1	0.92	0.10	42,42,42,42	0
57	MG	1A	3339	1/1	0.92	0.08	40,40,40,40	0
57	MG	2A	3139	1/1	0.92	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3147	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3148	1/1	0.92	0.16	46,46,46,46	0
57	MG	2A	3428	1/1	0.92	0.29	62,62,62,62	0
57	MG	1A	3124	1/1	0.92	0.10	41,41,41,41	0
57	MG	2B	218	1/1	0.92	0.16	67,67,67,67	0
57	MG	1A	3854	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3581	1/1	0.92	0.16	57,57,57,57	0
57	MG	2D	306	1/1	0.92	0.09	63,63,63,63	0
57	MG	2E	304	1/1	0.92	0.20	43,43,43,43	0
57	MG	2E	305	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	3341	1/1	0.92	0.14	40,40,40,40	0
57	MG	2F	301	1/1	0.92	0.07	54,54,54,54	0
57	MG	2A	3160	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3436	1/1	0.92	0.11	41,41,41,41	0
57	MG	2O	201	1/1	0.92	0.16	64,64,64,64	0
57	MG	2O	202	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3441	1/1	0.92	0.16	61,61,61,61	0
57	MG	1B	228	1/1	0.92	0.09	55,55,55,55	0
57	MG	1A	3299	1/1	0.92	0.26	64,64,64,64	0
57	MG	2W	201	1/1	0.92	0.14	48,48,48,48	0
57	MG	1a	1730	1/1	0.92	0.08	46,46,46,46	0
57	MG	1A	3586	1/1	0.92	0.21	50,50,50,50	0
57	MG	2A	3171	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3587	1/1	0.92	0.17	50,50,50,50	0
57	MG	27	102	1/1	0.92	0.10	53,53,53,53	0
57	MG	27	103	1/1	0.92	0.42	41,41,41,41	0
57	MG	1A	3588	1/1	0.92	0.19	45,45,45,45	0
57	MG	1A	3074	1/1	0.92	0.22	57,57,57,57	0
57	MG	2A	3178	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3465	1/1	0.92	0.10	40,40,40,40	0
57	MG	1A	3354	1/1	0.92	0.17	39,39,39,39	0
57	MG	1A	3002	1/1	0.92	0.09	47,47,47,47	0
57	MG	2a	1607	1/1	0.92	0.15	59,59,59,59	0
57	MG	2A	3182	1/1	0.92	0.21	56,56,56,56	0
57	MG	1A	3887	1/1	0.92	0.07	38,38,38,38	0
57	MG	2A	3185	1/1	0.92	0.21	57,57,57,57	0
57	MG	2A	3186	1/1	0.92	0.09	58,58,58,58	0
57	MG	2a	1615	1/1	0.92	0.11	58,58,58,58	0
57	MG	1a	1758	1/1	0.92	0.16	58,58,58,58	0
57	MG	1A	3362	1/1	0.92	0.37	53,53,53,53	0
57	MG	2a	1620	1/1	0.92	0.15	65,65,65,65	0
57	MG	1A	3603	1/1	0.92	0.42	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3611	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3490	1/1	0.92	0.07	43,43,43,43	0
57	MG	1A	3626	1/1	0.92	0.12	56,56,56,56	0
57	MG	2A	3198	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3496	1/1	0.92	0.18	44,44,44,44	0
57	MG	2A	3498	1/1	0.92	0.09	71,71,71,71	0
57	MG	1P	205	1/1	0.92	0.15	54,54,54,54	0
57	MG	1A	3907	1/1	0.92	0.09	24,24,24,24	0
57	MG	1A	3456	1/1	0.92	0.08	51,51,51,51	0
57	MG	1A	3915	1/1	0.92	0.09	60,60,60,60	0
57	MG	1R	206	1/1	0.92	0.07	32,32,32,32	0
57	MG	1a	1779	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3366	1/1	0.92	0.06	32,32,32,32	0
57	MG	2A	3214	1/1	0.92	0.13	41,41,41,41	0
57	MG	1a	1783	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3533	1/1	0.92	0.12	44,44,44,44	0
57	MG	1A	3001	1/1	0.92	0.07	39,39,39,39	0
57	MG	2A	3218	1/1	0.92	0.12	56,56,56,56	0
57	MG	2A	3541	1/1	0.92	0.14	44,44,44,44	0
57	MG	2a	1644	1/1	0.92	0.07	63,63,63,63	0
57	MG	1X	106	1/1	0.92	0.08	53,53,53,53	0
57	MG	1a	1792	1/1	0.92	0.15	74,74,74,74	0
57	MG	1A	3041	1/1	0.92	0.13	49,49,49,49	0
57	MG	10	104	1/1	0.92	0.12	61,61,61,61	0
57	MG	2a	1650	1/1	0.92	0.13	73,73,73,73	0
57	MG	2A	3229	1/1	0.92	0.13	57,57,57,57	0
57	MG	10	106	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3372	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3260	1/1	0.92	0.11	51,51,51,51	0
57	MG	1A	3305	1/1	0.92	0.23	58,58,58,58	0
57	MG	1A	3307	1/1	0.92	0.13	43,43,43,43	0
57	MG	1A	3661	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3662	1/1	0.92	0.08	46,46,46,46	0
57	MG	1A	3475	1/1	0.92	0.24	42,42,42,42	0
57	MG	1A	3477	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3067	1/1	0.92	0.08	30,30,30,30	0
57	MG	2a	1669	1/1	0.92	0.23	54,54,54,54	0
57	MG	1b	301	1/1	0.92	0.14	70,70,70,70	0
57	MG	17	105	1/1	0.92	0.26	55,55,55,55	0
57	MG	18	104	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	3389	1/1	0.92	0.13	54,54,54,54	0
57	MG	2A	3605	1/1	0.92	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3263	1/1	0.92	0.08	44,44,44,44	0
57	MG	2A	3610	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3951	1/1	0.92	0.07	29,29,29,29	0
57	MG	1A	3397	1/1	0.92	0.22	60,60,60,60	0
57	MG	2A	3618	1/1	0.92	0.09	41,41,41,41	0
57	MG	1a	1613	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3068	1/1	0.92	0.23	51,51,51,51	0
57	MG	2a	1691	1/1	0.92	0.15	52,52,52,52	0
57	MG	2A	3636	1/1	0.92	0.09	38,38,38,38	0
57	MG	1A	3166	1/1	0.92	0.12	41,41,41,41	0
57	MG	1x	101	1/1	0.92	0.27	65,65,65,65	0
57	MG	1A	3710	1/1	0.92	0.09	21,21,21,21	0
57	MG	2A	3267	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3269	1/1	0.92	0.22	61,61,61,61	0
57	MG	2a	1704	1/1	0.92	0.10	80,80,80,80	0
57	MG	1A	3713	1/1	0.92	0.10	40,40,40,40	0
57	MG	2A	3274	1/1	0.92	0.09	80,80,80,80	0
57	MG	1A	3327	1/1	0.92	0.10	32,32,32,32	0
57	MG	2A	3662	1/1	0.92	0.13	73,73,73,73	0
57	MG	1x	112	1/1	0.92	0.24	54,54,54,54	0
57	MG	1A	3506	1/1	0.92	0.09	65,65,65,65	0
57	MG	2A	3284	1/1	0.92	0.22	67,67,67,67	0
57	MG	2A	3285	1/1	0.92	0.20	51,51,51,51	0
57	MG	2A	3287	1/1	0.92	0.11	52,52,52,52	0
57	MG	2A	3003	1/1	0.92	0.28	59,59,59,59	0
57	MG	2A	3005	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3015	1/1	0.92	0.26	54,54,54,54	0
57	MG	1A	3719	1/1	0.92	0.09	21,21,21,21	0
57	MG	1A	3328	1/1	0.92	0.19	58,58,58,58	0
57	MG	2A	3298	1/1	0.92	0.16	64,64,64,64	0
57	MG	2A	3683	1/1	0.92	0.13	32,32,32,32	0
57	MG	2A	3023	1/1	0.92	0.20	53,53,53,53	0
57	MG	2A	3685	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3686	1/1	0.92	0.15	77,77,77,77	0
57	MG	2A	3688	1/1	0.92	0.20	53,53,53,53	0
57	MG	1A	3409	1/1	0.92	0.23	43,43,43,43	0
57	MG	1A	3410	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3249	1/1	0.92	0.09	49,49,49,49	0
57	MG	2a	1739	1/1	0.92	0.24	74,74,74,74	0
57	MG	1A	3280	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3528	1/1	0.92	0.12	54,54,54,54	0
57	MG	1a	1646	1/1	0.92	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3705	1/1	0.92	0.09	49,49,49,49	0
57	MG	1A	4002	1/1	0.92	0.07	67,67,67,67	0
57	MG	2A	3711	1/1	0.92	0.13	45,45,45,45	0
57	MG	2A	3307	1/1	0.92	0.17	39,39,39,39	0
57	MG	2a	1752	1/1	0.92	0.06	65,65,65,65	0
57	MG	2a	1753	1/1	0.92	0.18	62,62,62,62	0
57	MG	1A	4005	1/1	0.92	0.08	56,56,56,56	0
57	MG	2A	3310	1/1	0.92	0.12	70,70,70,70	0
57	MG	1A	3766	1/1	0.92	0.12	37,37,37,37	0
57	MG	1a	1653	1/1	0.92	0.16	48,48,48,48	0
57	MG	2A	3723	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3048	1/1	0.92	0.13	31,31,31,31	0
57	MG	2A	3049	1/1	0.92	0.15	40,40,40,40	0
57	MG	1A	4010	1/1	0.92	0.16	51,51,51,51	0
57	MG	1A	4012	1/1	0.92	0.13	48,48,48,48	0
57	MG	2A	3053	1/1	0.92	0.25	62,62,62,62	0
57	MG	1a	1657	1/1	0.92	0.08	53,53,53,53	0
57	MG	2a	1772	1/1	0.92	0.07	52,52,52,52	0
57	MG	2A	3740	1/1	0.92	0.15	46,46,46,46	0
57	MG	2A	3056	1/1	0.92	0.13	55,55,55,55	0
57	MG	2a	1779	1/1	0.92	0.17	55,55,55,55	0
57	MG	2A	3744	1/1	0.92	0.12	67,67,67,67	0
57	MG	2A	3328	1/1	0.92	0.16	81,81,81,81	0
57	MG	1A	3416	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3750	1/1	0.92	0.14	47,47,47,47	0
57	MG	2A	3058	1/1	0.92	0.11	55,55,55,55	0
57	MG	1A	3417	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3758	1/1	0.92	0.19	57,57,57,57	0
57	MG	2a	1790	1/1	0.92	0.17	60,60,60,60	0
57	MG	2A	3761	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3418	1/1	0.92	0.11	50,50,50,50	0
57	MG	2A	3768	1/1	0.92	0.23	60,60,60,60	0
57	MG	1A	3534	1/1	0.92	0.29	32,32,32,32	0
57	MG	1A	3803	1/1	0.92	0.07	59,59,59,59	0
57	MG	2A	3774	1/1	0.92	0.14	59,59,59,59	0
57	MG	2a	1799	1/1	0.92	0.27	59,59,59,59	0
57	MG	2A	3341	1/1	0.92	0.11	55,55,55,55	0
57	MG	1A	3536	1/1	0.92	0.29	55,55,55,55	0
57	MG	1A	3540	1/1	0.92	0.10	29,29,29,29	0
57	MG	2A	3074	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3078	1/1	0.92	0.19	55,55,55,55	0
57	MG	2a	1807	1/1	0.92	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
57	MG	2A	3354	1/1	0.92	0.08	40,40,40,40	0
57	MG	1a	1671	1/1	0.92	0.18	53,53,53,53	0
57	MG	1A	3811	1/1	0.92	0.08	46,46,46,46	0
57	MG	1a	1674	1/1	0.92	0.20	45,45,45,45	0
57	MG	1A	3421	1/1	0.92	0.20	41,41,41,41	0
57	MG	2a	1816	1/1	0.92	0.15	43,43,43,43	0
57	MG	1A	3548	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3816	1/1	0.92	0.09	40,40,40,40	0
57	MG	2a	1820	1/1	0.92	0.13	55,55,55,55	0
57	MG	1a	1680	1/1	0.92	0.10	60,60,60,60	0
57	MG	1a	1681	1/1	0.92	0.17	51,51,51,51	0
57	MG	2d	301	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	4071	1/1	0.92	0.07	46,46,46,46	0
57	MG	2A	3807	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3814	1/1	0.92	0.16	58,58,58,58	0
57	MG	2A	3816	1/1	0.92	0.08	54,54,54,54	0
57	MG	2A	3368	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3817	1/1	0.92	0.43	41,41,41,41	0
57	MG	2l	202	1/1	0.92	0.18	69,69,69,69	0
57	MG	1A	3827	1/1	0.92	0.19	52,52,52,52	0
57	MG	2q	201	1/1	0.92	0.20	66,66,66,66	0
57	MG	2A	3374	1/1	0.92	0.17	58,58,58,58	0
57	MG	2r	101	1/1	0.92	0.08	61,61,61,61	0
57	MG	2t	201	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	4076	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	4079	1/1	0.92	0.15	56,56,56,56	0
57	MG	1a	1691	1/1	0.92	0.23	53,53,53,53	0
57	MG	2A	3104	1/1	0.92	0.15	47,47,47,47	0
57	MG	1a	1693	1/1	0.92	0.25	50,50,50,50	0
57	MG	1A	3549	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3281	1/1	0.92	0.13	48,48,48,48	0
57	MG	1A	3836	1/1	0.92	0.15	45,45,45,45	0
57	MG	1A	4085	1/1	0.92	0.26	42,42,42,42	0
57	MG	1A	3556	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3390	1/1	0.92	0.06	51,51,51,51	0
57	MG	2A	3395	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3853	1/1	0.92	0.26	62,62,62,62	0
57	MG	1A	3838	1/1	0.92	0.10	29,29,29,29	0
57	MG	27	101	1/1	0.93	0.10	48,48,48,48	0
57	MG	1a	1687	1/1	0.93	0.28	49,49,49,49	0
57	MG	2A	3568	1/1	0.93	0.10	40,40,40,40	0
57	MG	1B	229	1/1	0.93	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
57	MG	1A	3236	1/1	0.93	0.08	32,32,32,32	0
57	MG	2A	3574	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3440	1/1	0.93	0.14	55,55,55,55	0
57	MG	2A	3063	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3291	1/1	0.93	0.21	59,59,59,59	0
57	MG	2A	3582	1/1	0.93	0.07	38,38,38,38	0
57	MG	1A	3368	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3083	1/1	0.93	0.19	25,25,25,25	0
57	MG	2A	3587	1/1	0.93	0.10	55,55,55,55	0
57	MG	2A	3068	1/1	0.93	0.29	60,60,60,60	0
57	MG	1A	3120	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3450	1/1	0.93	0.06	28,28,28,28	0
57	MG	2A	3072	1/1	0.93	0.08	57,57,57,57	0
57	MG	1E	311	1/1	0.93	0.12	45,45,45,45	0
57	MG	1E	312	1/1	0.93	0.04	46,46,46,46	0
57	MG	1A	3732	1/1	0.93	0.10	60,60,60,60	0
57	MG	2A	3607	1/1	0.93	0.07	33,33,33,33	0
57	MG	1F	305	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3121	1/1	0.93	0.11	37,37,37,37	0
57	MG	1a	1711	1/1	0.93	0.14	54,54,54,54	0
57	MG	1A	3745	1/1	0.93	0.08	19,19,19,19	0
57	MG	1A	3748	1/1	0.93	0.07	17,17,17,17	0
57	MG	1N	201	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3622	1/1	0.93	0.16	44,44,44,44	0
57	MG	1N	204	1/1	0.93	0.13	53,53,53,53	0
57	MG	2A	3626	1/1	0.93	0.09	52,52,52,52	0
57	MG	1a	1718	1/1	0.93	0.22	60,60,60,60	0
57	MG	1A	3373	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3638	1/1	0.93	0.08	46,46,46,46	0
57	MG	2A	3639	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3317	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3759	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3183	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3647	1/1	0.93	0.11	40,40,40,40	0
57	MG	2A	3100	1/1	0.93	0.13	34,34,34,34	0
57	MG	2A	3652	1/1	0.93	0.15	49,49,49,49	0
57	MG	1P	206	1/1	0.93	0.13	48,48,48,48	0
57	MG	1A	3190	1/1	0.93	0.15	25,25,25,25	0
57	MG	2A	3657	1/1	0.93	0.12	58,58,58,58	0
57	MG	1a	1729	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3661	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3106	1/1	0.93	0.18	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3950	1/1	0.93	0.15	42,42,42,42	0
57	MG	2A	3330	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	1732	1/1	0.93	0.12	40,40,40,40	0
57	MG	1a	1734	1/1	0.93	0.08	46,46,46,46	0
57	MG	1A	3769	1/1	0.93	0.08	24,24,24,24	0
57	MG	2A	3336	1/1	0.93	0.21	58,58,58,58	0
57	MG	2A	3337	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3382	1/1	0.93	0.06	52,52,52,52	0
57	MG	1A	3956	1/1	0.93	0.08	45,45,45,45	0
57	MG	1A	3084	1/1	0.93	0.09	33,33,33,33	0
57	MG	2a	1670	1/1	0.93	0.19	58,58,58,58	0
57	MG	1a	1739	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3345	1/1	0.93	0.13	39,39,39,39	0
57	MG	1U	203	1/1	0.93	0.19	63,63,63,63	0
57	MG	2A	3123	1/1	0.93	0.07	74,74,74,74	0
57	MG	1U	206	1/1	0.93	0.15	48,48,48,48	0
57	MG	2A	3135	1/1	0.93	0.15	39,39,39,39	0
57	MG	1a	1752	1/1	0.93	0.10	56,56,56,56	0
57	MG	1a	1754	1/1	0.93	0.11	38,38,38,38	0
57	MG	1a	1756	1/1	0.93	0.20	57,57,57,57	0
57	MG	1U	209	1/1	0.93	0.17	38,38,38,38	0
57	MG	2a	1687	1/1	0.93	0.23	57,57,57,57	0
57	MG	2A	3694	1/1	0.93	0.06	41,41,41,41	0
57	MG	1U	210	1/1	0.93	0.08	37,37,37,37	0
57	MG	2A	3151	1/1	0.93	0.13	59,59,59,59	0
57	MG	2A	3703	1/1	0.93	0.10	32,32,32,32	0
57	MG	1V	206	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3059	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3961	1/1	0.93	0.07	49,49,49,49	0
57	MG	2a	1698	1/1	0.93	0.07	74,74,74,74	0
57	MG	2a	1700	1/1	0.93	0.23	60,60,60,60	0
57	MG	1Z	301	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3370	1/1	0.93	0.15	66,66,66,66	0
57	MG	2A	3371	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3163	1/1	0.93	0.12	39,39,39,39	0
57	MG	2A	3721	1/1	0.93	0.14	48,48,48,48	0
57	MG	1A	3796	1/1	0.93	0.15	45,45,45,45	0
57	MG	1a	1773	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3800	1/1	0.93	0.08	21,21,21,21	0
57	MG	1A	3469	1/1	0.93	0.07	47,47,47,47	0
57	MG	2A	3377	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3169	1/1	0.93	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1776	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3308	1/1	0.93	0.25	52,52,52,52	0
57	MG	1A	3981	1/1	0.93	0.07	27,27,27,27	0
57	MG	1A	3312	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3020	1/1	0.93	0.14	43,43,43,43	0
57	MG	1A	3320	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3401	1/1	0.93	0.08	38,38,38,38	0
57	MG	15	107	1/1	0.93	0.07	30,30,30,30	0
57	MG	2A	3391	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3097	1/1	0.93	0.18	41,41,41,41	0
57	MG	1A	3045	1/1	0.93	0.16	51,51,51,51	0
57	MG	2A	3759	1/1	0.93	0.08	63,63,63,63	0
57	MG	1A	3111	1/1	0.93	0.08	30,30,30,30	0
57	MG	18	102	1/1	0.93	0.16	34,34,34,34	0
57	MG	2A	3406	1/1	0.93	0.11	44,44,44,44	0
57	MG	2A	3769	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3617	1/1	0.93	0.17	54,54,54,54	0
57	MG	2A	3411	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	4003	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3415	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	3618	1/1	0.93	0.14	36,36,36,36	0
57	MG	2a	1747	1/1	0.93	0.26	63,63,63,63	0
57	MG	2A	3778	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3192	1/1	0.93	0.47	65,65,65,65	0
57	MG	1A	3205	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3783	1/1	0.93	0.10	77,77,77,77	0
57	MG	1A	3835	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3155	1/1	0.93	0.38	36,36,36,36	0
57	MG	2A	3427	1/1	0.93	0.23	54,54,54,54	0
57	MG	2A	3788	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3503	1/1	0.93	0.20	55,55,55,55	0
57	MG	1A	3635	1/1	0.93	0.06	39,39,39,39	0
57	MG	1A	3411	1/1	0.93	0.10	27,27,27,27	0
57	MG	1A	3215	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3266	1/1	0.93	0.11	45,45,45,45	0
57	MG	1j	201	1/1	0.93	0.30	58,58,58,58	0
57	MG	1A	4031	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3644	1/1	0.93	0.10	43,43,43,43	0
57	MG	2A	3803	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3851	1/1	0.93	0.08	22,22,22,22	0
57	MG	2A	3813	1/1	0.93	0.14	49,49,49,49	0
57	MG	2a	1780	1/1	0.93	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1632	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	4057	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3508	1/1	0.93	0.13	49,49,49,49	0
57	MG	1A	4059	1/1	0.93	0.07	38,38,38,38	0
57	MG	2A	3825	1/1	0.93	0.08	61,61,61,61	0
57	MG	1A	4065	1/1	0.93	0.24	54,54,54,54	0
57	MG	1w	105	1/1	0.93	0.07	54,54,54,54	0
57	MG	1a	1643	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3857	1/1	0.93	0.10	34,34,34,34	0
57	MG	2a	1793	1/1	0.93	0.11	51,51,51,51	0
57	MG	1A	4068	1/1	0.93	0.19	61,61,61,61	0
57	MG	1A	3649	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3861	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3652	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3002	1/1	0.93	0.25	46,46,46,46	0
57	MG	1A	3866	1/1	0.93	0.14	43,43,43,43	0
57	MG	2A	3474	1/1	0.93	0.24	42,42,42,42	0
57	MG	2A	3475	1/1	0.93	0.30	51,51,51,51	0
57	MG	2A	3477	1/1	0.93	0.26	53,53,53,53	0
57	MG	2A	3478	1/1	0.93	0.14	51,51,51,51	0
57	MG	1A	3510	1/1	0.93	0.28	43,43,43,43	0
57	MG	2A	3480	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3481	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3220	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3157	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3077	1/1	0.93	0.23	48,48,48,48	0
57	MG	2A	3243	1/1	0.93	0.07	51,51,51,51	0
57	MG	2A	3244	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3524	1/1	0.93	0.07	29,29,29,29	0
57	MG	1A	3525	1/1	0.93	0.22	48,48,48,48	0
57	MG	2a	1819	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3249	1/1	0.93	0.07	46,46,46,46	0
57	MG	2A	3250	1/1	0.93	0.06	53,53,53,53	0
57	MG	1A	3881	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3502	1/1	0.93	0.13	60,60,60,60	0
57	MG	2B	216	1/1	0.93	0.09	54,54,54,54	0
57	MG	1A	3671	1/1	0.93	0.13	32,32,32,32	0
57	MG	1A	3673	1/1	0.93	0.06	21,21,21,21	0
57	MG	2A	3507	1/1	0.93	0.11	35,35,35,35	0
57	MG	1A	3230	1/1	0.93	0.14	48,48,48,48	0
57	MG	2D	301	1/1	0.93	0.15	53,53,53,53	0
57	MG	1A	3282	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
57	MG	2E	302	1/1	0.93	0.06	43,43,43,43	0
57	MG	2E	303	1/1	0.93	0.16	52,52,52,52	0
57	MG	1A	3283	1/1	0.93	0.19	34,34,34,34	0
57	MG	2A	3524	1/1	0.93	0.08	52,52,52,52	0
57	MG	1a	1673	1/1	0.93	0.19	52,52,52,52	0
57	MG	1A	3162	1/1	0.93	0.18	50,50,50,50	0
57	MG	1A	3292	1/1	0.93	0.17	41,41,41,41	0
57	MG	1B	212	1/1	0.93	0.10	43,43,43,43	0
57	MG	2A	3268	1/1	0.93	0.17	76,76,76,76	0
57	MG	2w	103	1/1	0.93	0.06	77,77,77,77	0
57	MG	1A	3904	1/1	0.93	0.29	34,34,34,34	0
57	MG	1A	3297	1/1	0.93	0.16	41,41,41,41	0
57	MG	1A	3909	1/1	0.93	0.15	44,44,44,44	0
57	MG	1B	224	1/1	0.93	0.05	36,36,36,36	0
57	MG	2A	3551	1/1	0.93	0.13	42,42,42,42	0
57	MG	2A	3553	1/1	0.93	0.14	42,42,42,42	0
57	MG	1A	3298	1/1	0.93	0.06	29,29,29,29	0
57	MG	2x	106	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3437	1/1	0.93	0.16	48,48,48,48	0
57	MG	20	102	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3282	1/1	0.93	0.07	50,50,50,50	0
59	ERY	2A	3857	51/51	0.93	0.13	26,54,66,69	0
57	MG	2A	3205	1/1	0.94	0.08	59,59,59,59	0
57	MG	2B	209	1/1	0.94	0.08	65,65,65,65	0
57	MG	2B	210	1/1	0.94	0.19	55,55,55,55	0
57	MG	1A	3765	1/1	0.94	0.10	15,15,15,15	0
57	MG	2A	3473	1/1	0.94	0.06	58,58,58,58	0
57	MG	1A	3562	1/1	0.94	0.13	36,36,36,36	0
57	MG	1a	1785	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3564	1/1	0.94	0.15	43,43,43,43	0
57	MG	1A	3345	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3772	1/1	0.94	0.09	38,38,38,38	0
57	MG	2A	3217	1/1	0.94	0.28	40,40,40,40	0
57	MG	1A	3346	1/1	0.94	0.05	34,34,34,34	0
57	MG	2A	3482	1/1	0.94	0.18	42,42,42,42	0
57	MG	1A	3570	1/1	0.94	0.09	31,31,31,31	0
57	MG	1A	3572	1/1	0.94	0.07	48,48,48,48	0
57	MG	15	108	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3218	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	3348	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3492	1/1	0.94	0.06	38,38,38,38	0
57	MG	2E	306	1/1	0.94	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3219	1/1	0.94	0.16	38,38,38,38	0
57	MG	2A	3494	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3156	1/1	0.94	0.07	29,29,29,29	0
57	MG	1a	1805	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3497	1/1	0.94	0.07	44,44,44,44	0
57	MG	1A	3285	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3447	1/1	0.94	0.11	47,47,47,47	0
57	MG	1a	1808	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3024	1/1	0.94	0.15	32,32,32,32	0
57	MG	2U	202	1/1	0.94	0.05	41,41,41,41	0
57	MG	18	107	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	4019	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3510	1/1	0.94	0.16	44,44,44,44	0
57	MG	1a	1605	1/1	0.94	0.08	63,63,63,63	0
57	MG	1A	4020	1/1	0.94	0.10	30,30,30,30	0
57	MG	20	103	1/1	0.94	0.11	65,65,65,65	0
57	MG	1a	1609	1/1	0.94	0.06	38,38,38,38	0
57	MG	25	101	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3521	1/1	0.94	0.06	35,35,35,35	0
57	MG	2A	3523	1/1	0.94	0.10	39,39,39,39	0
57	MG	1a	1610	1/1	0.94	0.08	61,61,61,61	0
57	MG	27	104	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3526	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3245	1/1	0.94	0.09	55,55,55,55	0
57	MG	1a	1611	1/1	0.94	0.11	28,28,28,28	0
57	MG	1A	3363	1/1	0.94	0.21	55,55,55,55	0
57	MG	2A	3248	1/1	0.94	0.09	51,51,51,51	0
57	MG	1a	1614	1/1	0.94	0.05	60,60,60,60	0
57	MG	1A	3815	1/1	0.94	0.08	59,59,59,59	0
57	MG	2a	1608	1/1	0.94	0.08	56,56,56,56	0
57	MG	2A	3537	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	4024	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3364	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3287	1/1	0.94	0.08	58,58,58,58	0
57	MG	1a	1624	1/1	0.94	0.21	44,44,44,44	0
57	MG	2a	1616	1/1	0.94	0.09	67,67,67,67	0
57	MG	1a	1625	1/1	0.94	0.18	43,43,43,43	0
57	MG	2A	3554	1/1	0.94	0.10	46,46,46,46	0
57	MG	2A	3259	1/1	0.94	0.08	70,70,70,70	0
57	MG	2A	3557	1/1	0.94	0.10	41,41,41,41	0
57	MG	2A	3559	1/1	0.94	0.07	32,32,32,32	0
57	MG	1a	1626	1/1	0.94	0.22	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	110	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3819	1/1	0.94	0.08	18,18,18,18	0
57	MG	1A	4038	1/1	0.94	0.12	42,42,42,42	0
57	MG	2A	3265	1/1	0.94	0.08	58,58,58,58	0
57	MG	2a	1629	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3570	1/1	0.94	0.07	39,39,39,39	0
57	MG	1A	3821	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3826	1/1	0.94	0.18	48,48,48,48	0
57	MG	1a	1631	1/1	0.94	0.19	55,55,55,55	0
57	MG	2A	3271	1/1	0.94	0.10	43,43,43,43	0
57	MG	2A	3272	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3580	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3009	1/1	0.94	0.13	57,57,57,57	0
57	MG	1A	3592	1/1	0.94	0.13	34,34,34,34	0
57	MG	2A	3016	1/1	0.94	0.22	48,48,48,48	0
57	MG	1A	3288	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3832	1/1	0.94	0.06	41,41,41,41	0
57	MG	2A	3280	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	4060	1/1	0.94	0.10	31,31,31,31	0
57	MG	2A	3027	1/1	0.94	0.22	51,51,51,51	0
57	MG	1A	3112	1/1	0.94	0.15	40,40,40,40	0
57	MG	1A	4066	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3296	1/1	0.94	0.23	41,41,41,41	0
57	MG	2a	1649	1/1	0.94	0.11	70,70,70,70	0
57	MG	1A	3025	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	3604	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3037	1/1	0.94	0.09	33,33,33,33	0
57	MG	2a	1653	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3611	1/1	0.94	0.18	41,41,41,41	0
57	MG	1A	3231	1/1	0.94	0.06	48,48,48,48	0
57	MG	1A	3612	1/1	0.94	0.10	21,21,21,21	0
57	MG	1A	3613	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3468	1/1	0.94	0.19	45,45,45,45	0
57	MG	2A	3046	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	3377	1/1	0.94	0.27	37,37,37,37	0
57	MG	1A	4078	1/1	0.94	0.15	45,45,45,45	0
57	MG	2a	1664	1/1	0.94	0.18	44,44,44,44	0
57	MG	2A	3628	1/1	0.94	0.11	41,41,41,41	0
57	MG	2a	1667	1/1	0.94	0.30	57,57,57,57	0
57	MG	2A	3631	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3623	1/1	0.94	0.17	16,16,16,16	0
57	MG	1A	3048	1/1	0.94	0.07	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3627	1/1	0.94	0.12	32,32,32,32	0
57	MG	1A	3859	1/1	0.94	0.13	58,58,58,58	0
57	MG	2A	3640	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	4083	1/1	0.94	0.07	54,54,54,54	0
57	MG	2A	3308	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	4084	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3234	1/1	0.94	0.19	53,53,53,53	0
57	MG	2A	3311	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3313	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3472	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3473	1/1	0.94	0.18	61,61,61,61	0
57	MG	2a	1689	1/1	0.94	0.19	58,58,58,58	0
57	MG	2A	3061	1/1	0.94	0.17	48,48,48,48	0
57	MG	1B	205	1/1	0.94	0.21	51,51,51,51	0
57	MG	2A	3659	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3636	1/1	0.94	0.08	17,17,17,17	0
57	MG	1A	3474	1/1	0.94	0.26	46,46,46,46	0
57	MG	1A	3061	1/1	0.94	0.12	58,58,58,58	0
57	MG	1A	3062	1/1	0.94	0.19	38,38,38,38	0
57	MG	1a	1679	1/1	0.94	0.07	71,71,71,71	0
57	MG	1A	3478	1/1	0.94	0.13	41,41,41,41	0
57	MG	1A	3387	1/1	0.94	0.16	37,37,37,37	0
57	MG	1A	3181	1/1	0.94	0.09	47,47,47,47	0
57	MG	2A	3077	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3331	1/1	0.94	0.07	64,64,64,64	0
57	MG	1B	215	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3880	1/1	0.94	0.09	25,25,25,25	0
57	MG	1B	217	1/1	0.94	0.07	54,54,54,54	0
57	MG	2A	3085	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3122	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3338	1/1	0.94	0.06	49,49,49,49	0
57	MG	1A	3247	1/1	0.94	0.06	51,51,51,51	0
57	MG	2a	1716	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3392	1/1	0.94	0.29	50,50,50,50	0
57	MG	1A	3659	1/1	0.94	0.08	37,37,37,37	0
57	MG	2A	3342	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3497	1/1	0.94	0.13	59,59,59,59	0
57	MG	1A	3891	1/1	0.94	0.16	33,33,33,33	0
57	MG	2a	1724	1/1	0.94	0.13	55,55,55,55	0
57	MG	1a	1696	1/1	0.94	0.10	56,56,56,56	0
57	MG	1a	1697	1/1	0.94	0.12	44,44,44,44	0
57	MG	2A	3352	1/1	0.94	0.06	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1729	1/1	0.94	0.10	52,52,52,52	0
57	MG	2a	1730	1/1	0.94	0.22	59,59,59,59	0
57	MG	1A	3395	1/1	0.94	0.08	41,41,41,41	0
57	MG	2A	3704	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3896	1/1	0.94	0.13	45,45,45,45	0
57	MG	1a	1701	1/1	0.94	0.15	61,61,61,61	0
57	MG	1a	1702	1/1	0.94	0.15	41,41,41,41	0
57	MG	2A	3712	1/1	0.94	0.07	41,41,41,41	0
57	MG	2A	3102	1/1	0.94	0.07	56,56,56,56	0
57	MG	2a	1740	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3715	1/1	0.94	0.06	51,51,51,51	0
57	MG	1A	3663	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3188	1/1	0.94	0.27	40,40,40,40	0
57	MG	2A	3362	1/1	0.94	0.16	58,58,58,58	0
57	MG	1D	301	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3063	1/1	0.94	0.18	33,33,33,33	0
57	MG	1E	303	1/1	0.94	0.17	32,32,32,32	0
57	MG	1E	308	1/1	0.94	0.08	21,21,21,21	0
57	MG	1A	3127	1/1	0.94	0.39	42,42,42,42	0
57	MG	1A	3315	1/1	0.94	0.15	33,33,33,33	0
57	MG	2A	3732	1/1	0.94	0.08	49,49,49,49	0
57	MG	2A	3114	1/1	0.94	0.09	56,56,56,56	0
57	MG	2a	1757	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3675	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3736	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3251	1/1	0.94	0.09	26,26,26,26	0
57	MG	2a	1762	1/1	0.94	0.22	57,57,57,57	0
57	MG	1A	3091	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3095	1/1	0.94	0.18	41,41,41,41	0
57	MG	1G	202	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3124	1/1	0.94	0.10	52,52,52,52	0
57	MG	2a	1768	1/1	0.94	0.10	73,73,73,73	0
57	MG	1a	1722	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3701	1/1	0.94	0.09	25,25,25,25	0
57	MG	2A	3380	1/1	0.94	0.05	46,46,46,46	0
57	MG	2a	1774	1/1	0.94	0.07	63,63,63,63	0
57	MG	2A	3136	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3131	1/1	0.94	0.18	39,39,39,39	0
57	MG	2a	1778	1/1	0.94	0.11	37,37,37,37	0
57	MG	1A	3141	1/1	0.94	0.14	18,18,18,18	0
57	MG	2A	3385	1/1	0.94	0.05	52,52,52,52	0
57	MG	1A	3412	1/1	0.94	0.09	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1731	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3258	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3008	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3716	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3773	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3051	1/1	0.94	0.23	38,38,38,38	0
57	MG	1A	3022	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3398	1/1	0.94	0.23	53,53,53,53	0
57	MG	1R	202	1/1	0.94	0.10	27,27,27,27	0
57	MG	2A	3400	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3781	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3401	1/1	0.94	0.28	43,43,43,43	0
57	MG	2A	3402	1/1	0.94	0.23	48,48,48,48	0
57	MG	1A	3208	1/1	0.94	0.09	40,40,40,40	0
57	MG	1R	205	1/1	0.94	0.13	29,29,29,29	0
57	MG	1a	1745	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3419	1/1	0.94	0.08	48,48,48,48	0
57	MG	2a	1802	1/1	0.94	0.10	39,39,39,39	0
57	MG	2A	3413	1/1	0.94	0.29	54,54,54,54	0
57	MG	1a	1748	1/1	0.94	0.10	53,53,53,53	0
57	MG	1a	1751	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3416	1/1	0.94	0.28	45,45,45,45	0
57	MG	2A	3797	1/1	0.94	0.16	51,51,51,51	0
57	MG	1A	3420	1/1	0.94	0.15	28,28,28,28	0
57	MG	2a	1810	1/1	0.94	0.21	56,56,56,56	0
57	MG	2A	3418	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3726	1/1	0.94	0.10	22,22,22,22	0
57	MG	1a	1755	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3337	1/1	0.94	0.17	42,42,42,42	0
57	MG	2A	3175	1/1	0.94	0.19	49,49,49,49	0
57	MG	2A	3808	1/1	0.94	0.06	29,29,29,29	0
57	MG	2A	3425	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3176	1/1	0.94	0.13	42,42,42,42	0
57	MG	1U	204	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3210	1/1	0.94	0.11	49,49,49,49	0
57	MG	1a	1759	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3823	1/1	0.94	0.09	52,52,52,52	0
57	MG	1a	1760	1/1	0.94	0.17	50,50,50,50	0
57	MG	2f	202	1/1	0.94	0.09	63,63,63,63	0
57	MG	1A	3212	1/1	0.94	0.12	55,55,55,55	0
57	MG	1a	1764	1/1	0.94	0.07	55,55,55,55	0
57	MG	2A	3437	1/1	0.94	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3832	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3743	1/1	0.94	0.07	60,60,60,60	0
57	MG	2A	3439	1/1	0.94	0.06	50,50,50,50	0
57	MG	1a	1766	1/1	0.94	0.08	65,65,65,65	0
57	MG	1V	202	1/1	0.94	0.30	49,49,49,49	0
57	MG	2q	203	1/1	0.94	0.15	60,60,60,60	0
57	MG	2A	3443	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3545	1/1	0.94	0.23	48,48,48,48	0
57	MG	1V	207	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3843	1/1	0.94	0.16	49,49,49,49	0
57	MG	2A	3844	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3190	1/1	0.94	0.18	43,43,43,43	0
57	MG	2A	3453	1/1	0.94	0.14	68,68,68,68	0
57	MG	2A	3849	1/1	0.94	0.09	53,53,53,53	0
57	MG	1W	203	1/1	0.94	0.15	42,42,42,42	0
57	MG	1W	207	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3104	1/1	0.94	0.12	33,33,33,33	0
57	MG	1A	3425	1/1	0.94	0.09	41,41,41,41	0
57	MG	2B	201	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	3753	1/1	0.94	0.10	38,38,38,38	0
57	MG	2A	3461	1/1	0.94	0.08	54,54,54,54	0
57	MG	2z	101	1/1	0.94	0.07	50,50,50,50	0
57	MG	10	103	1/1	0.94	0.11	43,43,43,43	0
57	MG	1A	3217	1/1	0.94	0.13	36,36,36,36	0
57	MG	2A	3202	1/1	0.94	0.06	49,49,49,49	0
57	MG	1A	3430	1/1	0.94	0.16	36,36,36,36	0
57	MG	1F	304	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3908	1/1	0.95	0.09	23,23,23,23	0
57	MG	1A	3375	1/1	0.95	0.13	50,50,50,50	0
57	MG	2A	3839	1/1	0.95	0.10	41,41,41,41	0
57	MG	1A	3544	1/1	0.95	0.14	49,49,49,49	0
57	MG	2A	3167	1/1	0.95	0.10	48,48,48,48	0
57	MG	1G	201	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3912	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3711	1/1	0.95	0.09	41,41,41,41	0
57	MG	2A	3450	1/1	0.95	0.20	39,39,39,39	0
57	MG	2A	3451	1/1	0.95	0.11	38,38,38,38	0
57	MG	1I	201	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3376	1/1	0.95	0.17	38,38,38,38	0
57	MG	1N	203	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3715	1/1	0.95	0.08	50,50,50,50	0
57	MG	1a	1743	1/1	0.95	0.09	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3855	1/1	0.95	0.15	63,63,63,63	0
57	MG	2A	3856	1/1	0.95	0.07	52,52,52,52	0
57	MG	1a	1744	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3919	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3179	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3462	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3317	1/1	0.95	0.14	47,47,47,47	0
57	MG	1P	204	1/1	0.95	0.19	35,35,35,35	0
57	MG	2A	3467	1/1	0.95	0.10	40,40,40,40	0
57	MG	1a	1750	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3925	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3318	1/1	0.95	0.12	37,37,37,37	0
57	MG	2A	3471	1/1	0.95	0.15	55,55,55,55	0
57	MG	1A	3551	1/1	0.95	0.12	23,23,23,23	0
57	MG	1Q	206	1/1	0.95	0.05	39,39,39,39	0
57	MG	1A	3552	1/1	0.95	0.08	42,42,42,42	0
57	MG	1R	201	1/1	0.95	0.18	38,38,38,38	0
57	MG	2A	3476	1/1	0.95	0.18	28,28,28,28	0
57	MG	1A	3049	1/1	0.95	0.07	34,34,34,34	0
57	MG	2A	3191	1/1	0.95	0.12	69,69,69,69	0
57	MG	1A	3724	1/1	0.95	0.12	53,53,53,53	0
57	MG	1A	3268	1/1	0.95	0.07	51,51,51,51	0
57	MG	1a	1762	1/1	0.95	0.09	49,49,49,49	0
57	MG	2D	304	1/1	0.95	0.21	47,47,47,47	0
57	MG	2A	3196	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3452	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3321	1/1	0.95	0.17	34,34,34,34	0
57	MG	1A	3386	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3946	1/1	0.95	0.10	32,32,32,32	0
57	MG	1A	3738	1/1	0.95	0.14	51,51,51,51	0
57	MG	2E	308	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3948	1/1	0.95	0.06	29,29,29,29	0
57	MG	1A	3233	1/1	0.95	0.27	35,35,35,35	0
57	MG	1A	3567	1/1	0.95	0.06	38,38,38,38	0
57	MG	2F	303	1/1	0.95	0.12	57,57,57,57	0
57	MG	1A	3569	1/1	0.95	0.17	46,46,46,46	0
57	MG	2A	3211	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3953	1/1	0.95	0.10	53,53,53,53	0
57	MG	2P	201	1/1	0.95	0.05	43,43,43,43	0
57	MG	2A	3213	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3090	1/1	0.95	0.07	38,38,38,38	0
57	MG	2R	203	1/1	0.95	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3501	1/1	0.95	0.14	45,45,45,45	0
57	MG	2T	203	1/1	0.95	0.05	38,38,38,38	0
57	MG	1W	202	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3503	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3460	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3752	1/1	0.95	0.05	26,26,26,26	0
57	MG	1X	101	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3958	1/1	0.95	0.09	53,53,53,53	0
57	MG	1X	107	1/1	0.95	0.08	48,48,48,48	0
57	MG	2I	3501	1/1	0.95	0.48	51,51,51,51	0
57	MG	1A	3573	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3517	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3518	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3519	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3235	1/1	0.95	0.13	39,39,39,39	0
57	MG	2A	3228	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3522	1/1	0.95	0.10	32,32,32,32	0
57	MG	28	102	1/1	0.95	0.25	56,56,56,56	0
57	MG	2a	1601	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3761	1/1	0.95	0.11	55,55,55,55	0
57	MG	1A	3576	1/1	0.95	0.10	34,34,34,34	0
57	MG	1A	3966	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3763	1/1	0.95	0.13	49,49,49,49	0
57	MG	1A	3326	1/1	0.95	0.07	43,43,43,43	0
57	MG	10	109	1/1	0.95	0.13	60,60,60,60	0
57	MG	1A	3972	1/1	0.95	0.15	37,37,37,37	0
57	MG	1I	101	1/1	0.95	0.15	38,38,38,38	0
57	MG	2a	1611	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3976	1/1	0.95	0.16	61,61,61,61	0
57	MG	13	101	1/1	0.95	0.17	37,37,37,37	0
57	MG	2A	3539	1/1	0.95	0.08	37,37,37,37	0
57	MG	13	103	1/1	0.95	0.07	49,49,49,49	0
57	MG	2A	3542	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3979	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3580	1/1	0.95	0.23	35,35,35,35	0
57	MG	2A	3549	1/1	0.95	0.08	40,40,40,40	0
57	MG	15	104	1/1	0.95	0.27	32,32,32,32	0
57	MG	1A	3983	1/1	0.95	0.09	42,42,42,42	0
57	MG	1a	1810	1/1	0.95	0.13	59,59,59,59	0
57	MG	1a	1811	1/1	0.95	0.06	51,51,51,51	0
57	MG	1A	3466	1/1	0.95	0.11	37,37,37,37	0
57	MG	2A	3558	1/1	0.95	0.13	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1d	301	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3560	1/1	0.95	0.17	59,59,59,59	0
57	MG	1e	201	1/1	0.95	0.27	56,56,56,56	0
57	MG	1A	3037	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3393	1/1	0.95	0.13	62,62,62,62	0
57	MG	2A	3254	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3990	1/1	0.95	0.05	32,32,32,32	0
57	MG	1m	3001	1/1	0.95	0.05	46,46,46,46	0
57	MG	16	102	1/1	0.95	0.14	62,62,62,62	0
57	MG	2A	3573	1/1	0.95	0.07	28,28,28,28	0
57	MG	1n	103	1/1	0.95	0.19	46,46,46,46	0
57	MG	1A	3773	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3394	1/1	0.95	0.27	49,49,49,49	0
57	MG	2A	3577	1/1	0.95	0.06	28,28,28,28	0
57	MG	1A	3997	1/1	0.95	0.06	36,36,36,36	0
57	MG	2A	3579	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3776	1/1	0.95	0.05	21,21,21,21	0
57	MG	1A	4000	1/1	0.95	0.14	41,41,41,41	0
57	MG	1A	3779	1/1	0.95	0.05	57,57,57,57	0
57	MG	1a	1601	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3781	1/1	0.95	0.09	22,22,22,22	0
57	MG	2A	3588	1/1	0.95	0.13	35,35,35,35	0
57	MG	2A	3591	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3592	1/1	0.95	0.06	41,41,41,41	0
57	MG	2A	3593	1/1	0.95	0.07	53,53,53,53	0
57	MG	1a	1603	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3596	1/1	0.95	0.08	24,24,24,24	0
57	MG	1x	104	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3789	1/1	0.95	0.06	24,24,24,24	0
57	MG	1A	3093	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3795	1/1	0.95	0.12	49,49,49,49	0
57	MG	1x	111	1/1	0.95	0.26	53,53,53,53	0
57	MG	2A	3603	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3284	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3799	1/1	0.95	0.10	19,19,19,19	0
57	MG	2A	3608	1/1	0.95	0.09	24,24,24,24	0
57	MG	2a	1668	1/1	0.95	0.10	47,47,47,47	0
57	MG	2A	3281	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3060	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3245	1/1	0.95	0.04	47,47,47,47	0
57	MG	1a	1615	1/1	0.95	0.10	36,36,36,36	0
57	MG	2A	3613	1/1	0.95	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3286	1/1	0.95	0.09	64,64,64,64	0
57	MG	2A	3615	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3616	1/1	0.95	0.16	63,63,63,63	0
57	MG	2A	3006	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3591	1/1	0.95	0.16	42,42,42,42	0
57	MG	2a	1681	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3010	1/1	0.95	0.15	48,48,48,48	0
57	MG	2a	1683	1/1	0.95	0.18	51,51,51,51	0
57	MG	2A	3011	1/1	0.95	0.12	40,40,40,40	0
57	MG	2a	1685	1/1	0.95	0.16	46,46,46,46	0
57	MG	2A	3625	1/1	0.95	0.20	42,42,42,42	0
57	MG	2A	3012	1/1	0.95	0.04	49,49,49,49	0
57	MG	2A	3013	1/1	0.95	0.17	32,32,32,32	0
57	MG	2A	3630	1/1	0.95	0.17	54,54,54,54	0
57	MG	1a	1620	1/1	0.95	0.08	53,53,53,53	0
57	MG	2a	1692	1/1	0.95	0.20	61,61,61,61	0
57	MG	2A	3633	1/1	0.95	0.15	32,32,32,32	0
57	MG	1A	3808	1/1	0.95	0.63	32,32,32,32	0
57	MG	1A	4022	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3335	1/1	0.95	0.41	42,42,42,42	0
57	MG	1A	3597	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3025	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3203	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3158	1/1	0.95	0.11	25,25,25,25	0
57	MG	2A	3645	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3291	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	4034	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	4036	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3651	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3033	1/1	0.95	0.06	44,44,44,44	0
57	MG	2A	3653	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3005	1/1	0.95	0.06	44,44,44,44	0
57	MG	2a	1712	1/1	0.95	0.07	51,51,51,51	0
57	MG	2A	3036	1/1	0.95	0.07	50,50,50,50	0
57	MG	2a	1714	1/1	0.95	0.12	57,57,57,57	0
57	MG	1A	3075	1/1	0.95	0.06	37,37,37,37	0
57	MG	2A	3312	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	4040	1/1	0.95	0.09	32,32,32,32	0
57	MG	2a	1718	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3040	1/1	0.95	0.20	44,44,44,44	0
57	MG	1A	3484	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	4045	1/1	0.95	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1722	1/1	0.95	0.09	72,72,72,72	0
57	MG	2A	3669	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	4051	1/1	0.95	0.06	54,54,54,54	0
57	MG	1A	3485	1/1	0.95	0.13	49,49,49,49	0
57	MG	1a	1642	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3488	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3824	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3342	1/1	0.95	0.14	41,41,41,41	0
57	MG	2a	1731	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3491	1/1	0.95	0.09	38,38,38,38	0
57	MG	2A	3679	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3413	1/1	0.95	0.07	41,41,41,41	0
57	MG	2a	1735	1/1	0.95	0.28	60,60,60,60	0
57	MG	1A	3098	1/1	0.95	0.10	35,35,35,35	0
57	MG	2A	3055	1/1	0.95	0.13	52,52,52,52	0
57	MG	1A	3495	1/1	0.95	0.06	51,51,51,51	0
57	MG	2A	3332	1/1	0.95	0.14	47,47,47,47	0
57	MG	1A	3167	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3632	1/1	0.95	0.09	29,29,29,29	0
57	MG	2A	3687	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3213	1/1	0.95	0.19	40,40,40,40	0
57	MG	1A	3052	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3504	1/1	0.95	0.10	41,41,41,41	0
57	MG	2a	1746	1/1	0.95	0.23	62,62,62,62	0
57	MG	1a	1661	1/1	0.95	0.14	64,64,64,64	0
57	MG	1a	1664	1/1	0.95	0.16	50,50,50,50	0
57	MG	1A	3178	1/1	0.95	0.15	32,32,32,32	0
57	MG	2a	1751	1/1	0.95	0.13	49,49,49,49	0
57	MG	1A	4077	1/1	0.95	0.06	45,45,45,45	0
57	MG	2A	3069	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3701	1/1	0.95	0.08	47,47,47,47	0
57	MG	2a	1755	1/1	0.95	0.15	76,76,76,76	0
57	MG	1A	3079	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3358	1/1	0.95	0.20	40,40,40,40	0
57	MG	1a	1669	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3135	1/1	0.95	0.12	30,30,30,30	0
57	MG	2A	3075	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3076	1/1	0.95	0.11	33,33,33,33	0
57	MG	1A	3852	1/1	0.95	0.12	25,25,25,25	0
57	MG	1A	3139	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3855	1/1	0.95	0.13	36,36,36,36	0
57	MG	2A	3082	1/1	0.95	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3719	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3648	1/1	0.95	0.08	64,64,64,64	0
57	MG	2A	3359	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3185	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3516	1/1	0.95	0.21	46,46,46,46	0
57	MG	1A	3518	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3863	1/1	0.95	0.18	53,53,53,53	0
57	MG	2A	3728	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3028	1/1	0.95	0.22	69,69,69,69	0
57	MG	1A	3144	1/1	0.95	0.45	40,40,40,40	0
57	MG	2a	1781	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3660	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3369	1/1	0.95	0.12	53,53,53,53	0
57	MG	1A	3521	1/1	0.95	0.20	43,43,43,43	0
57	MG	1A	3523	1/1	0.95	0.19	44,44,44,44	0
57	MG	2A	3739	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3367	1/1	0.95	0.10	49,49,49,49	0
57	MG	1B	213	1/1	0.95	0.16	50,50,50,50	0
57	MG	2a	1789	1/1	0.95	0.19	60,60,60,60	0
57	MG	1A	3310	1/1	0.95	0.22	32,32,32,32	0
57	MG	2A	3745	1/1	0.95	0.08	54,54,54,54	0
57	MG	2A	3746	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3431	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3878	1/1	0.95	0.06	26,26,26,26	0
57	MG	1A	3879	1/1	0.95	0.10	30,30,30,30	0
57	MG	2A	3752	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3432	1/1	0.95	0.12	29,29,29,29	0
57	MG	1A	3529	1/1	0.95	0.14	44,44,44,44	0
57	MG	2A	3756	1/1	0.95	0.14	65,65,65,65	0
57	MG	1B	225	1/1	0.95	0.20	49,49,49,49	0
57	MG	1A	3882	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3434	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3762	1/1	0.95	0.07	48,48,48,48	0
57	MG	2A	3764	1/1	0.95	0.08	52,52,52,52	0
57	MG	2a	1806	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3765	1/1	0.95	0.06	35,35,35,35	0
57	MG	2A	3111	1/1	0.95	0.20	50,50,50,50	0
57	MG	1A	3679	1/1	0.95	0.08	18,18,18,18	0
57	MG	1A	3680	1/1	0.95	0.09	21,21,21,21	0
57	MG	1a	1704	1/1	0.95	0.08	50,50,50,50	0
57	MG	1A	3682	1/1	0.95	0.06	16,16,16,16	0
57	MG	1a	1707	1/1	0.95	0.32	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3117	1/1	0.95	0.14	38,38,38,38	0
57	MG	2A	3394	1/1	0.95	0.12	28,28,28,28	0
57	MG	1A	3265	1/1	0.95	0.11	47,47,47,47	0
57	MG	1A	3314	1/1	0.95	0.23	50,50,50,50	0
57	MG	1B	235	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3018	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3126	1/1	0.95	0.12	64,64,64,64	0
57	MG	2A	3128	1/1	0.95	0.13	43,43,43,43	0
57	MG	2A	3131	1/1	0.95	0.05	40,40,40,40	0
57	MG	2A	3133	1/1	0.95	0.10	46,46,46,46	0
57	MG	2f	201	1/1	0.95	0.11	54,54,54,54	0
57	MG	1A	3695	1/1	0.95	0.08	22,22,22,22	0
57	MG	2A	3407	1/1	0.95	0.30	53,53,53,53	0
57	MG	2A	3409	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3899	1/1	0.95	0.15	60,60,60,60	0
57	MG	1D	312	1/1	0.95	0.07	28,28,28,28	0
57	MG	2A	3412	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3796	1/1	0.95	0.07	41,41,41,41	0
57	MG	2o	101	1/1	0.95	0.14	54,54,54,54	0
57	MG	1E	301	1/1	0.95	0.17	44,44,44,44	0
57	MG	1A	3316	1/1	0.95	0.23	53,53,53,53	0
57	MG	2A	3141	1/1	0.95	0.14	37,37,37,37	0
57	MG	2A	3145	1/1	0.95	0.22	40,40,40,40	0
57	MG	2A	3146	1/1	0.95	0.07	35,35,35,35	0
57	MG	1E	305	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3805	1/1	0.95	0.11	48,48,48,48	0
57	MG	1E	307	1/1	0.95	0.08	41,41,41,41	0
57	MG	2A	3420	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3902	1/1	0.95	0.09	40,40,40,40	0
57	MG	2A	3150	1/1	0.95	0.11	54,54,54,54	0
57	MG	1A	3903	1/1	0.95	0.15	29,29,29,29	0
57	MG	2A	3153	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3439	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3156	1/1	0.95	0.09	63,63,63,63	0
57	MG	2A	3157	1/1	0.95	0.13	67,67,67,67	0
57	MG	1a	1724	1/1	0.95	0.15	50,50,50,50	0
57	MG	2A	3431	1/1	0.95	0.18	43,43,43,43	0
57	MG	2A	3828	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3542	1/1	0.95	0.11	32,32,32,32	0
57	MG	1a	1727	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3162	1/1	0.95	0.16	41,41,41,41	0
57	MG	2A	3835	1/1	0.95	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3103	1/1	0.96	0.05	56,56,56,56	0
57	MG	2E	301	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	4075	1/1	0.96	0.06	46,46,46,46	0
57	MG	2A	3266	1/1	0.96	0.11	51,51,51,51	0
57	MG	2A	3547	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3868	1/1	0.96	0.15	31,31,31,31	0
57	MG	2A	3020	1/1	0.96	0.11	42,42,42,42	0
57	MG	1a	1634	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3869	1/1	0.96	0.28	39,39,39,39	0
57	MG	2A	3024	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3163	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3026	1/1	0.96	0.04	42,42,42,42	0
57	MG	2F	304	1/1	0.96	0.07	33,33,33,33	0
57	MG	2A	3275	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3449	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3562	1/1	0.96	0.05	35,35,35,35	0
57	MG	2A	3277	1/1	0.96	0.15	46,46,46,46	0
57	MG	1a	1639	1/1	0.96	0.08	46,46,46,46	0
57	MG	1a	1640	1/1	0.96	0.10	49,49,49,49	0
57	MG	2R	201	1/1	0.96	0.04	46,46,46,46	0
57	MG	2A	3567	1/1	0.96	0.11	46,46,46,46	0
57	MG	1a	1641	1/1	0.96	0.06	58,58,58,58	0
57	MG	1A	3691	1/1	0.96	0.06	23,23,23,23	0
57	MG	2U	201	1/1	0.96	0.13	55,55,55,55	0
57	MG	2A	3032	1/1	0.96	0.05	41,41,41,41	0
57	MG	2V	201	1/1	0.96	0.07	62,62,62,62	0
57	MG	1A	3085	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3547	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3698	1/1	0.96	0.07	22,22,22,22	0
57	MG	1A	3378	1/1	0.96	0.04	38,38,38,38	0
57	MG	2A	3288	1/1	0.96	0.11	53,53,53,53	0
57	MG	1A	3703	1/1	0.96	0.09	19,19,19,19	0
57	MG	2A	3039	1/1	0.96	0.05	55,55,55,55	0
57	MG	1A	3132	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3455	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3293	1/1	0.96	0.16	62,62,62,62	0
57	MG	2A	3042	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3585	1/1	0.96	0.05	41,41,41,41	0
57	MG	1B	204	1/1	0.96	0.04	30,30,30,30	0
57	MG	1A	3214	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3709	1/1	0.96	0.07	24,24,24,24	0
57	MG	28	103	1/1	0.96	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	207	1/1	0.96	0.27	47,47,47,47	0
57	MG	1A	3554	1/1	0.96	0.06	46,46,46,46	0
57	MG	1A	3886	1/1	0.96	0.06	33,33,33,33	0
57	MG	1a	1662	1/1	0.96	0.05	33,33,33,33	0
57	MG	2A	3051	1/1	0.96	0.07	60,60,60,60	0
57	MG	1a	1663	1/1	0.96	0.14	51,51,51,51	0
57	MG	2A	3598	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3457	1/1	0.96	0.05	46,46,46,46	0
57	MG	2a	1609	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3888	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3712	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3168	1/1	0.96	0.10	30,30,30,30	0
57	MG	1A	3714	1/1	0.96	0.05	43,43,43,43	0
57	MG	2A	3604	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3558	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3897	1/1	0.96	0.04	31,31,31,31	0
57	MG	2a	1617	1/1	0.96	0.08	66,66,66,66	0
57	MG	1A	3134	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3384	1/1	0.96	0.04	48,48,48,48	0
57	MG	1A	3172	1/1	0.96	0.23	29,29,29,29	0
57	MG	1A	3175	1/1	0.96	0.04	22,22,22,22	0
57	MG	1A	3720	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3066	1/1	0.96	0.06	35,35,35,35	0
57	MG	1B	227	1/1	0.96	0.09	54,54,54,54	0
57	MG	2A	3322	1/1	0.96	0.08	85,85,85,85	0
57	MG	2A	3323	1/1	0.96	0.15	47,47,47,47	0
57	MG	1A	3323	1/1	0.96	0.20	43,43,43,43	0
57	MG	1A	3273	1/1	0.96	0.13	24,24,24,24	0
57	MG	1A	3390	1/1	0.96	0.13	55,55,55,55	0
57	MG	1A	3571	1/1	0.96	0.06	50,50,50,50	0
57	MG	2A	3073	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3274	1/1	0.96	0.45	35,35,35,35	0
57	MG	1a	1683	1/1	0.96	0.12	44,44,44,44	0
57	MG	1A	3911	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3731	1/1	0.96	0.12	56,56,56,56	0
57	MG	1A	3110	1/1	0.96	0.25	33,33,33,33	0
57	MG	1A	3574	1/1	0.96	0.07	40,40,40,40	0
57	MG	1D	303	1/1	0.96	0.08	33,33,33,33	0
57	MG	1D	306	1/1	0.96	0.09	35,35,35,35	0
57	MG	1a	1692	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3179	1/1	0.96	0.11	38,38,38,38	0
57	MG	2a	1643	1/1	0.96	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3740	1/1	0.96	0.06	47,47,47,47	0
57	MG	2A	3642	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3742	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3644	1/1	0.96	0.34	39,39,39,39	0
57	MG	1A	3227	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3090	1/1	0.96	0.15	47,47,47,47	0
57	MG	1A	3926	1/1	0.96	0.11	39,39,39,39	0
57	MG	2A	3648	1/1	0.96	0.11	67,67,67,67	0
57	MG	1A	3578	1/1	0.96	0.27	27,27,27,27	0
57	MG	1A	3928	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3348	1/1	0.96	0.08	51,51,51,51	0
57	MG	1E	310	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3929	1/1	0.96	0.06	55,55,55,55	0
57	MG	2a	1657	1/1	0.96	0.14	56,56,56,56	0
57	MG	1A	3930	1/1	0.96	0.08	44,44,44,44	0
57	MG	1E	313	1/1	0.96	0.07	48,48,48,48	0
57	MG	1a	1706	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3931	1/1	0.96	0.05	35,35,35,35	0
57	MG	2A	3660	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3746	1/1	0.96	0.12	26,26,26,26	0
57	MG	2a	1665	1/1	0.96	0.22	43,43,43,43	0
57	MG	1A	3023	1/1	0.96	0.04	17,17,17,17	0
57	MG	2A	3105	1/1	0.96	0.07	59,59,59,59	0
57	MG	2A	3665	1/1	0.96	0.09	56,56,56,56	0
57	MG	2A	3668	1/1	0.96	0.06	58,58,58,58	0
57	MG	2A	3360	1/1	0.96	0.17	46,46,46,46	0
57	MG	1F	307	1/1	0.96	0.09	29,29,29,29	0
57	MG	1A	3229	1/1	0.96	0.11	45,45,45,45	0
57	MG	2A	3363	1/1	0.96	0.13	43,43,43,43	0
57	MG	1A	3072	1/1	0.96	0.27	37,37,37,37	0
57	MG	2A	3674	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3182	1/1	0.96	0.12	60,60,60,60	0
57	MG	1A	3754	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3757	1/1	0.96	0.09	25,25,25,25	0
57	MG	1A	3943	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3402	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3143	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3036	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3483	1/1	0.96	0.06	43,43,43,43	0
57	MG	2a	1686	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3186	1/1	0.96	0.14	55,55,55,55	0
57	MG	2A	3120	1/1	0.96	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3121	1/1	0.96	0.20	64,64,64,64	0
57	MG	1O	204	1/1	0.96	0.07	63,63,63,63	0
57	MG	1P	203	1/1	0.96	0.19	29,29,29,29	0
57	MG	1a	1726	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3125	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3407	1/1	0.96	0.05	45,45,45,45	0
57	MG	1A	3768	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3129	1/1	0.96	0.17	50,50,50,50	0
57	MG	2A	3696	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3698	1/1	0.96	0.07	39,39,39,39	0
57	MG	2a	1701	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3130	1/1	0.96	0.07	72,72,72,72	0
57	MG	1A	3952	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3132	1/1	0.96	0.11	43,43,43,43	0
57	MG	1Q	202	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3486	1/1	0.96	0.07	39,39,39,39	0
57	MG	1Q	205	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3708	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3289	1/1	0.96	0.09	29,29,29,29	0
57	MG	2A	3392	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3290	1/1	0.96	0.21	40,40,40,40	0
57	MG	1A	3490	1/1	0.96	0.17	49,49,49,49	0
57	MG	2A	3140	1/1	0.96	0.20	38,38,38,38	0
57	MG	1A	3016	1/1	0.96	0.19	51,51,51,51	0
57	MG	2A	3142	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3189	1/1	0.96	0.06	46,46,46,46	0
57	MG	1A	3294	1/1	0.96	0.15	31,31,31,31	0
57	MG	1A	3240	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3783	1/1	0.96	0.06	26,26,26,26	0
57	MG	2A	3405	1/1	0.96	0.09	41,41,41,41	0
57	MG	1S	202	1/1	0.96	0.14	57,57,57,57	0
57	MG	1A	3965	1/1	0.96	0.08	41,41,41,41	0
57	MG	2A	3408	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3496	1/1	0.96	0.12	54,54,54,54	0
57	MG	2A	3731	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	3094	1/1	0.96	0.07	18,18,18,18	0
57	MG	2A	3733	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3501	1/1	0.96	0.12	31,31,31,31	0
57	MG	1A	3971	1/1	0.96	0.05	30,30,30,30	0
57	MG	1a	1753	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3615	1/1	0.96	0.04	48,48,48,48	0
57	MG	1V	201	1/1	0.96	0.31	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3974	1/1	0.96	0.07	29,29,29,29	0
57	MG	2A	3161	1/1	0.96	0.23	38,38,38,38	0
57	MG	2A	3743	1/1	0.96	0.13	55,55,55,55	0
57	MG	1A	3975	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3616	1/1	0.96	0.09	23,23,23,23	0
57	MG	1W	201	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3350	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3748	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3422	1/1	0.96	0.08	53,53,53,53	0
57	MG	1a	1761	1/1	0.96	0.05	35,35,35,35	0
57	MG	1A	3351	1/1	0.96	0.15	48,48,48,48	0
57	MG	1W	204	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3426	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3619	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3352	1/1	0.96	0.07	46,46,46,46	0
57	MG	1X	105	1/1	0.96	0.05	38,38,38,38	0
57	MG	2A	3172	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3192	1/1	0.96	0.23	25,25,25,25	0
57	MG	2A	3432	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3007	1/1	0.96	0.08	26,26,26,26	0
57	MG	2A	3766	1/1	0.96	0.08	47,47,47,47	0
57	MG	1a	1770	1/1	0.96	0.10	65,65,65,65	0
57	MG	1a	1771	1/1	0.96	0.05	67,67,67,67	0
57	MG	1A	3630	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3355	1/1	0.96	0.08	46,46,46,46	0
57	MG	1Z	302	1/1	0.96	0.06	57,57,57,57	0
57	MG	2a	1761	1/1	0.96	0.09	41,41,41,41	0
57	MG	2A	3440	1/1	0.96	0.10	42,42,42,42	0
57	MG	10	101	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3356	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3509	1/1	0.96	0.08	41,41,41,41	0
57	MG	2A	3777	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3183	1/1	0.96	0.06	46,46,46,46	0
57	MG	2A	3447	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3357	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3511	1/1	0.96	0.04	35,35,35,35	0
57	MG	1A	3637	1/1	0.96	0.07	35,35,35,35	0
57	MG	1a	1781	1/1	0.96	0.12	44,44,44,44	0
57	MG	2a	1776	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	3820	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3194	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3787	1/1	0.96	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4004	1/1	0.96	0.13	50,50,50,50	0
57	MG	2A	3456	1/1	0.96	0.12	69,69,69,69	0
57	MG	2A	3790	1/1	0.96	0.06	41,41,41,41	0
57	MG	1a	1788	1/1	0.96	0.10	40,40,40,40	0
57	MG	11	102	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3514	1/1	0.96	0.15	33,33,33,33	0
57	MG	12	101	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3359	1/1	0.96	0.16	33,33,33,33	0
57	MG	2A	3197	1/1	0.96	0.06	48,48,48,48	0
57	MG	2A	3799	1/1	0.96	0.06	34,34,34,34	0
57	MG	13	102	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	4009	1/1	0.96	0.06	48,48,48,48	0
57	MG	13	104	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3517	1/1	0.96	0.14	30,30,30,30	0
57	MG	1A	3828	1/1	0.96	0.10	48,48,48,48	0
57	MG	15	103	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3829	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3809	1/1	0.96	0.05	52,52,52,52	0
57	MG	2A	3812	1/1	0.96	0.16	54,54,54,54	0
57	MG	1A	3151	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3428	1/1	0.96	0.13	45,45,45,45	0
57	MG	2A	3210	1/1	0.96	0.14	42,42,42,42	0
57	MG	1A	3196	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3834	1/1	0.96	0.13	46,46,46,46	0
57	MG	1A	3650	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3153	1/1	0.96	0.08	36,36,36,36	0
57	MG	17	103	1/1	0.96	0.10	31,31,31,31	0
57	MG	17	104	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3006	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3829	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3365	1/1	0.96	0.09	39,39,39,39	0
57	MG	2A	3484	1/1	0.96	0.11	43,43,43,43	0
57	MG	2A	3219	1/1	0.96	0.21	59,59,59,59	0
57	MG	2A	3834	1/1	0.96	0.09	55,55,55,55	0
57	MG	2A	3221	1/1	0.96	0.12	42,42,42,42	0
57	MG	18	103	1/1	0.96	0.19	49,49,49,49	0
57	MG	2A	3489	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3839	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3081	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3842	1/1	0.96	0.07	46,46,46,46	0
57	MG	2a	1823	1/1	0.96	0.13	59,59,59,59	0
57	MG	1n	101	1/1	0.96	0.27	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4037	1/1	0.96	0.06	50,50,50,50	0
57	MG	2A	3230	1/1	0.96	0.15	51,51,51,51	0
57	MG	1A	3306	1/1	0.96	0.13	49,49,49,49	0
57	MG	1A	3009	1/1	0.96	0.07	32,32,32,32	0
57	MG	1r	101	1/1	0.96	0.18	51,51,51,51	0
57	MG	1A	3029	1/1	0.96	0.15	24,24,24,24	0
57	MG	2A	3235	1/1	0.96	0.07	47,47,47,47	0
57	MG	1a	1604	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3848	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3849	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	4046	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3508	1/1	0.96	0.20	50,50,50,50	0
57	MG	1A	4048	1/1	0.96	0.09	18,18,18,18	0
57	MG	1A	4050	1/1	0.96	0.08	23,23,23,23	0
57	MG	2A	3515	1/1	0.96	0.08	46,46,46,46	0
57	MG	1a	1612	1/1	0.96	0.04	67,67,67,67	0
57	MG	1A	3850	1/1	0.96	0.05	50,50,50,50	0
57	MG	1A	4053	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3530	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3309	1/1	0.96	0.08	34,34,34,34	0
57	MG	1a	1618	1/1	0.96	0.04	52,52,52,52	0
57	MG	1A	3668	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3160	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3129	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3858	1/1	0.96	0.07	57,57,57,57	0
57	MG	2A	3004	1/1	0.96	0.35	59,59,59,59	0
57	MG	1A	3672	1/1	0.96	0.11	21,21,21,21	0
57	MG	1A	3444	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3445	1/1	0.96	0.34	44,44,44,44	0
57	MG	1A	3539	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3864	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3374	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	4073	1/1	0.96	0.12	42,42,42,42	0
59	ERY	1A	4087	51/51	0.96	0.10	25,42,54,59	0
57	MG	2A	3014	1/1	0.96	0.11	41,41,41,41	0
60	ZN	14	102	1/1	0.96	0.11	118,118,118,118	0
60	ZN	24	501	1/1	0.96	0.13	137,137,137,137	0
60	ZN	2n	501	1/1	0.96	0.05	94,94,94,94	0
57	MG	2E	307	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3042	1/1	0.97	0.04	21,21,21,21	0
57	MG	1a	1645	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3728	1/1	0.97	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3198	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3043	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3590	1/1	0.97	0.10	24,24,24,24	0
57	MG	2F	305	1/1	0.97	0.18	51,51,51,51	0
57	MG	2A	3295	1/1	0.97	0.10	55,55,55,55	0
57	MG	1a	1650	1/1	0.97	0.13	48,48,48,48	0
57	MG	2A	3297	1/1	0.97	0.25	35,35,35,35	0
57	MG	1a	1651	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3901	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3360	1/1	0.97	0.15	39,39,39,39	0
57	MG	1A	3500	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3593	1/1	0.97	0.05	38,38,38,38	0
57	MG	2T	201	1/1	0.97	0.09	57,57,57,57	0
57	MG	1A	3159	1/1	0.97	0.08	36,36,36,36	0
57	MG	1a	1658	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3741	1/1	0.97	0.06	34,34,34,34	0
57	MG	1B	219	1/1	0.97	0.07	45,45,45,45	0
57	MG	1B	221	1/1	0.97	0.04	40,40,40,40	0
57	MG	1B	222	1/1	0.97	0.06	36,36,36,36	0
57	MG	1B	223	1/1	0.97	0.05	30,30,30,30	0
57	MG	2X	101	1/1	0.97	0.06	68,68,68,68	0
57	MG	1A	3080	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3064	1/1	0.97	0.12	41,41,41,41	0
57	MG	2A	3060	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3054	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3601	1/1	0.97	0.14	26,26,26,26	0
57	MG	1A	3747	1/1	0.97	0.07	27,27,27,27	0
57	MG	23	102	1/1	0.97	0.06	56,56,56,56	0
57	MG	1A	3602	1/1	0.97	0.24	34,34,34,34	0
57	MG	1B	230	1/1	0.97	0.08	41,41,41,41	0
57	MG	1A	3429	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3319	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3918	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3751	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3921	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3922	1/1	0.97	0.04	17,17,17,17	0
57	MG	1A	3013	1/1	0.97	0.14	23,23,23,23	0
57	MG	1B	237	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3605	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3606	1/1	0.97	0.04	38,38,38,38	0
57	MG	1D	304	1/1	0.97	0.15	47,47,47,47	0
57	MG	1D	305	1/1	0.97	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3617	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3755	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3619	1/1	0.97	0.12	61,61,61,61	0
57	MG	1D	308	1/1	0.97	0.17	31,31,31,31	0
57	MG	2A	3080	1/1	0.97	0.10	46,46,46,46	0
57	MG	1D	310	1/1	0.97	0.04	45,45,45,45	0
57	MG	1A	3756	1/1	0.97	0.07	47,47,47,47	0
57	MG	2A	3084	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3607	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3608	1/1	0.97	0.04	28,28,28,28	0
57	MG	1a	1690	1/1	0.97	0.22	51,51,51,51	0
57	MG	1E	302	1/1	0.97	0.16	35,35,35,35	0
57	MG	2A	3634	1/1	0.97	0.13	50,50,50,50	0
57	MG	2A	3635	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3609	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3610	1/1	0.97	0.06	34,34,34,34	0
57	MG	2a	1623	1/1	0.97	0.10	44,44,44,44	0
57	MG	2A	3091	1/1	0.97	0.04	44,44,44,44	0
57	MG	2A	3344	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3252	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3253	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3433	1/1	0.97	0.14	55,55,55,55	0
57	MG	2A	3350	1/1	0.97	0.26	42,42,42,42	0
57	MG	1A	3936	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3937	1/1	0.97	0.05	44,44,44,44	0
57	MG	1a	1699	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3938	1/1	0.97	0.08	58,58,58,58	0
57	MG	1A	3767	1/1	0.97	0.06	35,35,35,35	0
57	MG	1F	302	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3614	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3204	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3942	1/1	0.97	0.04	40,40,40,40	0
57	MG	1F	308	1/1	0.97	0.28	35,35,35,35	0
57	MG	1F	309	1/1	0.97	0.07	48,48,48,48	0
57	MG	2A	3656	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	3164	1/1	0.97	0.16	36,36,36,36	0
57	MG	2A	3109	1/1	0.97	0.14	43,43,43,43	0
57	MG	1A	3771	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3945	1/1	0.97	0.06	47,47,47,47	0
57	MG	1a	1712	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3313	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3107	1/1	0.97	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1G	204	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3667	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3515	1/1	0.97	0.13	33,33,33,33	0
57	MG	1A	3109	1/1	0.97	0.33	31,31,31,31	0
57	MG	1N	202	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3777	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3778	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3625	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3056	1/1	0.97	0.19	41,41,41,41	0
57	MG	1O	203	1/1	0.97	0.08	56,56,56,56	0
57	MG	1A	3954	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3677	1/1	0.97	0.16	38,38,38,38	0
57	MG	1A	3782	1/1	0.97	0.06	28,28,28,28	0
57	MG	2a	1662	1/1	0.97	0.09	48,48,48,48	0
57	MG	2A	3127	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3381	1/1	0.97	0.07	55,55,55,55	0
57	MG	1A	3211	1/1	0.97	0.14	46,46,46,46	0
57	MG	1A	3784	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3787	1/1	0.97	0.04	52,52,52,52	0
57	MG	1A	3628	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3960	1/1	0.97	0.10	54,54,54,54	0
57	MG	2A	3387	1/1	0.97	0.07	51,51,51,51	0
57	MG	1a	1733	1/1	0.97	0.05	39,39,39,39	0
57	MG	2a	1672	1/1	0.97	0.08	64,64,64,64	0
57	MG	1A	3629	1/1	0.97	0.09	31,31,31,31	0
57	MG	2A	3689	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3794	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3963	1/1	0.97	0.06	68,68,68,68	0
57	MG	1A	3169	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3393	1/1	0.97	0.11	51,51,51,51	0
57	MG	2a	1679	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3442	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3797	1/1	0.97	0.05	17,17,17,17	0
57	MG	1A	3443	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3397	1/1	0.97	0.21	39,39,39,39	0
57	MG	1A	3633	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3262	1/1	0.97	0.27	42,42,42,42	0
57	MG	1A	3802	1/1	0.97	0.06	40,40,40,40	0
57	MG	1a	1746	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3973	1/1	0.97	0.07	21,21,21,21	0
57	MG	2A	3707	1/1	0.97	0.10	53,53,53,53	0
57	MG	1U	201	1/1	0.97	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3709	1/1	0.97	0.05	51,51,51,51	0
57	MG	1a	1749	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3137	1/1	0.97	0.23	31,31,31,31	0
57	MG	2A	3152	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3804	1/1	0.97	0.04	41,41,41,41	0
57	MG	1U	205	1/1	0.97	0.04	40,40,40,40	0
57	MG	1A	3805	1/1	0.97	0.06	38,38,38,38	0
57	MG	1U	207	1/1	0.97	0.19	30,30,30,30	0
57	MG	1U	208	1/1	0.97	0.28	33,33,33,33	0
57	MG	1A	3806	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3138	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3982	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3034	1/1	0.97	0.33	31,31,31,31	0
57	MG	2A	3724	1/1	0.97	0.14	45,45,45,45	0
57	MG	2A	3725	1/1	0.97	0.05	45,45,45,45	0
57	MG	1V	204	1/1	0.97	0.14	38,38,38,38	0
57	MG	1V	205	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3984	1/1	0.97	0.14	17,17,17,17	0
57	MG	2A	3729	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	3527	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3216	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3069	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3643	1/1	0.97	0.06	39,39,39,39	0
57	MG	1a	1767	1/1	0.97	0.10	54,54,54,54	0
57	MG	1A	3113	1/1	0.97	0.08	31,31,31,31	0
57	MG	1W	205	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3993	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3645	1/1	0.97	0.06	22,22,22,22	0
57	MG	1X	103	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3269	1/1	0.97	0.11	29,29,29,29	0
57	MG	2A	3742	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3453	1/1	0.97	0.10	47,47,47,47	0
57	MG	2a	1725	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3271	1/1	0.97	0.08	37,37,37,37	0
57	MG	2A	3433	1/1	0.97	0.23	46,46,46,46	0
57	MG	1Y	201	1/1	0.97	0.14	43,43,43,43	0
57	MG	1A	3011	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3822	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3823	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3651	1/1	0.97	0.06	37,37,37,37	0
57	MG	10	102	1/1	0.97	0.17	46,46,46,46	0
57	MG	2A	3753	1/1	0.97	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1782	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3825	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	4006	1/1	0.97	0.07	61,61,61,61	0
57	MG	2A	3757	1/1	0.97	0.08	42,42,42,42	0
57	MG	10	105	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3146	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3446	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	4008	1/1	0.97	0.09	44,44,44,44	0
57	MG	1a	1791	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3537	1/1	0.97	0.13	26,26,26,26	0
57	MG	2A	3193	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3655	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3538	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	4013	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	4015	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3771	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3331	1/1	0.97	0.04	30,30,30,30	0
57	MG	1A	4018	1/1	0.97	0.04	47,47,47,47	0
57	MG	1A	3831	1/1	0.97	0.16	29,29,29,29	0
57	MG	1A	3221	1/1	0.97	0.04	31,31,31,31	0
57	MG	1a	1803	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3541	1/1	0.97	0.11	35,35,35,35	0
57	MG	2A	3463	1/1	0.97	0.12	45,45,45,45	0
57	MG	2A	3204	1/1	0.97	0.04	52,52,52,52	0
57	MG	2A	3780	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3278	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3334	1/1	0.97	0.12	41,41,41,41	0
57	MG	1A	3092	1/1	0.97	0.19	47,47,47,47	0
57	MG	2A	3209	1/1	0.97	0.19	62,62,62,62	0
57	MG	1A	3666	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3462	1/1	0.97	0.09	51,51,51,51	0
57	MG	15	105	1/1	0.97	0.30	35,35,35,35	0
57	MG	1A	4030	1/1	0.97	0.11	47,47,47,47	0
57	MG	2a	1770	1/1	0.97	0.05	68,68,68,68	0
57	MG	1A	3336	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3464	1/1	0.97	0.25	30,30,30,30	0
57	MG	1A	4035	1/1	0.97	0.09	16,16,16,16	0
57	MG	2A	3792	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3465	1/1	0.97	0.15	41,41,41,41	0
57	MG	1A	3225	1/1	0.97	0.06	21,21,21,21	0
57	MG	1A	3398	1/1	0.97	0.10	37,37,37,37	0
57	MG	2A	3220	1/1	0.97	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1l	202	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3676	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3553	1/1	0.97	0.15	36,36,36,36	0
57	MG	2A	3224	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3485	1/1	0.97	0.07	44,44,44,44	0
57	MG	18	101	1/1	0.97	0.10	48,48,48,48	0
57	MG	2A	3804	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3399	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3116	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3684	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	3184	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3810	1/1	0.97	0.12	38,38,38,38	0
57	MG	2a	1792	1/1	0.97	0.12	33,33,33,33	0
57	MG	2A	3811	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	4049	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3119	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3560	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3693	1/1	0.97	0.07	29,29,29,29	0
57	MG	1A	4054	1/1	0.97	0.04	25,25,25,25	0
57	MG	1w	106	1/1	0.97	0.06	66,66,66,66	0
57	MG	1A	4056	1/1	0.97	0.07	44,44,44,44	0
57	MG	2A	3824	1/1	0.97	0.07	26,26,26,26	0
57	MG	1A	3561	1/1	0.97	0.34	34,34,34,34	0
57	MG	1a	1606	1/1	0.97	0.16	60,60,60,60	0
57	MG	1A	3150	1/1	0.97	0.16	26,26,26,26	0
57	MG	1x	106	1/1	0.97	0.11	51,51,51,51	0
57	MG	1x	108	1/1	0.97	0.08	22,22,22,22	0
57	MG	1a	1608	1/1	0.97	0.15	56,56,56,56	0
57	MG	2A	3831	1/1	0.97	0.12	55,55,55,55	0
57	MG	1A	3696	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3697	1/1	0.97	0.05	55,55,55,55	0
57	MG	2A	3509	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	4063	1/1	0.97	0.09	53,53,53,53	0
57	MG	2a	1813	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3862	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3512	1/1	0.97	0.17	54,54,54,54	0
57	MG	1A	3187	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3699	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3700	1/1	0.97	0.04	25,25,25,25	0
57	MG	2A	3251	1/1	0.97	0.23	45,45,45,45	0
57	MG	1a	1616	1/1	0.97	0.04	42,42,42,42	0
57	MG	1A	3405	1/1	0.97	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
57	MG	2A	3007	1/1	0.97	0.06	40,40,40,40	0
57	MG	2a	1824	1/1	0.97	0.13	47,47,47,47	0
57	MG	2A	3008	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3256	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3702	1/1	0.97	0.15	26,26,26,26	0
57	MG	2A	3525	1/1	0.97	0.08	28,28,28,28	0
57	MG	1a	1619	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3343	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3528	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3476	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3705	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3532	1/1	0.97	0.14	44,44,44,44	0
57	MG	1A	3012	1/1	0.97	0.11	32,32,32,32	0
57	MG	1A	3707	1/1	0.97	0.04	17,17,17,17	0
57	MG	2A	3535	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3408	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3152	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3538	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3019	1/1	0.97	0.06	35,35,35,35	0
57	MG	1A	3039	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3481	1/1	0.97	0.08	26,26,26,26	0
57	MG	2A	3022	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3482	1/1	0.97	0.13	28,28,28,28	0
57	MG	1A	3191	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3349	1/1	0.97	0.09	53,53,53,53	0
57	MG	1A	3154	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3552	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3238	1/1	0.97	0.20	33,33,33,33	0
57	MG	1A	3487	1/1	0.97	0.07	39,39,39,39	0
57	MG	1a	1635	1/1	0.97	0.22	67,67,67,67	0
57	MG	1A	4086	1/1	0.97	0.20	36,36,36,36	0
57	MG	1A	3239	1/1	0.97	0.15	47,47,47,47	0
57	MG	1A	3076	1/1	0.97	0.04	33,33,33,33	0
57	MG	2D	305	1/1	0.97	0.21	45,45,45,45	0
57	MG	1A	3123	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3283	1/1	0.97	0.07	53,53,53,53	0
57	MG	2A	3034	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	3242	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3019	1/1	0.97	0.19	41,41,41,41	0
57	MG	1A	3895	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3244	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3347	1/1	0.98	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4052	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3349	1/1	0.98	0.07	39,39,39,39	0
57	MG	1a	1675	1/1	0.98	0.15	44,44,44,44	0
57	MG	1T	203	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3385	1/1	0.98	0.06	25,25,25,25	0
57	MG	1U	202	1/1	0.98	0.10	29,29,29,29	0
57	MG	1A	3106	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3760	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	4055	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3920	1/1	0.98	0.05	38,38,38,38	0
57	MG	2A	3763	1/1	0.98	0.03	39,39,39,39	0
57	MG	1A	3807	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3017	1/1	0.98	0.12	54,54,54,54	0
57	MG	1A	3550	1/1	0.98	0.18	33,33,33,33	0
57	MG	1a	1685	1/1	0.98	0.11	35,35,35,35	0
57	MG	2A	3555	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3035	1/1	0.98	0.15	37,37,37,37	0
57	MG	1A	3170	1/1	0.98	0.04	42,42,42,42	0
57	MG	1U	211	1/1	0.98	0.35	34,34,34,34	0
57	MG	1A	3621	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3813	1/1	0.98	0.05	50,50,50,50	0
57	MG	2A	3561	1/1	0.98	0.06	35,35,35,35	0
57	MG	1V	203	1/1	0.98	0.21	28,28,28,28	0
57	MG	1A	3493	1/1	0.98	0.06	30,30,30,30	0
57	MG	2A	3564	1/1	0.98	0.07	38,38,38,38	0
57	MG	2A	3017	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3624	1/1	0.98	0.10	30,30,30,30	0
57	MG	1A	3293	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3207	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3818	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3295	1/1	0.98	0.18	35,35,35,35	0
57	MG	1A	3557	1/1	0.98	0.26	46,46,46,46	0
57	MG	1A	3140	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3559	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3499	1/1	0.98	0.16	24,24,24,24	0
57	MG	1A	3209	1/1	0.98	0.25	31,31,31,31	0
57	MG	1a	1703	1/1	0.98	0.08	52,52,52,52	0
57	MG	1X	102	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3003	1/1	0.98	0.03	27,27,27,27	0
57	MG	1X	104	1/1	0.98	0.05	33,33,33,33	0
57	MG	2A	3581	1/1	0.98	0.10	40,40,40,40	0
57	MG	1A	3563	1/1	0.98	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3795	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3396	1/1	0.98	0.04	30,30,30,30	0
57	MG	2A	3207	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3173	1/1	0.98	0.32	40,40,40,40	0
57	MG	1A	3174	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3727	1/1	0.98	0.12	52,52,52,52	0
57	MG	1A	3638	1/1	0.98	0.03	21,21,21,21	0
57	MG	1A	3729	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3142	1/1	0.98	0.09	35,35,35,35	0
57	MG	2a	1693	1/1	0.98	0.04	57,57,57,57	0
57	MG	2A	3594	1/1	0.98	0.06	47,47,47,47	0
57	MG	1A	3568	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3806	1/1	0.98	0.09	39,39,39,39	0
57	MG	1B	202	1/1	0.98	0.11	38,38,38,38	0
57	MG	1A	3451	1/1	0.98	0.06	35,35,35,35	0
57	MG	2a	1699	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3733	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3734	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	3176	1/1	0.98	0.08	25,25,25,25	0
57	MG	1A	3177	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3840	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3015	1/1	0.98	0.14	26,26,26,26	0
57	MG	1A	3646	1/1	0.98	0.06	17,17,17,17	0
57	MG	1A	3843	1/1	0.98	0.12	44,44,44,44	0
57	MG	2A	3819	1/1	0.98	0.13	62,62,62,62	0
57	MG	2A	3606	1/1	0.98	0.11	55,55,55,55	0
57	MG	2A	3225	1/1	0.98	0.27	32,32,32,32	0
57	MG	2A	3404	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3010	1/1	0.98	0.06	34,34,34,34	0
57	MG	1a	1728	1/1	0.98	0.04	50,50,50,50	0
57	MG	1A	3259	1/1	0.98	0.12	33,33,33,33	0
57	MG	12	102	1/1	0.98	0.11	45,45,45,45	0
57	MG	1A	3744	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3847	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	3512	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3145	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3087	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3040	1/1	0.98	0.12	27,27,27,27	0
57	MG	15	101	1/1	0.98	0.10	33,33,33,33	0
57	MG	15	102	1/1	0.98	0.08	33,33,33,33	0
57	MG	2A	3621	1/1	0.98	0.07	44,44,44,44	0
57	MG	1B	220	1/1	0.98	0.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3653	1/1	0.98	0.07	40,40,40,40	0
57	MG	2A	3624	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3853	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3969	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3627	1/1	0.98	0.12	48,48,48,48	0
57	MG	2A	3067	1/1	0.98	0.05	38,38,38,38	0
57	MG	2A	3845	1/1	0.98	0.11	39,39,39,39	0
57	MG	2A	3629	1/1	0.98	0.08	35,35,35,35	0
57	MG	2A	3847	1/1	0.98	0.08	30,30,30,30	0
57	MG	1A	3750	1/1	0.98	0.04	49,49,49,49	0
57	MG	1A	3089	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3856	1/1	0.98	0.06	39,39,39,39	0
57	MG	2A	3851	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3311	1/1	0.98	0.08	40,40,40,40	0
57	MG	1A	3656	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	3222	1/1	0.98	0.11	42,42,42,42	0
57	MG	1A	3977	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3978	1/1	0.98	0.06	55,55,55,55	0
57	MG	17	106	1/1	0.98	0.03	35,35,35,35	0
57	MG	1A	3658	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3980	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3583	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3031	1/1	0.98	0.06	40,40,40,40	0
57	MG	2a	1749	1/1	0.98	0.14	44,44,44,44	0
57	MG	2A	3081	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3758	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3032	1/1	0.98	0.12	21,21,21,21	0
57	MG	1B	238	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3760	1/1	0.98	0.14	49,49,49,49	0
57	MG	1A	3226	1/1	0.98	0.16	30,30,30,30	0
57	MG	2A	3650	1/1	0.98	0.05	57,57,57,57	0
57	MG	1A	3867	1/1	0.98	0.04	25,25,25,25	0
57	MG	2A	3263	1/1	0.98	0.22	36,36,36,36	0
57	MG	1A	3522	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3664	1/1	0.98	0.04	32,32,32,32	0
57	MG	1D	307	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3070	1/1	0.98	0.12	19,19,19,19	0
57	MG	2a	1763	1/1	0.98	0.10	58,58,58,58	0
57	MG	2A	3448	1/1	0.98	0.05	45,45,45,45	0
57	MG	1D	309	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3995	1/1	0.98	0.07	28,28,28,28	0
57	MG	2D	302	1/1	0.98	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3270	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3871	1/1	0.98	0.13	24,24,24,24	0
57	MG	2A	3096	1/1	0.98	0.05	46,46,46,46	0
57	MG	2A	3663	1/1	0.98	0.03	33,33,33,33	0
57	MG	1A	3872	1/1	0.98	0.08	36,36,36,36	0
57	MG	2a	1773	1/1	0.98	0.10	43,43,43,43	0
57	MG	1A	3071	1/1	0.98	0.06	22,22,22,22	0
57	MG	2A	3666	1/1	0.98	0.09	52,52,52,52	0
57	MG	1A	3667	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3043	1/1	0.98	0.08	26,26,26,26	0
57	MG	2A	3458	1/1	0.98	0.03	28,28,28,28	0
57	MG	1E	304	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3272	1/1	0.98	0.06	41,41,41,41	0
57	MG	1E	306	1/1	0.98	0.04	35,35,35,35	0
57	MG	1A	3670	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3073	1/1	0.98	0.05	14,14,14,14	0
57	MG	1E	309	1/1	0.98	0.12	16,16,16,16	0
57	MG	1A	3369	1/1	0.98	0.05	24,24,24,24	0
57	MG	2F	306	1/1	0.98	0.11	49,49,49,49	0
57	MG	1A	3594	1/1	0.98	0.12	21,21,21,21	0
57	MG	1A	3595	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	3596	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3883	1/1	0.98	0.04	33,33,33,33	0
57	MG	1a	1786	1/1	0.98	0.04	43,43,43,43	0
57	MG	1a	1787	1/1	0.98	0.08	50,50,50,50	0
57	MG	1A	3057	1/1	0.98	0.12	25,25,25,25	0
57	MG	2R	202	1/1	0.98	0.05	44,44,44,44	0
57	MG	1F	303	1/1	0.98	0.19	34,34,34,34	0
57	MG	2R	204	1/1	0.98	0.05	36,36,36,36	0
57	MG	1A	3276	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3125	1/1	0.98	0.22	31,31,31,31	0
57	MG	2A	3118	1/1	0.98	0.06	47,47,47,47	0
57	MG	1a	1793	1/1	0.98	0.05	55,55,55,55	0
57	MG	1F	306	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3780	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3683	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	4017	1/1	0.98	0.05	39,39,39,39	0
57	MG	1F	310	1/1	0.98	0.08	36,36,36,36	0
57	MG	2Y	201	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3889	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	3126	1/1	0.98	0.22	34,34,34,34	0
57	MG	2A	3697	1/1	0.98	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1801	1/1	0.98	0.09	59,59,59,59	0
57	MG	1F	313	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3685	1/1	0.98	0.06	46,46,46,46	0
57	MG	1A	3893	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3279	1/1	0.98	0.07	39,39,39,39	0
57	MG	2a	1815	1/1	0.98	0.12	45,45,45,45	0
57	MG	26	101	1/1	0.98	0.14	41,41,41,41	0
57	MG	2A	3491	1/1	0.98	0.08	34,34,34,34	0
57	MG	1A	3785	1/1	0.98	0.06	48,48,48,48	0
57	MG	2A	3706	1/1	0.98	0.09	55,55,55,55	0
57	MG	1H	201	1/1	0.98	0.13	41,41,41,41	0
57	MG	1A	3786	1/1	0.98	0.10	18,18,18,18	0
57	MG	1A	3044	1/1	0.98	0.08	30,30,30,30	0
57	MG	1A	3788	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	4028	1/1	0.98	0.04	22,22,22,22	0
57	MG	2a	1825	1/1	0.98	0.09	53,53,53,53	0
57	MG	2A	3138	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	4029	1/1	0.98	0.03	41,41,41,41	0
57	MG	2A	3714	1/1	0.98	0.05	42,42,42,42	0
57	MG	2A	3500	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3535	1/1	0.98	0.08	24,24,24,24	0
57	MG	1a	1649	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3790	1/1	0.98	0.03	39,39,39,39	0
57	MG	2A	3143	1/1	0.98	0.22	44,44,44,44	0
57	MG	2A	3320	1/1	0.98	0.06	45,45,45,45	0
57	MG	2A	3506	1/1	0.98	0.14	45,45,45,45	0
57	MG	2l	203	1/1	0.98	0.06	63,63,63,63	0
57	MG	2A	3144	1/1	0.98	0.20	46,46,46,46	0
57	MG	1A	4033	1/1	0.98	0.11	58,58,58,58	0
57	MG	1A	3791	1/1	0.98	0.04	35,35,35,35	0
57	MG	1P	202	1/1	0.98	0.15	28,28,28,28	0
57	MG	1a	1654	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	3792	1/1	0.98	0.08	20,20,20,20	0
57	MG	1A	3692	1/1	0.98	0.07	22,22,22,22	0
57	MG	1A	3426	1/1	0.98	0.16	36,36,36,36	0
57	MG	1A	3033	1/1	0.98	0.05	28,28,28,28	0
57	MG	1Q	201	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3099	1/1	0.98	0.10	24,24,24,24	0
57	MG	1Q	203	1/1	0.98	0.09	40,40,40,40	0
57	MG	1A	3046	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	4042	1/1	0.98	0.03	26,26,26,26	0
57	MG	1A	4043	1/1	0.98	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3738	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3102	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3078	1/1	0.98	0.05	18,18,18,18	0
57	MG	1A	3381	1/1	0.98	0.06	62,62,62,62	0
57	MG	1A	4047	1/1	0.98	0.11	11,11,11,11	0
57	MG	1x	103	1/1	0.98	0.14	52,52,52,52	0
57	MG	1R	204	1/1	0.98	0.11	26,26,26,26	0
57	MG	2A	3530	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3914	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3047	1/1	0.98	0.04	28,28,28,28	0
57	MG	1x	107	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3165	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3105	1/1	0.98	0.07	27,27,27,27	0
60	ZN	25	102	1/1	0.98	0.03	80,80,80,80	0
57	MG	2A	3751	1/1	0.98	0.07	58,58,58,58	0
57	MG	1A	4064	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3764	1/1	0.99	0.06	28,28,28,28	0
57	MG	1A	4011	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3640	1/1	0.99	0.09	34,34,34,34	0
57	MG	2A	3545	1/1	0.99	0.05	37,37,37,37	0
57	MG	2A	3546	1/1	0.99	0.03	25,25,25,25	0
57	MG	2A	3702	1/1	0.99	0.07	34,34,34,34	0
57	MG	1A	3117	1/1	0.99	0.06	49,49,49,49	0
57	MG	2A	3548	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	4014	1/1	0.99	0.06	26,26,26,26	0
57	MG	1a	1740	1/1	0.99	0.04	27,27,27,27	0
57	MG	1a	1741	1/1	0.99	0.08	25,25,25,25	0
57	MG	1A	3118	1/1	0.99	0.06	22,22,22,22	0
57	MG	2A	3154	1/1	0.99	0.08	31,31,31,31	0
57	MG	1D	302	1/1	0.99	0.04	26,26,26,26	0
57	MG	2A	3632	1/1	0.99	0.02	39,39,39,39	0
57	MG	1A	3577	1/1	0.99	0.03	38,38,38,38	0
57	MG	2A	3092	1/1	0.99	0.04	37,37,37,37	0
57	MG	1A	3620	1/1	0.99	0.08	37,37,37,37	0
57	MG	2D	303	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3344	1/1	0.99	0.13	41,41,41,41	0
57	MG	2A	3716	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3970	1/1	0.99	0.08	22,22,22,22	0
57	MG	1A	3622	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3735	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3736	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3737	1/1	0.99	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3775	1/1	0.99	0.03	51,51,51,51	0
57	MG	1A	3275	1/1	0.99	0.27	29,29,29,29	0
57	MG	1A	4026	1/1	0.99	0.07	24,24,24,24	0
57	MG	1A	3892	1/1	0.99	0.06	43,43,43,43	0
57	MG	1A	3498	1/1	0.99	0.13	26,26,26,26	0
57	MG	1A	3082	1/1	0.99	0.18	33,33,33,33	0
57	MG	1A	3674	1/1	0.99	0.12	17,17,17,17	0
57	MG	2A	3572	1/1	0.99	0.03	36,36,36,36	0
57	MG	1T	202	1/1	0.99	0.14	40,40,40,40	0
57	MG	1A	3038	1/1	0.99	0.13	18,18,18,18	0
57	MG	1A	4032	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3026	1/1	0.99	0.05	39,39,39,39	0
57	MG	1A	3677	1/1	0.99	0.10	20,20,20,20	0
57	MG	2A	3815	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3678	1/1	0.99	0.06	21,21,21,21	0
57	MG	1A	3985	1/1	0.99	0.08	30,30,30,30	0
57	MG	2A	3818	1/1	0.99	0.08	21,21,21,21	0
57	MG	1A	3986	1/1	0.99	0.07	32,32,32,32	0
57	MG	2A	3820	1/1	0.99	0.09	57,57,57,57	0
57	MG	1A	3330	1/1	0.99	0.05	40,40,40,40	0
57	MG	2A	3822	1/1	0.99	0.05	45,45,45,45	0
57	MG	1A	3014	1/1	0.99	0.04	30,30,30,30	0
57	MG	2A	3583	1/1	0.99	0.06	34,34,34,34	0
57	MG	1A	3681	1/1	0.99	0.04	24,24,24,24	0
57	MG	1A	4041	1/1	0.99	0.02	23,23,23,23	0
57	MG	17	101	1/1	0.99	0.03	27,27,27,27	0
57	MG	17	102	1/1	0.99	0.05	25,25,25,25	0
57	MG	2A	3513	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3589	1/1	0.99	0.02	27,27,27,27	0
57	MG	2A	3590	1/1	0.99	0.06	31,31,31,31	0
57	MG	2A	3514	1/1	0.99	0.08	58,58,58,58	0
57	MG	1A	3133	1/1	0.99	0.19	35,35,35,35	0
57	MG	1A	3991	1/1	0.99	0.04	23,23,23,23	0
57	MG	1A	3086	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3906	1/1	0.99	0.02	29,29,29,29	0
57	MG	1A	3994	1/1	0.99	0.05	21,21,21,21	0
57	MG	1a	1715	1/1	0.99	0.04	49,49,49,49	0
57	MG	1A	3021	1/1	0.99	0.03	20,20,20,20	0
57	MG	1A	3136	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3686	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3998	1/1	0.99	0.07	25,25,25,25	0
57	MG	1A	3237	1/1	0.99	0.08	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3688	1/1	0.99	0.09	22,22,22,22	0
57	MG	1A	3689	1/1	0.99	0.05	17,17,17,17	0
57	MG	1A	3913	1/1	0.99	0.05	30,30,30,30	0
57	MG	1W	206	1/1	0.99	0.07	24,24,24,24	0
57	MG	1A	3721	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3197	1/1	0.99	0.05	18,18,18,18	0
57	MG	2A	3464	1/1	0.99	0.06	48,48,48,48	0
57	MG	1A	3723	1/1	0.99	0.07	40,40,40,40	0
57	MG	1A	3224	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3270	1/1	0.99	0.21	26,26,26,26	0
57	MG	1A	3100	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	4061	1/1	0.99	0.11	41,41,41,41	0
60	ZN	1Y	203	1/1	0.99	0.03	69,69,69,69	0
57	MG	1A	4062	1/1	0.99	0.08	33,33,33,33	0
60	ZN	15	110	1/1	0.99	0.04	43,43,43,43	0
60	ZN	16	103	1/1	0.99	0.03	41,41,41,41	0
60	ZN	19	501	1/1	0.99	0.09	56,56,56,56	0
60	ZN	1n	104	1/1	0.99	0.03	55,55,55,55	0
60	ZN	2Y	202	1/1	0.99	0.03	103,103,103,103	0
57	MG	1A	3108	1/1	0.99	0.08	25,25,25,25	0
57	MG	2A	3540	1/1	0.99	0.07	32,32,32,32	0
60	ZN	26	102	1/1	0.99	0.04	59,59,59,59	0
60	ZN	29	501	1/1	0.99	0.03	66,66,66,66	0
57	MG	2A	3695	1/1	0.99	0.03	45,45,45,45	0
61	SF4	1d	302	8/8	0.99	0.04	46,48,60,61	0
61	SF4	2d	303	8/8	0.99	0.03	57,71,80,82	0
57	MG	2A	3550	1/1	1.00	0.10	29,29,29,29	0
57	MG	1A	3924	1/1	1.00	0.05	17,17,17,17	0
57	MG	1P	201	1/1	1.00	0.10	26,26,26,26	0
57	MG	1A	3798	1/1	1.00	0.04	22,22,22,22	0
57	MG	1a	1790	1/1	1.00	0.03	37,37,37,37	0
57	MG	1A	3905	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.