



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 05:51 AM EDT

PDB ID : 8CVK / pdb_00008cvk
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNA^{phe}, peptidyl P-site fMRC-NH-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.50Å resolution
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Deposited on : 2022-05-18
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

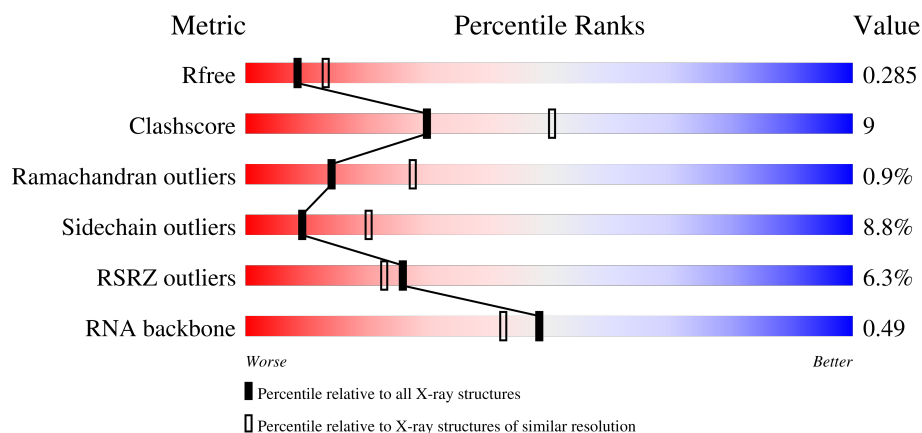
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 66% 27% 6%
1	2A	2915	4% 58% 31% 7%
2	1B	121	67% 31%
2	2B	121	56% 35% 8%

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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	2w	76	
55	1x	77	
55	2x	77	
56	1z	3	
56	2z	3	
57	1y	76	
57	2y	76	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300017 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 MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Phe-NH-tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1603	722	287	518	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMRC-NH-tRNA^{met} 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-NH-tRNA^{met} 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 a RNA chain called E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1098	Total	Mg	0	0
			1098	1098		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	12	Total 12	Mg 12	0	0
58	1E	13	Total 13	Mg 13	0	0
58	1F	14	Total 14	Mg 14	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	6	Total 6	Mg 6	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	4	Total 4	Mg 4	0	0
58	1Q	8	Total 8	Mg 8	0	0
58	1R	4	Total 4	Mg 4	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	4	Total 4	Mg 4	0	0
58	1U	9	Total 9	Mg 9	0	0
58	1V	7	Total 7	Mg 7	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	6	Total 6	Mg 6	0	0
58	1Y	5	Total 5	Mg 5	0	0
58	1Z	2	Total 2	Mg 2	0	0
58	10	9	Total 9	Mg 9	0	0
58	11	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	12	3	Total 3	Mg 3	0	0
58	13	3	Total 3	Mg 3	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	7	Total 7	Mg 7	0	0
58	16	1	Total 1	Mg 1	0	0
58	17	4	Total 4	Mg 4	0	0
58	18	9	Total 9	Mg 9	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	214	Total 214	Mg 214	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1k	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1v	1	Total 1	Mg 1	0	0
58	1w	8	Total 8	Mg 8	0	0
58	1x	12	Total 12	Mg 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2A	870	Total 870	Mg 870	0	0
58	2B	20	Total 20	Mg 20	0	0
58	2D	8	Total 8	Mg 8	0	0
58	2E	10	Total 10	Mg 10	0	0
58	2F	8	Total 8	Mg 8	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2O	1	Total 1	Mg 1	0	0
58	2P	2	Total 2	Mg 2	0	0
58	2Q	2	Total 2	Mg 2	0	0
58	2R	1	Total 1	Mg 1	0	0
58	2T	1	Total 1	Mg 1	0	0
58	2U	2	Total 2	Mg 2	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	4	Total 4	Mg 4	0	0
58	2X	3	Total 3	Mg 3	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	2	Total 2	Mg 2	0	0
58	23	3	Total 3	Mg 3	0	0
58	25	5	Total 5	Mg 5	0	0
58	26	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	27	3	Total 3	Mg 3	0	0
58	28	3	Total 3	Mg 3	0	0
58	29	1	Total 1	Mg 1	0	0
58	2a	235	Total 235	Mg 235	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2i	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2k	1	Total 1	Mg 1	0	0
58	2l	4	Total 4	Mg 4	0	0
58	2n	2	Total 2	Mg 2	0	0
58	2q	3	Total 3	Mg 3	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	1	Total 1	Mg 1	0	0
58	2v	3	Total 3	Mg 3	0	0
58	2w	5	Total 5	Mg 5	0	0
58	2x	7	Total 7	Mg 7	0	0
58	2y	1	Total 1	Mg 1	0	0

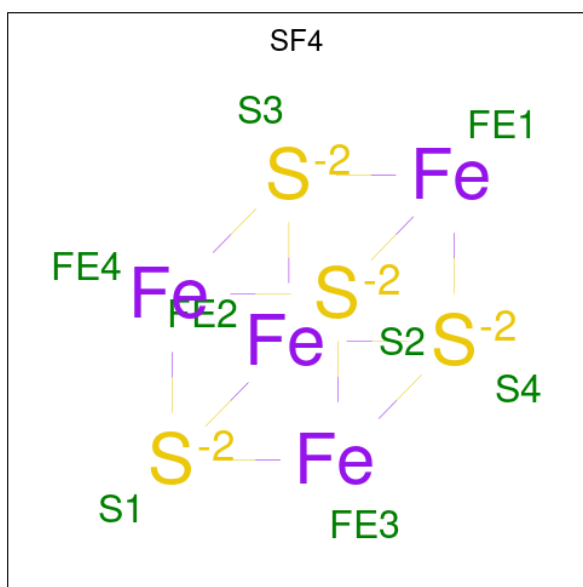
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0
59	2A	1	Total K 1 1	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
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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	1968	Total	O	0	0
			1968	1968		
62	1B	61	Total	O	0	0
			61	61		
62	1D	31	Total	O	0	0
			31	31		
62	1E	29	Total	O	0	0
			29	29		
62	1F	22	Total	O	0	0
			22	22		
62	1G	2	Total	O	0	0
			2	2		
62	1H	2	Total	O	0	0
			2	2		
62	1I	1	Total	O	0	0
			1	1		
62	1N	5	Total	O	0	0
			5	5		
62	1O	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	20	Total 20	O 20	0	0
62	1Q	6	Total 6	O 6	0	0
62	1R	15	Total 15	O 15	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	8	Total 8	O 8	0	0
62	1U	11	Total 11	O 11	0	0
62	1V	7	Total 7	O 7	0	0
62	1W	5	Total 5	O 5	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	14	Total 14	O 14	0	0
62	11	10	Total 10	O 10	0	0
62	12	3	Total 3	O 3	0	0
62	13	5	Total 5	O 5	0	0
62	14	1	Total 1	O 1	0	0
62	15	7	Total 7	O 7	0	0
62	16	3	Total 3	O 3	0	0
62	17	10	Total 10	O 10	0	0
62	18	10	Total 10	O 10	0	0
62	1a	340	Total 340	O 340	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1b	1	Total 1	O 1	0	0
62	1e	2	Total 2	O 2	0	0
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	8	Total 8	O 8	0	0
62	1m	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	4	Total 4	O 4	0	0
62	1w	9	Total 9	O 9	0	0
62	1x	9	Total 9	O 9	0	0
62	1z	1	Total 1	O 1	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1091	Total 1091	O 1091	0	0
62	2B	23	Total 23	O 23	0	0
62	2D	21	Total 21	O 21	0	0
62	2E	11	Total 11	O 11	0	0
62	2F	13	Total 13	O 13	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	13	Total 13	O 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2Q	1	Total	O	0	0
			1	1		
62	2R	4	Total	O	0	0
			4	4		
62	2T	6	Total	O	0	0
			6	6		
62	2U	3	Total	O	0	0
			3	3		
62	2W	1	Total	O	0	0
			1	1		
62	2X	3	Total	O	0	0
			3	3		
62	2Y	1	Total	O	0	0
			1	1		
62	2Z	1	Total	O	0	0
			1	1		
62	20	4	Total	O	0	0
			4	4		
62	21	9	Total	O	0	0
			9	9		
62	23	2	Total	O	0	0
			2	2		
62	25	1	Total	O	0	0
			1	1		
62	27	4	Total	O	0	0
			4	4		
62	28	3	Total	O	0	0
			3	3		
62	29	1	Total	O	0	0
			1	1		
62	2a	216	Total	O	0	0
			216	216		
62	2d	2	Total	O	0	0
			2	2		
62	2e	1	Total	O	0	0
			1	1		
62	2i	1	Total	O	0	0
			1	1		
62	2j	2	Total	O	0	0
			2	2		
62	2l	6	Total	O	0	0
			6	6		

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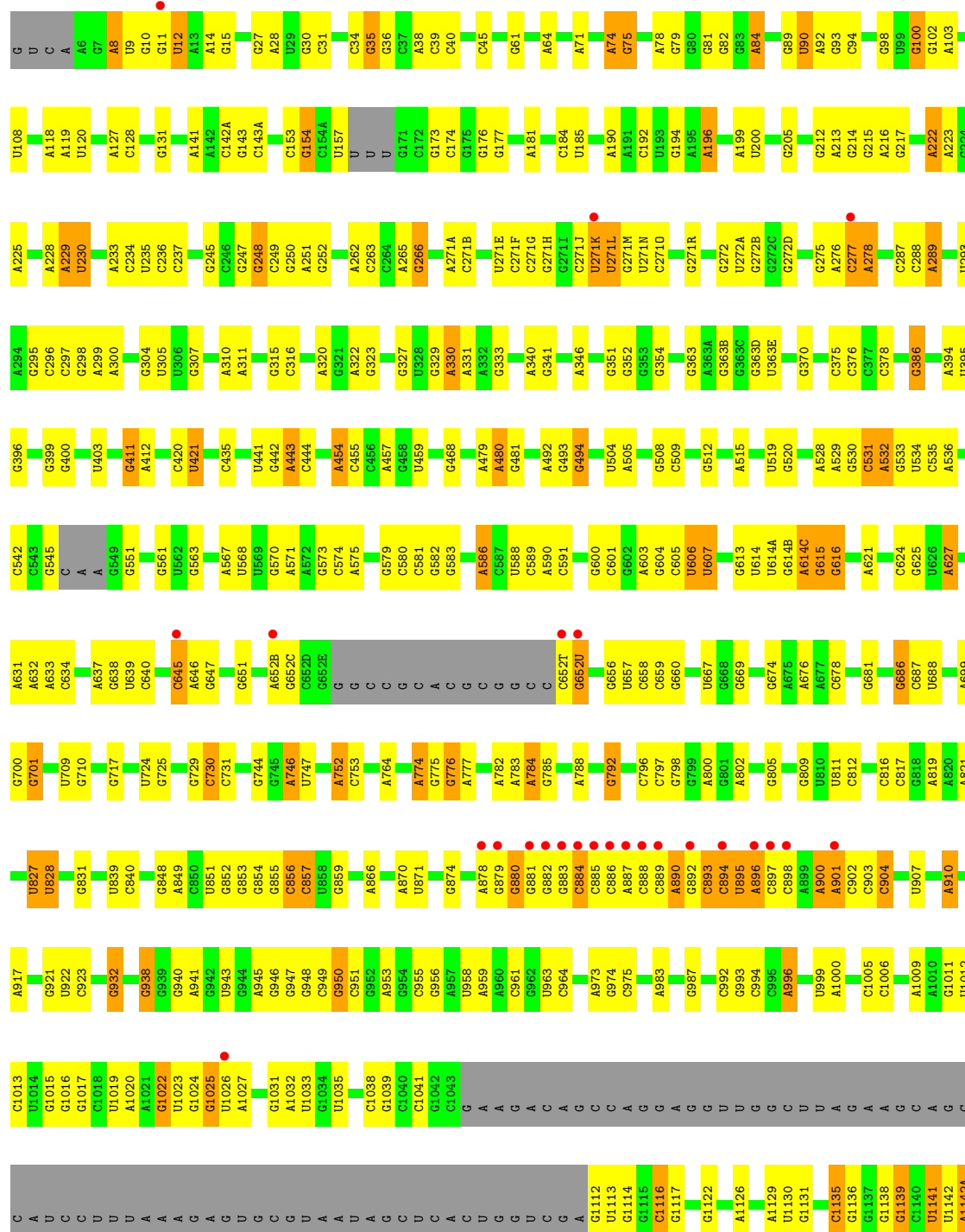
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2p	1	Total 1	O 1	0	0
62	2q	1	Total 1	O 1	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	1	Total 1	O 1	0	0
62	2v	1	Total 1	O 1	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	4	Total 4	O 4	0	0
62	2z	1	Total 1	O 1	0	0
62	2y	1	Total 1	O 1	0	0

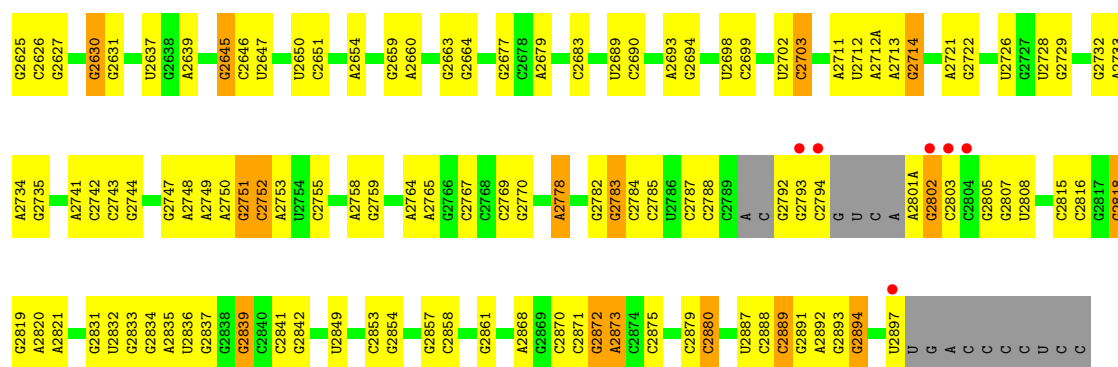
G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	A1128	G1135	G1136	G1137	G1138	G1139	G1149	C1150	A1155	A1156	G1164	U1165	C1166	U1167	G1168	G1171	G1173	U1174	U1175	A1177	C1179	G1180	C1181	G1183	G1184	G1187	U1188	A1189	A1220	G1243	G1244	G1248	G1252	A1253	G1256	U1263																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G1264	A1265	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	A1276	G1277	A1278	U1292	C1293	C1297	U1300	A1301	G1302	G1303	G1309	C1315	C1320	A1321	G1332	G1339	C1345	U1352	A1356	A1359	A1360	G1364	A1365	G1368	G1369	G1370	G1371	U1372	G1376	A1379	G1380	A1384	G1385																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
A1395	U1396	C1399	U1405	U1406	G1416	C1417	G1418	A1419	U1420	G1421	U1518	G1519	G1526	G1527	G1529	C1531	C1532	G	U	A	C	G1537	G1538	G1539	G1428	G1429	C1430	U1431	A1436	A1439	A1442	A1445	G1450	A1452	U1453	G1455	A1460	G1461	C1467	C1468	G1482	C1493	A1494	U1497	U1503	C1504	C1505	C1506	A1507	A1508	C1509	A1509A	U1512	C1513																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
G1651	A1654	G1663	A1664	A1665	G1666	A1669	C1670	G1674	U1680	G1681	G1682	G1683	C1684	U1688	U1693	G1696	G1697	A1698	G1699	A1700	G1701	G1702	G1703	U1709	C1710	G1580	G1581	C1582	A1583	C1584	A1586	A1587	C1588	C1589	G1593	G1594	G1595	U1602	A1603	C1607	A1608	A1609	A1632	G1633	G1647	C1648																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A1786	C1790	A1791	G1792	U1796	C1797	G1799	A1800	G1801	A1802	A1803	A1812	G1813	G1814	A1815	G1816	G1817	G1823	G1824	A1825	A1829	C1830	C1844	G1845	G1846	A1847	U1851	C1852	A1853	A1854	C1866	A1876	A1877	G1878	A1889	G1899	A1900	G1906	U1911	U1915	U1916	U1917	A1918	A1919	C1920	C2055																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G1929	G1930	A1937	A1938	U1939	G1942	U1955	U1963	A1964	C1965	A1966	C1967	U2006	G2007	U2008	G2009	G2010	G2101	C2102	G2103	G2104	C2105	G2106	U1991	G1992	U1993	C1996	G1997	A2001	U2011	G2012	C2021	C2022	U2023	G2024	C2025	C2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	G2038	C2043	C2055																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G2056	A2059	G2061	C2064	C2065	C2066	G2069	U2074	U2075	U2079	U2096	G2097	U2098	G2100	G2101	C2102	G2103	G2104	C2105	G2106	U1991	G1992	U1993	C1996	G1997	A2001	U2011	G2012	C2021	C2022	U2023	G2024	C2025	C2026	G2027	U2028	G2029	A2030	A2031	G2032	A2033	G2038	C2043	C2055																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
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• Molecule 1: 23S Ribosomal RNA

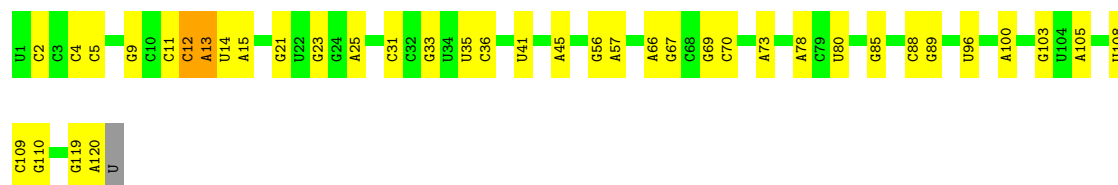


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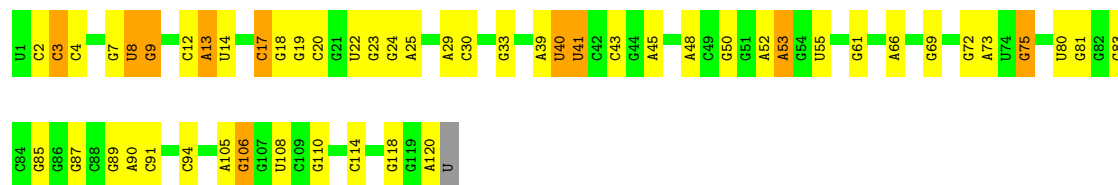
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 67% 31% ..



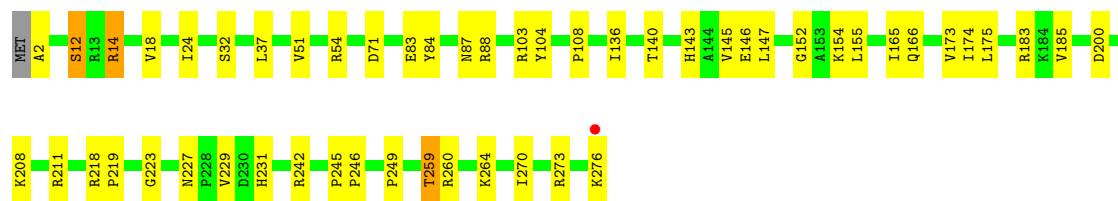
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 56% 35% 8% .



• Molecule 3: 50S ribosomal protein L2

Chain 1D: 81% 18% .



• Molecule 3: 50S ribosomal protein L2

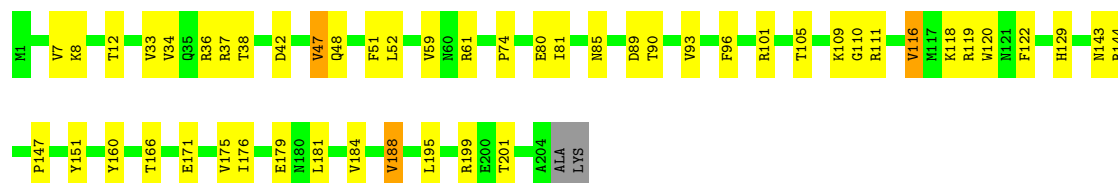
Chain 2D: 80% 18% .





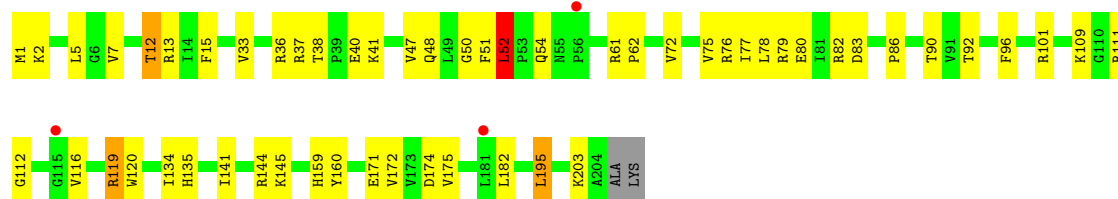
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 75% 23% ..



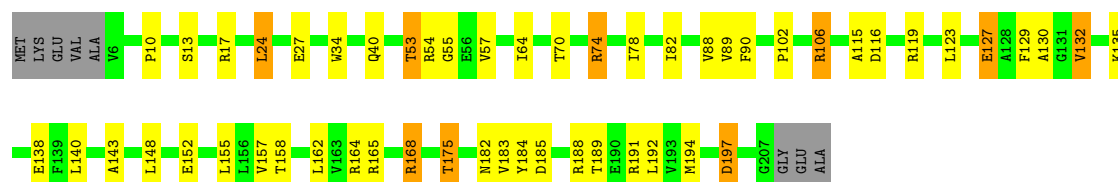
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 72% 25% ..



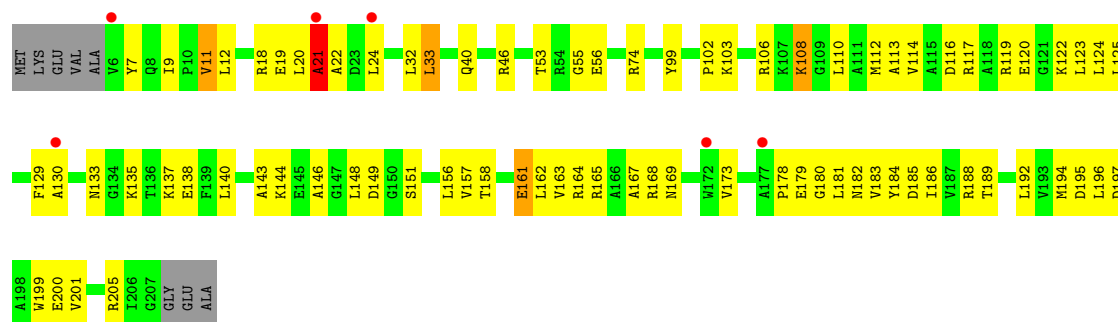
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 71% 21% . .



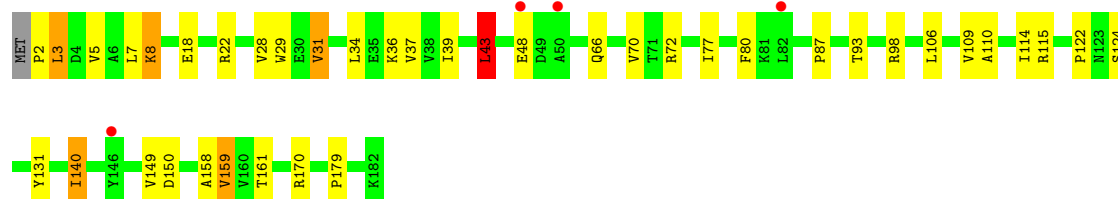
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 3% 58% 36% . .



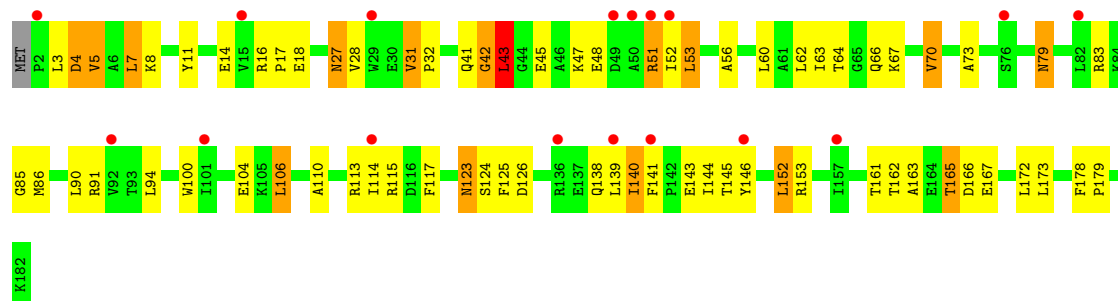
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 



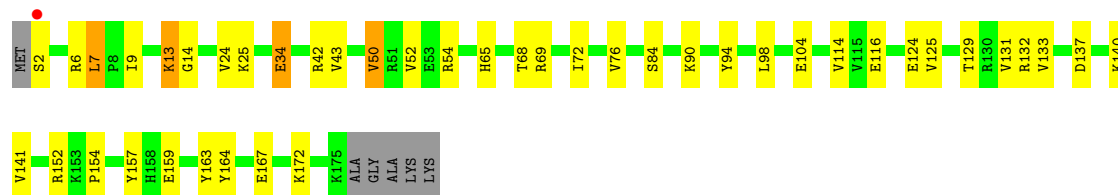
- Molecule 6: 50S ribosomal protein L5

Chain 2G: 



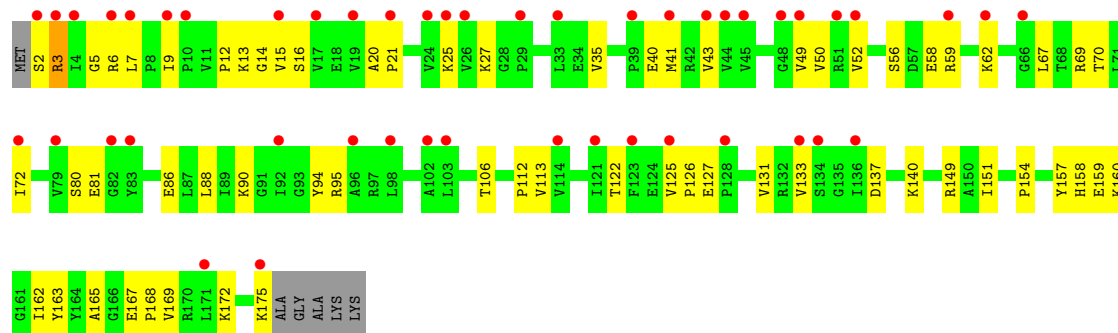
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 

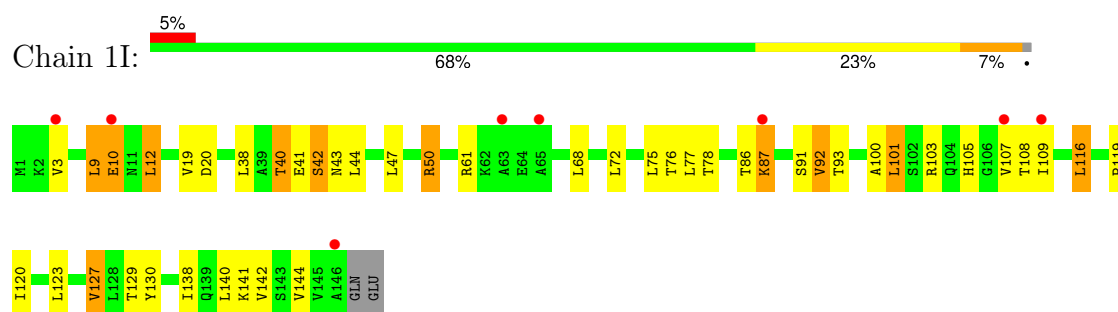


- Molecule 7: 50S ribosomal protein L6

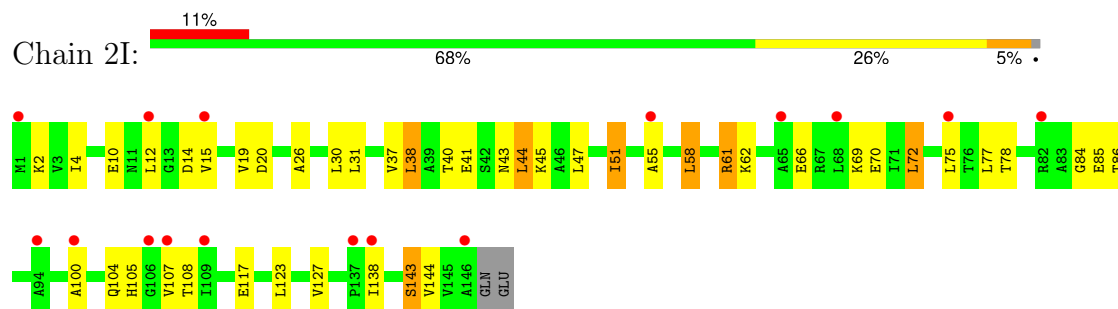
Chain 2H: 



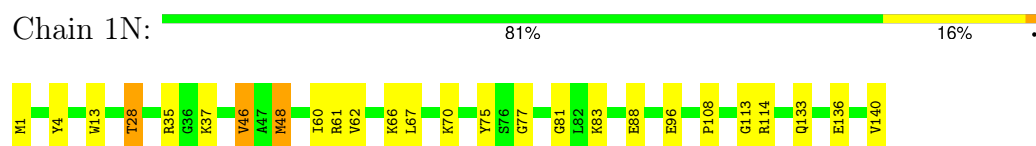
- Molecule 8: 50S ribosomal protein L9



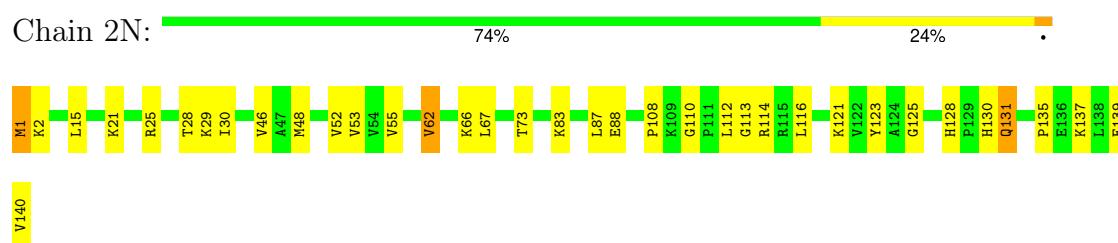
- Molecule 8: 50S ribosomal protein L9



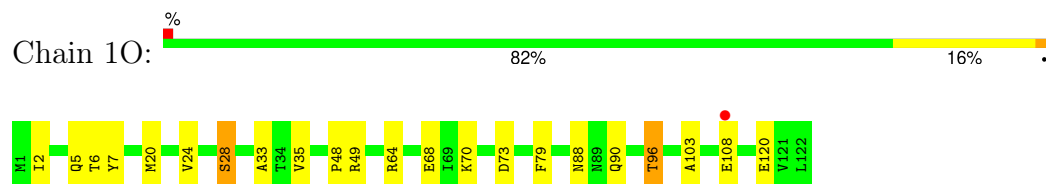
- Molecule 9: 50S ribosomal protein L13



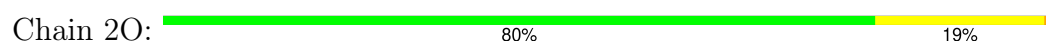
- Molecule 9: 50S ribosomal protein L13

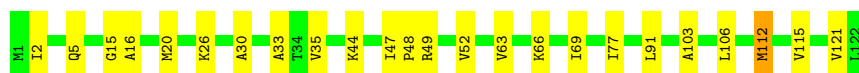


- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14





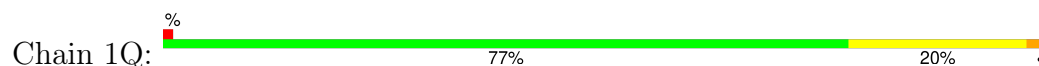
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



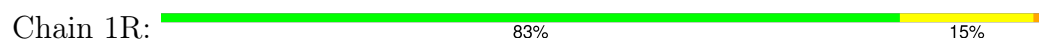
- Molecule 12: 50S ribosomal protein L16



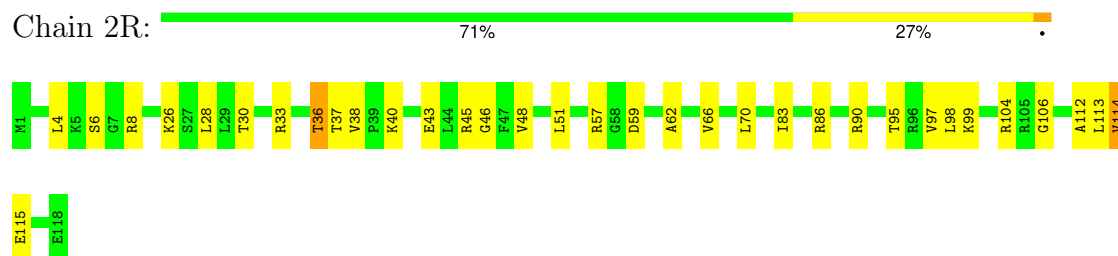
- Molecule 12: 50S ribosomal protein L16



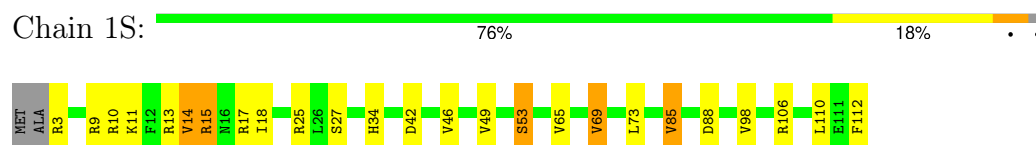
- Molecule 13: 50S ribosomal protein L17



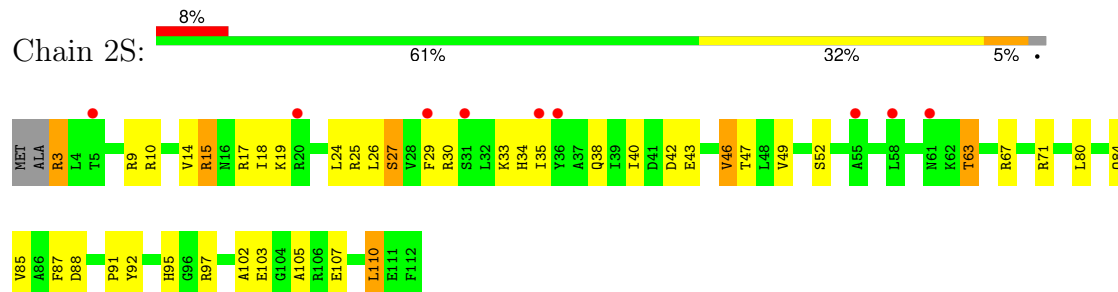
- Molecule 13: 50S ribosomal protein L17



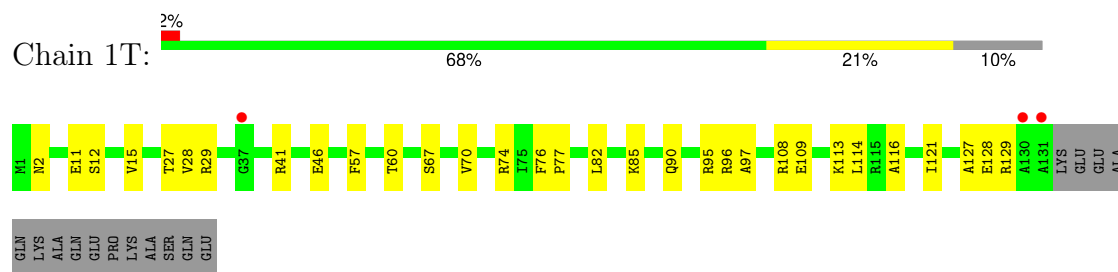
- Molecule 14: 50S ribosomal protein L18



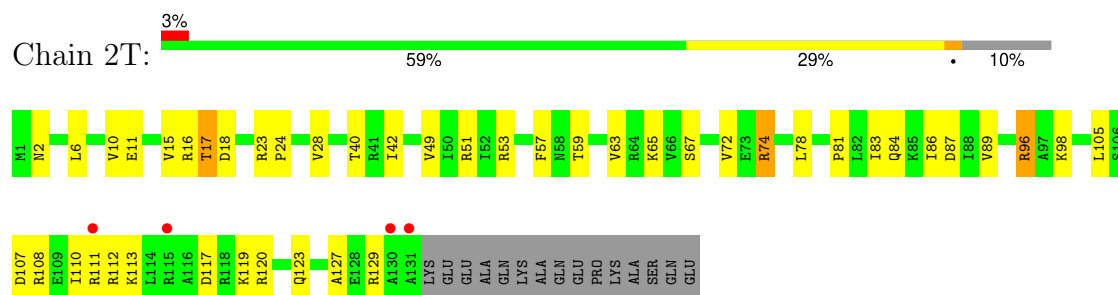
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



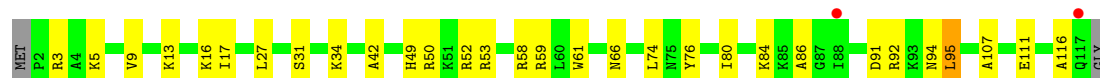
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  81% 18% .



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  2% 73% 25% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V:  80% 17% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  4% 72% 24% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  2% 81% 17% ..



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  3% 86% 12% ..

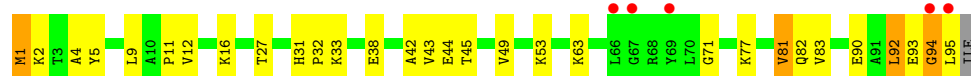


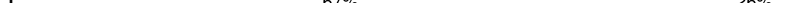
- Molecule 19: 50S ribosomal protein L23

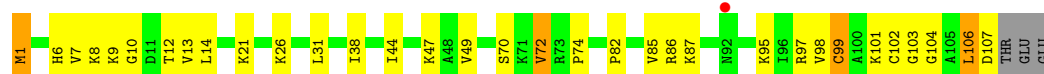
Chain 1X:  2% 77% 21% ..

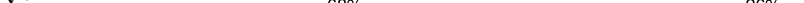


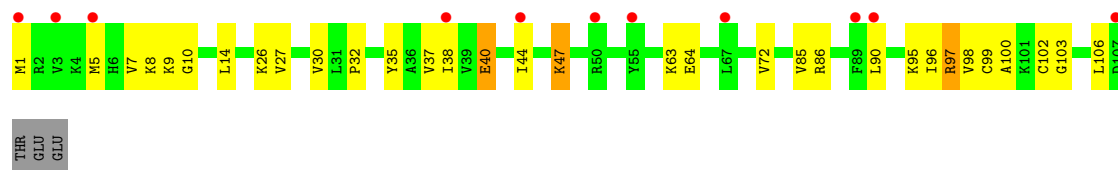
- Molecule 19: 50S ribosomal protein L23

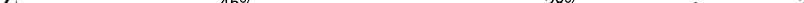


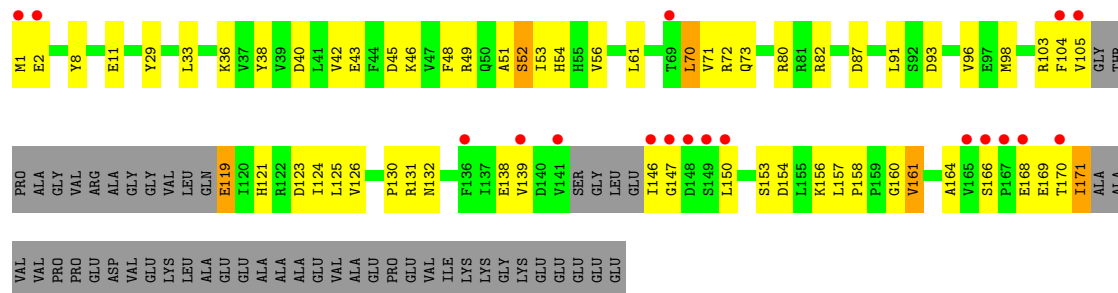
- Chain 1Y:  67% 26%

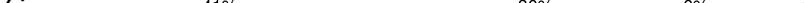


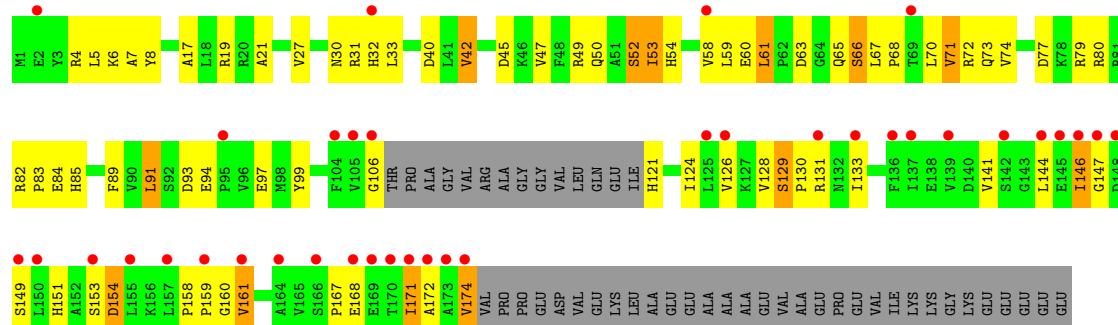
- Chain 2Y: 



- Chain 1Z: 

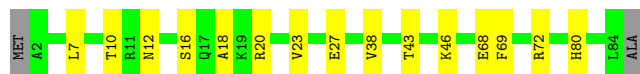


- Chain 2Z: 



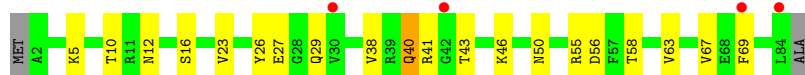
- Molecule 22: 50S ribosomal protein L27

Chain 10:  80% 18%



- Molecule 22: 50S ribosomal protein L27

Chain 20:  5% 74% 22%



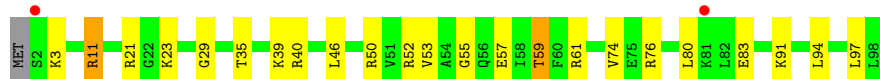
- Molecule 23: 50S ribosomal protein L28

Chain 11:  % 77% 18%



- Molecule 23: 50S ribosomal protein L28

Chain 21:  2% 76% 21%



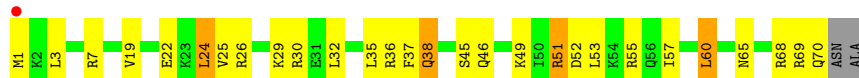
- Molecule 24: 50S ribosomal protein L29

Chain 12:  81% 17%



- Molecule 24: 50S ribosomal protein L29

Chain 22:  % 58% 33% 6%

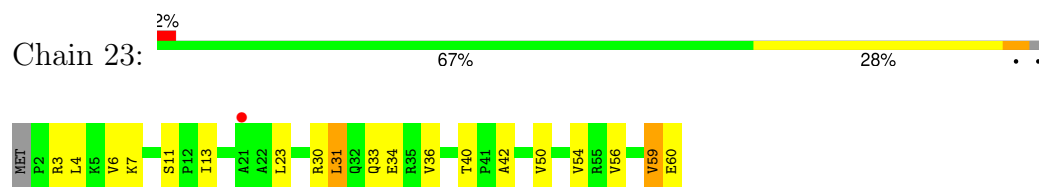


- Molecule 25: 50S ribosomal protein L30

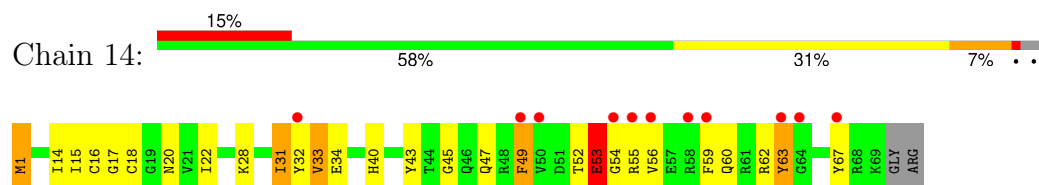
Chain 13:  65% 30%



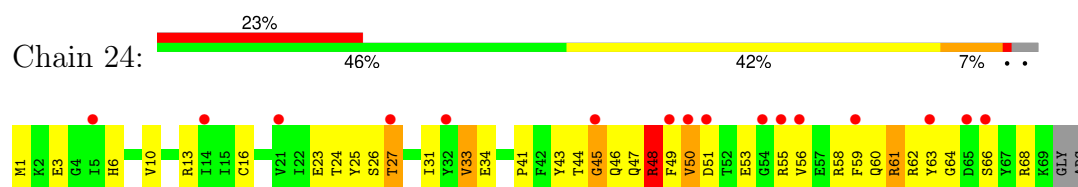
- Molecule 25: 50S ribosomal protein L30



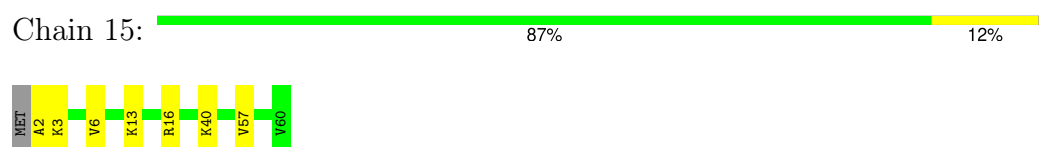
- Molecule 26: 50S ribosomal protein L31



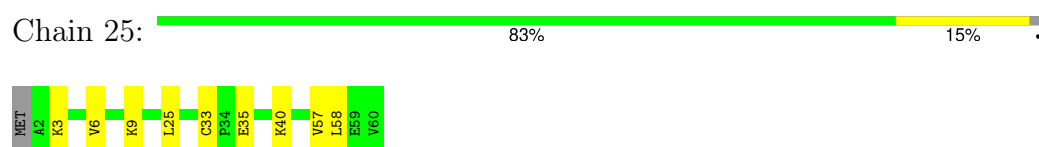
- Molecule 26: 50S ribosomal protein L31



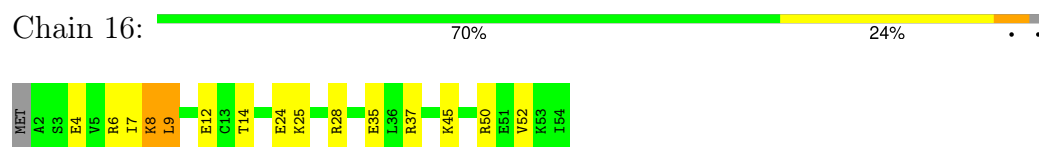
- Molecule 27: 50S ribosomal protein L32



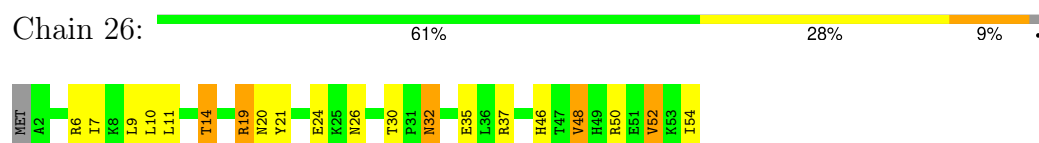
- Molecule 27: 50S ribosomal protein L32



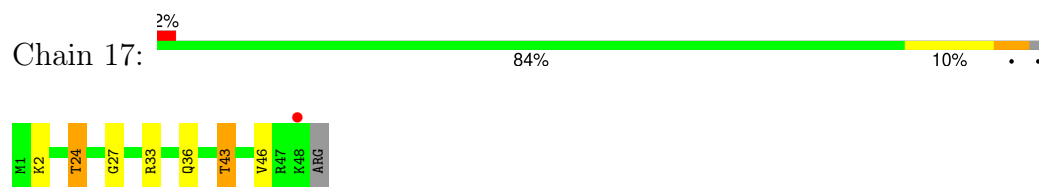
- Molecule 28: 50S ribosomal protein L33



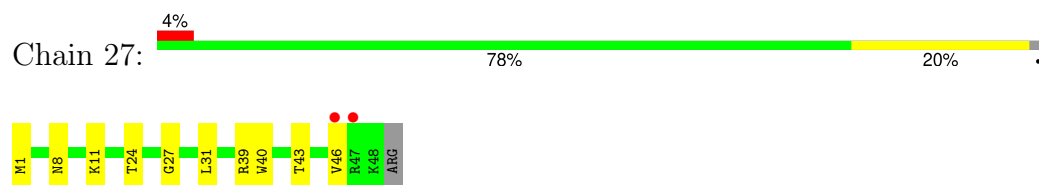
- Molecule 28: 50S ribosomal protein L33



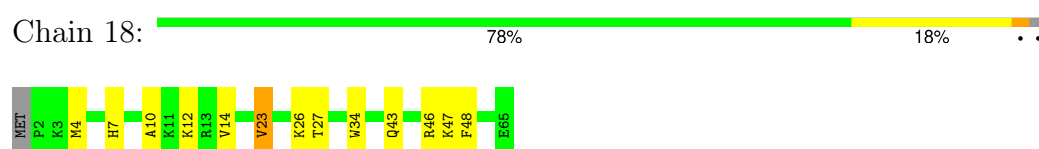
- Molecule 29: 50S ribosomal protein L34



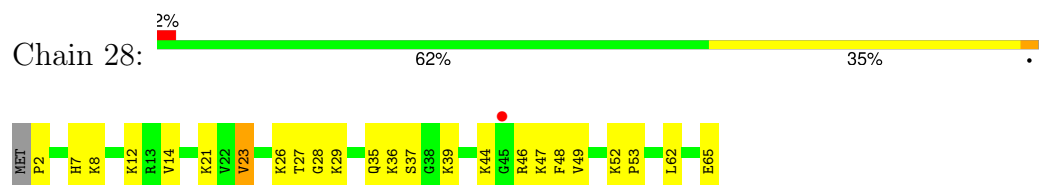
- Molecule 29: 50S ribosomal protein L34



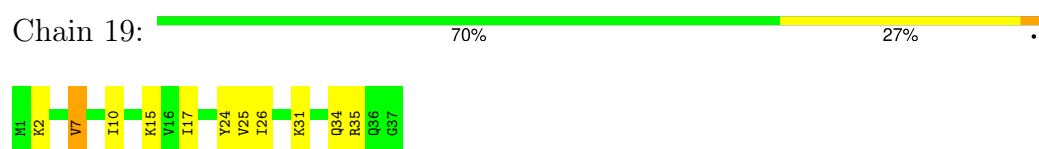
- Molecule 30: 50S ribosomal protein L35



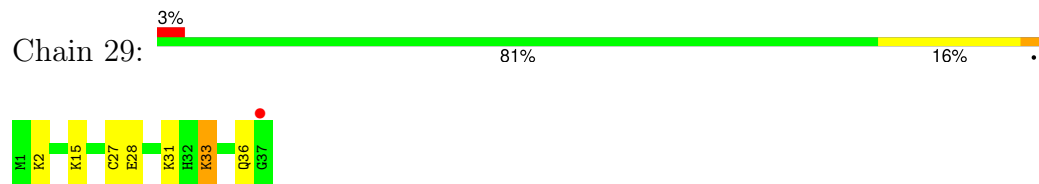
- Molecule 30: 50S ribosomal protein L35



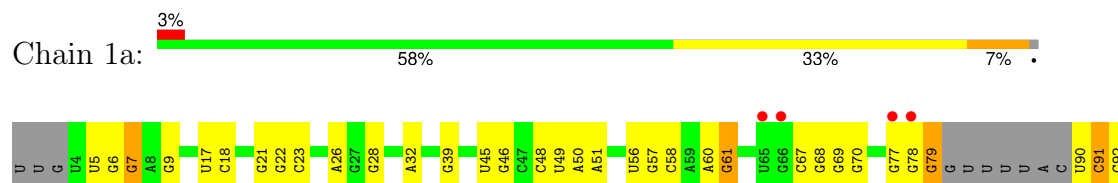
- Molecule 31: 50S ribosomal protein L36

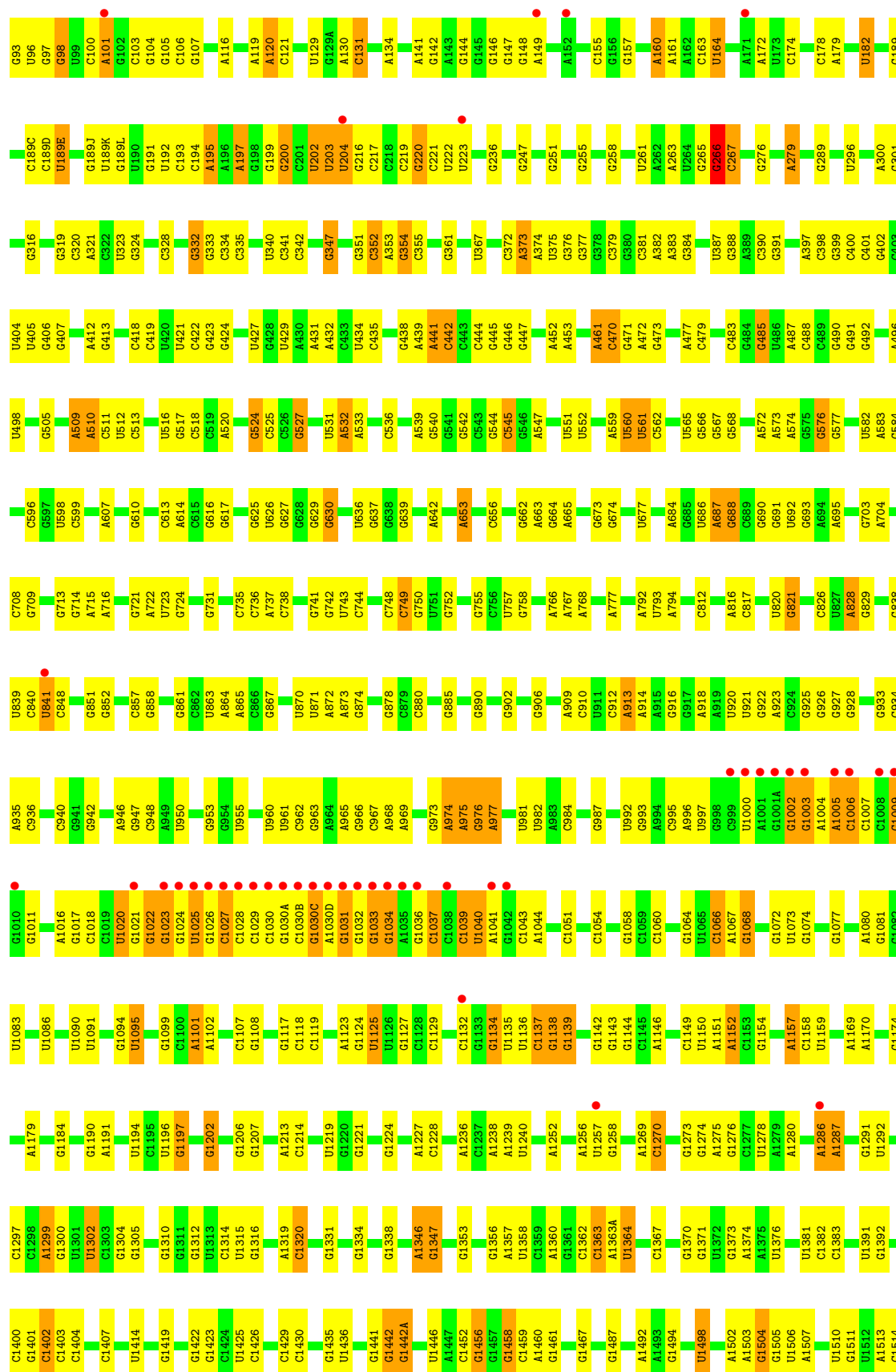


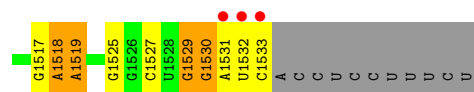
- Molecule 31: 50S ribosomal protein L36



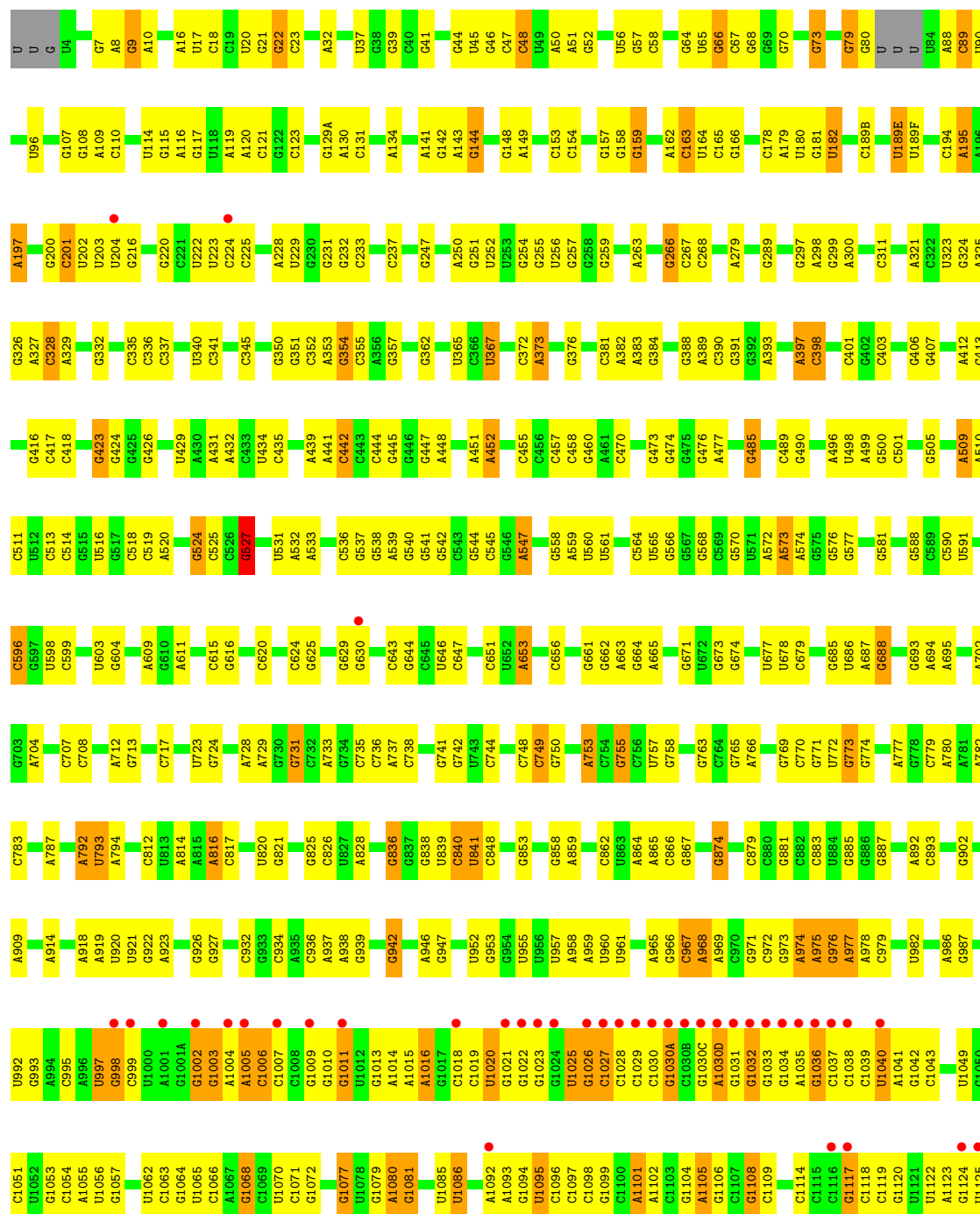
- Molecule 32: 16S Ribosomal RNA

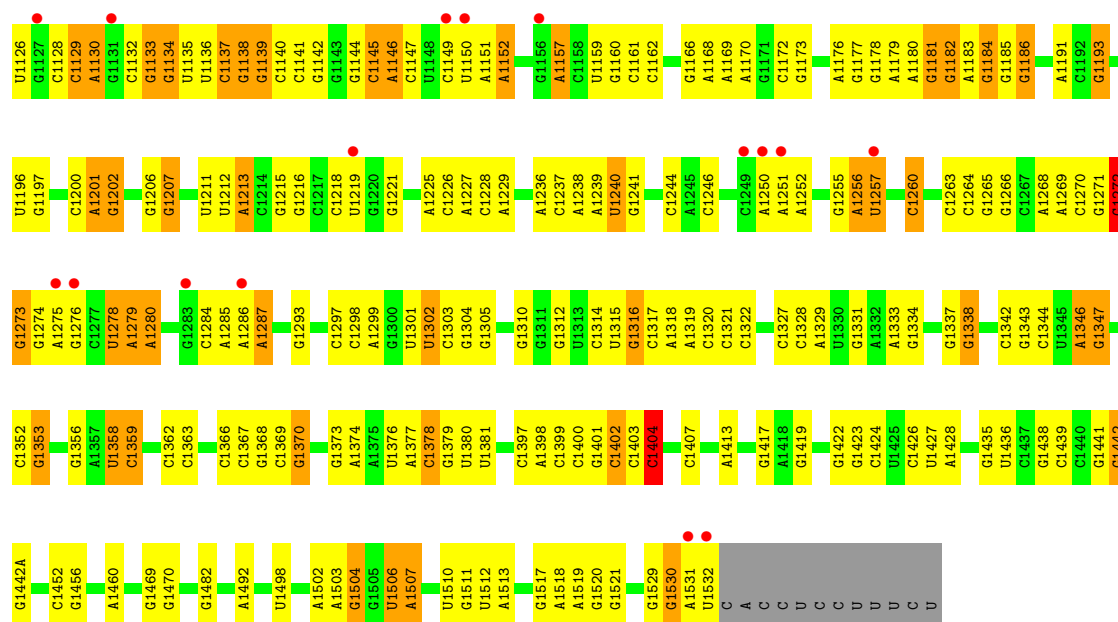




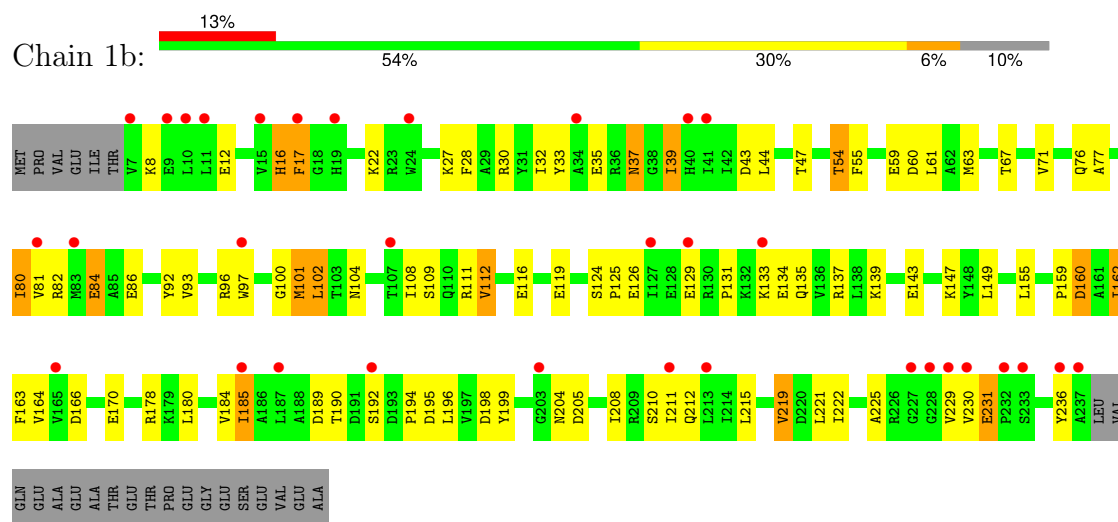


- Molecule 32: 16S Ribosomal RNA

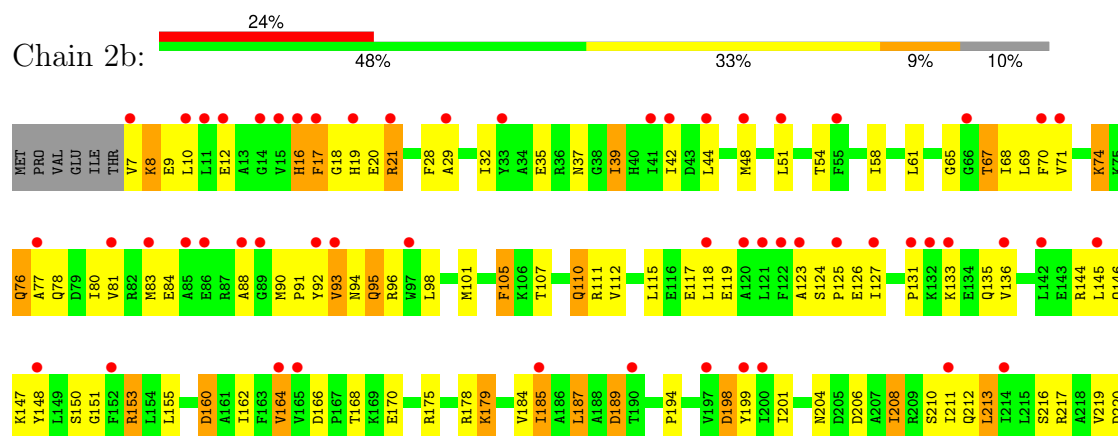


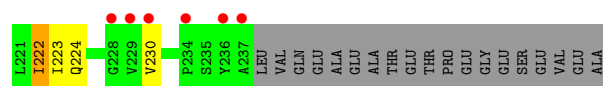


• Molecule 33: 30S ribosomal protein S2

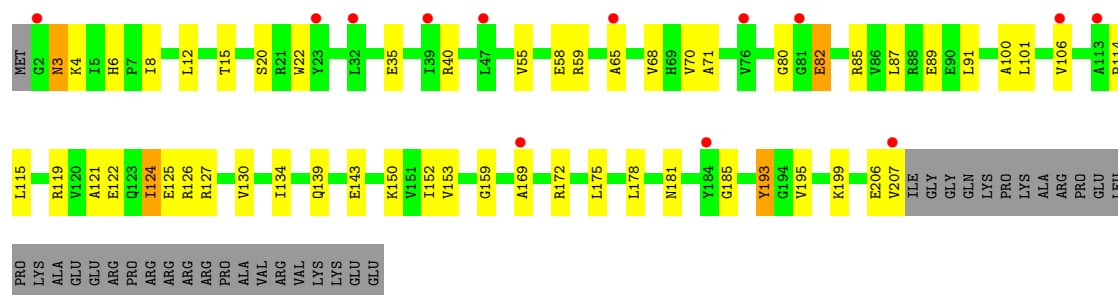


• Molecule 33: 30S ribosomal protein S2

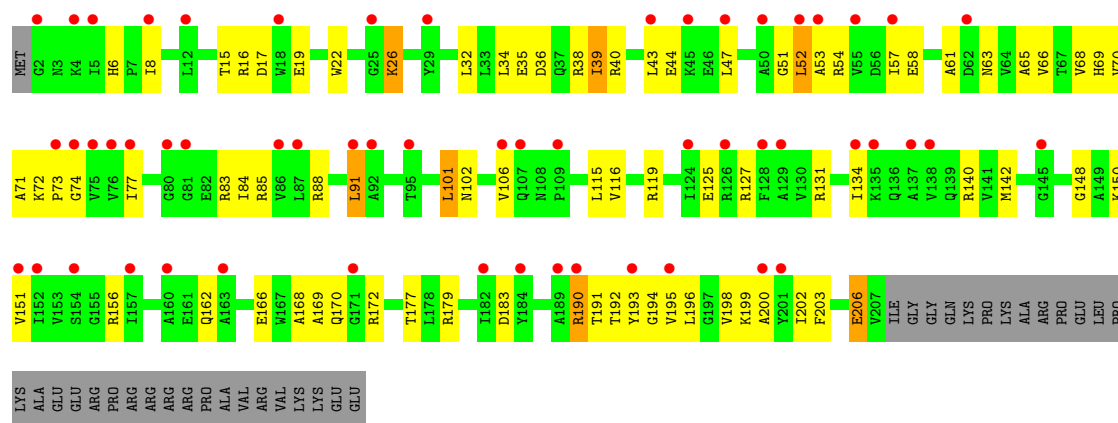




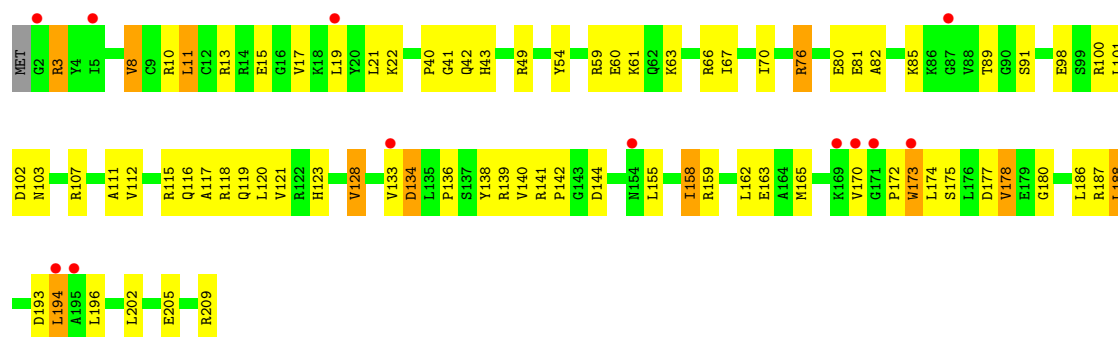
• Molecule 34: 30S ribosomal protein S3



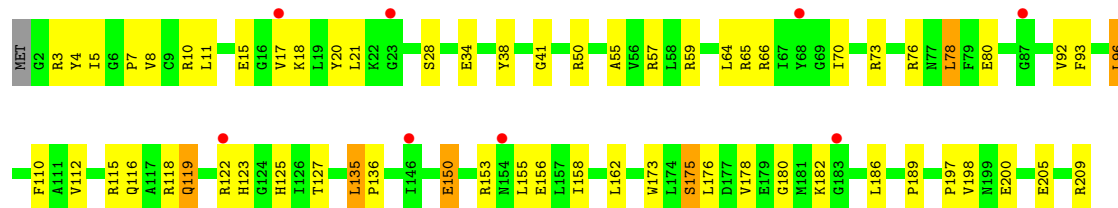
• Molecule 34: 30S ribosomal protein S3



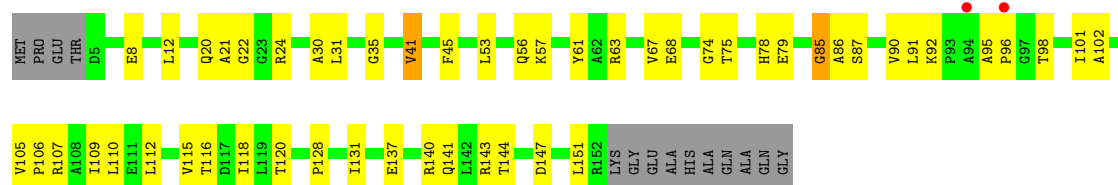
• Molecule 35: 30S ribosomal protein S4



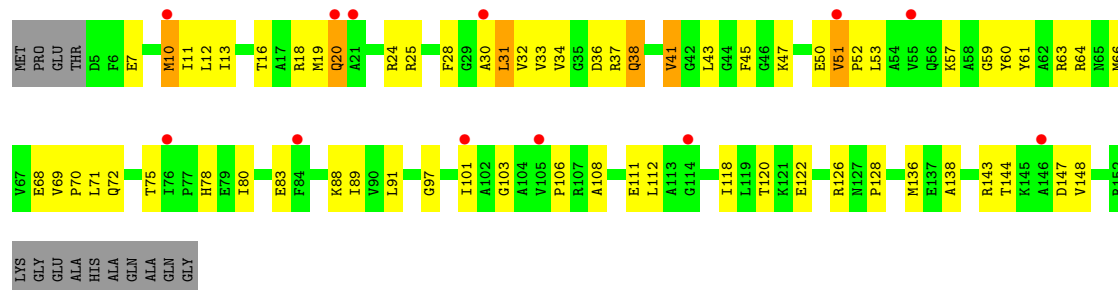
• Molecule 35: 30S ribosomal protein S4



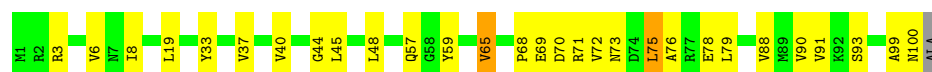
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



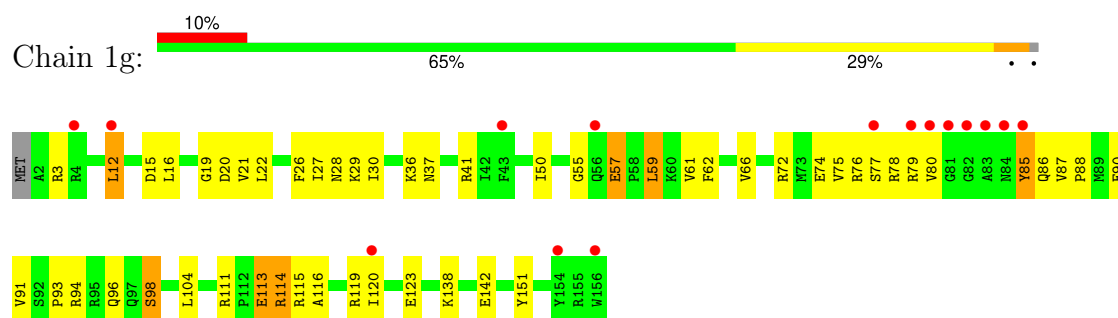
- Molecule 37: 30S ribosomal protein S6



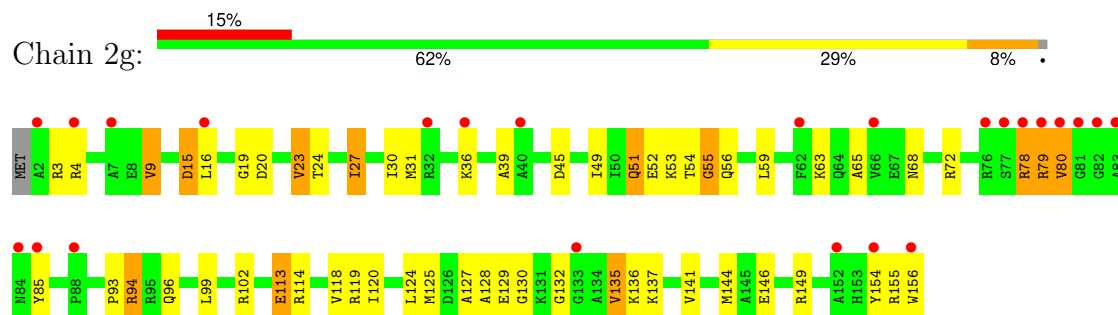
- Molecule 37: 30S ribosomal protein S6



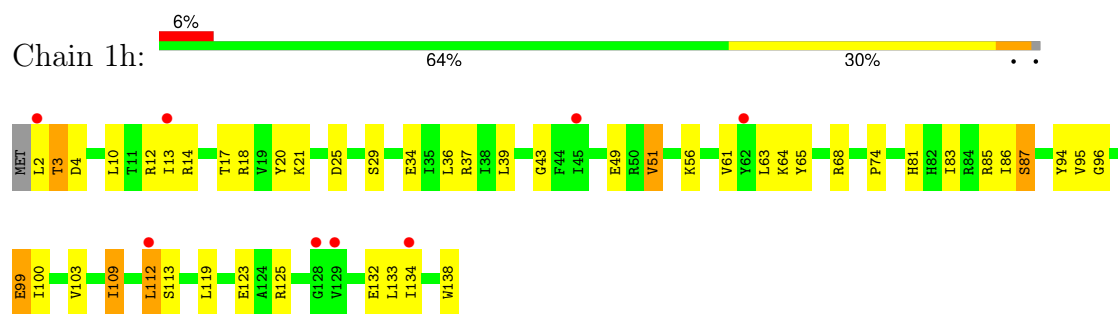
- Molecule 38: 30S ribosomal protein S7



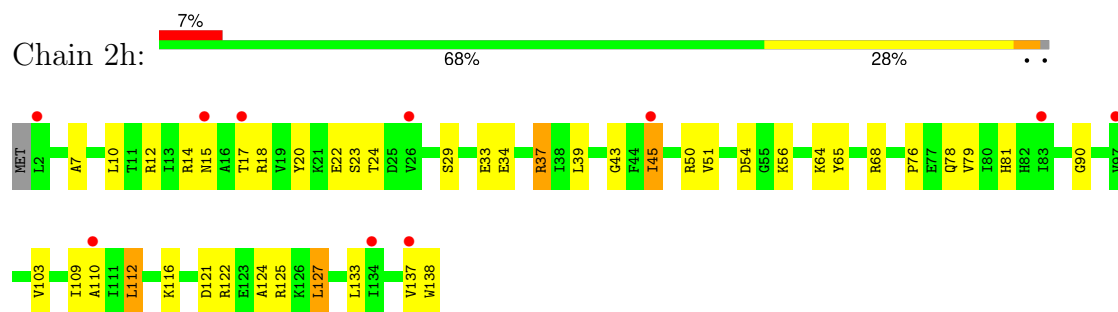
- Molecule 38: 30S ribosomal protein S7



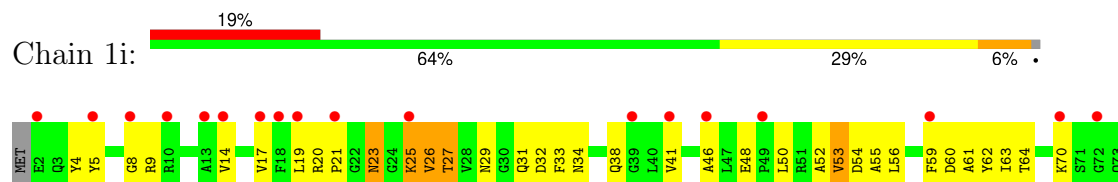
- Molecule 39: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S8

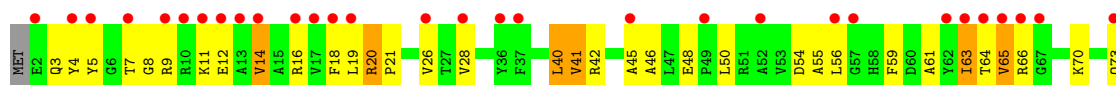


- Molecule 40: 30S ribosomal protein S9

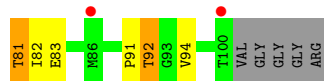
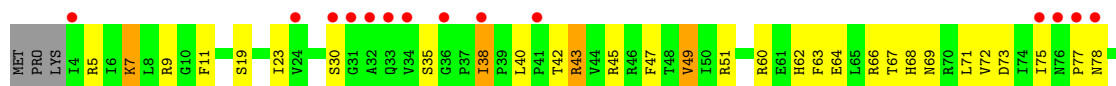




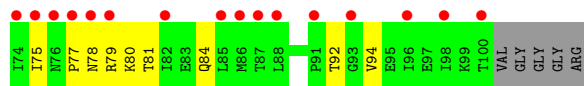
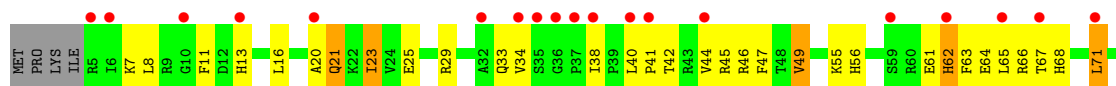
- Molecule 40: 30S ribosomal protein S9



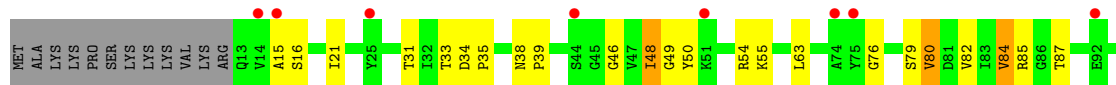
- Molecule 41: 30S ribosomal protein S10



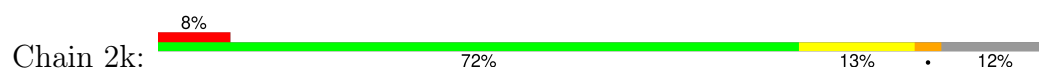
- Molecule 41: 30S ribosomal protein S10

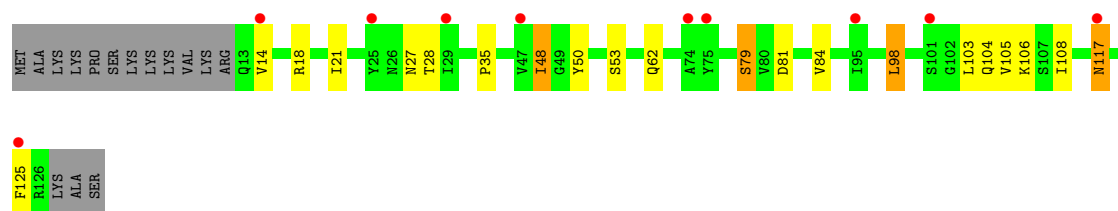


- Molecule 42: 30S ribosomal protein S11

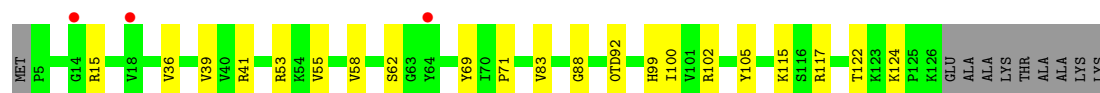
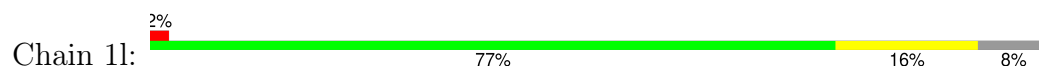


- Molecule 42: 30S ribosomal protein S11

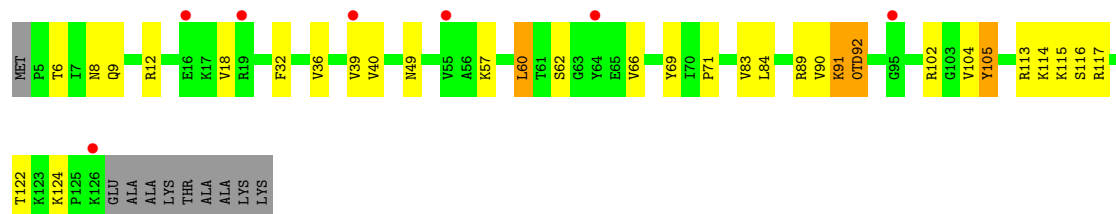




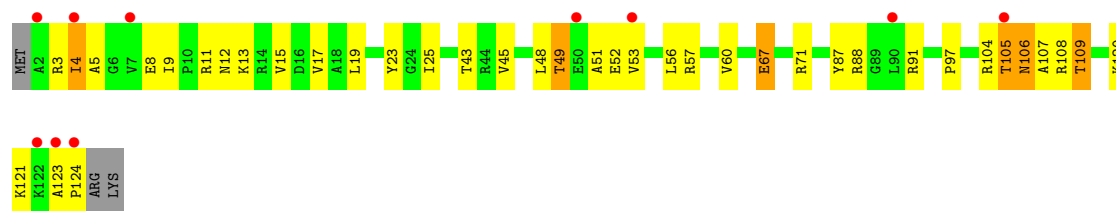
- Molecule 43: 30S ribosomal protein S12



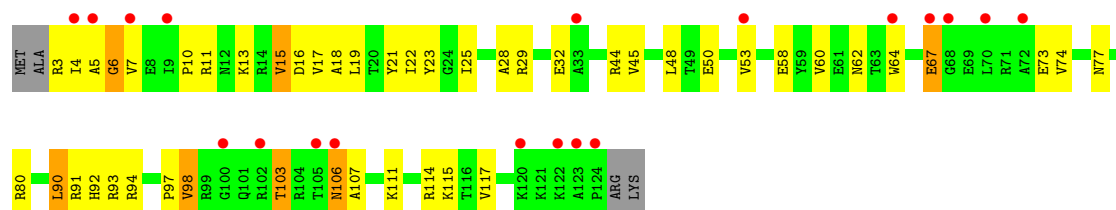
- Molecule 43: 30S ribosomal protein S12



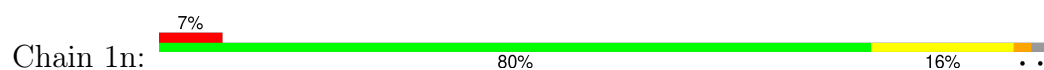
- Molecule 44: 30S ribosomal protein S13



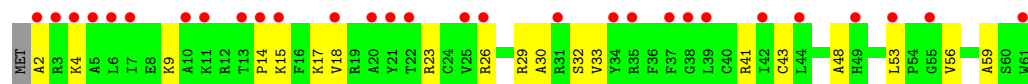
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



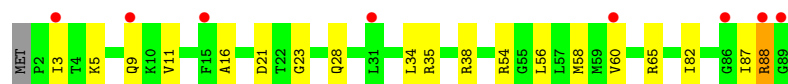
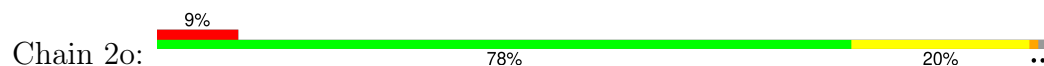
- Molecule 45: 30S ribosomal protein S14 type Z



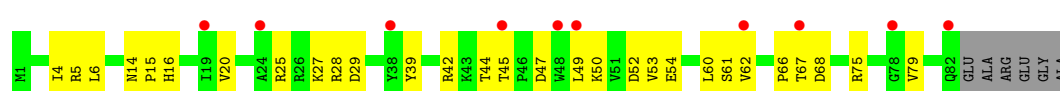
- Molecule 46: 30S ribosomal protein S15



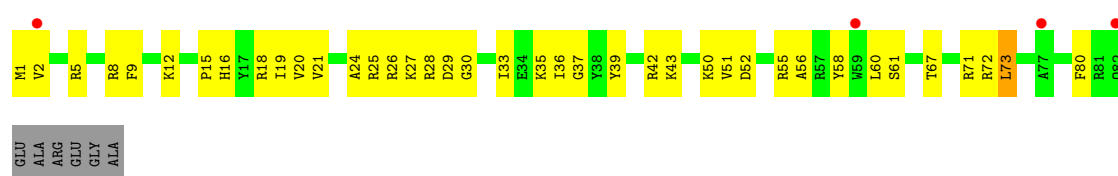
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

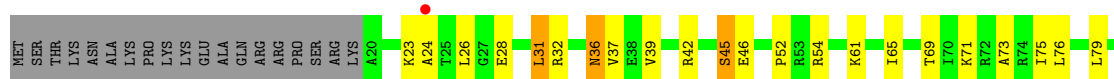




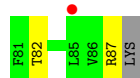
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

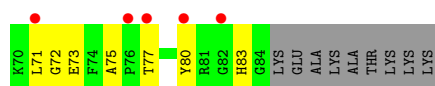


- Molecule 50: 30S ribosomal protein S19

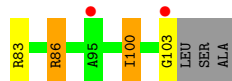
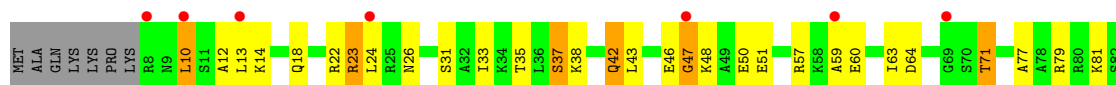


- Molecule 50: 30S ribosomal protein S19

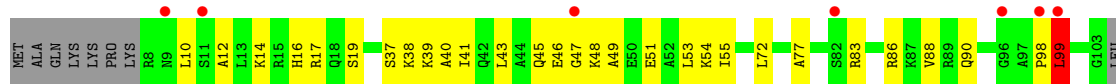




- Molecule 51: 30S ribosomal protein S20



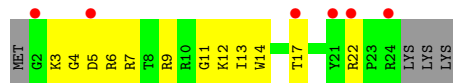
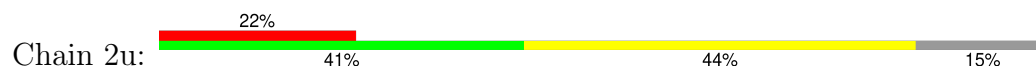
- Molecule 51: 30S ribosomal protein S20



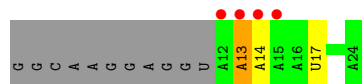
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

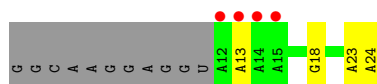


- Molecule 53: MF-mRNA



- Molecule 53: MF-mRNA

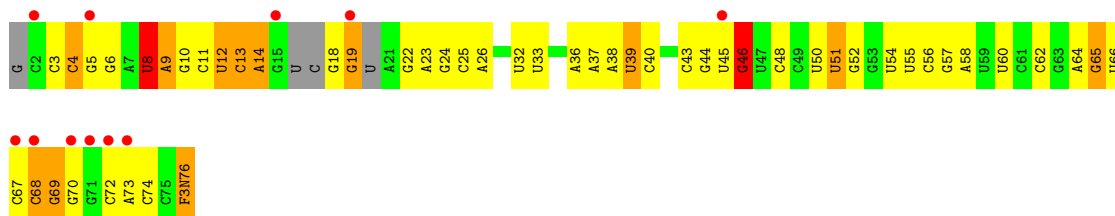




● Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe



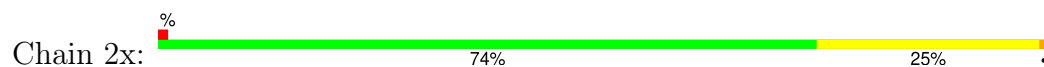
● Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe



● Molecule 55: P-site Peptidyl-tRNA fMRC-NH-tRNAmet RNA-part



● Molecule 55: P-site Peptidyl-tRNA fMRC-NH-tRNAmet RNA-part



● Molecule 56: P-site Peptidyl-tRNA fMRC-NH-tRNAmet Peptide-part

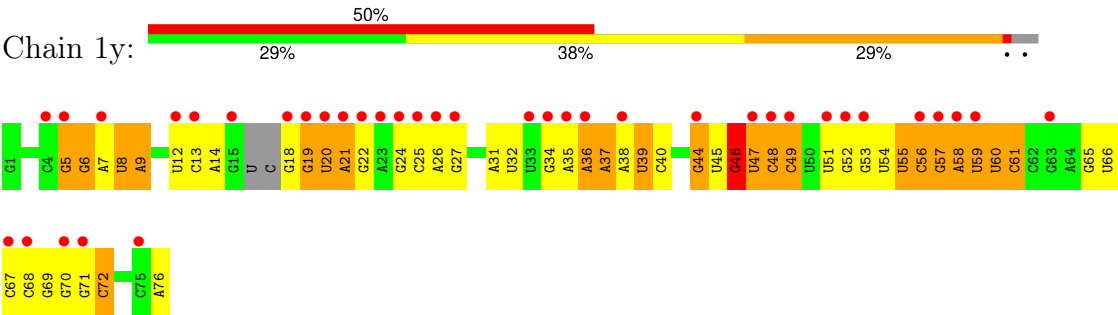


● Molecule 56: P-site Peptidyl-tRNA fMRC-NH-tRNAmet Peptide-part

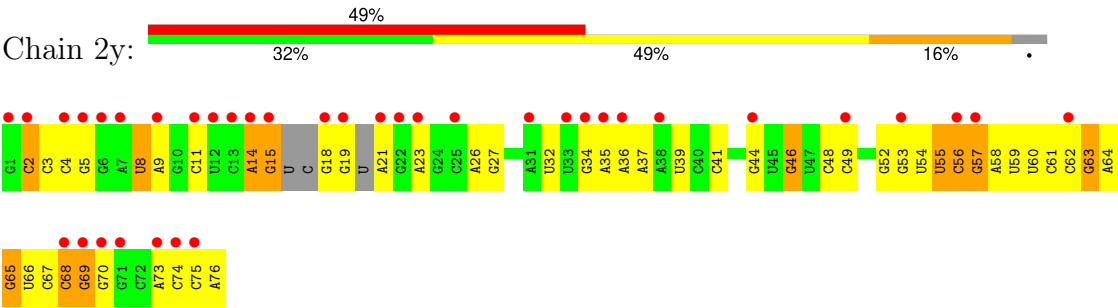




● Molecule 57: E-site Deacylated tRNAphe



● Molecule 57: E-site Deacylated tRNAphe



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.16Å 452.74Å 623.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	128.40 – 2.50 128.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (128.40-2.50) 99.6 (128.40-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.235 , 0.284 0.237 , 0.285	Depositor DCC
R_{free} test set	101013 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	300017	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: OMU, PSU, MA6, MIA, OMG, G7M, 5MU, FME, SF4, 5MC, M2G, K, 4SU, 4OC, OMC, MG, F3N, 2MG, 2MA, ZN, UR3, 8AN, 0TD

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	0.27	1/69011 (0.0%)	0.47	2/107720 (0.0%)
1	2A	0.21	0/67295	0.41	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.38	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.43	0/2149
5	1F	0.25	0/1618	0.48	0/2191
5	2F	0.20	0/1614	0.46	2/2186 (0.1%)
6	1G	0.22	0/1448	0.47	1/1957 (0.1%)
6	2G	0.18	0/1453	0.41	0/1963
7	1H	0.21	0/1356	0.42	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.19	0/1112	0.46	0/1514
8	2I	0.17	0/1079	0.40	0/1475
9	1N	0.24	0/1144	0.45	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.23	0/943	0.47	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.25	0/1152	0.54	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.24	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.26	0/982	0.47	0/1312
13	2R	0.20	0/982	0.43	0/1312
14	1S	0.23	0/883	0.47	0/1176
14	2S	0.22	0/880	0.46	0/1172
15	1T	0.23	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.42	0/1468
16	1U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.24	0/782	0.48	0/1049
17	2V	0.18	0/782	0.41	0/1049
18	1W	0.26	0/897	0.44	0/1205
18	2W	0.21	0/897	0.41	0/1205
19	1X	0.25	0/764	0.53	2/1025 (0.2%)
19	2X	0.22	0/764	0.51	2/1025 (0.2%)
20	1Y	0.21	0/819	0.45	0/1095
20	2Y	0.19	0/819	0.42	0/1095
21	1Z	0.21	0/1267	0.48	0/1717
21	2Z	0.20	0/1299	0.42	0/1763
22	10	0.26	0/662	0.49	0/881
22	20	0.21	0/662	0.43	0/881
23	11	0.25	0/762	0.45	0/1014
23	21	0.21	0/762	0.42	0/1014
24	12	0.24	0/590	0.45	0/781
24	22	0.19	0/590	0.37	0/781
25	13	0.26	0/474	0.50	0/635
25	23	0.17	0/469	0.41	0/630
26	14	0.26	0/565	0.58	0/761
26	24	0.21	0/545	0.51	0/737
27	15	0.30	0/469	0.53	0/635
27	25	0.21	0/469	0.48	0/635
28	16	0.26	0/460	0.47	0/613
28	26	0.20	0/456	0.44	0/608
29	17	0.28	0/426	0.53	0/561
29	27	0.25	0/426	0.52	0/561
30	18	0.27	0/525	0.49	0/691
30	28	0.19	0/525	0.39	0/691
31	19	0.24	0/310	0.53	0/407
31	29	0.19	0/310	0.39	0/407
32	1a	0.20	0/35795	0.39	2/55864 (0.0%)
32	2a	0.19	0/35886	0.38	1/56005 (0.0%)
33	1b	0.22	0/1881	0.48	0/2542
33	2b	0.22	0/1860	0.51	1/2518 (0.0%)
34	1c	0.19	0/1572	0.41	0/2126
34	2c	0.21	0/1566	0.43	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.46	0/2284
36	1e	0.21	0/1145	0.51	1/1543 (0.1%)
36	2e	0.21	0/1149	0.49	0/1548
37	1f	0.19	0/823	0.39	0/1115
37	2f	0.18	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.41	0/1679
38	2g	0.19	0/1254	0.43	0/1683
39	1h	0.19	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.47	0/1346
40	2i	0.20	0/997	0.49	0/1343
41	1j	0.20	0/722	0.48	1/982 (0.1%)
41	2j	0.22	0/727	0.57	1/988 (0.1%)
42	1k	0.20	0/844	0.43	0/1145
42	2k	0.18	0/848	0.38	0/1149
43	1l	0.21	0/937	0.41	0/1260
43	2l	0.20	0/937	0.43	0/1260
44	1m	0.20	0/969	0.51	0/1302
44	2m	0.19	0/961	0.45	0/1291
45	1n	0.19	0/501	0.42	0/664
45	2n	0.19	0/501	0.41	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.18	0/739	0.41	0/985
47	1p	0.18	0/697	0.43	0/939
47	2p	0.21	0/693	0.48	0/935
48	1q	0.19	0/836	0.42	0/1117
48	2q	0.18	0/836	0.43	0/1117
49	1r	0.20	0/560	0.39	0/746
49	2r	0.17	0/560	0.39	0/746
50	1s	0.18	0/667	0.46	0/900
50	2s	0.23	0/661	0.54	0/893
51	1t	0.20	0/730	0.50	0/965
51	2t	0.21	0/729	0.44	0/965
52	1u	0.19	0/203	0.42	0/266
52	2u	0.20	0/203	0.47	0/266
53	1v	0.21	0/310	0.30	0/480
53	2v	0.20	0/310	0.35	0/480
54	1w	0.30	1/1581 (0.1%)	0.46	0/2458
54	2w	0.30	2/1531 (0.1%)	0.43	0/2379
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.26	1/1723 (0.1%)	0.40	0/2684
56	1z	0.51	0/16	0.92	0/19
56	2z	0.31	0/16	0.79	0/19
57	1y	0.33	2/1606 (0.1%)	0.41	0/2497
57	2y	0.33	2/1583 (0.1%)	0.45	1/2459 (0.0%)
All	All	0.23	9/316666 (0.0%)	0.43	18/474075 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1y	46	G7M	O3'-P	5.74	1.61	1.56
54	1w	46	G7M	O3'-P	5.60	1.61	1.56
54	2w	46	G7M	O3'-P	5.55	1.61	1.56
57	2y	46	G7M	O3'-P	5.50	1.61	1.56
54	2w	8	4SU	O3'-P	5.38	1.61	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	2j	23	ILE	N-CA-C	-8.03	106.08	113.71
33	2b	222	ILE	N-CA-C	-6.93	106.03	112.96
41	1j	82	ILE	N-CA-C	-6.57	104.46	113.00
1	1A	1992	G	C2'-C3'-O3'	6.55	119.33	109.50
36	1e	109	ILE	N-CA-C	-6.26	106.70	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	583	0
1	2A	60322	0	30426	693	0
2	1B	2577	0	1305	27	0
2	2B	2575	0	1303	35	0
3	1D	2136	0	2218	33	0
3	2D	2136	0	2218	39	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	30	0
5	1F	1583	0	1625	34	0
5	2F	1579	0	1619	55	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	49	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	33	0
8	1I	1097	0	1140	24	0
8	2I	1064	0	1082	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	18	0
10	1O	933	0	996	16	0
10	2O	933	0	996	17	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	34	0
12	1Q	1122	0	1179	24	0
12	2Q	1122	0	1179	33	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	21	0
14	1S	873	0	926	15	0
14	2S	870	0	923	41	0
15	1T	1091	0	1151	15	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	20	0
17	1V	771	0	830	16	0
17	2V	771	0	830	16	0
18	1W	886	0	940	13	0
18	2W	886	0	940	7	0
19	1X	750	0	814	14	0
19	2X	750	0	814	20	0
20	1Y	806	0	881	21	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	38	0
21	2Z	1271	0	1273	47	0
22	10	653	0	673	11	0
22	20	653	0	674	16	0
23	11	755	0	826	14	0
23	21	755	0	826	18	0
24	12	588	0	643	4	0
24	22	588	0	643	20	0
25	13	469	0	518	16	0
25	23	464	0	514	14	0
26	14	552	0	533	20	0
26	24	532	0	503	22	0
27	15	455	0	465	4	0
27	25	455	0	465	4	0
28	16	453	0	473	6	0
28	26	449	0	469	13	0
29	17	418	0	467	6	0
29	27	418	0	467	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	18	517	0	582	11	0
30	28	517	0	582	18	0
31	19	307	0	335	6	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	378	0
32	2a	32327	0	16338	480	0
33	1b	1846	0	1867	54	0
33	2b	1825	0	1828	76	0
34	1c	1548	0	1535	33	0
34	2c	1542	0	1517	54	0
35	1d	1655	0	1672	51	0
35	2d	1674	0	1714	42	0
36	1e	1129	0	1185	31	0
36	2e	1133	0	1191	44	0
37	1f	810	0	804	12	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	32	0
38	2g	1235	0	1248	34	0
39	1h	1088	0	1126	30	0
39	2h	1088	0	1126	23	0
40	1i	983	0	986	29	0
40	2i	978	0	966	43	0
41	1j	709	0	650	21	0
41	2j	714	0	672	27	0
42	1k	829	0	825	20	0
42	2k	833	0	834	9	0
43	1l	932	0	981	8	0
43	2l	932	0	980	20	0
44	1m	958	0	1002	26	0
44	2m	950	0	988	35	0
45	1n	492	0	529	8	0
45	2n	492	0	529	14	0
46	1o	728	0	760	16	0
46	2o	728	0	760	13	0
47	1p	681	0	697	20	0
47	2p	677	0	686	24	0
48	1q	823	0	891	20	0
48	2q	823	0	891	16	0
49	1r	555	0	618	13	0
49	2r	555	0	618	22	0
50	1s	652	0	662	17	0
50	2s	646	0	644	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1t	728	0	798	26	0
51	2t	727	0	796	17	0
52	1u	199	0	208	7	0
52	2u	199	0	208	8	0
53	1v	277	0	140	3	0
53	2v	277	0	140	4	0
54	1w	1603	0	828	26	0
54	2w	1555	0	797	30	0
55	1x	1646	0	839	11	0
55	2x	1646	0	838	11	0
56	1z	27	0	28	0	0
56	2z	27	0	28	0	0
57	1y	1585	0	803	43	0
57	2y	1565	0	793	39	0
58	10	9	0	0	0	0
58	11	6	0	0	0	0
58	12	3	0	0	0	0
58	13	3	0	0	0	0
58	14	1	0	0	0	0
58	15	7	0	0	0	0
58	16	1	0	0	0	0
58	17	4	0	0	0	0
58	18	9	0	0	0	0
58	19	1	0	0	0	0
58	1A	1098	0	0	0	0
58	1B	37	0	0	0	0
58	1D	12	0	0	0	0
58	1E	13	0	0	0	0
58	1F	14	0	0	0	0
58	1G	5	0	0	0	0
58	1I	1	0	0	0	0
58	1N	6	0	0	0	0
58	1O	5	0	0	0	0
58	1P	4	0	0	0	0
58	1Q	8	0	0	0	0
58	1R	4	0	0	0	0
58	1S	3	0	0	0	0
58	1T	4	0	0	0	0
58	1U	9	0	0	0	0
58	1V	7	0	0	0	0
58	1W	7	0	0	0	0
58	1X	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1Y	5	0	0	0	0
58	1Z	2	0	0	0	0
58	1a	214	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1k	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	8	0	0	0	0
58	1x	12	0	0	0	0
58	20	2	0	0	0	0
58	23	3	0	0	0	0
58	25	5	0	0	0	0
58	26	1	0	0	0	0
58	27	3	0	0	0	0
58	28	3	0	0	0	0
58	29	1	0	0	0	0
58	2A	870	0	0	0	0
58	2B	20	0	0	0	0
58	2D	8	0	0	0	0
58	2E	10	0	0	0	0
58	2F	8	0	0	0	0
58	2G	1	0	0	0	0
58	2O	1	0	0	0	0
58	2P	2	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	1	0	0	0	0
58	2T	1	0	0	0	0
58	2U	2	0	0	0	0
58	2V	2	0	0	0	0
58	2W	4	0	0	0	0
58	2X	3	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	235	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2i	1	0	0	0	0
58	2j	1	0	0	0	0
58	2k	1	0	0	0	0
58	2l	4	0	0	0	0
58	2n	2	0	0	0	0
58	2q	3	0	0	0	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	3	0	0	0	0
58	2w	5	0	0	0	0
58	2x	7	0	0	0	0
58	2y	1	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	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
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	14	0	0	1	0
62	11	10	0	0	0	0
62	12	3	0	0	0	0
62	13	5	0	0	0	0
62	14	1	0	0	0	0
62	15	7	0	0	0	0
62	16	3	0	0	0	0
62	17	10	0	0	1	0
62	18	10	0	0	0	0
62	1A	1968	0	0	96	0
62	1B	61	0	0	4	0
62	1D	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1E	29	0	0	0	0
62	1F	22	0	0	1	0
62	1G	2	0	0	0	0
62	1H	2	0	0	0	0
62	1I	1	0	0	0	0
62	1N	5	0	0	1	0
62	1O	6	0	0	0	0
62	1P	20	0	0	2	0
62	1Q	6	0	0	0	0
62	1R	15	0	0	5	0
62	1S	5	0	0	0	0
62	1T	8	0	0	0	0
62	1U	11	0	0	0	0
62	1V	7	0	0	1	0
62	1W	5	0	0	0	0
62	1X	5	0	0	0	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	340	0	0	24	0
62	1b	1	0	0	1	0
62	1e	2	0	0	0	0
62	1f	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	8	0	0	0	0
62	1m	1	0	0	1	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	4	0	0	0	0
62	1w	9	0	0	0	0
62	1x	9	0	0	1	0
62	1y	1	0	0	0	0
62	1z	1	0	0	0	0
62	20	4	0	0	0	0
62	21	9	0	0	0	0
62	23	2	0	0	0	0
62	25	1	0	0	0	0
62	27	4	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1091	0	0	77	0
62	2B	23	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2D	21	0	0	2	0
62	2E	11	0	0	0	0
62	2F	13	0	0	0	0
62	2O	2	0	0	0	0
62	2P	13	0	0	2	0
62	2Q	1	0	0	0	0
62	2R	4	0	0	0	0
62	2T	6	0	0	0	0
62	2U	3	0	0	0	0
62	2W	1	0	0	0	0
62	2X	3	0	0	0	0
62	2Y	1	0	0	0	0
62	2Z	1	0	0	0	0
62	2a	216	0	0	17	0
62	2d	2	0	0	0	0
62	2e	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	2	0	0	0	0
62	2l	6	0	0	0	0
62	2p	1	0	0	0	0
62	2q	1	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	0	0
62	2v	1	0	0	0	0
62	2w	3	0	0	0	0
62	2x	4	0	0	1	0
62	2y	1	0	0	0	0
62	2z	1	0	0	0	0
All	All	300017	0	196778	4035	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 9.

The worst 5 of 4035 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	1.25	1.31
1:2A:2143:C:N4	1:2A:2148:G:H1	1.34	1.22
1:1A:1082:U:O4	1:1A:1086:A:N1	1.89	1.05
1:1A:1054:A:H61	1:1A:1105:U:H3	1.03	1.01
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.27	0.99

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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	253 (93%)	19 (7%)	1 (0%)	30	49
4	1E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24	43
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	43
5	1F	200/210 (95%)	192 (96%)	7 (4%)	1 (0%)	24	43
5	2F	200/210 (95%)	185 (92%)	13 (6%)	2 (1%)	12	24
6	1G	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	21	38
6	2G	179/182 (98%)	150 (84%)	25 (14%)	4 (2%)	5	9
7	1H	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	10	20
8	1I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	18	34
8	2I	144/148 (97%)	127 (88%)	16 (11%)	1 (1%)	18	34
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	128 (93%)	9 (6%)	1 (1%)	18	34
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	31
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	136 (92%)	8 (5%)	3 (2%)	6	10
11	2P	147/150 (98%)	131 (89%)	13 (9%)	3 (2%)	6	10
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	4 (3%)	1 (1%)	14	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	14	27
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	24
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	24
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	22
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	22
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	148/206 (72%)	129 (87%)	17 (12%)	2 (1%)	9	17
21	2Z	156/206 (76%)	124 (80%)	28 (18%)	4 (3%)	4	7
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	22
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	0
26	24	67/71 (94%)	50 (75%)	15 (22%)	2 (3%)	3	5
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	195 (85%)	25 (11%)	9 (4%)	2	3
33	2b	229/256 (90%)	178 (78%)	42 (18%)	9 (4%)	2	3
34	1c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	24	43
34	2c	204/239 (85%)	170 (83%)	32 (16%)	2 (1%)	12	24
35	1d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	24	43
35	2d	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	9	17
36	2e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	9	17
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	18	34
38	2g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	6	10
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	31
40	2i	125/128 (98%)	105 (84%)	19 (15%)	1 (1%)	16	31
41	1j	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	11	22
41	2j	94/105 (90%)	77 (82%)	14 (15%)	3 (3%)	3	4
42	1k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14	27
42	2k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14	27
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	16	31
43	2l	119/132 (90%)	112 (94%)	5 (4%)	2 (2%)	7	13
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	7	13
44	2m	120/126 (95%)	106 (88%)	11 (9%)	3 (2%)	4	7
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	20
46	2o	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	10	20
47	1p	80/88 (91%)	77 (96%)	2 (2%)	1 (1%)	9	18
47	2p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9	18
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	5	9
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	81 (86%)	12 (13%)	1 (1%)	11	22
51	2t	94/106 (89%)	85 (90%)	8 (8%)	1 (1%)	11	22
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
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%)	10433 (92%)	839 (7%)	98 (1%)	14	27

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	29	LYS
21	1Z	53	ILE
23	11	3	LYS
26	14	53	GLU
26	14	62	ARG

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%)	205 (95%)	10 (5%)	23	47
3	2D	215/218 (99%)	202 (94%)	13 (6%)	17	36
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	31
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10	22
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	14
5	2F	159/166 (96%)	149 (94%)	10 (6%)	16	34
6	1G	143/156 (92%)	132 (92%)	11 (8%)	12	25
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	4
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	30
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	19
8	1I	113/124 (91%)	92 (81%)	21 (19%)	1	3
8	2I	105/124 (85%)	84 (80%)	21 (20%)	1	2
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	37
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14	31
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	64
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	54
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	29
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	24
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	41
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	49
13	1R	101/101 (100%)	97 (96%)	4 (4%)	28	54
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	44
14	1S	86/88 (98%)	76 (88%)	10 (12%)	5	11
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	14
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	42
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	24
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	51
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	41
17	1V	80/82 (98%)	77 (96%)	3 (4%)	29	56
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	12
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	82
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	32
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
20	2Y	85/91 (93%)	71 (84%)	14 (16%)	2	4
21	1Z	135/179 (75%)	119 (88%)	16 (12%)	5	11
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5	11
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	62
23	11	80/83 (96%)	73 (91%)	7 (9%)	9	20
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	26
24	12	65/67 (97%)	60 (92%)	5 (8%)	12	25
24	22	65/67 (97%)	57 (88%)	8 (12%)	4	10
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	37
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	36
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	8
26	24	53/63 (84%)	40 (76%)	13 (24%)	1	1
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	24
28	16	51/52 (98%)	44 (86%)	7 (14%)	3	7
28	26	50/52 (96%)	41 (82%)	9 (18%)	2	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	27
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	45
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	39
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	39
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	37
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	192/220 (87%)	165 (86%)	27 (14%)	3	7
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2	4
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8	19
34	2c	140/188 (74%)	129 (92%)	11 (8%)	11	24
35	1d	169/181 (93%)	148 (88%)	21 (12%)	4	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11	23
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	34
36	2e	114/123 (93%)	104 (91%)	10 (9%)	9	20
37	1f	84/90 (93%)	74 (88%)	10 (12%)	5	11
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18	37
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	5
38	2g	120/127 (94%)	101 (84%)	19 (16%)	2	5
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14	29
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	17
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	9
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	5
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	11
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	8
42	2k	83/99 (84%)	73 (88%)	10 (12%)	5	10
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	34
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	18
44	1m	93/101 (92%)	85 (91%)	8 (9%)	10	21
44	2m	92/101 (91%)	82 (89%)	10 (11%)	6	13
45	1n	49/50 (98%)	47 (96%)	2 (4%)	27	53
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	35
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	43
46	2o	78/80 (98%)	77 (99%)	1 (1%)	61	82
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	27
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	42
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	42
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	11
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14	31
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	21
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	60 (86%)	10 (14%)	3	6
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	51
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	39
56	1z	2/2 (100%)	2 (100%)	0	100	100
56	2z	2/2 (100%)	2 (100%)	0	100	100
All	All	9307/10068 (92%)	8485 (91%)	822 (9%)	9	20

5 of 822 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	2H	95	ARG
20	2Y	97	ARG
47	2p	67	THR
8	2I	51	ILE
7	2H	70	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
42	2k	22	HIS
44	2m	77	ASN
50	2s	57	HIS
37	1f	57	GLN
36	1e	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	444 (15%)	30 (1%)
1	2A	2791/2915 (95%)	459 (16%)	25 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1497/1521 (98%)	242 (16%)	0
32	2a	1501/1521 (98%)	276 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	0	0
54	1w	71/76 (93%)	24 (33%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	2w	68/76 (89%)	23 (33%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
57	1y	72/76 (94%)	27 (37%)	0
57	2y	70/76 (92%)	22 (31%)	0
All	All	9345/9620 (97%)	1563 (16%)	55 (0%)

5 of 1563 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	27	G
1	1A	34	C

5 of 55 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2689	U
1	2A	271(M)	G
1	2A	2689	U
1	2A	1913	A
1	1A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.18	2 (7%)
1	2MA	1A	2503	58,1	22,25,26	1.52	4 (18%)	32,37,40	2.22	8 (25%)
43	0TD	2l	92	43	8,9,10	4.54	1 (12%)	6,11,13	4.13	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1939	1	19,22,23	1.49	6 (31%)	27,32,35	2.21	6 (22%)
55	PSU	1x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.93	3 (14%)
32	M2G	1a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.87	5 (15%)
32	5MC	1a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.21	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.32	2 (11%)	21,30,33	2.18	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	1.00	1 (4%)
1	2MA	2A	2503	58,1	22,25,26	1.45	4 (18%)	32,37,40	2.40	9 (28%)
1	PSU	1A	1917	1	18,21,22	1.39	4 (22%)	21,30,33	2.25	4 (19%)
32	4OC	2a	1402	32,58	20,23,24	0.75	0	25,32,35	1.00	3 (12%)
1	PSU	1A	2605	58,1	18,21,22	1.41	2 (11%)	21,30,33	2.08	4 (19%)
1	PSU	2A	2605	1	18,21,22	1.41	3 (16%)	21,30,33	2.07	4 (19%)
57	4SU	1y	8	57	18,21,22	1.75	4 (22%)	25,30,33	2.18	5 (20%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.84	0
55	5MU	1x	54	55	19,22,23	1.36	4 (21%)	27,32,35	2.06	6 (22%)
54	4SU	1w	8	54	18,21,22	1.93	5 (27%)	25,30,33	1.89	5 (20%)
55	8AN	1x	76	55,58,56	21,24,25	1.52	3 (14%)	26,35,38	2.52	11 (42%)
55	8AN	2x	76	55,58,56	21,24,25	1.42	3 (14%)	26,35,38	2.50	11 (42%)
32	5MC	1a	1407	32	19,22,23	1.69	2 (10%)	26,32,35	1.16	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.04	1 (4%)
57	PSU	2y	32	57	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
55	4SU	1x	8	55	18,21,22	2.14	5 (27%)	25,30,33	1.62	6 (24%)
1	5MC	2A	1942	1	19,22,23	1.69	3 (15%)	26,32,35	1.17	3 (11%)
57	G7M	1y	46	57	23,26,27	1.50	4 (17%)	34,39,42	1.81	5 (14%)
32	2MG	2a	1207	32	23,26,27	1.23	4 (17%)	33,38,41	2.28	9 (27%)
32	M2G	2a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.83	6 (18%)
32	UR3	2a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.69	2 (7%)
57	PSU	1y	39	57	18,21,22	1.43	2 (11%)	21,30,33	1.94	4 (19%)
54	PSU	2w	39	54	18,21,22	1.32	2 (11%)	21,30,33	2.12	5 (23%)
54	G7M	1w	46	54	23,26,27	1.52	4 (17%)	34,39,42	1.66	4 (11%)
54	F3N	2w	76	54,1	33,36,37	1.44	4 (12%)	41,51,54	1.74	9 (21%)
32	5MC	1a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.09	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.09	4 (19%)
57	MIA	1y	37	57	21,24,32	1.61	4 (19%)	30,35,47	2.09	7 (23%)
1	5MU	2A	1939	58,1	19,22,23	1.39	5 (26%)	27,32,35	2.45	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PSU	2y	55	57	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
54	4SU	2w	8	54	18,21,22	1.77	4 (22%)	25,30,33	2.46	5 (20%)
1	OMG	2A	2251	55,1	23,26,27	1.23	3 (13%)	32,38,41	1.96	6 (18%)
32	5MC	2a	967	32,58	19,22,23	1.63	2 (10%)	26,32,35	1.10	2 (7%)
57	PSU	1y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
1	5MC	2A	1962	58,1	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
32	G7M	2a	527	32,58	23,26,27	1.45	4 (17%)	34,39,42	1.59	4 (11%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	6.99	3 (50%)
1	OMU	1A	2552	58,1	19,22,23	1.23	2 (10%)	25,31,34	1.79	6 (24%)
1	5MC	1A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.22	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.09	7 (25%)
1	5MC	1A	1962	1	19,22,23	1.78	3 (15%)	26,32,35	1.20	3 (11%)
57	MIA	2y	37	57	21,24,32	1.59	3 (14%)	30,35,47	2.05	8 (26%)
54	MIA	2w	37	54	24,27,32	2.09	6 (25%)	32,39,47	2.79	12 (37%)
56	FME	2z	1	56	8,9,10	1.00	0	8,9,11	1.68	2 (25%)
32	G7M	1a	527	32,58	23,26,27	1.54	3 (13%)	34,39,42	1.77	5 (14%)
54	PSU	1w	55	54	18,21,22	1.44	2 (11%)	21,30,33	2.04	4 (19%)
55	5MC	2x	32	55	19,22,23	1.72	3 (15%)	26,32,35	1.29	4 (15%)
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.18	3 (11%)
54	PSU	1w	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.24	5 (23%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.14	8 (29%)
54	5MU	1w	54	54	19,22,23	1.29	5 (26%)	27,32,35	2.13	6 (22%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	2.28	6 (22%)
56	FME	1z	1	56	8,9,10	1.03	0	8,9,11	1.85	3 (37%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.01	4 (19%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
57	PSU	1y	32	57	18,21,22	1.35	2 (11%)	21,30,33	1.95	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.04	4 (19%)
57	PSU	2y	39	42,57	18,21,22	1.31	2 (11%)	21,30,33	2.13	3 (14%)
57	G7M	2y	46	57	23,26,27	1.57	3 (13%)	34,39,42	1.89	4 (11%)
57	5MU	1y	54	57	19,22,23	1.42	4 (21%)	27,32,35	2.03	7 (25%)
54	PSU	1w	32	54	18,21,22	1.38	3 (16%)	21,30,33	1.89	4 (19%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.08	9 (27%)
1	OMU	2A	2552	58,1	19,22,23	1.16	2 (10%)	25,31,34	1.91	6 (24%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.00	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	MIA	1w	37	54	28,31,32	2.27	6 (21%)	38,44,47	2.83	13 (34%)
1	OMG	1A	2251	55,58,1	23,26,27	1.23	3 (13%)	32,38,41	1.97	6 (18%)
54	G7M	2w	46	54	23,26,27	1.47	2 (8%)	34,39,42	1.68	5 (14%)
57	4SU	2y	8	57	18,21,22	1.84	4 (22%)	25,30,33	2.30	4 (16%)
55	4SU	2x	8	55,58	18,21,22	2.10	6 (33%)	25,30,33	1.56	5 (20%)
32	5MC	1a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.15	2 (7%)
57	5MU	2y	54	57	19,22,23	1.41	5 (26%)	27,32,35	1.78	5 (18%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.85	3 (11%)
32	MA6	2a	1518	32	23,26,27	0.45	0	33,38,41	2.05	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.75	3 (15%)	26,32,35	1.20	3 (11%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.15	10 (30%)
32	PSU	1a	516	32	18,21,22	1.37	2 (11%)	21,30,33	2.08	5 (23%)
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	27,32,35	1.83	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.27	8 (24%)
32	MA6	2a	1519	32	23,26,27	0.47	0	33,38,41	2.18	9 (27%)
55	5MC	1x	32	55,58	19,22,23	1.67	3 (15%)	26,32,35	1.34	3 (11%)
54	F3N	1w	76	54,1	33,36,37	1.45	4 (12%)	41,51,54	1.79	10 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	1/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	2MA	2A	2503	58,1	-	2/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,58	-	0/9/29/30	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	1/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	55,58,56	-	3/7/25/26	0/3/3/3
55	8AN	2x	76	55,58,56	-	3/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	1/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
57	PSU	1y	39	57	-	1/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	F3N	2w	76	54,1	-	2/19/37/38	0/4/4/4
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	1/7/25/26	0/2/2/2
57	MIA	1y	37	57	-	1/7/25/34	0/3/3/3
1	5MU	2A	1939	58,1	-	0/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
32	5MC	2a	967	32,58	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	2/7/25/26	0/2/2/2
32	G7M	2a	527	32,58	-	3/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
57	MIA	2y	37	57	-	0/7/25/34	0/3/3/3
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
56	FME	2z	1	56	-	4/7/9/11	-
32	G7M	1a	527	32,58	-	3/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	4/7/9/11	-
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
57	PSU	1y	32	57	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
57	PSU	2y	39	42,57	-	0/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	2/7/25/26	0/3/3/3
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	5/15/33/34	0/3/3/3
1	OMG	1A	2251	55,58,1	-	1/9/27/28	0/3/3/3
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
57	4SU	2y	8	57	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,58	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
55	5MC	1x	32	55,58	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4

The worst 5 of 253 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.46	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.24	1.69	1.82
54	2w	37	MIA	C2-S10	-6.74	1.70	1.75
54	1w	37	MIA	C13-C14	6.64	1.52	1.32
54	1w	37	MIA	C2-S10	-6.54	1.70	1.75

The worst 5 of 450 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.61	72.51	102.36
54	2w	37	MIA	C5-C4-N3	-9.32	117.36	127.18
54	1w	37	MIA	C12-C13-C14	-9.27	110.37	127.01
43	2l	92	0TD	CSB-SB-CB	-9.13	85.95	102.36
1	2A	2503	2MA	C5-C4-N3	-8.24	118.50	127.18

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
57	1y	46	G7M	C4'-C5'-O5'-P

There are no ring outliers.

33 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2503	2MA	1	0
43	2l	92	0TD	1	0
1	1A	1939	5MU	1	0
1	1A	1917	PSU	1	0
32	2a	1402	4OC	1	0
57	1y	8	4SU	2	0
54	1w	8	4SU	1	0
55	1x	76	8AN	2	0
55	2x	76	8AN	2	0
32	1a	1402	4OC	2	0
55	1x	8	4SU	1	0
57	1y	46	G7M	4	0
32	2a	1207	2MG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1y	39	PSU	1	0
54	2w	39	PSU	1	0
54	1w	46	G7M	2	0
54	2w	76	F3N	2	0
57	1y	37	MIA	3	0
1	2A	1939	5MU	1	0
57	2y	55	PSU	5	0
54	2w	8	4SU	1	0
32	2a	967	5MC	1	0
57	1y	55	PSU	2	0
32	2a	527	G7M	1	0
1	1A	2552	OMU	1	0
32	2a	1404	5MC	1	0
54	1w	39	PSU	1	0
57	2y	46	G7M	2	0
32	1a	1518	MA6	1	0
1	2A	2552	OMU	1	0
54	2w	46	G7M	1	0
32	1a	1498	UR3	1	0
32	1a	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2784 ligands modelled in this entry, 2782 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	-0.44	158 (5%) 30 27	14, 30, 79, 88	0
1	2A	2789/2915 (95%)	0.02	128 (4%) 37 33	26, 48, 76, 86	0
2	1B	120/121 (99%)	-0.34	0 100 100	24, 42, 54, 75	0
2	2B	120/121 (99%)	0.50	0 100 100	47, 60, 68, 72	0
3	1D	275/276 (99%)	-0.11	1 (0%) 88 86	14, 31, 43, 63	0
3	2D	275/276 (99%)	0.21	3 (1%) 78 75	25, 41, 51, 68	0
4	1E	204/206 (99%)	-0.01	0 100 100	14, 35, 54, 63	0
4	2E	204/206 (99%)	0.50	3 (1%) 72 68	29, 49, 60, 66	0
5	1F	202/210 (96%)	0.03	0 100 100	14, 37, 56, 68	0
5	2F	202/210 (96%)	0.64	6 (2%) 52 48	28, 54, 64, 68	0
6	1G	181/182 (99%)	0.52	4 (2%) 62 58	33, 49, 61, 71	0
6	2G	181/182 (99%)	1.19	17 (9%) 14 12	50, 61, 68, 73	0
7	1H	174/180 (96%)	0.47	1 (0%) 85 83	33, 47, 55, 60	0
7	2H	174/180 (96%)	1.54	47 (27%) 1 1	56, 67, 73, 75	0
8	1I	146/148 (98%)	0.86	8 (5%) 30 27	37, 59, 66, 69	0
8	2I	146/148 (98%)	1.19	16 (10%) 10 8	44, 60, 68, 71	0
9	1N	140/140 (100%)	0.03	0 100 100	19, 34, 50, 59	0
9	2N	140/140 (100%)	0.67	0 100 100	38, 53, 63, 72	0
10	1O	122/122 (100%)	0.01	1 (0%) 82 80	24, 35, 49, 55	0
10	2O	122/122 (100%)	0.53	0 100 100	37, 48, 60, 63	0
11	1P	149/150 (99%)	0.11	1 (0%) 84 81	15, 39, 58, 64	0
11	2P	149/150 (99%)	0.74	7 (4%) 36 32	28, 54, 67, 71	0
12	1Q	141/141 (100%)	0.02	1 (0%) 84 81	19, 35, 47, 60	0
12	2Q	141/141 (100%)	0.82	11 (7%) 19 17	35, 52, 62, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.16	0 100 100	22, 31, 39, 48	0
13	2R	118/118 (100%)	0.26	0 100 100	34, 44, 53, 60	0
14	1S	110/112 (98%)	0.22	0 100 100	30, 40, 51, 54	0
14	2S	110/112 (98%)	1.06	9 (8%) 17 15	47, 56, 63, 68	0
15	1T	131/146 (89%)	0.19	3 (2%) 61 57	27, 39, 57, 65	0
15	2T	131/146 (89%)	0.56	4 (3%) 51 47	39, 51, 61, 65	0
16	1U	116/118 (98%)	-0.28	0 100 100	17, 26, 42, 51	0
16	2U	116/118 (98%)	0.58	2 (1%) 69 65	35, 50, 61, 66	0
17	1V	101/101 (100%)	-0.11	0 100 100	19, 36, 50, 57	0
17	2V	101/101 (100%)	0.93	4 (3%) 42 38	36, 57, 63, 71	0
18	1W	112/113 (99%)	-0.24	2 (1%) 67 64	17, 27, 43, 67	0
18	2W	112/113 (99%)	0.36	3 (2%) 56 51	30, 41, 56, 82	0
19	1X	95/96 (98%)	0.04	2 (2%) 63 59	21, 31, 51, 68	0
19	2X	95/96 (98%)	0.75	5 (5%) 32 28	36, 49, 61, 71	0
20	1Y	107/110 (97%)	0.36	1 (0%) 81 78	28, 43, 57, 66	0
20	2Y	107/110 (97%)	1.11	11 (10%) 12 10	48, 59, 67, 72	0
21	1Z	154/206 (74%)	0.88	18 (11%) 9 7	35, 52, 69, 72	0
21	2Z	160/206 (77%)	1.51	37 (23%) 2 1	47, 64, 72, 75	0
22	10	83/85 (97%)	-0.10	0 100 100	20, 30, 41, 53	0
22	20	83/85 (97%)	0.69	4 (4%) 35 31	34, 50, 58, 64	0
23	11	97/98 (98%)	0.11	1 (1%) 79 76	21, 38, 58, 62	0
23	21	97/98 (98%)	0.52	2 (2%) 63 59	32, 45, 60, 66	0
24	12	70/72 (97%)	0.16	0 100 100	27, 39, 52, 63	0
24	22	70/72 (97%)	0.86	1 (1%) 73 70	47, 56, 63, 66	0
25	13	59/60 (98%)	-0.03	0 100 100	17, 31, 52, 60	0
25	23	59/60 (98%)	0.64	1 (1%) 69 65	43, 54, 63, 66	0
26	14	69/71 (97%)	1.00	11 (15%) 5 4	42, 60, 71, 75	0
26	24	69/71 (97%)	1.47	16 (23%) 2 1	60, 67, 73, 79	0
27	15	59/60 (98%)	-0.00	0 100 100	15, 30, 57, 62	0
27	25	59/60 (98%)	0.40	0 100 100	27, 43, 61, 65	0
28	16	53/54 (98%)	-0.12	0 100 100	26, 35, 44, 50	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.50	0 100 100	39, 49, 55, 58	0
29	17	48/49 (97%)	-0.32	1 (2%) 63 59	15, 21, 43, 50	0
29	27	48/49 (97%)	0.12	2 (4%) 40 36	27, 35, 55, 61	0
30	18	64/65 (98%)	-0.16	0 100 100	21, 27, 35, 46	0
30	28	64/65 (98%)	0.49	1 (1%) 70 67	38, 45, 51, 54	0
31	19	37/37 (100%)	-0.10	0 100 100	26, 34, 42, 50	0
31	29	37/37 (100%)	0.92	1 (2%) 56 51	45, 55, 60, 62	0
32	1a	1488/1521 (97%)	0.34	50 (3%) 48 43	27, 55, 75, 87	0
32	2a	1491/1521 (98%)	0.56	56 (3%) 44 39	40, 62, 76, 87	0
33	1b	231/256 (90%)	1.19	33 (14%) 6 5	50, 63, 70, 78	0
33	2b	231/256 (90%)	1.56	61 (26%) 1 1	58, 67, 72, 77	0
34	1c	206/239 (86%)	0.96	13 (6%) 26 23	49, 58, 66, 73	0
34	2c	206/239 (86%)	1.57	56 (27%) 1 1	59, 66, 72, 76	0
35	1d	208/209 (99%)	0.83	12 (5%) 29 25	43, 57, 64, 67	0
35	2d	208/209 (99%)	0.82	8 (3%) 44 39	47, 57, 64, 72	0
36	1e	148/162 (91%)	0.65	2 (1%) 73 70	40, 53, 60, 64	0
36	2e	148/162 (91%)	1.08	12 (8%) 18 15	50, 60, 65, 68	0
37	1f	100/101 (99%)	0.57	0 100 100	46, 55, 61, 62	0
37	2f	100/101 (99%)	0.75	1 (1%) 79 76	47, 56, 62, 64	0
38	1g	155/156 (99%)	0.98	15 (9%) 13 11	49, 58, 68, 76	0
38	2g	155/156 (99%)	1.33	24 (15%) 5 4	54, 65, 70, 76	0
39	1h	137/138 (99%)	0.87	8 (5%) 29 25	45, 55, 61, 63	0
39	2h	137/138 (99%)	1.09	10 (7%) 21 19	51, 61, 66, 71	0
40	1i	127/128 (99%)	1.36	24 (18%) 3 2	44, 63, 69, 71	0
40	2i	127/128 (99%)	1.75	43 (33%) 1 1	57, 67, 72, 73	0
41	1j	97/105 (92%)	1.29	16 (16%) 4 3	45, 62, 69, 73	0
41	2j	96/105 (91%)	1.80	35 (36%) 1 1	58, 68, 72, 73	0
42	1k	114/129 (88%)	0.81	8 (7%) 22 20	32, 54, 62, 69	0
42	2k	114/129 (88%)	1.13	10 (8%) 15 14	48, 60, 66, 70	0
43	1l	121/132 (91%)	0.42	3 (2%) 58 54	33, 44, 54, 60	0
43	2l	121/132 (91%)	0.76	7 (5%) 29 25	44, 53, 61, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.96	10 (8%) 18 15	46, 57, 63, 68	0
44	2m	122/126 (96%)	1.43	19 (15%) 5 4	56, 64, 69, 72	0
45	1n	60/61 (98%)	1.05	4 (6%) 24 21	50, 55, 62, 62	0
45	2n	60/61 (98%)	2.12	29 (48%) 0 0	60, 67, 70, 73	0
46	1o	88/89 (98%)	0.91	6 (6%) 23 20	40, 53, 62, 68	0
46	2o	88/89 (98%)	1.10	8 (9%) 15 13	48, 58, 64, 67	0
47	1p	82/88 (93%)	1.23	10 (12%) 8 7	46, 58, 64, 69	0
47	2p	82/88 (93%)	0.86	4 (4%) 35 31	49, 57, 64, 67	0
48	1q	99/105 (94%)	0.92	3 (3%) 52 48	43, 54, 63, 67	0
48	2q	99/105 (94%)	0.99	5 (5%) 33 29	51, 57, 64, 68	0
49	1r	68/88 (77%)	0.59	2 (2%) 53 49	46, 54, 63, 66	0
49	2r	68/88 (77%)	0.85	5 (7%) 20 18	49, 57, 65, 69	0
50	1s	83/93 (89%)	1.05	6 (7%) 21 19	49, 58, 66, 70	0
50	2s	83/93 (89%)	1.44	18 (21%) 2 2	60, 66, 71, 73	0
51	1t	96/106 (90%)	1.10	9 (9%) 14 12	50, 58, 65, 73	0
51	2t	96/106 (90%)	1.01	7 (7%) 21 19	46, 57, 68, 75	0
52	1u	23/27 (85%)	1.32	3 (13%) 7 6	50, 54, 58, 60	0
52	2u	23/27 (85%)	1.81	6 (26%) 1 1	62, 65, 69, 73	0
53	1v	13/24 (54%)	0.78	4 (30%) 1 1	38, 42, 76, 78	0
53	2v	13/24 (54%)	1.16	4 (30%) 1 1	52, 59, 79, 87	0
54	1w	66/76 (86%)	1.04	6 (9%) 15 13	22, 68, 79, 83	0
54	2w	64/76 (84%)	1.26	11 (17%) 4 3	37, 75, 81, 85	0
55	1x	72/77 (93%)	0.23	0 100 100	19, 51, 68, 75	0
55	2x	72/77 (93%)	0.49	1 (1%) 73 70	35, 61, 70, 80	0
56	1z	2/3 (66%)	-0.60	0 100 100	18, 18, 18, 19	0
56	2z	2/3 (66%)	-0.73	0 100 100	31, 31, 31, 32	0
57	1y	67/76 (88%)	2.15	38 (56%) 0 0	54, 80, 85, 86	0
57	2y	66/76 (86%)	2.09	37 (56%) 0 0	62, 82, 86, 87	0
All	All	20875/21754 (95%)	0.43	1317 (6%) 26 23	14, 52, 72, 88	0

The worst 5 of 1317 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	1n	2	ALA	6.3
21	1Z	141	VAL	6.2
38	2g	80	VAL	6.1
1	2A	2146	C	5.8
1	2A	883	G	5.5

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
57	4SU	2y	8	20/21	0.54	0.21	76,88,95,107	0
57	G7M	2y	46	24/25	0.56	0.18	76,84,87,99	0
57	PSU	1y	55	20/21	0.59	0.18	79,84,91,100	0
54	G7M	2w	46	24/25	0.61	0.18	64,76,88,99	0
57	G7M	1y	46	24/25	0.65	0.17	64,78,86,92	0
57	5MU	1y	54	21/22	0.65	0.15	74,80,86,95	0
57	MIA	2y	37	22/30	0.67	0.17	71,77,91,104	0
57	4SU	1y	8	20/21	0.67	0.16	76,80,94,101	0
57	MIA	1y	37	22/30	0.67	0.21	69,78,88,96	0
57	PSU	1y	39	20/21	0.69	0.18	70,81,84,85	0
57	5MU	2y	54	21/22	0.70	0.17	67,76,83,95	0
54	G7M	1w	46	24/25	0.73	0.16	66,70,84,96	0
57	PSU	2y	39	20/21	0.73	0.15	74,80,87,90	0
57	PSU	2y	55	20/21	0.74	0.16	74,80,85,87	0
57	PSU	2y	32	20/21	0.75	0.16	73,79,83,89	0
57	PSU	1y	32	20/21	0.76	0.15	70,76,88,96	0
54	4SU	2w	8	20/21	0.86	0.13	67,74,82,83	0
54	PSU	2w	55	20/21	0.86	0.12	58,68,76,77	0
54	5MU	2w	54	21/22	0.88	0.12	56,63,68,71	0
54	4SU	1w	8	20/21	0.88	0.14	56,70,78,81	0
55	5MU	2x	54	21/22	0.89	0.14	59,65,69,71	0
54	MIA	2w	37	25/30	0.89	0.14	52,60,67,87	0
54	PSU	2w	32	20/21	0.90	0.13	52,65,81,85	0
1	5MU	2A	1915	21/22	0.90	0.12	50,58,62,64	0
55	4SU	2x	8	20/21	0.90	0.12	57,62,65,71	0
55	PSU	2x	55	20/21	0.91	0.11	55,59,68,73	0
32	2MG	2a	1207	24/25	0.91	0.12	59,68,70,71	0
55	5MC	2x	32	21/22	0.91	0.13	51,58,64,70	0
43	0TD	2l	92	10/11	0.91	0.13	47,51,57,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	M2G	2a	966	25/26	0.92	0.14	45,56,64,76	0
55	PSU	1x	55	20/21	0.92	0.11	45,51,64,67	0
54	PSU	1w	32	20/21	0.93	0.11	46,52,59,63	0
32	G7M	2a	527	24/25	0.93	0.12	47,53,58,61	0
32	2MG	1a	1207	24/25	0.93	0.10	48,56,59,63	0
43	0TD	1l	92	10/11	0.93	0.10	39,42,47,58	0
32	5MC	2a	1400	21/22	0.93	0.12	48,55,60,63	0
1	PSU	2A	1911	20/21	0.93	0.10	42,50,54,57	0
54	PSU	1w	55	20/21	0.93	0.10	40,60,66,67	0
55	5MU	1x	54	21/22	0.93	0.11	52,56,62,68	0
54	MIA	1w	37	29/30	0.94	0.12	35,44,52,76	0
1	5MC	2A	1942	21/22	0.94	0.11	44,49,56,57	0
54	PSU	2w	39	20/21	0.94	0.10	47,62,68,68	0
32	4OC	2a	1402	22/23	0.94	0.10	47,50,54,56	0
55	4SU	1x	8	20/21	0.94	0.10	49,54,59,60	0
1	PSU	2A	1917	20/21	0.94	0.09	43,55,58,58	0
32	5MC	2a	967	21/22	0.94	0.11	51,56,64,66	0
1	OMC	2A	1920	21/22	0.94	0.10	48,51,56,63	0
56	FME	2z	1	10/11	0.94	0.10	29,35,42,48	0
1	5MU	1A	1915	21/22	0.95	0.09	34,41,45,50	0
32	5MC	2a	1404	21/22	0.95	0.10	42,48,51,52	0
32	5MC	2a	1407	21/22	0.95	0.10	36,43,50,52	0
55	5MC	1x	32	21/22	0.95	0.11	34,42,49,55	0
32	5MC	1a	1400	21/22	0.95	0.11	36,43,46,48	0
32	G7M	1a	527	24/25	0.95	0.09	33,39,46,48	0
32	PSU	2a	516	20/21	0.95	0.09	47,58,63,64	0
32	M2G	1a	966	25/26	0.96	0.09	33,42,46,50	0
1	PSU	1A	1917	20/21	0.96	0.08	33,39,43,45	0
1	5MC	1A	1942	21/22	0.96	0.09	29,36,40,47	0
32	4OC	1a	1402	22/23	0.96	0.10	30,38,42,46	0
32	5MC	1a	1407	21/22	0.96	0.08	27,35,39,42	0
54	PSU	1w	39	20/21	0.96	0.09	30,52,60,67	0
32	MA6	1a	1519	24/25	0.96	0.10	31,36,42,49	0
32	PSU	1a	516	20/21	0.96	0.08	38,46,50,50	0
1	5MC	2A	1962	21/22	0.96	0.09	24,38,43,48	0
54	5MU	1w	54	21/22	0.96	0.10	34,50,54,57	0
32	UR3	2a	1498	21/22	0.96	0.10	46,49,53,53	0
32	MA6	2a	1518	24/25	0.96	0.10	42,48,53,53	0
32	MA6	2a	1519	24/25	0.96	0.11	42,50,53,55	0
54	F3N	2w	76	33/34	0.96	0.09	26,33,36,38	0
56	FME	1z	1	10/11	0.96	0.09	19,23,25,35	0
1	PSU	1A	1911	20/21	0.96	0.09	33,42,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	8AN	1x	76	22/23	0.97	0.07	14,18,23,33	0
32	5MC	1a	1404	21/22	0.97	0.10	26,32,38,39	0
1	OMU	2A	2552	21/22	0.97	0.09	27,36,43,46	0
55	8AN	2x	76	22/23	0.97	0.09	24,35,41,42	0
1	PSU	2A	2605	20/21	0.97	0.07	24,30,35,35	0
32	5MC	1a	967	21/22	0.97	0.09	37,43,48,53	0
32	UR3	1a	1498	21/22	0.97	0.09	29,35,39,40	0
1	5MU	1A	1939	21/22	0.98	0.06	15,22,28,30	0
1	OMC	1A	1920	21/22	0.98	0.07	26,39,44,47	0
1	5MC	1A	1962	21/22	0.98	0.07	23,28,32,36	0
32	MA6	1a	1518	24/25	0.98	0.09	28,35,37,41	0
1	OMG	1A	2251	24/25	0.98	0.06	15,20,22,24	0
1	2MA	1A	2503	23/24	0.98	0.06	12,14,17,18	0
1	5MU	2A	1939	21/22	0.98	0.07	24,30,34,35	0
1	OMU	1A	2552	21/22	0.98	0.06	17,24,27,28	0
54	F3N	1w	76	33/34	0.98	0.08	13,19,21,25	0
1	PSU	1A	2605	20/21	0.98	0.06	15,20,24,24	0
1	OMG	2A	2251	24/25	0.98	0.08	25,32,38,43	0
1	2MA	2A	2503	23/24	0.98	0.07	23,29,32,34	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	229	1/1	0.49	0.18	66,66,66,66	0
58	MG	2B	220	1/1	0.59	0.22	77,77,77,77	0
58	MG	1a	1766	1/1	0.63	0.22	68,68,68,68	0
58	MG	1A	3798	1/1	0.67	0.21	67,67,67,67	0
58	MG	2v	101	1/1	0.67	0.23	75,75,75,75	0
58	MG	1Y	203	1/1	0.68	0.13	66,66,66,66	0
58	MG	2a	1811	1/1	0.68	0.18	69,69,69,69	0
58	MG	1A	3903	1/1	0.68	0.23	66,66,66,66	0
58	MG	1A	4030	1/1	0.69	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3829	1/1	0.70	0.12	31,31,31,31	0
58	MG	1B	230	1/1	0.71	0.23	75,75,75,75	0
58	MG	2a	1741	1/1	0.71	0.17	69,69,69,69	0
58	MG	2A	3646	1/1	0.72	0.20	43,43,43,43	0
58	MG	2a	1781	1/1	0.72	0.18	56,56,56,56	0
58	MG	1A	3855	1/1	0.72	0.14	51,51,51,51	0
58	MG	2A	3051	1/1	0.72	0.21	65,65,65,65	0
58	MG	1A	3995	1/1	0.73	0.11	27,27,27,27	0
58	MG	1A	3414	1/1	0.73	0.28	68,68,68,68	0
58	MG	1A	4072	1/1	0.73	0.18	47,47,47,47	0
58	MG	2a	1826	1/1	0.73	0.25	59,59,59,59	0
58	MG	1A	4090	1/1	0.73	0.23	81,81,81,81	0
58	MG	10	107	1/1	0.74	0.23	54,54,54,54	0
58	MG	2a	1773	1/1	0.74	0.17	59,59,59,59	0
58	MG	2A	3788	1/1	0.74	0.21	60,60,60,60	0
58	MG	2A	3562	1/1	0.74	0.17	44,44,44,44	0
58	MG	2A	3579	1/1	0.74	0.23	54,54,54,54	0
58	MG	2a	1626	1/1	0.74	0.24	65,65,65,65	0
58	MG	1a	1744	1/1	0.75	0.18	64,64,64,64	0
58	MG	1A	3981	1/1	0.75	0.12	54,54,54,54	0
58	MG	1A	3796	1/1	0.75	0.11	44,44,44,44	0
58	MG	1A	4002	1/1	0.75	0.15	41,41,41,41	0
58	MG	1E	311	1/1	0.75	0.17	54,54,54,54	0
58	MG	1U	209	1/1	0.75	0.35	59,59,59,59	0
58	MG	1A	3713	1/1	0.75	0.15	34,34,34,34	0
58	MG	1A	3949	1/1	0.75	0.16	36,36,36,36	0
58	MG	1a	1782	1/1	0.76	0.12	57,57,57,57	0
58	MG	2A	3682	1/1	0.76	0.17	57,57,57,57	0
58	MG	2B	211	1/1	0.77	0.30	77,77,77,77	0
58	MG	1A	3074	1/1	0.77	0.18	54,54,54,54	0
58	MG	2a	1611	1/1	0.77	0.19	64,64,64,64	0
58	MG	2A	3605	1/1	0.77	0.13	34,34,34,34	0
58	MG	1A	3617	1/1	0.77	0.13	26,26,26,26	0
58	MG	2A	3667	1/1	0.77	0.16	64,64,64,64	0
58	MG	1A	4032	1/1	0.77	0.15	57,57,57,57	0
58	MG	1A	4055	1/1	0.77	0.23	61,61,61,61	0
58	MG	1a	1737	1/1	0.77	0.23	68,68,68,68	0
58	MG	2A	3843	1/1	0.77	0.20	54,54,54,54	0
58	MG	18	107	1/1	0.78	0.19	55,55,55,55	0
58	MG	1A	4025	1/1	0.78	0.15	59,59,59,59	0
58	MG	2A	3393	1/1	0.78	0.13	59,59,59,59	0
58	MG	1A	3691	1/1	0.78	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3734	1/1	0.78	0.17	47,47,47,47	0
58	MG	1A	3673	1/1	0.78	0.10	33,33,33,33	0
58	MG	2A	3165	1/1	0.79	0.39	62,62,62,62	0
58	MG	2a	1622	1/1	0.79	0.16	76,76,76,76	0
58	MG	2A	3357	1/1	0.79	0.18	58,58,58,58	0
58	MG	1A	3861	1/1	0.79	0.16	65,65,65,65	0
58	MG	1a	1745	1/1	0.79	0.16	54,54,54,54	0
58	MG	1A	3960	1/1	0.79	0.21	52,52,52,52	0
58	MG	2a	1803	1/1	0.79	0.15	65,65,65,65	0
58	MG	1A	3766	1/1	0.79	0.10	19,19,19,19	0
58	MG	2a	1814	1/1	0.79	0.14	61,61,61,61	0
58	MG	1A	3988	1/1	0.79	0.14	56,56,56,56	0
58	MG	2A	3660	1/1	0.79	0.15	66,66,66,66	0
58	MG	1A	4017	1/1	0.80	0.08	38,38,38,38	0
58	MG	1a	1805	1/1	0.80	0.15	56,56,56,56	0
58	MG	1A	4033	1/1	0.80	0.12	42,42,42,42	0
58	MG	2A	3801	1/1	0.80	0.14	57,57,57,57	0
58	MG	2A	3593	1/1	0.80	0.20	65,65,65,65	0
58	MG	2a	1796	1/1	0.80	0.15	64,64,64,64	0
58	MG	2A	3105	1/1	0.80	0.16	65,65,65,65	0
58	MG	1A	3651	1/1	0.80	0.14	63,63,63,63	0
58	MG	2A	3283	1/1	0.80	0.17	49,49,49,49	0
58	MG	2Q	202	1/1	0.80	0.17	52,52,52,52	0
58	MG	1A	3932	1/1	0.80	0.08	22,22,22,22	0
58	MG	2x	104	1/1	0.80	0.21	61,61,61,61	0
58	MG	2A	3313	1/1	0.81	0.16	61,61,61,61	0
58	MG	25	102	1/1	0.81	0.19	57,57,57,57	0
58	MG	2A	3317	1/1	0.81	0.13	57,57,57,57	0
58	MG	1A	3167	1/1	0.81	0.12	49,49,49,49	0
58	MG	2A	3718	1/1	0.81	0.15	57,57,57,57	0
58	MG	1A	3360	1/1	0.81	0.22	65,65,65,65	0
58	MG	2A	3747	1/1	0.81	0.14	57,57,57,57	0
58	MG	2A	3761	1/1	0.81	0.17	62,62,62,62	0
58	MG	2a	1792	1/1	0.81	0.14	53,53,53,53	0
58	MG	1A	3103	1/1	0.81	0.12	53,53,53,53	0
58	MG	1A	3532	1/1	0.81	0.10	37,37,37,37	0
58	MG	1A	3851	1/1	0.81	0.13	59,59,59,59	0
58	MG	1A	3966	1/1	0.81	0.10	43,43,43,43	0
58	MG	2A	3865	1/1	0.81	0.19	52,52,52,52	0
58	MG	2n	102	1/1	0.81	0.31	70,70,70,70	0
58	MG	2A	3624	1/1	0.81	0.16	62,62,62,62	0
58	MG	1A	3698	1/1	0.81	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2D	304	1/1	0.82	0.17	53,53,53,53	0
58	MG	1A	4039	1/1	0.82	0.10	45,45,45,45	0
58	MG	1A	3810	1/1	0.82	0.14	46,46,46,46	0
58	MG	1A	4024	1/1	0.82	0.15	47,47,47,47	0
58	MG	2A	3191	1/1	0.82	0.24	69,69,69,69	0
58	MG	2A	3247	1/1	0.82	0.23	68,68,68,68	0
58	MG	2a	1650	1/1	0.82	0.24	60,60,60,60	0
58	MG	1A	4081	1/1	0.82	0.15	27,27,27,27	0
58	MG	1A	3646	1/1	0.82	0.11	35,35,35,35	0
58	MG	1A	4092	1/1	0.82	0.13	41,41,41,41	0
58	MG	2A	3342	1/1	0.82	0.25	70,70,70,70	0
58	MG	1A	3542	1/1	0.82	0.29	63,63,63,63	0
58	MG	1A	3954	1/1	0.82	0.11	61,61,61,61	0
58	MG	2A	3481	1/1	0.82	0.17	54,54,54,54	0
58	MG	2A	3486	1/1	0.82	0.14	56,56,56,56	0
58	MG	2a	1819	1/1	0.82	0.23	68,68,68,68	0
58	MG	1E	301	1/1	0.82	0.19	55,55,55,55	0
58	MG	2A	3572	1/1	0.82	0.11	30,30,30,30	0
58	MG	1a	1793	1/1	0.82	0.16	71,71,71,71	0
58	MG	1A	3306	1/1	0.82	0.35	59,59,59,59	0
58	MG	2A	3796	1/1	0.83	0.16	52,52,52,52	0
58	MG	1A	3720	1/1	0.83	0.12	51,51,51,51	0
58	MG	2A	3355	1/1	0.83	0.19	61,61,61,61	0
58	MG	1A	3755	1/1	0.83	0.15	57,57,57,57	0
58	MG	2A	3854	1/1	0.83	0.14	59,59,59,59	0
58	MG	2A	3855	1/1	0.83	0.17	71,71,71,71	0
58	MG	1A	3312	1/1	0.83	0.14	58,58,58,58	0
58	MG	2A	3423	1/1	0.83	0.13	49,49,49,49	0
58	MG	2A	3429	1/1	0.83	0.17	56,56,56,56	0
58	MG	2A	3473	1/1	0.83	0.18	66,66,66,66	0
58	MG	1A	3991	1/1	0.83	0.10	29,29,29,29	0
58	MG	1a	1770	1/1	0.83	0.12	72,72,72,72	0
58	MG	2A	3506	1/1	0.83	0.18	53,53,53,53	0
58	MG	1A	3862	1/1	0.83	0.11	63,63,63,63	0
58	MG	1a	1785	1/1	0.83	0.12	40,40,40,40	0
58	MG	2a	1628	1/1	0.83	0.14	57,57,57,57	0
58	MG	1A	3886	1/1	0.83	0.17	25,25,25,25	0
58	MG	2a	1722	1/1	0.83	0.14	66,66,66,66	0
58	MG	1A	3891	1/1	0.83	0.13	22,22,22,22	0
58	MG	1a	1811	1/1	0.83	0.20	63,63,63,63	0
58	MG	2A	3611	1/1	0.83	0.19	63,63,63,63	0
58	MG	1A	3769	1/1	0.83	0.12	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3780	1/1	0.83	0.11	18,18,18,18	0
58	MG	1R	204	1/1	0.83	0.19	42,42,42,42	0
58	MG	1A	3667	1/1	0.83	0.08	18,18,18,18	0
58	MG	2A	3246	1/1	0.83	0.17	64,64,64,64	0
58	MG	1A	3467	1/1	0.83	0.23	60,60,60,60	0
58	MG	1A	3959	1/1	0.83	0.11	48,48,48,48	0
58	MG	2A	3285	1/1	0.83	0.27	61,61,61,61	0
58	MG	1A	3716	1/1	0.83	0.17	38,38,38,38	0
58	MG	1a	1623	1/1	0.83	0.12	49,49,49,49	0
58	MG	1a	1759	1/1	0.84	0.22	62,62,62,62	0
58	MG	2A	3250	1/1	0.84	0.22	63,63,63,63	0
58	MG	2B	215	1/1	0.84	0.22	56,56,56,56	0
58	MG	2A	3268	1/1	0.84	0.10	65,65,65,65	0
58	MG	2A	3603	1/1	0.84	0.17	55,55,55,55	0
58	MG	1A	3899	1/1	0.84	0.15	40,40,40,40	0
58	MG	1A	4064	1/1	0.84	0.12	36,36,36,36	0
58	MG	2A	3619	1/1	0.84	0.13	47,47,47,47	0
58	MG	2A	3298	1/1	0.84	0.24	53,53,53,53	0
58	MG	1A	3069	1/1	0.84	0.18	55,55,55,55	0
58	MG	1A	3922	1/1	0.84	0.09	20,20,20,20	0
58	MG	1A	3872	1/1	0.84	0.09	40,40,40,40	0
58	MG	2a	1680	1/1	0.84	0.22	54,54,54,54	0
58	MG	2a	1701	1/1	0.84	0.27	58,58,58,58	0
58	MG	1A	3131	1/1	0.84	0.10	41,41,41,41	0
58	MG	2A	3704	1/1	0.84	0.15	69,69,69,69	0
58	MG	2a	1772	1/1	0.84	0.12	55,55,55,55	0
58	MG	18	109	1/1	0.84	0.19	58,58,58,58	0
58	MG	1x	104	1/1	0.84	0.10	59,59,59,59	0
58	MG	1A	3887	1/1	0.84	0.12	54,54,54,54	0
58	MG	2A	3104	1/1	0.84	0.13	52,52,52,52	0
58	MG	2A	3764	1/1	0.84	0.17	51,51,51,51	0
58	MG	2A	3438	1/1	0.84	0.20	55,55,55,55	0
58	MG	1a	1685	1/1	0.84	0.11	57,57,57,57	0
58	MG	2A	3112	1/1	0.84	0.12	56,56,56,56	0
58	MG	1A	3080	1/1	0.84	0.18	52,52,52,52	0
58	MG	1A	4040	1/1	0.84	0.12	37,37,37,37	0
58	MG	2A	3512	1/1	0.84	0.10	45,45,45,45	0
58	MG	2w	105	1/1	0.84	0.13	60,60,60,60	0
58	MG	1E	309	1/1	0.84	0.09	19,19,19,19	0
58	MG	1a	1761	1/1	0.85	0.14	50,50,50,50	0
58	MG	2A	3795	1/1	0.85	0.12	39,39,39,39	0
58	MG	1A	3405	1/1	0.85	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3799	1/1	0.85	0.12	55,55,55,55	0
58	MG	2A	3365	1/1	0.85	0.13	64,64,64,64	0
58	MG	1A	4010	1/1	0.85	0.14	53,53,53,53	0
58	MG	1B	213	1/1	0.85	0.15	63,63,63,63	0
58	MG	1A	4011	1/1	0.85	0.07	25,25,25,25	0
58	MG	1A	3778	1/1	0.85	0.09	18,18,18,18	0
58	MG	2A	3443	1/1	0.85	0.18	58,58,58,58	0
58	MG	2B	203	1/1	0.85	0.16	63,63,63,63	0
58	MG	1B	233	1/1	0.85	0.10	41,41,41,41	0
58	MG	1A	3938	1/1	0.85	0.13	54,54,54,54	0
58	MG	1A	3948	1/1	0.85	0.10	25,25,25,25	0
58	MG	1A	4026	1/1	0.85	0.09	49,49,49,49	0
58	MG	2A	3511	1/1	0.85	0.11	63,63,63,63	0
58	MG	2A	3096	1/1	0.85	0.14	49,49,49,49	0
58	MG	2A	3519	1/1	0.85	0.18	52,52,52,52	0
58	MG	2a	1617	1/1	0.85	0.13	54,54,54,54	0
58	MG	1A	3538	1/1	0.85	0.16	40,40,40,40	0
58	MG	1A	3876	1/1	0.85	0.16	42,42,42,42	0
58	MG	1A	3885	1/1	0.85	0.13	26,26,26,26	0
58	MG	2A	3128	1/1	0.85	0.23	63,63,63,63	0
58	MG	2a	1662	1/1	0.85	0.24	55,55,55,55	0
58	MG	2A	3136	1/1	0.85	0.12	50,50,50,50	0
58	MG	1Z	301	1/1	0.85	0.12	59,59,59,59	0
58	MG	1A	3343	1/1	0.85	0.26	49,49,49,49	0
58	MG	2A	3212	1/1	0.85	0.29	64,64,64,64	0
58	MG	2A	3621	1/1	0.85	0.16	46,46,46,46	0
58	MG	1A	3565	1/1	0.85	0.20	57,57,57,57	0
58	MG	1A	4041	1/1	0.85	0.13	30,30,30,30	0
58	MG	2a	1788	1/1	0.85	0.23	57,57,57,57	0
58	MG	1A	4043	1/1	0.85	0.14	42,42,42,42	0
58	MG	1A	3742	1/1	0.85	0.09	32,32,32,32	0
58	MG	1a	1716	1/1	0.85	0.25	59,59,59,59	0
58	MG	1A	3173	1/1	0.85	0.15	57,57,57,57	0
58	MG	2A	3710	1/1	0.85	0.19	55,55,55,55	0
58	MG	2a	1816	1/1	0.85	0.16	56,56,56,56	0
58	MG	1a	1740	1/1	0.85	0.13	64,64,64,64	0
58	MG	2A	3719	1/1	0.85	0.14	43,43,43,43	0
58	MG	1A	3697	1/1	0.85	0.13	26,26,26,26	0
58	MG	2q	203	1/1	0.85	0.15	66,66,66,66	0
58	MG	1A	3915	1/1	0.85	0.11	47,47,47,47	0
58	MG	1A	4089	1/1	0.85	0.11	45,45,45,45	0
58	MG	2A	3351	1/1	0.85	0.28	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1750	1/1	0.86	0.21	69,69,69,69	0
58	MG	1A	3998	1/1	0.86	0.10	43,43,43,43	0
58	MG	2A	3860	1/1	0.86	0.21	68,68,68,68	0
58	MG	1A	3399	1/1	0.86	0.16	61,61,61,61	0
58	MG	2A	3583	1/1	0.86	0.13	41,41,41,41	0
58	MG	2B	206	1/1	0.86	0.21	57,57,57,57	0
58	MG	1P	204	1/1	0.86	0.20	46,46,46,46	0
58	MG	1Q	207	1/1	0.86	0.12	39,39,39,39	0
58	MG	1A	3627	1/1	0.86	0.12	59,59,59,59	0
58	MG	2A	3302	1/1	0.86	0.11	48,48,48,48	0
58	MG	2A	3618	1/1	0.86	0.11	27,27,27,27	0
58	MG	2A	3310	1/1	0.86	0.12	57,57,57,57	0
58	MG	2a	1604	1/1	0.86	0.19	62,62,62,62	0
58	MG	2a	1606	1/1	0.86	0.16	56,56,56,56	0
58	MG	1A	3435	1/1	0.86	0.16	43,43,43,43	0
58	MG	1A	3184	1/1	0.86	0.17	47,47,47,47	0
58	MG	2a	1619	1/1	0.86	0.12	54,54,54,54	0
58	MG	2a	1621	1/1	0.86	0.25	58,58,58,58	0
58	MG	2A	3634	1/1	0.86	0.12	48,48,48,48	0
58	MG	1A	4078	1/1	0.86	0.13	45,45,45,45	0
58	MG	1A	4021	1/1	0.86	0.13	65,65,65,65	0
58	MG	2a	1644	1/1	0.86	0.21	57,57,57,57	0
58	MG	18	106	1/1	0.86	0.11	47,47,47,47	0
58	MG	1A	3663	1/1	0.86	0.11	40,40,40,40	0
58	MG	2a	1666	1/1	0.86	0.13	60,60,60,60	0
58	MG	2A	3687	1/1	0.86	0.12	53,53,53,53	0
58	MG	1A	3475	1/1	0.86	0.17	52,52,52,52	0
58	MG	2A	3369	1/1	0.86	0.09	69,69,69,69	0
58	MG	2A	3383	1/1	0.86	0.14	61,61,61,61	0
58	MG	2a	1757	1/1	0.86	0.09	79,79,79,79	0
58	MG	1A	3727	1/1	0.86	0.10	39,39,39,39	0
58	MG	2A	3733	1/1	0.86	0.13	51,51,51,51	0
58	MG	1a	1672	1/1	0.86	0.18	55,55,55,55	0
58	MG	1A	3730	1/1	0.86	0.19	59,59,59,59	0
58	MG	2A	3750	1/1	0.86	0.13	33,33,33,33	0
58	MG	2A	3123	1/1	0.86	0.28	68,68,68,68	0
58	MG	1a	1713	1/1	0.86	0.18	57,57,57,57	0
58	MG	1A	3841	1/1	0.86	0.14	67,67,67,67	0
58	MG	2A	3789	1/1	0.86	0.10	33,33,33,33	0
58	MG	1A	3846	1/1	0.86	0.11	46,46,46,46	0
58	MG	1A	3740	1/1	0.86	0.15	61,61,61,61	0
58	MG	2a	1820	1/1	0.86	0.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3204	1/1	0.86	0.20	66,66,66,66	0
58	MG	2a	1828	1/1	0.86	0.19	54,54,54,54	0
58	MG	2a	1829	1/1	0.86	0.13	53,53,53,53	0
58	MG	2a	1832	1/1	0.86	0.13	64,64,64,64	0
58	MG	2g	201	1/1	0.86	0.10	64,64,64,64	0
58	MG	1B	236	1/1	0.86	0.11	34,34,34,34	0
58	MG	2A	3223	1/1	0.86	0.13	55,55,55,55	0
58	MG	2A	3835	1/1	0.86	0.11	63,63,63,63	0
58	MG	2w	102	1/1	0.86	0.37	57,57,57,57	0
58	MG	2A	3841	1/1	0.86	0.15	64,64,64,64	0
58	MG	1A	3604	1/1	0.86	0.13	42,42,42,42	0
58	MG	1A	4047	1/1	0.87	0.10	32,32,32,32	0
58	MG	2A	3224	1/1	0.87	0.12	52,52,52,52	0
58	MG	1O	203	1/1	0.87	0.13	55,55,55,55	0
58	MG	1A	3577	1/1	0.87	0.14	41,41,41,41	0
58	MG	1A	3602	1/1	0.87	0.13	52,52,52,52	0
58	MG	1a	1764	1/1	0.87	0.15	61,61,61,61	0
58	MG	2E	310	1/1	0.87	0.13	52,52,52,52	0
58	MG	1A	4065	1/1	0.87	0.12	48,48,48,48	0
58	MG	2U	202	1/1	0.87	0.09	45,45,45,45	0
58	MG	1A	3252	1/1	0.87	0.13	51,51,51,51	0
58	MG	29	101	1/1	0.87	0.20	60,60,60,60	0
58	MG	2A	3288	1/1	0.87	0.14	61,61,61,61	0
58	MG	2a	1605	1/1	0.87	0.20	59,59,59,59	0
58	MG	2A	3292	1/1	0.87	0.28	53,53,53,53	0
58	MG	1A	3951	1/1	0.87	0.22	62,62,62,62	0
58	MG	1A	3677	1/1	0.87	0.09	28,28,28,28	0
58	MG	1A	3733	1/1	0.87	0.12	49,49,49,49	0
58	MG	1A	3734	1/1	0.87	0.15	48,48,48,48	0
58	MG	1A	3824	1/1	0.87	0.12	55,55,55,55	0
58	MG	2A	3673	1/1	0.87	0.10	61,61,61,61	0
58	MG	1x	102	1/1	0.87	0.13	52,52,52,52	0
58	MG	2a	1642	1/1	0.87	0.20	54,54,54,54	0
58	MG	1A	4097	1/1	0.87	0.10	49,49,49,49	0
58	MG	2a	1646	1/1	0.87	0.26	66,66,66,66	0
58	MG	2A	3002	1/1	0.87	0.16	45,45,45,45	0
58	MG	2a	1655	1/1	0.87	0.17	53,53,53,53	0
58	MG	1A	3978	1/1	0.87	0.15	64,64,64,64	0
58	MG	2A	3711	1/1	0.87	0.29	63,63,63,63	0
58	MG	2A	3717	1/1	0.87	0.18	47,47,47,47	0
58	MG	2A	3090	1/1	0.87	0.17	61,61,61,61	0
58	MG	2A	3368	1/1	0.87	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3723	1/1	0.87	0.11	58,58,58,58	0
58	MG	2a	1752	1/1	0.87	0.11	69,69,69,69	0
58	MG	2A	3091	1/1	0.87	0.11	58,58,58,58	0
58	MG	1B	226	1/1	0.87	0.12	54,54,54,54	0
58	MG	2A	3390	1/1	0.87	0.16	57,57,57,57	0
58	MG	2a	1780	1/1	0.87	0.13	49,49,49,49	0
58	MG	1A	3536	1/1	0.87	0.13	55,55,55,55	0
58	MG	2A	3399	1/1	0.87	0.09	58,58,58,58	0
58	MG	1a	1692	1/1	0.87	0.25	50,50,50,50	0
58	MG	2A	3768	1/1	0.87	0.18	42,42,42,42	0
58	MG	1a	1696	1/1	0.87	0.25	57,57,57,57	0
58	MG	1a	1709	1/1	0.87	0.11	55,55,55,55	0
58	MG	1A	3987	1/1	0.87	0.17	58,58,58,58	0
58	MG	2A	3453	1/1	0.87	0.18	60,60,60,60	0
58	MG	2A	3798	1/1	0.87	0.14	54,54,54,54	0
58	MG	1A	3254	1/1	0.87	0.11	63,63,63,63	0
58	MG	2A	3152	1/1	0.87	0.18	56,56,56,56	0
58	MG	2A	3802	1/1	0.87	0.11	58,58,58,58	0
58	MG	2A	3823	1/1	0.87	0.10	67,67,67,67	0
58	MG	2A	3162	1/1	0.87	0.25	63,63,63,63	0
58	MG	2a	1833	1/1	0.87	0.10	65,65,65,65	0
58	MG	1a	1734	1/1	0.87	0.13	39,39,39,39	0
58	MG	2A	3187	1/1	0.87	0.13	61,61,61,61	0
58	MG	1A	3745	1/1	0.87	0.09	47,47,47,47	0
58	MG	2A	3513	1/1	0.87	0.11	44,44,44,44	0
58	MG	1A	3006	1/1	0.87	0.12	48,48,48,48	0
58	MG	2A	3527	1/1	0.87	0.14	64,64,64,64	0
58	MG	1A	3211	1/1	0.87	0.10	59,59,59,59	0
58	MG	2A	3585	1/1	0.88	0.18	64,64,64,64	0
58	MG	1x	112	1/1	0.88	0.19	53,53,53,53	0
58	MG	2A	3595	1/1	0.88	0.18	73,73,73,73	0
58	MG	1A	3648	1/1	0.88	0.07	13,13,13,13	0
58	MG	2A	3308	1/1	0.88	0.17	62,62,62,62	0
58	MG	1A	3898	1/1	0.88	0.13	30,30,30,30	0
58	MG	1A	4054	1/1	0.88	0.12	42,42,42,42	0
58	MG	1D	312	1/1	0.88	0.15	29,29,29,29	0
58	MG	2A	3334	1/1	0.88	0.16	50,50,50,50	0
58	MG	2A	3336	1/1	0.88	0.10	44,44,44,44	0
58	MG	2A	3630	1/1	0.88	0.14	50,50,50,50	0
58	MG	1A	3473	1/1	0.88	0.13	54,54,54,54	0
58	MG	27	101	1/1	0.88	0.12	44,44,44,44	0
58	MG	1A	3902	1/1	0.88	0.08	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3649	1/1	0.88	0.11	35,35,35,35	0
58	MG	1A	3217	1/1	0.88	0.13	49,49,49,49	0
58	MG	1a	1725	1/1	0.88	0.10	56,56,56,56	0
58	MG	2A	3360	1/1	0.88	0.14	61,61,61,61	0
58	MG	2A	3680	1/1	0.88	0.13	51,51,51,51	0
58	MG	1A	3980	1/1	0.88	0.12	48,48,48,48	0
58	MG	2A	3684	1/1	0.88	0.11	53,53,53,53	0
58	MG	1A	3543	1/1	0.88	0.23	58,58,58,58	0
58	MG	2A	3703	1/1	0.88	0.21	63,63,63,63	0
58	MG	1A	4080	1/1	0.88	0.09	29,29,29,29	0
58	MG	2a	1637	1/1	0.88	0.20	61,61,61,61	0
58	MG	2A	3708	1/1	0.88	0.09	21,21,21,21	0
58	MG	2A	3382	1/1	0.88	0.18	58,58,58,58	0
58	MG	1A	4028	1/1	0.88	0.10	46,46,46,46	0
58	MG	1T	204	1/1	0.88	0.10	40,40,40,40	0
58	MG	2A	3392	1/1	0.88	0.21	59,59,59,59	0
58	MG	2a	1657	1/1	0.88	0.11	68,68,68,68	0
58	MG	1A	3875	1/1	0.88	0.15	44,44,44,44	0
58	MG	1Y	201	1/1	0.88	0.09	37,37,37,37	0
58	MG	2A	3421	1/1	0.88	0.30	65,65,65,65	0
58	MG	1A	3836	1/1	0.88	0.16	48,48,48,48	0
58	MG	2a	1709	1/1	0.88	0.24	56,56,56,56	0
58	MG	2A	3745	1/1	0.88	0.16	67,67,67,67	0
58	MG	2a	1729	1/1	0.88	0.14	55,55,55,55	0
58	MG	1A	3877	1/1	0.88	0.12	24,24,24,24	0
58	MG	2a	1748	1/1	0.88	0.13	58,58,58,58	0
58	MG	2a	1751	1/1	0.88	0.15	66,66,66,66	0
58	MG	2A	3205	1/1	0.88	0.11	52,52,52,52	0
58	MG	2A	3753	1/1	0.88	0.10	37,37,37,37	0
58	MG	2a	1758	1/1	0.88	0.12	62,62,62,62	0
58	MG	2a	1767	1/1	0.88	0.09	73,73,73,73	0
58	MG	2A	3759	1/1	0.88	0.11	51,51,51,51	0
58	MG	1A	3319	1/1	0.88	0.15	50,50,50,50	0
58	MG	2A	3215	1/1	0.88	0.13	62,62,62,62	0
58	MG	1A	3205	1/1	0.88	0.08	48,48,48,48	0
58	MG	1A	3784	1/1	0.88	0.09	34,34,34,34	0
58	MG	2a	1790	1/1	0.88	0.18	59,59,59,59	0
58	MG	2A	3242	1/1	0.88	0.13	61,61,61,61	0
58	MG	2A	3793	1/1	0.88	0.12	47,47,47,47	0
58	MG	2A	3491	1/1	0.88	0.19	54,54,54,54	0
58	MG	1B	227	1/1	0.88	0.11	41,41,41,41	0
58	MG	1a	1602	1/1	0.88	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
58	MG	1a	1622	1/1	0.88	0.24	54,54,54,54	0
58	MG	2A	3251	1/1	0.88	0.15	61,61,61,61	0
58	MG	2A	3514	1/1	0.88	0.13	34,34,34,34	0
58	MG	2A	3804	1/1	0.88	0.17	66,66,66,66	0
58	MG	2a	1827	1/1	0.88	0.21	65,65,65,65	0
58	MG	2A	3811	1/1	0.88	0.14	42,42,42,42	0
58	MG	2A	3813	1/1	0.88	0.11	52,52,52,52	0
58	MG	1A	4042	1/1	0.88	0.10	32,32,32,32	0
58	MG	2A	3824	1/1	0.88	0.10	52,52,52,52	0
58	MG	1a	1812	1/1	0.88	0.16	47,47,47,47	0
58	MG	2A	3536	1/1	0.88	0.11	55,55,55,55	0
58	MG	1w	106	1/1	0.88	0.15	56,56,56,56	0
58	MG	1a	1668	1/1	0.88	0.21	61,61,61,61	0
58	MG	2A	3851	1/1	0.88	0.10	43,43,43,43	0
58	MG	2A	3290	1/1	0.88	0.13	62,62,62,62	0
58	MG	1a	1671	1/1	0.88	0.11	52,52,52,52	0
58	MG	1A	3465	1/1	0.89	0.19	53,53,53,53	0
58	MG	1a	1754	1/1	0.89	0.09	42,42,42,42	0
58	MG	1A	4091	1/1	0.89	0.14	59,59,59,59	0
58	MG	1A	3175	1/1	0.89	0.15	50,50,50,50	0
58	MG	1A	3774	1/1	0.89	0.09	17,17,17,17	0
58	MG	2A	3856	1/1	0.89	0.11	50,50,50,50	0
58	MG	15	107	1/1	0.89	0.10	46,46,46,46	0
58	MG	2A	3863	1/1	0.89	0.09	54,54,54,54	0
58	MG	1B	207	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3871	1/1	0.89	0.17	51,51,51,51	0
58	MG	2A	3565	1/1	0.89	0.10	34,34,34,34	0
58	MG	1A	3775	1/1	0.89	0.11	39,39,39,39	0
58	MG	2B	207	1/1	0.89	0.11	57,57,57,57	0
58	MG	2A	3253	1/1	0.89	0.16	67,67,67,67	0
58	MG	2B	212	1/1	0.89	0.22	59,59,59,59	0
58	MG	2B	213	1/1	0.89	0.21	49,49,49,49	0
58	MG	1B	224	1/1	0.89	0.09	53,53,53,53	0
58	MG	2A	3269	1/1	0.89	0.14	49,49,49,49	0
58	MG	2A	3587	1/1	0.89	0.13	47,47,47,47	0
58	MG	2A	3279	1/1	0.89	0.09	45,45,45,45	0
58	MG	2P	201	1/1	0.89	0.15	53,53,53,53	0
58	MG	1A	3567	1/1	0.89	0.25	55,55,55,55	0
58	MG	1a	1802	1/1	0.89	0.08	58,58,58,58	0
58	MG	2A	3286	1/1	0.89	0.10	55,55,55,55	0
58	MG	1A	3395	1/1	0.89	0.24	26,26,26,26	0
58	MG	28	101	1/1	0.89	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3289	1/1	0.89	0.15	42,42,42,42	0
58	MG	1A	3590	1/1	0.89	0.10	43,43,43,43	0
58	MG	1a	1625	1/1	0.89	0.18	55,55,55,55	0
58	MG	2A	3293	1/1	0.89	0.12	50,50,50,50	0
58	MG	2a	1607	1/1	0.89	0.15	56,56,56,56	0
58	MG	2A	3629	1/1	0.89	0.15	56,56,56,56	0
58	MG	2A	3294	1/1	0.89	0.21	54,54,54,54	0
58	MG	1a	1636	1/1	0.89	0.22	67,67,67,67	0
58	MG	1w	108	1/1	0.89	0.11	67,67,67,67	0
58	MG	2A	3306	1/1	0.89	0.13	49,49,49,49	0
58	MG	1A	3999	1/1	0.89	0.14	45,45,45,45	0
58	MG	1B	231	1/1	0.89	0.12	68,68,68,68	0
58	MG	2a	1632	1/1	0.89	0.11	52,52,52,52	0
58	MG	1A	4001	1/1	0.89	0.09	33,33,33,33	0
58	MG	2A	3679	1/1	0.89	0.10	43,43,43,43	0
58	MG	1a	1679	1/1	0.89	0.17	57,57,57,57	0
58	MG	2A	3322	1/1	0.89	0.13	53,53,53,53	0
58	MG	2a	1649	1/1	0.89	0.14	55,55,55,55	0
58	MG	2A	3008	1/1	0.89	0.11	53,53,53,53	0
58	MG	2A	3031	1/1	0.89	0.12	59,59,59,59	0
58	MG	2A	3693	1/1	0.89	0.11	52,52,52,52	0
58	MG	2A	3701	1/1	0.89	0.11	53,53,53,53	0
58	MG	2A	3340	1/1	0.89	0.09	49,49,49,49	0
58	MG	2a	1678	1/1	0.89	0.32	61,61,61,61	0
58	MG	2A	3032	1/1	0.89	0.10	50,50,50,50	0
58	MG	2A	3045	1/1	0.89	0.12	51,51,51,51	0
58	MG	2A	3709	1/1	0.89	0.17	66,66,66,66	0
58	MG	2A	3352	1/1	0.89	0.19	49,49,49,49	0
58	MG	1a	1681	1/1	0.89	0.16	56,56,56,56	0
58	MG	2a	1735	1/1	0.89	0.27	56,56,56,56	0
58	MG	2A	3356	1/1	0.89	0.28	57,57,57,57	0
58	MG	2a	1747	1/1	0.89	0.11	52,52,52,52	0
58	MG	2A	3058	1/1	0.89	0.19	55,55,55,55	0
58	MG	1A	4044	1/1	0.89	0.10	48,48,48,48	0
58	MG	2A	3720	1/1	0.89	0.17	58,58,58,58	0
58	MG	2A	3722	1/1	0.89	0.10	51,51,51,51	0
58	MG	1A	3208	1/1	0.89	0.10	44,44,44,44	0
58	MG	1A	4009	1/1	0.89	0.10	59,59,59,59	0
58	MG	2A	3100	1/1	0.89	0.17	53,53,53,53	0
58	MG	1a	1704	1/1	0.89	0.16	60,60,60,60	0
58	MG	1a	1705	1/1	0.89	0.16	57,57,57,57	0
58	MG	1a	1706	1/1	0.89	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3001	1/1	0.89	0.11	37,37,37,37	0
58	MG	1A	3805	1/1	0.89	0.09	12,12,12,12	0
58	MG	1A	3259	1/1	0.89	0.11	59,59,59,59	0
58	MG	2A	3409	1/1	0.89	0.13	56,56,56,56	0
58	MG	1a	1717	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3816	1/1	0.89	0.10	49,49,49,49	0
58	MG	1A	4022	1/1	0.89	0.10	60,60,60,60	0
58	MG	2A	3166	1/1	0.89	0.16	56,56,56,56	0
58	MG	2a	1817	1/1	0.89	0.13	60,60,60,60	0
58	MG	2A	3173	1/1	0.89	0.23	61,61,61,61	0
58	MG	2A	3185	1/1	0.89	0.13	49,49,49,49	0
58	MG	2A	3467	1/1	0.89	0.10	47,47,47,47	0
58	MG	1A	3822	1/1	0.89	0.13	64,64,64,64	0
58	MG	2A	3800	1/1	0.89	0.09	68,68,68,68	0
58	MG	2A	3479	1/1	0.89	0.19	63,63,63,63	0
58	MG	1S	203	1/1	0.89	0.09	55,55,55,55	0
58	MG	2A	3803	1/1	0.89	0.13	73,73,73,73	0
58	MG	2A	3195	1/1	0.89	0.15	65,65,65,65	0
58	MG	2l	204	1/1	0.89	0.08	54,54,54,54	0
58	MG	2A	3487	1/1	0.89	0.23	58,58,58,58	0
58	MG	1A	3353	1/1	0.89	0.14	61,61,61,61	0
58	MG	2A	3492	1/1	0.89	0.13	51,51,51,51	0
58	MG	2v	103	1/1	0.89	0.28	50,50,50,50	0
58	MG	2A	3498	1/1	0.89	0.17	65,65,65,65	0
58	MG	1A	3454	1/1	0.89	0.12	48,48,48,48	0
58	MG	1a	1746	1/1	0.89	0.13	53,53,53,53	0
58	MG	1A	3956	1/1	0.90	0.09	54,54,54,54	0
58	MG	1a	1620	1/1	0.90	0.11	46,46,46,46	0
58	MG	2B	218	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	4056	1/1	0.90	0.07	12,12,12,12	0
58	MG	1A	3363	1/1	0.90	0.14	51,51,51,51	0
58	MG	2D	308	1/1	0.90	0.09	48,48,48,48	0
58	MG	1A	3821	1/1	0.90	0.12	60,60,60,60	0
58	MG	2F	305	1/1	0.90	0.12	46,46,46,46	0
58	MG	1A	3681	1/1	0.90	0.06	15,15,15,15	0
58	MG	1a	1643	1/1	0.90	0.17	55,55,55,55	0
58	MG	1a	1658	1/1	0.90	0.16	55,55,55,55	0
58	MG	2W	201	1/1	0.90	0.12	50,50,50,50	0
58	MG	23	103	1/1	0.90	0.08	41,41,41,41	0
58	MG	2A	3651	1/1	0.90	0.16	38,38,38,38	0
58	MG	25	105	1/1	0.90	0.15	61,61,61,61	0
58	MG	2A	3343	1/1	0.90	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3344	1/1	0.90	0.14	65,65,65,65	0
58	MG	2A	3670	1/1	0.90	0.11	59,59,59,59	0
58	MG	2a	1603	1/1	0.90	0.19	57,57,57,57	0
58	MG	2A	3345	1/1	0.90	0.12	53,53,53,53	0
58	MG	2A	3350	1/1	0.90	0.09	57,57,57,57	0
58	MG	1A	3272	1/1	0.90	0.12	37,37,37,37	0
58	MG	2A	3681	1/1	0.90	0.14	55,55,55,55	0
58	MG	1a	1669	1/1	0.90	0.24	57,57,57,57	0
58	MG	2a	1612	1/1	0.90	0.10	46,46,46,46	0
58	MG	2A	3353	1/1	0.90	0.11	60,60,60,60	0
58	MG	1A	3301	1/1	0.90	0.29	54,54,54,54	0
58	MG	1A	3548	1/1	0.90	0.21	52,52,52,52	0
58	MG	1A	3842	1/1	0.90	0.13	24,24,24,24	0
58	MG	1A	3704	1/1	0.90	0.07	19,19,19,19	0
58	MG	1A	3989	1/1	0.90	0.18	46,46,46,46	0
58	MG	1A	3172	1/1	0.90	0.11	37,37,37,37	0
58	MG	2a	1633	1/1	0.90	0.34	56,56,56,56	0
58	MG	1A	3410	1/1	0.90	0.14	49,49,49,49	0
58	MG	1A	3996	1/1	0.90	0.11	46,46,46,46	0
58	MG	1B	208	1/1	0.90	0.18	64,64,64,64	0
58	MG	1A	3997	1/1	0.90	0.08	42,42,42,42	0
58	MG	1A	3413	1/1	0.90	0.13	52,52,52,52	0
58	MG	2A	3171	1/1	0.90	0.13	62,62,62,62	0
58	MG	2A	3397	1/1	0.90	0.09	57,57,57,57	0
58	MG	1A	3721	1/1	0.90	0.17	50,50,50,50	0
58	MG	1a	1715	1/1	0.90	0.16	46,46,46,46	0
58	MG	2a	1663	1/1	0.90	0.18	61,61,61,61	0
58	MG	1A	3587	1/1	0.90	0.08	48,48,48,48	0
58	MG	1A	3019	1/1	0.90	0.16	36,36,36,36	0
58	MG	2A	3737	1/1	0.90	0.07	54,54,54,54	0
58	MG	2a	1687	1/1	0.90	0.17	52,52,52,52	0
58	MG	1A	3595	1/1	0.90	0.09	33,33,33,33	0
58	MG	2a	1704	1/1	0.90	0.21	60,60,60,60	0
58	MG	2a	1705	1/1	0.90	0.15	48,48,48,48	0
58	MG	2a	1706	1/1	0.90	0.14	48,48,48,48	0
58	MG	2a	1707	1/1	0.90	0.16	58,58,58,58	0
58	MG	1A	3427	1/1	0.90	0.17	54,54,54,54	0
58	MG	2a	1712	1/1	0.90	0.10	61,61,61,61	0
58	MG	2a	1719	1/1	0.90	0.23	59,59,59,59	0
58	MG	1A	3318	1/1	0.90	0.15	45,45,45,45	0
58	MG	1A	4012	1/1	0.90	0.06	14,14,14,14	0
58	MG	2a	1733	1/1	0.90	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3458	1/1	0.90	0.12	55,55,55,55	0
58	MG	2a	1738	1/1	0.90	0.23	62,62,62,62	0
58	MG	1B	237	1/1	0.90	0.08	36,36,36,36	0
58	MG	2A	3469	1/1	0.90	0.12	61,61,61,61	0
58	MG	2A	3220	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1749	1/1	0.90	0.16	65,65,65,65	0
58	MG	1A	3608	1/1	0.90	0.10	51,51,51,51	0
58	MG	1A	3616	1/1	0.90	0.10	44,44,44,44	0
58	MG	2a	1756	1/1	0.90	0.17	65,65,65,65	0
58	MG	1A	3888	1/1	0.90	0.10	24,24,24,24	0
58	MG	1A	3020	1/1	0.90	0.16	37,37,37,37	0
58	MG	1G	204	1/1	0.90	0.07	48,48,48,48	0
58	MG	1A	3624	1/1	0.90	0.11	9,9,9,9	0
58	MG	2A	3497	1/1	0.90	0.09	42,42,42,42	0
58	MG	1A	3337	1/1	0.90	0.14	49,49,49,49	0
58	MG	2A	3252	1/1	0.90	0.14	57,57,57,57	0
58	MG	1A	3631	1/1	0.90	0.07	31,31,31,31	0
58	MG	1A	3633	1/1	0.90	0.13	53,53,53,53	0
58	MG	1A	3910	1/1	0.90	0.13	46,46,46,46	0
58	MG	2a	1795	1/1	0.90	0.10	54,54,54,54	0
58	MG	2A	3278	1/1	0.90	0.09	46,46,46,46	0
58	MG	2a	1800	1/1	0.90	0.15	61,61,61,61	0
58	MG	2A	3812	1/1	0.90	0.08	24,24,24,24	0
58	MG	2A	3517	1/1	0.90	0.15	51,51,51,51	0
58	MG	2A	3816	1/1	0.90	0.10	53,53,53,53	0
58	MG	1A	3914	1/1	0.90	0.08	48,48,48,48	0
58	MG	2A	3280	1/1	0.90	0.24	57,57,57,57	0
58	MG	1A	3637	1/1	0.90	0.09	38,38,38,38	0
58	MG	1A	3339	1/1	0.90	0.12	45,45,45,45	0
58	MG	1A	3150	1/1	0.90	0.17	29,29,29,29	0
58	MG	1a	1810	1/1	0.90	0.18	45,45,45,45	0
58	MG	2A	3575	1/1	0.90	0.12	52,52,52,52	0
58	MG	1A	3187	1/1	0.90	0.19	62,62,62,62	0
58	MG	2a	1830	1/1	0.90	0.16	49,49,49,49	0
58	MG	1A	3509	1/1	0.90	0.11	55,55,55,55	0
58	MG	1b	301	1/1	0.90	0.09	58,58,58,58	0
58	MG	2a	1835	1/1	0.90	0.18	51,51,51,51	0
58	MG	1v	101	1/1	0.90	0.27	64,64,64,64	0
58	MG	1l	104	1/1	0.90	0.08	31,31,31,31	0
58	MG	2A	3295	1/1	0.90	0.16	57,57,57,57	0
58	MG	2q	201	1/1	0.90	0.24	56,56,56,56	0
58	MG	1A	3804	1/1	0.90	0.12	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3355	1/1	0.90	0.15	54,54,54,54	0
58	MG	2A	3606	1/1	0.90	0.14	64,64,64,64	0
58	MG	2A	3608	1/1	0.90	0.11	48,48,48,48	0
58	MG	1A	4048	1/1	0.90	0.10	19,19,19,19	0
58	MG	1A	3026	1/1	0.90	0.15	57,57,57,57	0
58	MG	2x	105	1/1	0.90	0.08	39,39,39,39	0
58	MG	2y	101	1/1	0.90	0.09	58,58,58,58	0
58	MG	1A	3718	1/1	0.91	0.08	38,38,38,38	0
58	MG	2A	3442	1/1	0.91	0.11	55,55,55,55	0
58	MG	1A	3719	1/1	0.91	0.11	50,50,50,50	0
58	MG	2A	3449	1/1	0.91	0.18	45,45,45,45	0
58	MG	1a	1662	1/1	0.91	0.08	50,50,50,50	0
58	MG	1A	3983	1/1	0.91	0.09	56,56,56,56	0
58	MG	2A	3462	1/1	0.91	0.23	44,44,44,44	0
58	MG	1A	3843	1/1	0.91	0.07	29,29,29,29	0
58	MG	2A	3124	1/1	0.91	0.17	44,44,44,44	0
58	MG	1A	3404	1/1	0.91	0.09	41,41,41,41	0
58	MG	1A	3477	1/1	0.91	0.08	40,40,40,40	0
58	MG	1a	1675	1/1	0.91	0.10	52,52,52,52	0
58	MG	1a	1676	1/1	0.91	0.08	49,49,49,49	0
58	MG	1A	3854	1/1	0.91	0.09	36,36,36,36	0
58	MG	2A	3490	1/1	0.91	0.17	69,69,69,69	0
58	MG	1a	1680	1/1	0.91	0.14	44,44,44,44	0
58	MG	1A	3725	1/1	0.91	0.12	51,51,51,51	0
58	MG	1a	1682	1/1	0.91	0.10	55,55,55,55	0
58	MG	2A	3175	1/1	0.91	0.10	42,42,42,42	0
58	MG	2A	3178	1/1	0.91	0.07	41,41,41,41	0
58	MG	2A	3508	1/1	0.91	0.14	51,51,51,51	0
58	MG	1A	3857	1/1	0.91	0.09	44,44,44,44	0
58	MG	1a	1690	1/1	0.91	0.25	45,45,45,45	0
58	MG	2A	3190	1/1	0.91	0.19	62,62,62,62	0
58	MG	1a	1691	1/1	0.91	0.24	57,57,57,57	0
58	MG	1A	3506	1/1	0.91	0.10	28,28,28,28	0
58	MG	2E	301	1/1	0.91	0.14	52,52,52,52	0
58	MG	2E	306	1/1	0.91	0.08	29,29,29,29	0
58	MG	2A	3198	1/1	0.91	0.13	52,52,52,52	0
58	MG	2F	304	1/1	0.91	0.12	41,41,41,41	0
58	MG	2A	3524	1/1	0.91	0.12	41,41,41,41	0
58	MG	2A	3201	1/1	0.91	0.17	55,55,55,55	0
58	MG	2A	3203	1/1	0.91	0.17	57,57,57,57	0
58	MG	2A	3552	1/1	0.91	0.10	36,36,36,36	0
58	MG	1A	3507	1/1	0.91	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1700	1/1	0.91	0.20	56,56,56,56	0
58	MG	2A	3568	1/1	0.91	0.08	37,37,37,37	0
58	MG	1a	1701	1/1	0.91	0.18	53,53,53,53	0
58	MG	26	101	1/1	0.91	0.12	53,53,53,53	0
58	MG	1A	3201	1/1	0.91	0.09	39,39,39,39	0
58	MG	1A	3510	1/1	0.91	0.09	38,38,38,38	0
58	MG	2A	3221	1/1	0.91	0.14	42,42,42,42	0
58	MG	2a	1601	1/1	0.91	0.14	59,59,59,59	0
58	MG	1A	3529	1/1	0.91	0.11	54,54,54,54	0
58	MG	1A	4005	1/1	0.91	0.06	14,14,14,14	0
58	MG	1A	3210	1/1	0.91	0.08	46,46,46,46	0
58	MG	1A	3884	1/1	0.91	0.11	38,38,38,38	0
58	MG	2A	3600	1/1	0.91	0.10	49,49,49,49	0
58	MG	1A	3257	1/1	0.91	0.17	39,39,39,39	0
58	MG	1A	3749	1/1	0.91	0.09	15,15,15,15	0
58	MG	1A	3315	1/1	0.91	0.15	53,53,53,53	0
58	MG	2a	1618	1/1	0.91	0.28	63,63,63,63	0
58	MG	1A	3540	1/1	0.91	0.17	43,43,43,43	0
58	MG	2A	3610	1/1	0.91	0.15	53,53,53,53	0
58	MG	1A	3417	1/1	0.91	0.21	52,52,52,52	0
58	MG	2a	1625	1/1	0.91	0.12	50,50,50,50	0
58	MG	2A	3612	1/1	0.91	0.08	51,51,51,51	0
58	MG	2A	3617	1/1	0.91	0.09	23,23,23,23	0
58	MG	2a	1630	1/1	0.91	0.23	56,56,56,56	0
58	MG	2A	3254	1/1	0.91	0.18	61,61,61,61	0
58	MG	2A	3259	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3662	1/1	0.91	0.07	28,28,28,28	0
58	MG	2a	1641	1/1	0.91	0.09	54,54,54,54	0
58	MG	1a	1741	1/1	0.91	0.15	46,46,46,46	0
58	MG	2A	3627	1/1	0.91	0.09	53,53,53,53	0
58	MG	1A	3359	1/1	0.91	0.09	48,48,48,48	0
58	MG	1O	202	1/1	0.91	0.19	49,49,49,49	0
58	MG	1A	3777	1/1	0.91	0.06	18,18,18,18	0
58	MG	1A	3229	1/1	0.91	0.10	37,37,37,37	0
58	MG	2a	1656	1/1	0.91	0.22	56,56,56,56	0
58	MG	2A	3647	1/1	0.91	0.11	34,34,34,34	0
58	MG	2a	1658	1/1	0.91	0.09	67,67,67,67	0
58	MG	1Q	205	1/1	0.91	0.11	58,58,58,58	0
58	MG	2A	3650	1/1	0.91	0.10	51,51,51,51	0
58	MG	1A	4029	1/1	0.91	0.06	40,40,40,40	0
58	MG	2a	1674	1/1	0.91	0.11	51,51,51,51	0
58	MG	1A	3779	1/1	0.91	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
58	MG	2A	3663	1/1	0.91	0.11	51,51,51,51	0
58	MG	1A	3671	1/1	0.91	0.07	38,38,38,38	0
58	MG	2a	1688	1/1	0.91	0.11	60,60,60,60	0
58	MG	1A	3549	1/1	0.91	0.23	50,50,50,50	0
58	MG	1A	3794	1/1	0.91	0.07	39,39,39,39	0
58	MG	2A	3676	1/1	0.91	0.09	42,42,42,42	0
58	MG	1a	1781	1/1	0.91	0.10	39,39,39,39	0
58	MG	1W	202	1/1	0.91	0.17	44,44,44,44	0
58	MG	1W	207	1/1	0.91	0.09	26,26,26,26	0
58	MG	1A	3924	1/1	0.91	0.22	31,31,31,31	0
58	MG	2a	1713	1/1	0.91	0.11	58,58,58,58	0
58	MG	1a	1799	1/1	0.91	0.12	68,68,68,68	0
58	MG	2a	1721	1/1	0.91	0.24	67,67,67,67	0
58	MG	1a	1801	1/1	0.91	0.09	46,46,46,46	0
58	MG	2A	3688	1/1	0.91	0.20	49,49,49,49	0
58	MG	2A	3307	1/1	0.91	0.14	51,51,51,51	0
58	MG	1A	3929	1/1	0.91	0.11	41,41,41,41	0
58	MG	1A	3674	1/1	0.91	0.07	26,26,26,26	0
58	MG	10	102	1/1	0.91	0.11	40,40,40,40	0
58	MG	2A	3705	1/1	0.91	0.08	46,46,46,46	0
58	MG	1A	3936	1/1	0.91	0.07	32,32,32,32	0
58	MG	1A	3440	1/1	0.91	0.14	42,42,42,42	0
58	MG	2A	3327	1/1	0.91	0.21	65,65,65,65	0
58	MG	1A	3265	1/1	0.91	0.11	55,55,55,55	0
58	MG	2A	3716	1/1	0.91	0.08	29,29,29,29	0
58	MG	18	101	1/1	0.91	0.14	40,40,40,40	0
58	MG	1A	3569	1/1	0.91	0.10	47,47,47,47	0
58	MG	2a	1759	1/1	0.91	0.10	65,65,65,65	0
58	MG	1A	3457	1/1	0.91	0.12	59,59,59,59	0
58	MG	1A	3373	1/1	0.91	0.15	43,43,43,43	0
58	MG	1A	3466	1/1	0.91	0.14	60,60,60,60	0
58	MG	1x	109	1/1	0.91	0.08	63,63,63,63	0
58	MG	2A	3728	1/1	0.91	0.08	36,36,36,36	0
58	MG	2a	1786	1/1	0.91	0.17	56,56,56,56	0
58	MG	2A	3729	1/1	0.91	0.08	47,47,47,47	0
58	MG	2A	3731	1/1	0.91	0.08	48,48,48,48	0
58	MG	1a	1603	1/1	0.91	0.14	51,51,51,51	0
58	MG	1a	1609	1/1	0.91	0.12	40,40,40,40	0
58	MG	2A	3003	1/1	0.91	0.25	52,52,52,52	0
58	MG	2A	3739	1/1	0.91	0.11	49,49,49,49	0
58	MG	2A	3740	1/1	0.91	0.10	45,45,45,45	0
58	MG	2a	1808	1/1	0.91	0.14	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3742	1/1	0.91	0.09	53,53,53,53	0
58	MG	2A	3005	1/1	0.91	0.17	56,56,56,56	0
58	MG	1A	3705	1/1	0.91	0.09	18,18,18,18	0
58	MG	2A	3011	1/1	0.91	0.09	41,41,41,41	0
58	MG	2A	3017	1/1	0.91	0.16	40,40,40,40	0
58	MG	2A	3758	1/1	0.91	0.15	55,55,55,55	0
58	MG	2a	1823	1/1	0.91	0.18	59,59,59,59	0
58	MG	1A	3335	1/1	0.91	0.09	52,52,52,52	0
58	MG	2A	3364	1/1	0.91	0.13	54,54,54,54	0
58	MG	2A	3763	1/1	0.91	0.07	41,41,41,41	0
58	MG	1A	4067	1/1	0.91	0.10	38,38,38,38	0
58	MG	2A	3037	1/1	0.91	0.13	53,53,53,53	0
58	MG	2A	3043	1/1	0.91	0.19	51,51,51,51	0
58	MG	1A	3826	1/1	0.91	0.08	34,34,34,34	0
58	MG	1a	1627	1/1	0.91	0.20	52,52,52,52	0
58	MG	1a	1629	1/1	0.91	0.16	50,50,50,50	0
58	MG	2i	201	1/1	0.91	0.20	57,57,57,57	0
58	MG	2j	201	1/1	0.91	0.17	57,57,57,57	0
58	MG	2A	3066	1/1	0.91	0.12	54,54,54,54	0
58	MG	2A	3067	1/1	0.91	0.17	58,58,58,58	0
58	MG	2A	3082	1/1	0.91	0.15	53,53,53,53	0
58	MG	1A	3248	1/1	0.91	0.12	43,43,43,43	0
58	MG	2A	3408	1/1	0.91	0.12	53,53,53,53	0
58	MG	1a	1638	1/1	0.91	0.15	47,47,47,47	0
58	MG	2A	3415	1/1	0.91	0.18	47,47,47,47	0
58	MG	2w	104	1/1	0.91	0.18	65,65,65,65	0
58	MG	1a	1641	1/1	0.91	0.16	47,47,47,47	0
58	MG	2x	101	1/1	0.91	0.17	51,51,51,51	0
58	MG	2A	3097	1/1	0.91	0.16	53,53,53,53	0
58	MG	2A	3426	1/1	0.91	0.17	51,51,51,51	0
58	MG	2A	3098	1/1	0.91	0.09	38,38,38,38	0
58	MG	1A	3746	1/1	0.92	0.08	42,42,42,42	0
58	MG	1A	3092	1/1	0.92	0.10	47,47,47,47	0
58	MG	1A	3880	1/1	0.92	0.17	24,24,24,24	0
58	MG	1A	3518	1/1	0.92	0.09	47,47,47,47	0
58	MG	1A	3765	1/1	0.92	0.12	40,40,40,40	0
58	MG	2A	3192	1/1	0.92	0.08	48,48,48,48	0
58	MG	1F	305	1/1	0.92	0.08	36,36,36,36	0
58	MG	2A	3501	1/1	0.92	0.21	52,52,52,52	0
58	MG	1A	3528	1/1	0.92	0.17	57,57,57,57	0
58	MG	2A	3199	1/1	0.92	0.10	45,45,45,45	0
58	MG	2B	205	1/1	0.92	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
58	MG	1A	4014	1/1	0.92	0.10	33,33,33,33	0
58	MG	1A	3096	1/1	0.92	0.11	45,45,45,45	0
58	MG	1A	4018	1/1	0.92	0.09	37,37,37,37	0
58	MG	1A	3771	1/1	0.92	0.06	20,20,20,20	0
58	MG	2A	3209	1/1	0.92	0.09	47,47,47,47	0
58	MG	1A	3655	1/1	0.92	0.09	26,26,26,26	0
58	MG	2A	3520	1/1	0.92	0.12	33,33,33,33	0
58	MG	2A	3522	1/1	0.92	0.11	52,52,52,52	0
58	MG	2A	3214	1/1	0.92	0.24	65,65,65,65	0
58	MG	2A	3525	1/1	0.92	0.09	51,51,51,51	0
58	MG	1R	202	1/1	0.92	0.08	26,26,26,26	0
58	MG	2A	3218	1/1	0.92	0.14	45,45,45,45	0
58	MG	2E	307	1/1	0.92	0.10	53,53,53,53	0
58	MG	2A	3541	1/1	0.92	0.11	51,51,51,51	0
58	MG	2A	3547	1/1	0.92	0.09	42,42,42,42	0
58	MG	1a	1749	1/1	0.92	0.09	44,44,44,44	0
58	MG	2A	3560	1/1	0.92	0.11	37,37,37,37	0
58	MG	1A	4023	1/1	0.92	0.08	34,34,34,34	0
58	MG	1A	3326	1/1	0.92	0.15	43,43,43,43	0
58	MG	1a	1755	1/1	0.92	0.17	58,58,58,58	0
58	MG	2W	204	1/1	0.92	0.12	53,53,53,53	0
58	MG	2Z	301	1/1	0.92	0.12	64,64,64,64	0
58	MG	2A	3226	1/1	0.92	0.13	55,55,55,55	0
58	MG	2A	3240	1/1	0.92	0.14	51,51,51,51	0
58	MG	2A	3577	1/1	0.92	0.06	25,25,25,25	0
58	MG	1T	202	1/1	0.92	0.10	50,50,50,50	0
58	MG	1a	1760	1/1	0.92	0.09	62,62,62,62	0
58	MG	1A	3332	1/1	0.92	0.16	57,57,57,57	0
58	MG	1A	3334	1/1	0.92	0.10	47,47,47,47	0
58	MG	1V	202	1/1	0.92	0.22	33,33,33,33	0
58	MG	2A	3594	1/1	0.92	0.08	53,53,53,53	0
58	MG	1A	3040	1/1	0.92	0.13	43,43,43,43	0
58	MG	1A	3191	1/1	0.92	0.09	38,38,38,38	0
58	MG	1A	3420	1/1	0.92	0.09	38,38,38,38	0
58	MG	1A	4031	1/1	0.92	0.08	41,41,41,41	0
58	MG	1a	1791	1/1	0.92	0.10	54,54,54,54	0
58	MG	1A	3787	1/1	0.92	0.11	21,21,21,21	0
58	MG	2a	1613	1/1	0.92	0.13	62,62,62,62	0
58	MG	2a	1616	1/1	0.92	0.08	59,59,59,59	0
58	MG	1A	3226	1/1	0.92	0.10	38,38,38,38	0
58	MG	1A	3923	1/1	0.92	0.09	25,25,25,25	0
58	MG	1A	3342	1/1	0.92	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3689	1/1	0.92	0.11	53,53,53,53	0
58	MG	1A	3296	1/1	0.92	0.09	46,46,46,46	0
58	MG	1A	3446	1/1	0.92	0.13	52,52,52,52	0
58	MG	1A	3344	1/1	0.92	0.12	38,38,38,38	0
58	MG	2a	1627	1/1	0.92	0.09	53,53,53,53	0
58	MG	1a	1813	1/1	0.92	0.15	53,53,53,53	0
58	MG	1A	4045	1/1	0.92	0.07	32,32,32,32	0
58	MG	2A	3291	1/1	0.92	0.25	54,54,54,54	0
58	MG	1d	301	1/1	0.92	0.23	51,51,51,51	0
58	MG	2A	3633	1/1	0.92	0.09	32,32,32,32	0
58	MG	2a	1638	1/1	0.92	0.12	38,38,38,38	0
58	MG	1f	202	1/1	0.92	0.15	58,58,58,58	0
58	MG	1n	101	1/1	0.92	0.20	53,53,53,53	0
58	MG	1a	1601	1/1	0.92	0.12	49,49,49,49	0
58	MG	1w	103	1/1	0.92	0.16	65,65,65,65	0
58	MG	2A	3299	1/1	0.92	0.20	60,60,60,60	0
58	MG	1A	3455	1/1	0.92	0.08	36,36,36,36	0
58	MG	2A	3305	1/1	0.92	0.18	58,58,58,58	0
58	MG	2A	3662	1/1	0.92	0.08	53,53,53,53	0
58	MG	1A	3297	1/1	0.92	0.10	51,51,51,51	0
58	MG	1A	3199	1/1	0.92	0.07	36,36,36,36	0
58	MG	2a	1659	1/1	0.92	0.12	69,69,69,69	0
58	MG	2a	1660	1/1	0.92	0.22	55,55,55,55	0
58	MG	1a	1610	1/1	0.92	0.18	49,49,49,49	0
58	MG	1x	108	1/1	0.92	0.07	16,16,16,16	0
58	MG	2A	3312	1/1	0.92	0.16	36,36,36,36	0
58	MG	2a	1667	1/1	0.92	0.17	70,70,70,70	0
58	MG	2a	1673	1/1	0.92	0.11	48,48,48,48	0
58	MG	1a	1613	1/1	0.92	0.08	56,56,56,56	0
58	MG	1A	3952	1/1	0.92	0.06	43,43,43,43	0
58	MG	2A	3318	1/1	0.92	0.09	44,44,44,44	0
58	MG	2a	1684	1/1	0.92	0.13	60,60,60,60	0
58	MG	2A	3319	1/1	0.92	0.14	59,59,59,59	0
58	MG	1A	3591	1/1	0.92	0.07	40,40,40,40	0
58	MG	2A	3686	1/1	0.92	0.13	46,46,46,46	0
58	MG	2A	3325	1/1	0.92	0.12	52,52,52,52	0
58	MG	1A	3238	1/1	0.92	0.11	59,59,59,59	0
58	MG	2A	3691	1/1	0.92	0.20	51,51,51,51	0
58	MG	1A	3833	1/1	0.92	0.09	33,33,33,33	0
58	MG	2A	3694	1/1	0.92	0.13	40,40,40,40	0
58	MG	1A	3601	1/1	0.92	0.28	57,57,57,57	0
58	MG	2A	3339	1/1	0.92	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1628	1/1	0.92	0.15	39,39,39,39	0
58	MG	1A	4071	1/1	0.92	0.12	47,47,47,47	0
58	MG	2A	3023	1/1	0.92	0.10	57,57,57,57	0
58	MG	2a	1723	1/1	0.92	0.17	59,59,59,59	0
58	MG	2a	1724	1/1	0.92	0.31	60,60,60,60	0
58	MG	2a	1725	1/1	0.92	0.35	68,68,68,68	0
58	MG	1a	1630	1/1	0.92	0.25	59,59,59,59	0
58	MG	2a	1732	1/1	0.92	0.14	62,62,62,62	0
58	MG	1A	3961	1/1	0.92	0.11	51,51,51,51	0
58	MG	1A	3965	1/1	0.92	0.08	30,30,30,30	0
58	MG	1A	3837	1/1	0.92	0.14	42,42,42,42	0
58	MG	1A	3967	1/1	0.92	0.07	25,25,25,25	0
58	MG	2a	1742	1/1	0.92	0.12	47,47,47,47	0
58	MG	2A	3047	1/1	0.92	0.07	40,40,40,40	0
58	MG	2A	3354	1/1	0.92	0.20	61,61,61,61	0
58	MG	1a	1645	1/1	0.92	0.09	51,51,51,51	0
58	MG	2a	1750	1/1	0.92	0.09	51,51,51,51	0
58	MG	2A	3055	1/1	0.92	0.23	57,57,57,57	0
58	MG	1A	4088	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3358	1/1	0.92	0.11	48,48,48,48	0
58	MG	2A	3059	1/1	0.92	0.10	56,56,56,56	0
58	MG	2A	3060	1/1	0.92	0.16	49,49,49,49	0
58	MG	2A	3732	1/1	0.92	0.12	55,55,55,55	0
58	MG	2a	1763	1/1	0.92	0.10	48,48,48,48	0
58	MG	1A	3974	1/1	0.92	0.21	51,51,51,51	0
58	MG	2A	3366	1/1	0.92	0.29	43,43,43,43	0
58	MG	1A	3118	1/1	0.92	0.13	37,37,37,37	0
58	MG	2a	1777	1/1	0.92	0.13	56,56,56,56	0
58	MG	2A	3080	1/1	0.92	0.10	43,43,43,43	0
58	MG	2A	3372	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	3469	1/1	0.92	0.13	51,51,51,51	0
58	MG	1A	3313	1/1	0.92	0.10	36,36,36,36	0
58	MG	2A	3386	1/1	0.92	0.10	51,51,51,51	0
58	MG	2a	1791	1/1	0.92	0.17	58,58,58,58	0
58	MG	1A	3982	1/1	0.92	0.09	31,31,31,31	0
58	MG	2a	1793	1/1	0.92	0.13	53,53,53,53	0
58	MG	2A	3751	1/1	0.92	0.11	47,47,47,47	0
58	MG	1B	206	1/1	0.92	0.10	40,40,40,40	0
58	MG	2A	3756	1/1	0.92	0.08	37,37,37,37	0
58	MG	1A	3844	1/1	0.92	0.12	45,45,45,45	0
58	MG	2a	1805	1/1	0.92	0.11	56,56,56,56	0
58	MG	1A	3125	1/1	0.92	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1809	1/1	0.92	0.23	43,43,43,43	0
58	MG	2A	3760	1/1	0.92	0.08	48,48,48,48	0
58	MG	2a	1813	1/1	0.92	0.09	42,42,42,42	0
58	MG	1B	210	1/1	0.92	0.10	50,50,50,50	0
58	MG	2A	3405	1/1	0.92	0.07	63,63,63,63	0
58	MG	2A	3407	1/1	0.92	0.09	58,58,58,58	0
58	MG	2a	1818	1/1	0.92	0.13	54,54,54,54	0
58	MG	2A	3101	1/1	0.92	0.13	53,53,53,53	0
58	MG	1A	3376	1/1	0.92	0.10	27,27,27,27	0
58	MG	1B	222	1/1	0.92	0.09	40,40,40,40	0
58	MG	2a	1824	1/1	0.92	0.15	49,49,49,49	0
58	MG	2A	3790	1/1	0.92	0.10	59,59,59,59	0
58	MG	2A	3417	1/1	0.92	0.14	34,34,34,34	0
58	MG	1B	223	1/1	0.92	0.12	41,41,41,41	0
58	MG	2A	3115	1/1	0.92	0.17	46,46,46,46	0
58	MG	1A	3618	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3498	1/1	0.92	0.10	44,44,44,44	0
58	MG	2A	3125	1/1	0.92	0.06	41,41,41,41	0
58	MG	2a	1834	1/1	0.92	0.19	52,52,52,52	0
58	MG	2A	3439	1/1	0.92	0.10	41,41,41,41	0
58	MG	1A	3735	1/1	0.92	0.15	63,63,63,63	0
58	MG	1a	1693	1/1	0.92	0.15	46,46,46,46	0
58	MG	1A	3378	1/1	0.92	0.09	36,36,36,36	0
58	MG	2l	201	1/1	0.92	0.14	61,61,61,61	0
58	MG	2A	3155	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3457	1/1	0.92	0.14	44,44,44,44	0
58	MG	2A	3159	1/1	0.92	0.08	46,46,46,46	0
58	MG	2q	202	1/1	0.92	0.08	55,55,55,55	0
58	MG	1A	3316	1/1	0.92	0.17	45,45,45,45	0
58	MG	2A	3817	1/1	0.92	0.09	26,26,26,26	0
58	MG	2A	3818	1/1	0.92	0.10	34,34,34,34	0
58	MG	1A	3869	1/1	0.92	0.11	39,39,39,39	0
58	MG	1a	1703	1/1	0.92	0.10	45,45,45,45	0
58	MG	2A	3825	1/1	0.92	0.08	46,46,46,46	0
58	MG	1A	3744	1/1	0.92	0.15	37,37,37,37	0
58	MG	2A	3830	1/1	0.92	0.09	49,49,49,49	0
58	MG	1B	235	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3396	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3992	1/1	0.93	0.14	35,35,35,35	0
58	MG	1a	1695	1/1	0.93	0.22	56,56,56,56	0
58	MG	2A	3113	1/1	0.93	0.14	54,54,54,54	0
58	MG	2A	3419	1/1	0.93	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	234	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3122	1/1	0.93	0.07	43,43,43,43	0
58	MG	2A	3424	1/1	0.93	0.13	51,51,51,51	0
58	MG	1a	1697	1/1	0.93	0.14	46,46,46,46	0
58	MG	2A	3427	1/1	0.93	0.29	53,53,53,53	0
58	MG	2A	3428	1/1	0.93	0.21	48,48,48,48	0
58	MG	1a	1698	1/1	0.93	0.22	45,45,45,45	0
58	MG	2A	3431	1/1	0.93	0.23	55,55,55,55	0
58	MG	2A	3434	1/1	0.93	0.14	50,50,50,50	0
58	MG	2A	3436	1/1	0.93	0.09	46,46,46,46	0
58	MG	1a	1699	1/1	0.93	0.20	49,49,49,49	0
58	MG	2A	3126	1/1	0.93	0.07	39,39,39,39	0
58	MG	2A	3852	1/1	0.93	0.11	52,52,52,52	0
58	MG	2A	3441	1/1	0.93	0.26	50,50,50,50	0
58	MG	1A	3849	1/1	0.93	0.20	58,58,58,58	0
58	MG	2A	3129	1/1	0.93	0.12	50,50,50,50	0
58	MG	2A	3132	1/1	0.93	0.08	61,61,61,61	0
58	MG	2A	3861	1/1	0.93	0.09	37,37,37,37	0
58	MG	1A	3731	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3146	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3866	1/1	0.93	0.10	64,64,64,64	0
58	MG	2A	3867	1/1	0.93	0.15	46,46,46,46	0
58	MG	2A	3870	1/1	0.93	0.09	50,50,50,50	0
58	MG	1A	3325	1/1	0.93	0.11	46,46,46,46	0
58	MG	2A	3460	1/1	0.93	0.17	51,51,51,51	0
58	MG	1D	311	1/1	0.93	0.12	35,35,35,35	0
58	MG	2A	3156	1/1	0.93	0.08	26,26,26,26	0
58	MG	2A	3468	1/1	0.93	0.12	50,50,50,50	0
58	MG	2B	209	1/1	0.93	0.12	49,49,49,49	0
58	MG	2B	210	1/1	0.93	0.18	67,67,67,67	0
58	MG	1A	3082	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	3629	1/1	0.93	0.07	27,27,27,27	0
58	MG	2A	3474	1/1	0.93	0.14	44,44,44,44	0
58	MG	1A	3739	1/1	0.93	0.04	12,12,12,12	0
58	MG	1a	1710	1/1	0.93	0.13	50,50,50,50	0
58	MG	2A	3167	1/1	0.93	0.14	38,38,38,38	0
58	MG	2D	302	1/1	0.93	0.21	52,52,52,52	0
58	MG	1A	3361	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3489	1/1	0.93	0.16	58,58,58,58	0
58	MG	1E	313	1/1	0.93	0.06	40,40,40,40	0
58	MG	1A	3866	1/1	0.93	0.10	37,37,37,37	0
58	MG	1F	311	1/1	0.93	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1722	1/1	0.93	0.18	58,58,58,58	0
58	MG	2F	301	1/1	0.93	0.11	40,40,40,40	0
58	MG	1a	1723	1/1	0.93	0.14	55,55,55,55	0
58	MG	1F	312	1/1	0.93	0.18	29,29,29,29	0
58	MG	1a	1726	1/1	0.93	0.13	46,46,46,46	0
58	MG	1a	1729	1/1	0.93	0.12	45,45,45,45	0
58	MG	2R	201	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3510	1/1	0.93	0.09	36,36,36,36	0
58	MG	2A	3193	1/1	0.93	0.25	58,58,58,58	0
58	MG	1G	202	1/1	0.93	0.09	44,44,44,44	0
58	MG	2X	101	1/1	0.93	0.11	62,62,62,62	0
58	MG	2Y	201	1/1	0.93	0.12	47,47,47,47	0
58	MG	1A	3741	1/1	0.93	0.08	44,44,44,44	0
58	MG	20	102	1/1	0.93	0.13	50,50,50,50	0
58	MG	23	101	1/1	0.93	0.15	63,63,63,63	0
58	MG	1N	202	1/1	0.93	0.09	38,38,38,38	0
58	MG	25	101	1/1	0.93	0.19	57,57,57,57	0
58	MG	2A	3200	1/1	0.93	0.08	42,42,42,42	0
58	MG	25	103	1/1	0.93	0.07	39,39,39,39	0
58	MG	1A	3871	1/1	0.93	0.11	47,47,47,47	0
58	MG	1A	3362	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3873	1/1	0.93	0.09	40,40,40,40	0
58	MG	27	103	1/1	0.93	0.13	40,40,40,40	0
58	MG	1A	3531	1/1	0.93	0.09	33,33,33,33	0
58	MG	2A	3208	1/1	0.93	0.08	48,48,48,48	0
58	MG	1A	4015	1/1	0.93	0.10	23,23,23,23	0
58	MG	2A	3532	1/1	0.93	0.10	27,27,27,27	0
58	MG	1A	3638	1/1	0.93	0.05	19,19,19,19	0
58	MG	1a	1753	1/1	0.93	0.16	53,53,53,53	0
58	MG	2A	3542	1/1	0.93	0.12	44,44,44,44	0
58	MG	2A	3546	1/1	0.93	0.13	45,45,45,45	0
58	MG	2a	1609	1/1	0.93	0.17	51,51,51,51	0
58	MG	1A	3644	1/1	0.93	0.07	32,32,32,32	0
58	MG	2A	3550	1/1	0.93	0.10	36,36,36,36	0
58	MG	1A	3302	1/1	0.93	0.18	49,49,49,49	0
58	MG	1T	201	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3365	1/1	0.93	0.18	52,52,52,52	0
58	MG	1A	3763	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3566	1/1	0.93	0.09	54,54,54,54	0
58	MG	1a	1763	1/1	0.93	0.09	58,58,58,58	0
58	MG	1A	3764	1/1	0.93	0.10	44,44,44,44	0
58	MG	2a	1623	1/1	0.93	0.12	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3228	1/1	0.93	0.09	50,50,50,50	0
58	MG	1A	3249	1/1	0.93	0.15	51,51,51,51	0
58	MG	1a	1769	1/1	0.93	0.07	45,45,45,45	0
58	MG	2A	3580	1/1	0.93	0.10	32,32,32,32	0
58	MG	2A	3245	1/1	0.93	0.11	58,58,58,58	0
58	MG	2A	3584	1/1	0.93	0.09	49,49,49,49	0
58	MG	1V	204	1/1	0.93	0.07	40,40,40,40	0
58	MG	2a	1634	1/1	0.93	0.11	68,68,68,68	0
58	MG	1a	1773	1/1	0.93	0.10	58,58,58,58	0
58	MG	2A	3248	1/1	0.93	0.11	68,68,68,68	0
58	MG	2A	3249	1/1	0.93	0.14	64,64,64,64	0
58	MG	1a	1775	1/1	0.93	0.08	65,65,65,65	0
58	MG	2a	1643	1/1	0.93	0.12	60,60,60,60	0
58	MG	1A	3654	1/1	0.93	0.06	21,21,21,21	0
58	MG	1A	3267	1/1	0.93	0.15	44,44,44,44	0
58	MG	2a	1647	1/1	0.93	0.07	40,40,40,40	0
58	MG	1A	3661	1/1	0.93	0.10	38,38,38,38	0
58	MG	1A	3456	1/1	0.93	0.18	41,41,41,41	0
58	MG	2a	1654	1/1	0.93	0.10	45,45,45,45	0
58	MG	2A	3607	1/1	0.93	0.11	46,46,46,46	0
58	MG	2A	3255	1/1	0.93	0.14	51,51,51,51	0
58	MG	2A	3258	1/1	0.93	0.07	38,38,38,38	0
58	MG	1A	3900	1/1	0.93	0.07	19,19,19,19	0
58	MG	2A	3260	1/1	0.93	0.07	45,45,45,45	0
58	MG	2A	3267	1/1	0.93	0.11	49,49,49,49	0
58	MG	1A	3271	1/1	0.93	0.15	51,51,51,51	0
58	MG	1A	3384	1/1	0.93	0.21	37,37,37,37	0
58	MG	2a	1665	1/1	0.93	0.19	54,54,54,54	0
58	MG	2A	3274	1/1	0.93	0.20	49,49,49,49	0
58	MG	2A	3623	1/1	0.93	0.10	39,39,39,39	0
58	MG	2A	3275	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3626	1/1	0.93	0.14	57,57,57,57	0
58	MG	1A	3385	1/1	0.93	0.15	45,45,45,45	0
58	MG	1A	3912	1/1	0.93	0.08	27,27,27,27	0
58	MG	1A	3551	1/1	0.93	0.19	55,55,55,55	0
58	MG	2a	1686	1/1	0.93	0.10	52,52,52,52	0
58	MG	1A	3338	1/1	0.93	0.11	45,45,45,45	0
58	MG	1A	3919	1/1	0.93	0.12	22,22,22,22	0
58	MG	2a	1689	1/1	0.93	0.17	60,60,60,60	0
58	MG	2a	1698	1/1	0.93	0.09	61,61,61,61	0
58	MG	2A	3635	1/1	0.93	0.09	37,37,37,37	0
58	MG	2a	1703	1/1	0.93	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3139	1/1	0.93	0.13	50,50,50,50	0
58	MG	1A	3294	1/1	0.93	0.11	38,38,38,38	0
58	MG	2A	3648	1/1	0.93	0.13	47,47,47,47	0
58	MG	1A	3791	1/1	0.93	0.07	50,50,50,50	0
58	MG	1A	3926	1/1	0.93	0.08	26,26,26,26	0
58	MG	2a	1711	1/1	0.93	0.17	53,53,53,53	0
58	MG	1l	201	1/1	0.93	0.10	62,62,62,62	0
58	MG	2A	3656	1/1	0.93	0.13	54,54,54,54	0
58	MG	2a	1714	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3659	1/1	0.93	0.08	47,47,47,47	0
58	MG	2a	1720	1/1	0.93	0.11	51,51,51,51	0
58	MG	1a	1606	1/1	0.93	0.12	47,47,47,47	0
58	MG	1n	102	1/1	0.93	0.08	44,44,44,44	0
58	MG	1A	3792	1/1	0.93	0.07	29,29,29,29	0
58	MG	1w	102	1/1	0.93	0.09	50,50,50,50	0
58	MG	2A	3296	1/1	0.93	0.07	43,43,43,43	0
58	MG	1A	3684	1/1	0.93	0.05	14,14,14,14	0
58	MG	1A	3123	1/1	0.93	0.17	33,33,33,33	0
58	MG	2A	3677	1/1	0.93	0.09	56,56,56,56	0
58	MG	2A	3300	1/1	0.93	0.07	59,59,59,59	0
58	MG	1a	1615	1/1	0.93	0.09	47,47,47,47	0
58	MG	1a	1616	1/1	0.93	0.20	61,61,61,61	0
58	MG	1x	103	1/1	0.93	0.12	53,53,53,53	0
58	MG	2a	1746	1/1	0.93	0.24	51,51,51,51	0
58	MG	2A	3683	1/1	0.93	0.13	56,56,56,56	0
58	MG	1A	3062	1/1	0.93	0.07	36,36,36,36	0
58	MG	1x	106	1/1	0.93	0.16	50,50,50,50	0
58	MG	1A	3943	1/1	0.93	0.08	51,51,51,51	0
58	MG	1A	3947	1/1	0.93	0.06	46,46,46,46	0
58	MG	1a	1624	1/1	0.93	0.16	49,49,49,49	0
58	MG	2a	1753	1/1	0.93	0.08	58,58,58,58	0
58	MG	2A	3315	1/1	0.93	0.11	62,62,62,62	0
58	MG	2A	3316	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	3802	1/1	0.93	0.07	14,14,14,14	0
58	MG	2A	3702	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3694	1/1	0.93	0.06	20,20,20,20	0
58	MG	2a	1765	1/1	0.93	0.09	61,61,61,61	0
58	MG	2A	3004	1/1	0.93	0.11	35,35,35,35	0
58	MG	1A	3950	1/1	0.93	0.08	41,41,41,41	0
58	MG	2A	3706	1/1	0.93	0.12	51,51,51,51	0
58	MG	2A	3006	1/1	0.93	0.16	47,47,47,47	0
58	MG	2A	3326	1/1	0.93	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3479	1/1	0.93	0.07	49,49,49,49	0
58	MG	1A	3807	1/1	0.93	0.08	35,35,35,35	0
58	MG	2a	1787	1/1	0.93	0.11	57,57,57,57	0
58	MG	1A	3481	1/1	0.93	0.11	41,41,41,41	0
58	MG	2A	3020	1/1	0.93	0.11	55,55,55,55	0
58	MG	1A	3486	1/1	0.93	0.17	35,35,35,35	0
58	MG	2A	3341	1/1	0.93	0.21	62,62,62,62	0
58	MG	2A	3024	1/1	0.93	0.07	42,42,42,42	0
58	MG	2a	1794	1/1	0.93	0.11	54,54,54,54	0
58	MG	2A	3029	1/1	0.93	0.16	54,54,54,54	0
58	MG	1A	3599	1/1	0.93	0.15	45,45,45,45	0
58	MG	2a	1797	1/1	0.93	0.14	49,49,49,49	0
58	MG	2a	1798	1/1	0.93	0.14	47,47,47,47	0
58	MG	2A	3724	1/1	0.93	0.10	35,35,35,35	0
58	MG	2a	1801	1/1	0.93	0.11	57,57,57,57	0
58	MG	1A	3709	1/1	0.93	0.08	21,21,21,21	0
58	MG	2a	1804	1/1	0.93	0.15	51,51,51,51	0
58	MG	2A	3348	1/1	0.93	0.13	46,46,46,46	0
58	MG	2A	3034	1/1	0.93	0.10	34,34,34,34	0
58	MG	1A	3711	1/1	0.93	0.07	34,34,34,34	0
58	MG	1A	4095	1/1	0.93	0.22	49,49,49,49	0
58	MG	1a	1660	1/1	0.93	0.07	48,48,48,48	0
58	MG	1A	3490	1/1	0.93	0.10	39,39,39,39	0
58	MG	1A	3493	1/1	0.93	0.08	37,37,37,37	0
58	MG	2A	3052	1/1	0.93	0.06	39,39,39,39	0
58	MG	1A	3346	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3606	1/1	0.93	0.08	29,29,29,29	0
58	MG	1A	3976	1/1	0.93	0.09	47,47,47,47	0
58	MG	1A	3840	1/1	0.93	0.09	34,34,34,34	0
58	MG	2A	3064	1/1	0.93	0.09	56,56,56,56	0
58	MG	1A	3500	1/1	0.93	0.22	46,46,46,46	0
58	MG	2A	3367	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3757	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	3612	1/1	0.93	0.10	41,41,41,41	0
58	MG	2A	3071	1/1	0.93	0.13	44,44,44,44	0
58	MG	2A	3074	1/1	0.93	0.09	53,53,53,53	0
58	MG	2A	3380	1/1	0.93	0.19	43,43,43,43	0
58	MG	2A	3381	1/1	0.93	0.23	54,54,54,54	0
58	MG	1A	3412	1/1	0.93	0.24	51,51,51,51	0
58	MG	1B	225	1/1	0.93	0.07	41,41,41,41	0
58	MG	2A	3773	1/1	0.93	0.10	44,44,44,44	0
58	MG	2A	3781	1/1	0.93	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3783	1/1	0.93	0.08	54,54,54,54	0
58	MG	2A	3784	1/1	0.93	0.10	43,43,43,43	0
58	MG	2n	101	1/1	0.93	0.13	61,61,61,61	0
58	MG	1A	3322	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3389	1/1	0.93	0.08	53,53,53,53	0
58	MG	1a	1683	1/1	0.93	0.17	59,59,59,59	0
58	MG	2A	3095	1/1	0.93	0.09	36,36,36,36	0
58	MG	2A	3794	1/1	0.93	0.09	30,30,30,30	0
58	MG	1A	3845	1/1	0.93	0.14	51,51,51,51	0
58	MG	1a	1687	1/1	0.93	0.07	49,49,49,49	0
58	MG	2A	3398	1/1	0.93	0.13	48,48,48,48	0
58	MG	1a	1689	1/1	0.93	0.22	51,51,51,51	0
58	MG	2A	3400	1/1	0.93	0.10	60,60,60,60	0
58	MG	1A	3323	1/1	0.93	0.10	32,32,32,32	0
58	MG	1A	3847	1/1	0.93	0.07	35,35,35,35	0
58	MG	2x	107	1/1	0.93	0.13	32,32,32,32	0
58	MG	1A	3848	1/1	0.93	0.06	27,27,27,27	0
58	MG	1A	3497	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3770	1/1	0.94	0.09	34,34,34,34	0
58	MG	2A	3416	1/1	0.94	0.20	48,48,48,48	0
58	MG	2A	3821	1/1	0.94	0.06	31,31,31,31	0
58	MG	1A	3398	1/1	0.94	0.16	49,49,49,49	0
58	MG	1A	3641	1/1	0.94	0.08	45,45,45,45	0
58	MG	1a	1684	1/1	0.94	0.21	51,51,51,51	0
58	MG	2A	3110	1/1	0.94	0.07	44,44,44,44	0
58	MG	1A	3499	1/1	0.94	0.11	39,39,39,39	0
58	MG	2A	3833	1/1	0.94	0.07	31,31,31,31	0
58	MG	1A	4094	1/1	0.94	0.09	38,38,38,38	0
58	MG	2A	3839	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3931	1/1	0.94	0.08	48,48,48,48	0
58	MG	2A	3121	1/1	0.94	0.10	66,66,66,66	0
58	MG	2A	3844	1/1	0.94	0.06	33,33,33,33	0
58	MG	2A	3845	1/1	0.94	0.09	39,39,39,39	0
58	MG	2A	3847	1/1	0.94	0.12	37,37,37,37	0
58	MG	1A	4096	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3268	1/1	0.94	0.07	37,37,37,37	0
58	MG	1B	201	1/1	0.94	0.12	30,30,30,30	0
58	MG	1B	204	1/1	0.94	0.18	48,48,48,48	0
58	MG	1a	1694	1/1	0.94	0.18	47,47,47,47	0
58	MG	1A	3933	1/1	0.94	0.07	39,39,39,39	0
58	MG	2A	3440	1/1	0.94	0.22	43,43,43,43	0
58	MG	1A	3647	1/1	0.94	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3131	1/1	0.94	0.08	48,48,48,48	0
58	MG	1A	3501	1/1	0.94	0.14	59,59,59,59	0
58	MG	2A	3445	1/1	0.94	0.17	49,49,49,49	0
58	MG	2A	3868	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3939	1/1	0.94	0.07	51,51,51,51	0
58	MG	2A	3450	1/1	0.94	0.17	56,56,56,56	0
58	MG	2A	3141	1/1	0.94	0.12	52,52,52,52	0
58	MG	2A	3145	1/1	0.94	0.20	58,58,58,58	0
58	MG	1B	212	1/1	0.94	0.10	51,51,51,51	0
58	MG	2A	3147	1/1	0.94	0.20	36,36,36,36	0
58	MG	2B	208	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3149	1/1	0.94	0.12	49,49,49,49	0
58	MG	2A	3150	1/1	0.94	0.12	41,41,41,41	0
58	MG	1A	3063	1/1	0.94	0.10	37,37,37,37	0
58	MG	1B	215	1/1	0.94	0.07	39,39,39,39	0
58	MG	1a	1702	1/1	0.94	0.13	41,41,41,41	0
58	MG	1B	219	1/1	0.94	0.12	34,34,34,34	0
58	MG	1A	3140	1/1	0.94	0.05	21,21,21,21	0
58	MG	2B	219	1/1	0.94	0.13	52,52,52,52	0
58	MG	1A	3785	1/1	0.94	0.09	26,26,26,26	0
58	MG	2A	3483	1/1	0.94	0.10	41,41,41,41	0
58	MG	1A	3406	1/1	0.94	0.08	45,45,45,45	0
58	MG	2D	306	1/1	0.94	0.21	29,29,29,29	0
58	MG	1a	1707	1/1	0.94	0.08	32,32,32,32	0
58	MG	2A	3169	1/1	0.94	0.08	44,44,44,44	0
58	MG	2E	303	1/1	0.94	0.19	59,59,59,59	0
58	MG	1A	3789	1/1	0.94	0.08	38,38,38,38	0
58	MG	1A	3407	1/1	0.94	0.08	34,34,34,34	0
58	MG	2E	308	1/1	0.94	0.08	33,33,33,33	0
58	MG	1A	3273	1/1	0.94	0.11	54,54,54,54	0
58	MG	2A	3493	1/1	0.94	0.11	55,55,55,55	0
58	MG	2F	302	1/1	0.94	0.16	53,53,53,53	0
58	MG	2F	303	1/1	0.94	0.08	48,48,48,48	0
58	MG	1A	3520	1/1	0.94	0.16	37,37,37,37	0
58	MG	2A	3182	1/1	0.94	0.13	44,44,44,44	0
58	MG	2O	201	1/1	0.94	0.12	45,45,45,45	0
58	MG	2A	3500	1/1	0.94	0.13	46,46,46,46	0
58	MG	1A	3666	1/1	0.94	0.07	24,24,24,24	0
58	MG	1A	3524	1/1	0.94	0.08	41,41,41,41	0
58	MG	2T	201	1/1	0.94	0.08	52,52,52,52	0
58	MG	1a	1720	1/1	0.94	0.13	53,53,53,53	0
58	MG	2V	202	1/1	0.94	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3668	1/1	0.94	0.05	18,18,18,18	0
58	MG	1A	3670	1/1	0.94	0.08	48,48,48,48	0
58	MG	1a	1724	1/1	0.94	0.13	50,50,50,50	0
58	MG	1A	3525	1/1	0.94	0.09	59,59,59,59	0
58	MG	2A	3197	1/1	0.94	0.14	52,52,52,52	0
58	MG	1A	3141	1/1	0.94	0.21	20,20,20,20	0
58	MG	1A	3231	1/1	0.94	0.10	19,19,19,19	0
58	MG	1a	1730	1/1	0.94	0.08	40,40,40,40	0
58	MG	1a	1731	1/1	0.94	0.06	54,54,54,54	0
58	MG	2A	3202	1/1	0.94	0.06	34,34,34,34	0
58	MG	1a	1732	1/1	0.94	0.07	43,43,43,43	0
58	MG	1A	3968	1/1	0.94	0.09	55,55,55,55	0
58	MG	1A	3970	1/1	0.94	0.06	39,39,39,39	0
58	MG	1A	3971	1/1	0.94	0.10	16,16,16,16	0
58	MG	27	102	1/1	0.94	0.09	36,36,36,36	0
58	MG	2A	3537	1/1	0.94	0.08	24,24,24,24	0
58	MG	2A	3539	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	3235	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3211	1/1	0.94	0.08	51,51,51,51	0
58	MG	2a	1602	1/1	0.94	0.16	60,60,60,60	0
58	MG	1A	3817	1/1	0.94	0.15	41,41,41,41	0
58	MG	1E	312	1/1	0.94	0.10	28,28,28,28	0
58	MG	2A	3548	1/1	0.94	0.07	38,38,38,38	0
58	MG	1A	3236	1/1	0.94	0.08	48,48,48,48	0
58	MG	2A	3551	1/1	0.94	0.09	39,39,39,39	0
58	MG	2a	1608	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3217	1/1	0.94	0.06	36,36,36,36	0
58	MG	1A	3122	1/1	0.94	0.06	30,30,30,30	0
58	MG	1A	3425	1/1	0.94	0.06	41,41,41,41	0
58	MG	2A	3564	1/1	0.94	0.06	17,17,17,17	0
58	MG	1A	3350	1/1	0.94	0.13	31,31,31,31	0
58	MG	2A	3222	1/1	0.94	0.20	50,50,50,50	0
58	MG	1A	3433	1/1	0.94	0.08	54,54,54,54	0
58	MG	1A	3986	1/1	0.94	0.07	52,52,52,52	0
58	MG	2A	3573	1/1	0.94	0.08	36,36,36,36	0
58	MG	1A	3696	1/1	0.94	0.08	28,28,28,28	0
58	MG	1N	204	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3578	1/1	0.94	0.13	62,62,62,62	0
58	MG	2A	3230	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3231	1/1	0.94	0.24	47,47,47,47	0
58	MG	2A	3234	1/1	0.94	0.15	33,33,33,33	0
58	MG	2A	3237	1/1	0.94	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3239	1/1	0.94	0.16	41,41,41,41	0
58	MG	2A	3586	1/1	0.94	0.11	21,21,21,21	0
58	MG	1A	3352	1/1	0.94	0.24	50,50,50,50	0
58	MG	2a	1636	1/1	0.94	0.09	70,70,70,70	0
58	MG	1A	3438	1/1	0.94	0.12	27,27,27,27	0
58	MG	1O	204	1/1	0.94	0.09	49,49,49,49	0
58	MG	2a	1640	1/1	0.94	0.14	48,48,48,48	0
58	MG	1A	3990	1/1	0.94	0.07	20,20,20,20	0
58	MG	2A	3597	1/1	0.94	0.16	43,43,43,43	0
58	MG	1a	1767	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3701	1/1	0.94	0.09	21,21,21,21	0
58	MG	1A	3240	1/1	0.94	0.11	20,20,20,20	0
58	MG	1A	3441	1/1	0.94	0.12	37,37,37,37	0
58	MG	1A	3706	1/1	0.94	0.07	17,17,17,17	0
58	MG	1a	1776	1/1	0.94	0.13	52,52,52,52	0
58	MG	1a	1777	1/1	0.94	0.10	63,63,63,63	0
58	MG	1a	1780	1/1	0.94	0.07	63,63,63,63	0
58	MG	1A	3708	1/1	0.94	0.06	22,22,22,22	0
58	MG	2A	3615	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3443	1/1	0.94	0.08	51,51,51,51	0
58	MG	1a	1784	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3566	1/1	0.94	0.17	46,46,46,46	0
58	MG	2A	3263	1/1	0.94	0.10	58,58,58,58	0
58	MG	2A	3265	1/1	0.94	0.12	53,53,53,53	0
58	MG	1a	1787	1/1	0.94	0.09	61,61,61,61	0
58	MG	1A	3354	1/1	0.94	0.12	49,49,49,49	0
58	MG	1a	1792	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3270	1/1	0.94	0.07	71,71,71,71	0
58	MG	2A	3272	1/1	0.94	0.10	62,62,62,62	0
58	MG	1U	204	1/1	0.94	0.18	42,42,42,42	0
58	MG	1a	1796	1/1	0.94	0.07	46,46,46,46	0
58	MG	1a	1798	1/1	0.94	0.07	65,65,65,65	0
58	MG	2A	3641	1/1	0.94	0.08	35,35,35,35	0
58	MG	2A	3642	1/1	0.94	0.07	35,35,35,35	0
58	MG	1A	3715	1/1	0.94	0.09	33,33,33,33	0
58	MG	1A	3850	1/1	0.94	0.07	31,31,31,31	0
58	MG	2a	1692	1/1	0.94	0.17	48,48,48,48	0
58	MG	2a	1695	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3282	1/1	0.94	0.10	51,51,51,51	0
58	MG	1A	4007	1/1	0.94	0.09	60,60,60,60	0
58	MG	1W	201	1/1	0.94	0.09	37,37,37,37	0
58	MG	1A	3447	1/1	0.94	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3452	1/1	0.94	0.20	41,41,41,41	0
58	MG	1A	3310	1/1	0.94	0.23	48,48,48,48	0
58	MG	1A	3856	1/1	0.94	0.13	44,44,44,44	0
58	MG	1A	3589	1/1	0.94	0.07	37,37,37,37	0
58	MG	2a	1710	1/1	0.94	0.15	56,56,56,56	0
58	MG	1Z	302	1/1	0.94	0.07	37,37,37,37	0
58	MG	1f	201	1/1	0.94	0.14	42,42,42,42	0
58	MG	2A	3669	1/1	0.94	0.07	27,27,27,27	0
58	MG	1A	3860	1/1	0.94	0.07	29,29,29,29	0
58	MG	2a	1715	1/1	0.94	0.09	54,54,54,54	0
58	MG	10	103	1/1	0.94	0.09	38,38,38,38	0
58	MG	1A	3247	1/1	0.94	0.07	32,32,32,32	0
58	MG	2A	3297	1/1	0.94	0.14	48,48,48,48	0
58	MG	10	108	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3722	1/1	0.94	0.04	10,10,10,10	0
58	MG	1w	101	1/1	0.94	0.31	67,67,67,67	0
58	MG	2A	3301	1/1	0.94	0.12	56,56,56,56	0
58	MG	2a	1727	1/1	0.94	0.17	57,57,57,57	0
58	MG	14	101	1/1	0.94	0.06	51,51,51,51	0
58	MG	2A	3304	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	3198	1/1	0.94	0.21	41,41,41,41	0
58	MG	17	104	1/1	0.94	0.05	36,36,36,36	0
58	MG	1A	3726	1/1	0.94	0.14	40,40,40,40	0
58	MG	2a	1739	1/1	0.94	0.18	50,50,50,50	0
58	MG	1x	101	1/1	0.94	0.23	56,56,56,56	0
58	MG	1A	3314	1/1	0.94	0.22	50,50,50,50	0
58	MG	2a	1743	1/1	0.94	0.24	43,43,43,43	0
58	MG	1A	3597	1/1	0.94	0.12	46,46,46,46	0
58	MG	2A	3698	1/1	0.94	0.08	55,55,55,55	0
58	MG	2A	3700	1/1	0.94	0.09	34,34,34,34	0
58	MG	1A	3461	1/1	0.94	0.08	49,49,49,49	0
58	MG	1x	105	1/1	0.94	0.13	53,53,53,53	0
58	MG	1A	3463	1/1	0.94	0.13	51,51,51,51	0
58	MG	1A	3464	1/1	0.94	0.17	38,38,38,38	0
58	MG	1A	3603	1/1	0.94	0.13	46,46,46,46	0
58	MG	1a	1605	1/1	0.94	0.07	42,42,42,42	0
58	MG	2A	3001	1/1	0.94	0.23	51,51,51,51	0
58	MG	1A	3878	1/1	0.94	0.13	20,20,20,20	0
58	MG	1A	3152	1/1	0.94	0.21	39,39,39,39	0
58	MG	2a	1760	1/1	0.94	0.08	56,56,56,56	0
58	MG	1A	3250	1/1	0.94	0.08	50,50,50,50	0
58	MG	2A	3331	1/1	0.94	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3162	1/1	0.94	0.06	39,39,39,39	0
58	MG	2a	1770	1/1	0.94	0.09	61,61,61,61	0
58	MG	2A	3335	1/1	0.94	0.13	44,44,44,44	0
58	MG	1A	4038	1/1	0.94	0.08	35,35,35,35	0
58	MG	2A	3007	1/1	0.94	0.16	46,46,46,46	0
58	MG	2a	1778	1/1	0.94	0.12	39,39,39,39	0
58	MG	1A	3372	1/1	0.94	0.18	31,31,31,31	0
58	MG	1A	3613	1/1	0.94	0.08	16,16,16,16	0
58	MG	2a	1782	1/1	0.94	0.19	53,53,53,53	0
58	MG	2A	3015	1/1	0.94	0.09	36,36,36,36	0
58	MG	2A	3726	1/1	0.94	0.17	53,53,53,53	0
58	MG	2A	3016	1/1	0.94	0.09	53,53,53,53	0
58	MG	1a	1621	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3016	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3346	1/1	0.94	0.13	56,56,56,56	0
58	MG	1A	3889	1/1	0.94	0.06	39,39,39,39	0
58	MG	2A	3349	1/1	0.94	0.14	46,46,46,46	0
58	MG	1A	3168	1/1	0.94	0.13	47,47,47,47	0
58	MG	2A	3025	1/1	0.94	0.09	39,39,39,39	0
58	MG	1A	3894	1/1	0.94	0.09	17,17,17,17	0
58	MG	2A	3741	1/1	0.94	0.14	40,40,40,40	0
58	MG	1A	3895	1/1	0.94	0.08	19,19,19,19	0
58	MG	1A	3004	1/1	0.94	0.06	14,14,14,14	0
58	MG	1A	3753	1/1	0.94	0.18	47,47,47,47	0
58	MG	2A	3749	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	4050	1/1	0.94	0.06	34,34,34,34	0
58	MG	1A	4052	1/1	0.94	0.10	42,42,42,42	0
58	MG	1A	3754	1/1	0.94	0.10	49,49,49,49	0
58	MG	1a	1639	1/1	0.94	0.17	50,50,50,50	0
58	MG	2a	1812	1/1	0.94	0.12	50,50,50,50	0
58	MG	1A	3901	1/1	0.94	0.05	28,28,28,28	0
58	MG	1A	3002	1/1	0.94	0.09	48,48,48,48	0
58	MG	1A	3757	1/1	0.94	0.08	32,32,32,32	0
58	MG	1a	1647	1/1	0.94	0.08	41,41,41,41	0
58	MG	1a	1657	1/1	0.94	0.24	49,49,49,49	0
58	MG	1A	3905	1/1	0.94	0.08	24,24,24,24	0
58	MG	2A	3063	1/1	0.94	0.10	50,50,50,50	0
58	MG	2a	1822	1/1	0.94	0.11	48,48,48,48	0
58	MG	2A	3373	1/1	0.94	0.23	66,66,66,66	0
58	MG	2A	3771	1/1	0.94	0.12	50,50,50,50	0
58	MG	2A	3374	1/1	0.94	0.20	45,45,45,45	0
58	MG	2A	3775	1/1	0.94	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3776	1/1	0.94	0.14	65,65,65,65	0
58	MG	2A	3375	1/1	0.94	0.08	43,43,43,43	0
58	MG	2A	3377	1/1	0.94	0.17	49,49,49,49	0
58	MG	1A	3760	1/1	0.94	0.09	47,47,47,47	0
58	MG	2A	3785	1/1	0.94	0.07	31,31,31,31	0
58	MG	2A	3065	1/1	0.94	0.19	51,51,51,51	0
58	MG	1A	3266	1/1	0.94	0.14	46,46,46,46	0
58	MG	2f	202	1/1	0.94	0.12	51,51,51,51	0
58	MG	1a	1664	1/1	0.94	0.12	45,45,45,45	0
58	MG	2A	3791	1/1	0.94	0.09	63,63,63,63	0
58	MG	2A	3792	1/1	0.94	0.11	45,45,45,45	0
58	MG	2A	3068	1/1	0.94	0.07	37,37,37,37	0
58	MG	2A	3387	1/1	0.94	0.14	55,55,55,55	0
58	MG	1A	3392	1/1	0.94	0.12	17,17,17,17	0
58	MG	2A	3073	1/1	0.94	0.08	39,39,39,39	0
58	MG	1A	3215	1/1	0.94	0.08	28,28,28,28	0
58	MG	1A	4079	1/1	0.94	0.07	30,30,30,30	0
58	MG	1A	3918	1/1	0.94	0.12	23,23,23,23	0
58	MG	2t	201	1/1	0.94	0.12	44,44,44,44	0
58	MG	2A	3088	1/1	0.94	0.12	47,47,47,47	0
58	MG	1a	1674	1/1	0.94	0.23	57,57,57,57	0
58	MG	1A	3333	1/1	0.94	0.10	43,43,43,43	0
58	MG	2A	3403	1/1	0.94	0.10	58,58,58,58	0
58	MG	2A	3805	1/1	0.94	0.09	48,48,48,48	0
58	MG	2A	3808	1/1	0.94	0.07	45,45,45,45	0
58	MG	2A	3809	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	4086	1/1	0.94	0.18	52,52,52,52	0
58	MG	1a	1678	1/1	0.94	0.19	40,40,40,40	0
58	MG	1A	4087	1/1	0.94	0.09	36,36,36,36	0
58	MG	2A	3114	1/1	0.95	0.28	61,61,61,61	0
58	MG	2A	3406	1/1	0.95	0.09	32,32,32,32	0
58	MG	1A	3491	1/1	0.95	0.06	35,35,35,35	0
58	MG	2A	3120	1/1	0.95	0.14	38,38,38,38	0
58	MG	1A	3772	1/1	0.95	0.05	26,26,26,26	0
58	MG	2A	3414	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3934	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3773	1/1	0.95	0.07	23,23,23,23	0
58	MG	2A	3806	1/1	0.95	0.08	37,37,37,37	0
58	MG	1A	3284	1/1	0.95	0.15	21,21,21,21	0
58	MG	2A	3418	1/1	0.95	0.12	43,43,43,43	0
58	MG	1B	211	1/1	0.95	0.12	32,32,32,32	0
58	MG	2A	3420	1/1	0.95	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3634	1/1	0.95	0.07	19,19,19,19	0
58	MG	1A	3942	1/1	0.95	0.05	30,30,30,30	0
58	MG	1B	214	1/1	0.95	0.09	45,45,45,45	0
58	MG	2A	3425	1/1	0.95	0.22	51,51,51,51	0
58	MG	1A	3776	1/1	0.95	0.08	22,22,22,22	0
58	MG	1A	3946	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3133	1/1	0.95	0.09	32,32,32,32	0
58	MG	1B	221	1/1	0.95	0.05	45,45,45,45	0
58	MG	2A	3430	1/1	0.95	0.14	44,44,44,44	0
58	MG	2A	3140	1/1	0.95	0.12	34,34,34,34	0
58	MG	2A	3832	1/1	0.95	0.08	47,47,47,47	0
58	MG	2A	3432	1/1	0.95	0.11	48,48,48,48	0
58	MG	2A	3433	1/1	0.95	0.26	51,51,51,51	0
58	MG	2A	3836	1/1	0.95	0.06	50,50,50,50	0
58	MG	1A	3154	1/1	0.95	0.21	34,34,34,34	0
58	MG	1A	3340	1/1	0.95	0.06	32,32,32,32	0
58	MG	2A	3437	1/1	0.95	0.13	41,41,41,41	0
58	MG	1A	3411	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3643	1/1	0.95	0.07	17,17,17,17	0
58	MG	1A	3243	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3156	1/1	0.95	0.11	38,38,38,38	0
58	MG	2A	3151	1/1	0.95	0.18	46,46,46,46	0
58	MG	1B	228	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	3505	1/1	0.95	0.11	36,36,36,36	0
58	MG	2A	3446	1/1	0.95	0.29	55,55,55,55	0
58	MG	2A	3858	1/1	0.95	0.14	51,51,51,51	0
58	MG	2A	3448	1/1	0.95	0.21	35,35,35,35	0
58	MG	1A	3298	1/1	0.95	0.07	41,41,41,41	0
58	MG	2A	3158	1/1	0.95	0.05	64,64,64,64	0
58	MG	1A	3300	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3454	1/1	0.95	0.18	46,46,46,46	0
58	MG	2A	3455	1/1	0.95	0.25	47,47,47,47	0
58	MG	1A	3419	1/1	0.95	0.07	55,55,55,55	0
58	MG	2A	3163	1/1	0.95	0.09	52,52,52,52	0
58	MG	2A	3459	1/1	0.95	0.11	28,28,28,28	0
58	MG	2B	202	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3793	1/1	0.95	0.06	30,30,30,30	0
58	MG	2A	3461	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3962	1/1	0.95	0.07	38,38,38,38	0
58	MG	2A	3463	1/1	0.95	0.24	44,44,44,44	0
58	MG	1A	3027	1/1	0.95	0.12	59,59,59,59	0
58	MG	1A	3657	1/1	0.95	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3170	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3472	1/1	0.95	0.09	52,52,52,52	0
58	MG	1A	3658	1/1	0.95	0.14	44,44,44,44	0
58	MG	1A	3800	1/1	0.95	0.07	37,37,37,37	0
58	MG	2B	214	1/1	0.95	0.06	41,41,41,41	0
58	MG	2A	3476	1/1	0.95	0.16	60,60,60,60	0
58	MG	2B	217	1/1	0.95	0.11	43,43,43,43	0
58	MG	2A	3477	1/1	0.95	0.18	57,57,57,57	0
58	MG	2A	3174	1/1	0.95	0.14	53,53,53,53	0
58	MG	1A	3512	1/1	0.95	0.07	35,35,35,35	0
58	MG	2A	3482	1/1	0.95	0.09	34,34,34,34	0
58	MG	2A	3176	1/1	0.95	0.09	50,50,50,50	0
58	MG	1A	3513	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3514	1/1	0.95	0.09	17,17,17,17	0
58	MG	2A	3488	1/1	0.95	0.08	43,43,43,43	0
58	MG	2E	302	1/1	0.95	0.13	55,55,55,55	0
58	MG	1A	3806	1/1	0.95	0.06	30,30,30,30	0
58	MG	1A	3517	1/1	0.95	0.07	48,48,48,48	0
58	MG	1a	1736	1/1	0.95	0.06	46,46,46,46	0
58	MG	1A	3421	1/1	0.95	0.17	39,39,39,39	0
58	MG	1a	1738	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3495	1/1	0.95	0.11	46,46,46,46	0
58	MG	1F	306	1/1	0.95	0.05	25,25,25,25	0
58	MG	1A	3811	1/1	0.95	0.04	14,14,14,14	0
58	MG	2A	3499	1/1	0.95	0.15	47,47,47,47	0
58	MG	1a	1742	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3084	1/1	0.95	0.06	21,21,21,21	0
58	MG	1F	313	1/1	0.95	0.07	32,32,32,32	0
58	MG	2P	202	1/1	0.95	0.06	44,44,44,44	0
58	MG	2Q	201	1/1	0.95	0.05	45,45,45,45	0
58	MG	1A	3522	1/1	0.95	0.16	25,25,25,25	0
58	MG	1A	3985	1/1	0.95	0.04	33,33,33,33	0
58	MG	1A	3024	1/1	0.95	0.11	36,36,36,36	0
58	MG	2U	201	1/1	0.95	0.13	45,45,45,45	0
58	MG	1A	3430	1/1	0.95	0.08	39,39,39,39	0
58	MG	1O	201	1/1	0.95	0.12	55,55,55,55	0
58	MG	1A	3527	1/1	0.95	0.10	62,62,62,62	0
58	MG	2A	3515	1/1	0.95	0.11	40,40,40,40	0
58	MG	1A	3676	1/1	0.95	0.06	25,25,25,25	0
58	MG	2A	3518	1/1	0.95	0.08	17,17,17,17	0
58	MG	1A	3044	1/1	0.95	0.13	33,33,33,33	0
58	MG	20	101	1/1	0.95	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1O	205	1/1	0.95	0.15	47,47,47,47	0
58	MG	1A	3434	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3523	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3682	1/1	0.95	0.10	17,17,17,17	0
58	MG	1A	3838	1/1	0.95	0.12	53,53,53,53	0
58	MG	2A	3526	1/1	0.95	0.06	26,26,26,26	0
58	MG	2A	3216	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3529	1/1	0.95	0.07	50,50,50,50	0
58	MG	2A	3531	1/1	0.95	0.14	54,54,54,54	0
58	MG	1Q	208	1/1	0.95	0.14	34,34,34,34	0
58	MG	2A	3533	1/1	0.95	0.05	40,40,40,40	0
58	MG	2A	3534	1/1	0.95	0.07	29,29,29,29	0
58	MG	28	102	1/1	0.95	0.22	54,54,54,54	0
58	MG	28	103	1/1	0.95	0.12	45,45,45,45	0
58	MG	2A	3535	1/1	0.95	0.10	41,41,41,41	0
58	MG	1A	3530	1/1	0.95	0.05	34,34,34,34	0
58	MG	2A	3219	1/1	0.95	0.12	43,43,43,43	0
58	MG	1A	3133	1/1	0.95	0.09	55,55,55,55	0
58	MG	2A	3540	1/1	0.95	0.12	47,47,47,47	0
58	MG	1a	1771	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3256	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3543	1/1	0.95	0.11	47,47,47,47	0
58	MG	1a	1774	1/1	0.95	0.07	59,59,59,59	0
58	MG	1A	3692	1/1	0.95	0.05	21,21,21,21	0
58	MG	2a	1610	1/1	0.95	0.22	53,53,53,53	0
58	MG	1A	4000	1/1	0.95	0.05	39,39,39,39	0
58	MG	2A	3227	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3693	1/1	0.95	0.17	50,50,50,50	0
58	MG	2a	1614	1/1	0.95	0.23	61,61,61,61	0
58	MG	1A	3097	1/1	0.95	0.10	34,34,34,34	0
58	MG	1A	4003	1/1	0.95	0.09	7,7,7,7	0
58	MG	2A	3232	1/1	0.95	0.25	39,39,39,39	0
58	MG	1A	4004	1/1	0.95	0.13	16,16,16,16	0
58	MG	2a	1620	1/1	0.95	0.08	47,47,47,47	0
58	MG	2A	3235	1/1	0.95	0.07	41,41,41,41	0
58	MG	1A	3099	1/1	0.95	0.07	16,16,16,16	0
58	MG	1V	205	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3571	1/1	0.95	0.07	36,36,36,36	0
58	MG	1a	1786	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3241	1/1	0.95	0.19	40,40,40,40	0
58	MG	1A	3262	1/1	0.95	0.08	27,27,27,27	0
58	MG	2a	1629	1/1	0.95	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3244	1/1	0.95	0.16	41,41,41,41	0
58	MG	1A	3541	1/1	0.95	0.12	44,44,44,44	0
58	MG	1A	3700	1/1	0.95	0.09	54,54,54,54	0
58	MG	1X	106	1/1	0.95	0.12	50,50,50,50	0
58	MG	2A	3581	1/1	0.95	0.09	40,40,40,40	0
58	MG	1a	1794	1/1	0.95	0.06	56,56,56,56	0
58	MG	1A	3445	1/1	0.95	0.08	23,23,23,23	0
58	MG	1A	3703	1/1	0.95	0.11	41,41,41,41	0
58	MG	1A	3853	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3317	1/1	0.95	0.06	21,21,21,21	0
58	MG	2A	3589	1/1	0.95	0.09	42,42,42,42	0
58	MG	1A	3227	1/1	0.95	0.07	30,30,30,30	0
58	MG	1a	1803	1/1	0.95	0.10	52,52,52,52	0
58	MG	1A	3451	1/1	0.95	0.06	27,27,27,27	0
58	MG	1a	1808	1/1	0.95	0.07	48,48,48,48	0
58	MG	10	105	1/1	0.95	0.11	47,47,47,47	0
58	MG	2a	1651	1/1	0.95	0.08	46,46,46,46	0
58	MG	2a	1653	1/1	0.95	0.14	47,47,47,47	0
58	MG	1A	3707	1/1	0.95	0.13	35,35,35,35	0
58	MG	2A	3262	1/1	0.95	0.06	42,42,42,42	0
58	MG	1A	3367	1/1	0.95	0.12	35,35,35,35	0
58	MG	11	101	1/1	0.95	0.16	29,29,29,29	0
58	MG	2A	3266	1/1	0.95	0.07	42,42,42,42	0
58	MG	11	103	1/1	0.95	0.06	26,26,26,26	0
58	MG	1A	3552	1/1	0.95	0.09	51,51,51,51	0
58	MG	11	105	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3613	1/1	0.95	0.11	44,44,44,44	0
58	MG	12	102	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	3556	1/1	0.95	0.08	39,39,39,39	0
58	MG	15	105	1/1	0.95	0.08	21,21,21,21	0
58	MG	2a	1668	1/1	0.95	0.08	59,59,59,59	0
58	MG	2a	1669	1/1	0.95	0.19	59,59,59,59	0
58	MG	1A	3557	1/1	0.95	0.12	28,28,28,28	0
58	MG	2A	3276	1/1	0.95	0.07	54,54,54,54	0
58	MG	2a	1676	1/1	0.95	0.10	47,47,47,47	0
58	MG	1t	201	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3867	1/1	0.95	0.18	37,37,37,37	0
58	MG	2a	1681	1/1	0.95	0.15	51,51,51,51	0
58	MG	2a	1682	1/1	0.95	0.09	42,42,42,42	0
58	MG	2A	3625	1/1	0.95	0.06	39,39,39,39	0
58	MG	2a	1685	1/1	0.95	0.08	52,52,52,52	0
58	MG	1A	4027	1/1	0.95	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3281	1/1	0.95	0.10	54,54,54,54	0
58	MG	1A	3562	1/1	0.95	0.11	19,19,19,19	0
58	MG	1A	3370	1/1	0.95	0.11	41,41,41,41	0
58	MG	2a	1691	1/1	0.95	0.12	51,51,51,51	0
58	MG	1w	104	1/1	0.95	0.21	47,47,47,47	0
58	MG	2a	1694	1/1	0.95	0.20	48,48,48,48	0
58	MG	1w	105	1/1	0.95	0.20	52,52,52,52	0
58	MG	2A	3287	1/1	0.95	0.06	57,57,57,57	0
58	MG	2A	3636	1/1	0.95	0.06	48,48,48,48	0
58	MG	2A	3638	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3639	1/1	0.95	0.10	38,38,38,38	0
58	MG	1A	3186	1/1	0.95	0.07	55,55,55,55	0
58	MG	1w	107	1/1	0.95	0.15	40,40,40,40	0
58	MG	2A	3645	1/1	0.95	0.08	39,39,39,39	0
58	MG	1A	3320	1/1	0.95	0.12	25,25,25,25	0
58	MG	1A	3375	1/1	0.95	0.12	40,40,40,40	0
58	MG	1A	3458	1/1	0.95	0.10	43,43,43,43	0
58	MG	1a	1604	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	4036	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3582	1/1	0.95	0.14	26,26,26,26	0
58	MG	2A	3653	1/1	0.95	0.12	55,55,55,55	0
58	MG	2a	1717	1/1	0.95	0.15	57,57,57,57	0
58	MG	1a	1607	1/1	0.95	0.17	52,52,52,52	0
58	MG	1A	3460	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3045	1/1	0.95	0.07	26,26,26,26	0
58	MG	1x	110	1/1	0.95	0.09	58,58,58,58	0
58	MG	1x	111	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3666	1/1	0.95	0.07	45,45,45,45	0
58	MG	1a	1612	1/1	0.95	0.06	51,51,51,51	0
58	MG	1A	3882	1/1	0.95	0.09	23,23,23,23	0
58	MG	1A	3462	1/1	0.95	0.10	42,42,42,42	0
58	MG	1A	3233	1/1	0.95	0.12	35,35,35,35	0
58	MG	1a	1617	1/1	0.95	0.10	37,37,37,37	0
58	MG	2a	1734	1/1	0.95	0.08	61,61,61,61	0
58	MG	1A	3382	1/1	0.95	0.07	41,41,41,41	0
58	MG	2a	1737	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3117	1/1	0.95	0.12	27,27,27,27	0
58	MG	1A	4046	1/1	0.95	0.11	27,27,27,27	0
58	MG	1A	3196	1/1	0.95	0.24	25,25,25,25	0
58	MG	1A	3388	1/1	0.95	0.11	57,57,57,57	0
58	MG	2A	3314	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3012	1/1	0.95	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3685	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3327	1/1	0.95	0.16	35,35,35,35	0
58	MG	1A	3892	1/1	0.95	0.04	14,14,14,14	0
58	MG	1A	3472	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3329	1/1	0.95	0.13	47,47,47,47	0
58	MG	2A	3692	1/1	0.95	0.08	49,49,49,49	0
58	MG	2A	3320	1/1	0.95	0.11	48,48,48,48	0
58	MG	2a	1755	1/1	0.95	0.11	46,46,46,46	0
58	MG	2A	3321	1/1	0.95	0.09	58,58,58,58	0
58	MG	2A	3697	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3605	1/1	0.95	0.07	38,38,38,38	0
58	MG	2A	3699	1/1	0.95	0.10	43,43,43,43	0
58	MG	2A	3323	1/1	0.95	0.12	53,53,53,53	0
58	MG	2a	1761	1/1	0.95	0.10	43,43,43,43	0
58	MG	1a	1633	1/1	0.95	0.15	46,46,46,46	0
58	MG	1a	1635	1/1	0.95	0.17	49,49,49,49	0
58	MG	2A	3027	1/1	0.95	0.08	33,33,33,33	0
58	MG	2a	1768	1/1	0.95	0.10	44,44,44,44	0
58	MG	2A	3329	1/1	0.95	0.07	42,42,42,42	0
58	MG	2A	3330	1/1	0.95	0.06	44,44,44,44	0
58	MG	1A	4058	1/1	0.95	0.15	43,43,43,43	0
58	MG	2a	1775	1/1	0.95	0.18	51,51,51,51	0
58	MG	1A	4059	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3050	1/1	0.95	0.09	28,28,28,28	0
58	MG	2a	1779	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3033	1/1	0.95	0.05	29,29,29,29	0
58	MG	1a	1640	1/1	0.95	0.20	53,53,53,53	0
58	MG	2A	3712	1/1	0.95	0.11	52,52,52,52	0
58	MG	2a	1784	1/1	0.95	0.14	57,57,57,57	0
58	MG	2A	3713	1/1	0.95	0.21	52,52,52,52	0
58	MG	2A	3715	1/1	0.95	0.09	30,30,30,30	0
58	MG	1A	3476	1/1	0.95	0.11	43,43,43,43	0
58	MG	2a	1789	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3040	1/1	0.95	0.13	58,58,58,58	0
58	MG	1a	1642	1/1	0.95	0.17	53,53,53,53	0
58	MG	1A	3611	1/1	0.95	0.07	24,24,24,24	0
58	MG	1A	4068	1/1	0.95	0.10	10,10,10,10	0
58	MG	2A	3049	1/1	0.95	0.06	40,40,40,40	0
58	MG	2A	3050	1/1	0.95	0.09	21,21,21,21	0
58	MG	2A	3347	1/1	0.95	0.07	57,57,57,57	0
58	MG	1a	1646	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3747	1/1	0.95	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3054	1/1	0.95	0.10	49,49,49,49	0
58	MG	1a	1649	1/1	0.95	0.18	55,55,55,55	0
58	MG	2A	3056	1/1	0.95	0.08	33,33,33,33	0
58	MG	1a	1650	1/1	0.95	0.12	49,49,49,49	0
58	MG	1A	3276	1/1	0.95	0.08	20,20,20,20	0
58	MG	2A	3736	1/1	0.95	0.08	47,47,47,47	0
58	MG	1A	4076	1/1	0.95	0.04	25,25,25,25	0
58	MG	2A	3738	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	4077	1/1	0.95	0.09	51,51,51,51	0
58	MG	1a	1661	1/1	0.95	0.14	55,55,55,55	0
58	MG	1A	3277	1/1	0.95	0.04	33,33,33,33	0
58	MG	1a	1663	1/1	0.95	0.24	57,57,57,57	0
58	MG	1A	3906	1/1	0.95	0.11	38,38,38,38	0
58	MG	1a	1667	1/1	0.95	0.16	52,52,52,52	0
58	MG	2A	3070	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3615	1/1	0.95	0.10	19,19,19,19	0
58	MG	2a	1821	1/1	0.95	0.14	59,59,59,59	0
58	MG	1A	3403	1/1	0.95	0.09	24,24,24,24	0
58	MG	1A	4085	1/1	0.95	0.13	48,48,48,48	0
58	MG	2A	3755	1/1	0.95	0.17	41,41,41,41	0
58	MG	2a	1825	1/1	0.95	0.14	51,51,51,51	0
58	MG	2A	3371	1/1	0.95	0.10	40,40,40,40	0
58	MG	1A	3279	1/1	0.95	0.10	40,40,40,40	0
58	MG	2A	3081	1/1	0.95	0.11	40,40,40,40	0
58	MG	1A	3487	1/1	0.95	0.11	33,33,33,33	0
58	MG	2A	3085	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3762	1/1	0.95	0.05	16,16,16,16	0
58	MG	1A	3622	1/1	0.95	0.08	17,17,17,17	0
58	MG	1A	3488	1/1	0.95	0.06	39,39,39,39	0
58	MG	2A	3765	1/1	0.95	0.06	40,40,40,40	0
58	MG	1A	3626	1/1	0.95	0.06	23,23,23,23	0
58	MG	2A	3769	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	3489	1/1	0.95	0.07	38,38,38,38	0
58	MG	2A	3384	1/1	0.95	0.16	66,66,66,66	0
58	MG	2k	201	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3774	1/1	0.95	0.06	43,43,43,43	0
58	MG	1A	4093	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	3767	1/1	0.95	0.06	40,40,40,40	0
58	MG	2A	3780	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3388	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3927	1/1	0.95	0.08	59,59,59,59	0
58	MG	1A	3928	1/1	0.95	0.09	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3391	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3103	1/1	0.95	0.06	23,23,23,23	0
58	MG	2v	102	1/1	0.95	0.20	57,57,57,57	0
58	MG	1A	3628	1/1	0.95	0.09	20,20,20,20	0
58	MG	2A	3395	1/1	0.95	0.16	44,44,44,44	0
58	MG	2w	103	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3396	1/1	0.95	0.09	52,52,52,52	0
58	MG	1a	1686	1/1	0.95	0.19	53,53,53,53	0
58	MG	2A	3106	1/1	0.95	0.07	42,42,42,42	0
58	MG	2x	103	1/1	0.95	0.12	50,50,50,50	0
58	MG	1A	4099	1/1	0.95	0.19	47,47,47,47	0
58	MG	1A	3280	1/1	0.95	0.12	28,28,28,28	0
58	MG	1B	202	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3797	1/1	0.95	0.06	50,50,50,50	0
58	MG	1a	1795	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3857	1/1	0.96	0.11	51,51,51,51	0
58	MG	1A	4035	1/1	0.96	0.05	40,40,40,40	0
58	MG	2A	3859	1/1	0.96	0.05	36,36,36,36	0
58	MG	1a	1797	1/1	0.96	0.07	44,44,44,44	0
58	MG	1A	3341	1/1	0.96	0.17	49,49,49,49	0
58	MG	2A	3862	1/1	0.96	0.12	37,37,37,37	0
58	MG	2A	3502	1/1	0.96	0.17	46,46,46,46	0
58	MG	1A	3737	1/1	0.96	0.07	35,35,35,35	0
58	MG	11	106	1/1	0.96	0.06	36,36,36,36	0
58	MG	2A	3509	1/1	0.96	0.09	47,47,47,47	0
58	MG	12	101	1/1	0.96	0.06	44,44,44,44	0
58	MG	2A	3869	1/1	0.96	0.06	53,53,53,53	0
58	MG	2A	3229	1/1	0.96	0.19	41,41,41,41	0
58	MG	1A	3502	1/1	0.96	0.20	44,44,44,44	0
58	MG	2B	201	1/1	0.96	0.14	59,59,59,59	0
58	MG	12	103	1/1	0.96	0.05	34,34,34,34	0
58	MG	1a	1807	1/1	0.96	0.05	51,51,51,51	0
58	MG	1A	3614	1/1	0.96	0.06	31,31,31,31	0
58	MG	2A	3516	1/1	0.96	0.07	24,24,24,24	0
58	MG	15	101	1/1	0.96	0.15	15,15,15,15	0
58	MG	2A	3236	1/1	0.96	0.09	45,45,45,45	0
58	MG	15	102	1/1	0.96	0.15	31,31,31,31	0
58	MG	2A	3238	1/1	0.96	0.18	44,44,44,44	0
58	MG	1A	3105	1/1	0.96	0.07	21,21,21,21	0
58	MG	1A	3220	1/1	0.96	0.08	45,45,45,45	0
58	MG	17	103	1/1	0.96	0.08	25,25,25,25	0
58	MG	1A	3423	1/1	0.96	0.05	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3508	1/1	0.96	0.07	41,41,41,41	0
58	MG	2B	216	1/1	0.96	0.09	42,42,42,42	0
58	MG	18	103	1/1	0.96	0.06	33,33,33,33	0
58	MG	1k	201	1/1	0.96	0.16	38,38,38,38	0
58	MG	18	105	1/1	0.96	0.11	42,42,42,42	0
58	MG	1A	3890	1/1	0.96	0.05	24,24,24,24	0
58	MG	1A	3620	1/1	0.96	0.07	24,24,24,24	0
58	MG	18	108	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3221	1/1	0.96	0.15	28,28,28,28	0
58	MG	2D	307	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3222	1/1	0.96	0.13	36,36,36,36	0
58	MG	1A	3751	1/1	0.96	0.05	15,15,15,15	0
58	MG	1A	3897	1/1	0.96	0.05	28,28,28,28	0
58	MG	1A	3752	1/1	0.96	0.05	13,13,13,13	0
58	MG	2E	305	1/1	0.96	0.05	43,43,43,43	0
58	MG	2A	3256	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3223	1/1	0.96	0.06	30,30,30,30	0
58	MG	1A	3113	1/1	0.96	0.13	32,32,32,32	0
58	MG	1A	4057	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	3116	1/1	0.96	0.04	26,26,26,26	0
58	MG	1A	3158	1/1	0.96	0.14	31,31,31,31	0
58	MG	2A	3549	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	4060	1/1	0.96	0.07	41,41,41,41	0
58	MG	1A	4062	1/1	0.96	0.04	28,28,28,28	0
58	MG	2F	306	1/1	0.96	0.11	40,40,40,40	0
58	MG	2F	308	1/1	0.96	0.16	43,43,43,43	0
58	MG	1A	3758	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3554	1/1	0.96	0.07	32,32,32,32	0
58	MG	2A	3555	1/1	0.96	0.08	34,34,34,34	0
58	MG	2A	3559	1/1	0.96	0.07	53,53,53,53	0
58	MG	1A	3904	1/1	0.96	0.06	26,26,26,26	0
58	MG	1A	3437	1/1	0.96	0.06	32,32,32,32	0
58	MG	1x	107	1/1	0.96	0.07	40,40,40,40	0
58	MG	1a	1619	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3632	1/1	0.96	0.09	38,38,38,38	0
58	MG	1A	4069	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3569	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3907	1/1	0.96	0.05	25,25,25,25	0
58	MG	2A	3277	1/1	0.96	0.15	43,43,43,43	0
58	MG	1A	3908	1/1	0.96	0.05	28,28,28,28	0
58	MG	1A	4074	1/1	0.96	0.06	42,42,42,42	0
58	MG	1A	3909	1/1	0.96	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1626	1/1	0.96	0.13	53,53,53,53	0
58	MG	1A	3083	1/1	0.96	0.31	39,39,39,39	0
58	MG	1A	3911	1/1	0.96	0.12	29,29,29,29	0
58	MG	1A	3356	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3232	1/1	0.96	0.12	20,20,20,20	0
58	MG	1a	1631	1/1	0.96	0.17	38,38,38,38	0
58	MG	1A	3013	1/1	0.96	0.09	18,18,18,18	0
58	MG	1A	4084	1/1	0.96	0.07	38,38,38,38	0
58	MG	2A	3013	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3588	1/1	0.96	0.10	45,45,45,45	0
58	MG	1A	3526	1/1	0.96	0.13	40,40,40,40	0
58	MG	2A	3590	1/1	0.96	0.13	52,52,52,52	0
58	MG	1A	3642	1/1	0.96	0.06	22,22,22,22	0
58	MG	1A	3444	1/1	0.96	0.08	30,30,30,30	0
58	MG	2A	3019	1/1	0.96	0.12	28,28,28,28	0
58	MG	2A	3596	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3091	1/1	0.96	0.08	26,26,26,26	0
58	MG	2A	3022	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3066	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3309	1/1	0.96	0.14	42,42,42,42	0
58	MG	1A	3364	1/1	0.96	0.06	34,34,34,34	0
58	MG	1A	3124	1/1	0.96	0.08	30,30,30,30	0
58	MG	1A	3534	1/1	0.96	0.17	23,23,23,23	0
58	MG	2A	3609	1/1	0.96	0.09	41,41,41,41	0
58	MG	2A	3030	1/1	0.96	0.09	33,33,33,33	0
58	MG	1A	3095	1/1	0.96	0.05	34,34,34,34	0
58	MG	1a	1648	1/1	0.96	0.09	44,44,44,44	0
58	MG	1A	3537	1/1	0.96	0.17	40,40,40,40	0
58	MG	1A	3368	1/1	0.96	0.08	46,46,46,46	0
58	MG	2a	1615	1/1	0.96	0.13	49,49,49,49	0
58	MG	2A	3035	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3309	1/1	0.96	0.08	56,56,56,56	0
58	MG	2A	3036	1/1	0.96	0.04	26,26,26,26	0
58	MG	2A	3311	1/1	0.96	0.09	26,26,26,26	0
58	MG	2A	3622	1/1	0.96	0.10	28,28,28,28	0
58	MG	1a	1656	1/1	0.96	0.10	44,44,44,44	0
58	MG	1A	3660	1/1	0.96	0.08	33,33,33,33	0
58	MG	2A	3042	1/1	0.96	0.15	42,42,42,42	0
58	MG	1A	4098	1/1	0.96	0.05	39,39,39,39	0
58	MG	2A	3044	1/1	0.96	0.15	51,51,51,51	0
58	MG	1A	3783	1/1	0.96	0.06	54,54,54,54	0
58	MG	2A	3046	1/1	0.96	0.07	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3631	1/1	0.96	0.05	32,32,32,32	0
58	MG	2A	3632	1/1	0.96	0.06	42,42,42,42	0
58	MG	2a	1631	1/1	0.96	0.05	43,43,43,43	0
58	MG	1A	3539	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3183	1/1	0.96	0.10	30,30,30,30	0
58	MG	1B	203	1/1	0.96	0.06	31,31,31,31	0
58	MG	2a	1635	1/1	0.96	0.11	52,52,52,52	0
58	MG	1A	3941	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3129	1/1	0.96	0.06	23,23,23,23	0
58	MG	2A	3053	1/1	0.96	0.12	56,56,56,56	0
58	MG	2a	1639	1/1	0.96	0.21	49,49,49,49	0
58	MG	1A	3665	1/1	0.96	0.07	24,24,24,24	0
58	MG	1A	3185	1/1	0.96	0.16	39,39,39,39	0
58	MG	2A	3643	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3644	1/1	0.96	0.13	28,28,28,28	0
58	MG	2A	3328	1/1	0.96	0.14	41,41,41,41	0
58	MG	1A	3048	1/1	0.96	0.07	19,19,19,19	0
58	MG	1A	3544	1/1	0.96	0.15	40,40,40,40	0
58	MG	2a	1648	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3669	1/1	0.96	0.03	13,13,13,13	0
58	MG	1A	3795	1/1	0.96	0.06	37,37,37,37	0
58	MG	1A	3132	1/1	0.96	0.05	29,29,29,29	0
58	MG	2a	1652	1/1	0.96	0.06	64,64,64,64	0
58	MG	1A	3042	1/1	0.96	0.16	21,21,21,21	0
58	MG	2A	3652	1/1	0.96	0.05	38,38,38,38	0
58	MG	2A	3337	1/1	0.96	0.15	57,57,57,57	0
58	MG	1A	3550	1/1	0.96	0.06	39,39,39,39	0
58	MG	2A	3658	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	3380	1/1	0.96	0.12	31,31,31,31	0
58	MG	1A	3957	1/1	0.96	0.11	38,38,38,38	0
58	MG	2A	3661	1/1	0.96	0.13	37,37,37,37	0
58	MG	1A	3253	1/1	0.96	0.13	25,25,25,25	0
58	MG	1A	3553	1/1	0.96	0.08	44,44,44,44	0
58	MG	2a	1664	1/1	0.96	0.06	59,59,59,59	0
58	MG	2A	3665	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3678	1/1	0.96	0.04	32,32,32,32	0
58	MG	1A	3554	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3963	1/1	0.96	0.05	36,36,36,36	0
58	MG	2A	3078	1/1	0.96	0.07	19,19,19,19	0
58	MG	2a	1670	1/1	0.96	0.13	32,32,32,32	0
58	MG	2a	1671	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3079	1/1	0.96	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3675	1/1	0.96	0.09	43,43,43,43	0
58	MG	2a	1675	1/1	0.96	0.12	42,42,42,42	0
58	MG	1A	3808	1/1	0.96	0.09	53,53,53,53	0
58	MG	1A	3809	1/1	0.96	0.04	40,40,40,40	0
58	MG	2a	1679	1/1	0.96	0.05	38,38,38,38	0
58	MG	1A	3555	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3192	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3086	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3815	1/1	0.96	0.23	16,16,16,16	0
58	MG	1A	3686	1/1	0.96	0.11	42,42,42,42	0
58	MG	1A	3687	1/1	0.96	0.08	51,51,51,51	0
58	MG	2A	3094	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3820	1/1	0.96	0.06	48,48,48,48	0
58	MG	2A	3359	1/1	0.96	0.08	44,44,44,44	0
58	MG	2a	1690	1/1	0.96	0.13	50,50,50,50	0
58	MG	1A	3977	1/1	0.96	0.07	48,48,48,48	0
58	MG	2A	3361	1/1	0.96	0.08	44,44,44,44	0
58	MG	1D	302	1/1	0.96	0.07	33,33,33,33	0
58	MG	1A	3195	1/1	0.96	0.15	27,27,27,27	0
58	MG	2a	1697	1/1	0.96	0.22	49,49,49,49	0
58	MG	1A	3979	1/1	0.96	0.08	52,52,52,52	0
58	MG	1A	3135	1/1	0.96	0.07	28,28,28,28	0
58	MG	2a	1702	1/1	0.96	0.15	50,50,50,50	0
58	MG	2A	3102	1/1	0.96	0.10	45,45,45,45	0
58	MG	1A	3564	1/1	0.96	0.15	29,29,29,29	0
58	MG	2A	3370	1/1	0.96	0.12	41,41,41,41	0
58	MG	1A	3324	1/1	0.96	0.08	28,28,28,28	0
58	MG	1A	3827	1/1	0.96	0.08	25,25,25,25	0
58	MG	1A	3831	1/1	0.96	0.05	17,17,17,17	0
58	MG	2A	3107	1/1	0.96	0.14	43,43,43,43	0
58	MG	2A	3108	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3109	1/1	0.96	0.08	60,60,60,60	0
58	MG	2A	3707	1/1	0.96	0.11	57,57,57,57	0
58	MG	2A	3378	1/1	0.96	0.07	41,41,41,41	0
58	MG	2A	3379	1/1	0.96	0.22	57,57,57,57	0
58	MG	1A	3394	1/1	0.96	0.21	33,33,33,33	0
58	MG	1A	3835	1/1	0.96	0.08	43,43,43,43	0
58	MG	1F	308	1/1	0.96	0.12	20,20,20,20	0
58	MG	1a	1708	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3258	1/1	0.96	0.06	39,39,39,39	0
58	MG	2A	3117	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3118	1/1	0.96	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3197	1/1	0.96	0.19	26,26,26,26	0
58	MG	2a	1726	1/1	0.96	0.12	43,43,43,43	0
58	MG	1a	1712	1/1	0.96	0.19	51,51,51,51	0
58	MG	2a	1728	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	3573	1/1	0.96	0.14	53,53,53,53	0
58	MG	1a	1714	1/1	0.96	0.08	28,28,28,28	0
58	MG	1F	314	1/1	0.96	0.15	43,43,43,43	0
58	MG	1G	201	1/1	0.96	0.09	38,38,38,38	0
58	MG	1A	3839	1/1	0.96	0.07	42,42,42,42	0
58	MG	2a	1736	1/1	0.96	0.12	45,45,45,45	0
58	MG	2A	3727	1/1	0.96	0.08	23,23,23,23	0
58	MG	2A	3127	1/1	0.96	0.14	41,41,41,41	0
58	MG	1a	1719	1/1	0.96	0.08	28,28,28,28	0
58	MG	2a	1740	1/1	0.96	0.22	29,29,29,29	0
58	MG	1G	203	1/1	0.96	0.07	57,57,57,57	0
58	MG	1a	1721	1/1	0.96	0.12	48,48,48,48	0
58	MG	1A	3699	1/1	0.96	0.04	17,17,17,17	0
58	MG	2a	1744	1/1	0.96	0.17	48,48,48,48	0
58	MG	2A	3402	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	3993	1/1	0.96	0.08	18,18,18,18	0
58	MG	2A	3404	1/1	0.96	0.06	51,51,51,51	0
58	MG	2A	3134	1/1	0.96	0.05	32,32,32,32	0
58	MG	1A	3575	1/1	0.96	0.07	41,41,41,41	0
58	MG	1N	205	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3576	1/1	0.96	0.09	41,41,41,41	0
58	MG	2A	3142	1/1	0.96	0.12	42,42,42,42	0
58	MG	2A	3743	1/1	0.96	0.09	46,46,46,46	0
58	MG	2A	3410	1/1	0.96	0.13	31,31,31,31	0
58	MG	2A	3411	1/1	0.96	0.12	52,52,52,52	0
58	MG	2A	3748	1/1	0.96	0.06	53,53,53,53	0
58	MG	2A	3412	1/1	0.96	0.19	44,44,44,44	0
58	MG	2A	3413	1/1	0.96	0.12	33,33,33,33	0
58	MG	1a	1727	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3752	1/1	0.96	0.09	45,45,45,45	0
58	MG	1a	1728	1/1	0.96	0.09	51,51,51,51	0
58	MG	2a	1766	1/1	0.96	0.06	46,46,46,46	0
58	MG	1A	3702	1/1	0.96	0.05	35,35,35,35	0
58	MG	1A	3138	1/1	0.96	0.08	31,31,31,31	0
58	MG	1A	3578	1/1	0.96	0.23	36,36,36,36	0
58	MG	1A	3581	1/1	0.96	0.12	30,30,30,30	0
58	MG	1A	3264	1/1	0.96	0.06	41,41,41,41	0
58	MG	1Q	202	1/1	0.96	0.14	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3584	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3762	1/1	0.96	0.09	41,41,41,41	0
58	MG	1A	3330	1/1	0.96	0.07	32,32,32,32	0
58	MG	1a	1739	1/1	0.96	0.08	38,38,38,38	0
58	MG	2A	3160	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3331	1/1	0.96	0.07	34,34,34,34	0
58	MG	1R	201	1/1	0.96	0.11	35,35,35,35	0
58	MG	2A	3770	1/1	0.96	0.07	44,44,44,44	0
58	MG	2A	3164	1/1	0.96	0.04	24,24,24,24	0
58	MG	2A	3772	1/1	0.96	0.07	49,49,49,49	0
58	MG	1A	3057	1/1	0.96	0.10	36,36,36,36	0
58	MG	1A	3712	1/1	0.96	0.07	22,22,22,22	0
58	MG	1S	201	1/1	0.96	0.11	33,33,33,33	0
58	MG	2A	3168	1/1	0.96	0.09	43,43,43,43	0
58	MG	2A	3778	1/1	0.96	0.11	52,52,52,52	0
58	MG	1S	202	1/1	0.96	0.07	37,37,37,37	0
58	MG	1a	1747	1/1	0.96	0.04	49,49,49,49	0
58	MG	2A	3782	1/1	0.96	0.07	43,43,43,43	0
58	MG	1a	1748	1/1	0.96	0.05	43,43,43,43	0
58	MG	2A	3172	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3100	1/1	0.96	0.09	38,38,38,38	0
58	MG	2A	3787	1/1	0.96	0.07	44,44,44,44	0
58	MG	1A	3101	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3596	1/1	0.96	0.08	32,32,32,32	0
58	MG	1T	203	1/1	0.96	0.08	35,35,35,35	0
58	MG	1A	3143	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3179	1/1	0.96	0.19	50,50,50,50	0
58	MG	2a	1810	1/1	0.96	0.13	41,41,41,41	0
58	MG	2A	3181	1/1	0.96	0.05	37,37,37,37	0
58	MG	1U	203	1/1	0.96	0.12	30,30,30,30	0
58	MG	2A	3183	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3336	1/1	0.96	0.16	41,41,41,41	0
58	MG	2A	3451	1/1	0.96	0.14	42,42,42,42	0
58	MG	2A	3452	1/1	0.96	0.14	42,42,42,42	0
58	MG	1A	3600	1/1	0.96	0.14	25,25,25,25	0
58	MG	2A	3189	1/1	0.96	0.09	62,62,62,62	0
58	MG	1A	4016	1/1	0.96	0.04	36,36,36,36	0
58	MG	1A	3146	1/1	0.96	0.07	35,35,35,35	0
58	MG	1A	3863	1/1	0.96	0.05	12,12,12,12	0
58	MG	1V	206	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3194	1/1	0.96	0.06	49,49,49,49	0
58	MG	1a	1768	1/1	0.96	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3807	1/1	0.96	0.04	37,37,37,37	0
58	MG	2A	3196	1/1	0.96	0.16	41,41,41,41	0
58	MG	1A	4019	1/1	0.96	0.04	40,40,40,40	0
58	MG	2A	3810	1/1	0.96	0.05	49,49,49,49	0
58	MG	2A	3464	1/1	0.96	0.10	49,49,49,49	0
58	MG	2a	1831	1/1	0.96	0.10	57,57,57,57	0
58	MG	1A	3864	1/1	0.96	0.09	16,16,16,16	0
58	MG	1W	203	1/1	0.96	0.09	45,45,45,45	0
58	MG	2A	3815	1/1	0.96	0.06	28,28,28,28	0
58	MG	1W	205	1/1	0.96	0.09	36,36,36,36	0
58	MG	2d	301	1/1	0.96	0.22	54,54,54,54	0
58	MG	2e	201	1/1	0.96	0.05	60,60,60,60	0
58	MG	2A	3470	1/1	0.96	0.08	41,41,41,41	0
58	MG	1A	3015	1/1	0.96	0.08	26,26,26,26	0
58	MG	2A	3819	1/1	0.96	0.09	42,42,42,42	0
58	MG	1X	102	1/1	0.96	0.05	28,28,28,28	0
58	MG	1A	3723	1/1	0.96	0.08	47,47,47,47	0
58	MG	2A	3475	1/1	0.96	0.11	37,37,37,37	0
58	MG	1A	3868	1/1	0.96	0.11	40,40,40,40	0
58	MG	2A	3826	1/1	0.96	0.05	54,54,54,54	0
58	MG	2A	3827	1/1	0.96	0.09	53,53,53,53	0
58	MG	2A	3828	1/1	0.96	0.10	50,50,50,50	0
58	MG	1a	1779	1/1	0.96	0.06	46,46,46,46	0
58	MG	2A	3206	1/1	0.96	0.12	47,47,47,47	0
58	MG	2A	3480	1/1	0.96	0.12	40,40,40,40	0
58	MG	1Y	202	1/1	0.96	0.05	32,32,32,32	0
58	MG	1A	3494	1/1	0.96	0.10	46,46,46,46	0
58	MG	2A	3210	1/1	0.96	0.07	46,46,46,46	0
58	MG	2w	101	1/1	0.96	0.14	46,46,46,46	0
58	MG	1A	3495	1/1	0.96	0.16	32,32,32,32	0
58	MG	1A	3151	1/1	0.96	0.05	30,30,30,30	0
58	MG	2A	3213	1/1	0.96	0.07	50,50,50,50	0
58	MG	10	101	1/1	0.96	0.09	31,31,31,31	0
58	MG	1A	3415	1/1	0.96	0.12	42,42,42,42	0
58	MG	1A	3607	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3732	1/1	0.96	0.10	50,50,50,50	0
58	MG	1A	3275	1/1	0.96	0.10	44,44,44,44	0
58	MG	1A	3418	1/1	0.96	0.05	27,27,27,27	0
58	MG	1A	3879	1/1	0.96	0.05	32,32,32,32	0
60	ZN	2n	103	1/1	0.96	0.06	82,82,82,82	0
58	MG	1A	3964	1/1	0.97	0.04	38,38,38,38	0
58	MG	2D	301	1/1	0.97	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3582	1/1	0.97	0.04	23,23,23,23	0
58	MG	2D	303	1/1	0.97	0.14	34,34,34,34	0
58	MG	1a	1677	1/1	0.97	0.18	43,43,43,43	0
58	MG	1A	3246	1/1	0.97	0.11	39,39,39,39	0
58	MG	1A	3803	1/1	0.97	0.08	18,18,18,18	0
58	MG	1A	3659	1/1	0.97	0.07	25,25,25,25	0
58	MG	2A	3062	1/1	0.97	0.05	35,35,35,35	0
58	MG	1A	3176	1/1	0.97	0.05	30,30,30,30	0
58	MG	1A	3969	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3328	1/1	0.97	0.10	45,45,45,45	0
58	MG	2A	3591	1/1	0.97	0.05	32,32,32,32	0
58	MG	1A	3181	1/1	0.97	0.09	15,15,15,15	0
58	MG	1A	3972	1/1	0.97	0.07	26,26,26,26	0
58	MG	1A	3973	1/1	0.97	0.04	35,35,35,35	0
58	MG	2A	3069	1/1	0.97	0.07	25,25,25,25	0
58	MG	1E	305	1/1	0.97	0.11	22,22,22,22	0
58	MG	2A	3599	1/1	0.97	0.05	36,36,36,36	0
58	MG	1E	306	1/1	0.97	0.21	42,42,42,42	0
58	MG	2A	3602	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3072	1/1	0.97	0.08	45,45,45,45	0
58	MG	2F	307	1/1	0.97	0.18	44,44,44,44	0
58	MG	2A	3604	1/1	0.97	0.10	47,47,47,47	0
58	MG	2G	201	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3089	1/1	0.97	0.10	37,37,37,37	0
58	MG	1A	3422	1/1	0.97	0.08	34,34,34,34	0
58	MG	2A	3077	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3126	1/1	0.97	0.11	20,20,20,20	0
58	MG	1A	3424	1/1	0.97	0.06	44,44,44,44	0
58	MG	1F	303	1/1	0.97	0.09	20,20,20,20	0
58	MG	1A	3533	1/1	0.97	0.07	29,29,29,29	0
58	MG	1A	3058	1/1	0.97	0.10	16,16,16,16	0
58	MG	2A	3333	1/1	0.97	0.06	58,58,58,58	0
58	MG	2V	201	1/1	0.97	0.21	42,42,42,42	0
58	MG	2A	3083	1/1	0.97	0.07	36,36,36,36	0
58	MG	2A	3616	1/1	0.97	0.12	43,43,43,43	0
58	MG	2W	203	1/1	0.97	0.07	39,39,39,39	0
58	MG	1F	307	1/1	0.97	0.05	33,33,33,33	0
58	MG	1A	3130	1/1	0.97	0.16	31,31,31,31	0
58	MG	1F	310	1/1	0.97	0.08	33,33,33,33	0
58	MG	2A	3620	1/1	0.97	0.05	39,39,39,39	0
58	MG	2A	3338	1/1	0.97	0.07	68,68,68,68	0
58	MG	2A	3089	1/1	0.97	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3819	1/1	0.97	0.05	28,28,28,28	0
58	MG	23	102	1/1	0.97	0.06	33,33,33,33	0
58	MG	1A	3429	1/1	0.97	0.06	22,22,22,22	0
58	MG	1A	3984	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3061	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3431	1/1	0.97	0.04	35,35,35,35	0
58	MG	2A	3628	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3189	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3093	1/1	0.97	0.05	37,37,37,37	0
58	MG	2A	3099	1/1	0.97	0.04	37,37,37,37	0
58	MG	1A	3012	1/1	0.97	0.06	21,21,21,21	0
58	MG	1I	201	1/1	0.97	0.05	42,42,42,42	0
58	MG	1N	201	1/1	0.97	0.15	41,41,41,41	0
58	MG	1A	3436	1/1	0.97	0.17	41,41,41,41	0
58	MG	1a	1711	1/1	0.97	0.08	38,38,38,38	0
58	MG	2A	3637	1/1	0.97	0.11	49,49,49,49	0
58	MG	1A	3832	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	3193	1/1	0.97	0.18	30,30,30,30	0
58	MG	1N	206	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3546	1/1	0.97	0.14	34,34,34,34	0
58	MG	1A	3685	1/1	0.97	0.06	22,22,22,22	0
58	MG	1A	3260	1/1	0.97	0.12	18,18,18,18	0
58	MG	1A	3439	1/1	0.97	0.05	39,39,39,39	0
58	MG	1A	3688	1/1	0.97	0.05	20,20,20,20	0
58	MG	1A	3261	1/1	0.97	0.04	17,17,17,17	0
58	MG	2A	3363	1/1	0.97	0.07	48,48,48,48	0
58	MG	1A	3690	1/1	0.97	0.09	18,18,18,18	0
58	MG	1Q	203	1/1	0.97	0.06	24,24,24,24	0
58	MG	1A	3134	1/1	0.97	0.09	33,33,33,33	0
58	MG	1Q	206	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3442	1/1	0.97	0.05	37,37,37,37	0
58	MG	2A	3655	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3263	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3017	1/1	0.97	0.05	39,39,39,39	0
58	MG	1A	3695	1/1	0.97	0.04	23,23,23,23	0
58	MG	1A	3064	1/1	0.97	0.10	34,34,34,34	0
58	MG	1A	4008	1/1	0.97	0.06	46,46,46,46	0
58	MG	1A	3345	1/1	0.97	0.08	50,50,50,50	0
58	MG	2a	1624	1/1	0.97	0.16	52,52,52,52	0
58	MG	1a	1733	1/1	0.97	0.07	25,25,25,25	0
58	MG	1A	3005	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3130	1/1	0.97	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3559	1/1	0.97	0.08	37,37,37,37	0
58	MG	2A	3668	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3450	1/1	0.97	0.30	32,32,32,32	0
58	MG	1A	4013	1/1	0.97	0.05	22,22,22,22	0
58	MG	2A	3672	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3563	1/1	0.97	0.11	23,23,23,23	0
58	MG	2A	3135	1/1	0.97	0.05	25,25,25,25	0
58	MG	1U	201	1/1	0.97	0.06	27,27,27,27	0
58	MG	2A	3385	1/1	0.97	0.06	46,46,46,46	0
58	MG	2A	3137	1/1	0.97	0.12	33,33,33,33	0
58	MG	2A	3139	1/1	0.97	0.11	50,50,50,50	0
58	MG	1U	202	1/1	0.97	0.23	36,36,36,36	0
58	MG	1A	3347	1/1	0.97	0.07	33,33,33,33	0
58	MG	1a	1743	1/1	0.97	0.09	35,35,35,35	0
58	MG	2A	3143	1/1	0.97	0.14	31,31,31,31	0
58	MG	2A	3144	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3349	1/1	0.97	0.08	30,30,30,30	0
58	MG	2a	1645	1/1	0.97	0.19	54,54,54,54	0
58	MG	2A	3394	1/1	0.97	0.10	59,59,59,59	0
58	MG	1U	205	1/1	0.97	0.09	27,27,27,27	0
58	MG	2A	3689	1/1	0.97	0.11	45,45,45,45	0
58	MG	2A	3690	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3067	1/1	0.97	0.10	30,30,30,30	0
58	MG	2A	3148	1/1	0.97	0.05	25,25,25,25	0
58	MG	1V	201	1/1	0.97	0.22	25,25,25,25	0
58	MG	1A	3200	1/1	0.97	0.11	20,20,20,20	0
58	MG	2A	3696	1/1	0.97	0.10	22,22,22,22	0
58	MG	1A	3858	1/1	0.97	0.07	25,25,25,25	0
58	MG	2A	3401	1/1	0.97	0.07	43,43,43,43	0
58	MG	1A	4020	1/1	0.97	0.08	37,37,37,37	0
58	MG	2A	3154	1/1	0.97	0.11	44,44,44,44	0
58	MG	1A	3859	1/1	0.97	0.08	14,14,14,14	0
58	MG	1V	207	1/1	0.97	0.06	48,48,48,48	0
58	MG	2a	1661	1/1	0.97	0.06	52,52,52,52	0
58	MG	1A	3047	1/1	0.97	0.07	25,25,25,25	0
58	MG	1a	1757	1/1	0.97	0.06	42,42,42,42	0
58	MG	1a	1758	1/1	0.97	0.07	44,44,44,44	0
58	MG	2A	3161	1/1	0.97	0.11	32,32,32,32	0
58	MG	1A	3570	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3203	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3204	1/1	0.97	0.05	20,20,20,20	0
58	MG	1W	206	1/1	0.97	0.09	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3710	1/1	0.97	0.05	9,9,9,9	0
58	MG	1A	3459	1/1	0.97	0.06	43,43,43,43	0
58	MG	2a	1672	1/1	0.97	0.06	49,49,49,49	0
58	MG	1X	103	1/1	0.97	0.07	39,39,39,39	0
58	MG	1X	104	1/1	0.97	0.11	32,32,32,32	0
58	MG	1A	3274	1/1	0.97	0.15	29,29,29,29	0
58	MG	1A	3357	1/1	0.97	0.17	40,40,40,40	0
58	MG	2a	1677	1/1	0.97	0.08	35,35,35,35	0
58	MG	1A	3142	1/1	0.97	0.08	27,27,27,27	0
58	MG	1a	1772	1/1	0.97	0.07	58,58,58,58	0
58	MG	1A	3102	1/1	0.97	0.06	41,41,41,41	0
58	MG	2A	3721	1/1	0.97	0.04	38,38,38,38	0
58	MG	1A	3209	1/1	0.97	0.07	24,24,24,24	0
58	MG	2a	1683	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3585	1/1	0.97	0.08	21,21,21,21	0
58	MG	1A	3586	1/1	0.97	0.12	26,26,26,26	0
58	MG	2A	3725	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3278	1/1	0.97	0.12	39,39,39,39	0
58	MG	1A	3144	1/1	0.97	0.06	24,24,24,24	0
58	MG	1A	3145	1/1	0.97	0.07	9,9,9,9	0
58	MG	1A	3212	1/1	0.97	0.09	26,26,26,26	0
58	MG	2A	3730	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3593	1/1	0.97	0.07	31,31,31,31	0
58	MG	2A	3186	1/1	0.97	0.05	33,33,33,33	0
58	MG	10	109	1/1	0.97	0.04	31,31,31,31	0
58	MG	1A	3881	1/1	0.97	0.10	31,31,31,31	0
58	MG	2A	3435	1/1	0.97	0.25	47,47,47,47	0
58	MG	2a	1699	1/1	0.97	0.10	47,47,47,47	0
58	MG	11	102	1/1	0.97	0.09	32,32,32,32	0
58	MG	1A	3594	1/1	0.97	0.15	34,34,34,34	0
58	MG	1A	3728	1/1	0.97	0.04	29,29,29,29	0
58	MG	1A	3470	1/1	0.97	0.10	29,29,29,29	0
58	MG	1A	3471	1/1	0.97	0.07	24,24,24,24	0
58	MG	1A	3292	1/1	0.97	0.06	49,49,49,49	0
58	MG	1A	3293	1/1	0.97	0.14	26,26,26,26	0
58	MG	2a	1708	1/1	0.97	0.14	55,55,55,55	0
58	MG	1A	4049	1/1	0.97	0.04	27,27,27,27	0
58	MG	2A	3746	1/1	0.97	0.07	32,32,32,32	0
58	MG	13	102	1/1	0.97	0.14	49,49,49,49	0
58	MG	1A	3474	1/1	0.97	0.10	37,37,37,37	0
58	MG	1A	4051	1/1	0.97	0.10	36,36,36,36	0
58	MG	1a	1800	1/1	0.97	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3029	1/1	0.97	0.04	33,33,33,33	0
58	MG	2a	1716	1/1	0.97	0.18	51,51,51,51	0
58	MG	15	103	1/1	0.97	0.16	28,28,28,28	0
58	MG	2a	1718	1/1	0.97	0.08	51,51,51,51	0
58	MG	1A	4053	1/1	0.97	0.07	25,25,25,25	0
58	MG	2A	3754	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3295	1/1	0.97	0.05	27,27,27,27	0
58	MG	1a	1806	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3207	1/1	0.97	0.04	36,36,36,36	0
58	MG	2A	3456	1/1	0.97	0.06	43,43,43,43	0
58	MG	16	101	1/1	0.97	0.06	46,46,46,46	0
58	MG	17	101	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	3738	1/1	0.97	0.05	23,23,23,23	0
58	MG	1A	3216	1/1	0.97	0.12	38,38,38,38	0
58	MG	1A	3478	1/1	0.97	0.06	42,42,42,42	0
58	MG	2a	1730	1/1	0.97	0.17	41,41,41,41	0
58	MG	18	102	1/1	0.97	0.17	36,36,36,36	0
58	MG	1a	1814	1/1	0.97	0.04	41,41,41,41	0
58	MG	2A	3766	1/1	0.97	0.05	35,35,35,35	0
58	MG	2A	3767	1/1	0.97	0.09	33,33,33,33	0
58	MG	1A	3374	1/1	0.97	0.17	41,41,41,41	0
58	MG	1A	3480	1/1	0.97	0.04	33,33,33,33	0
58	MG	1e	201	1/1	0.97	0.12	59,59,59,59	0
58	MG	1e	202	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3076	1/1	0.97	0.05	15,15,15,15	0
58	MG	1A	4061	1/1	0.97	0.12	41,41,41,41	0
58	MG	1A	3106	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3609	1/1	0.97	0.06	34,34,34,34	0
58	MG	1l	202	1/1	0.97	0.10	49,49,49,49	0
58	MG	2a	1745	1/1	0.97	0.17	55,55,55,55	0
58	MG	1m	3001	1/1	0.97	0.04	51,51,51,51	0
58	MG	2A	3225	1/1	0.97	0.14	37,37,37,37	0
58	MG	2A	3478	1/1	0.97	0.05	17,17,17,17	0
58	MG	1A	3610	1/1	0.97	0.05	19,19,19,19	0
58	MG	1A	3110	1/1	0.97	0.06	22,22,22,22	0
58	MG	1A	3379	1/1	0.97	0.22	27,27,27,27	0
58	MG	1A	3077	1/1	0.97	0.15	32,32,32,32	0
58	MG	2A	3786	1/1	0.97	0.08	50,50,50,50	0
58	MG	2a	1754	1/1	0.97	0.10	53,53,53,53	0
58	MG	1A	3381	1/1	0.97	0.05	36,36,36,36	0
58	MG	2A	3484	1/1	0.97	0.05	49,49,49,49	0
58	MG	2A	3485	1/1	0.97	0.05	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3115	1/1	0.97	0.06	25,25,25,25	0
58	MG	1A	4073	1/1	0.97	0.04	12,12,12,12	0
58	MG	1a	1608	1/1	0.97	0.04	48,48,48,48	0
58	MG	1A	3492	1/1	0.97	0.07	43,43,43,43	0
58	MG	2a	1762	1/1	0.97	0.05	35,35,35,35	0
58	MG	1A	3756	1/1	0.97	0.10	30,30,30,30	0
58	MG	1A	3304	1/1	0.97	0.04	16,16,16,16	0
58	MG	1A	3305	1/1	0.97	0.12	39,39,39,39	0
58	MG	1a	1614	1/1	0.97	0.12	47,47,47,47	0
58	MG	2A	3494	1/1	0.97	0.07	39,39,39,39	0
58	MG	2a	1769	1/1	0.97	0.08	56,56,56,56	0
58	MG	1A	3759	1/1	0.97	0.04	31,31,31,31	0
58	MG	2A	3496	1/1	0.97	0.15	32,32,32,32	0
58	MG	1A	3913	1/1	0.97	0.14	14,14,14,14	0
58	MG	1A	3224	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	4083	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3621	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3917	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	3496	1/1	0.97	0.12	30,30,30,30	0
58	MG	2A	3504	1/1	0.97	0.14	31,31,31,31	0
58	MG	1A	3623	1/1	0.97	0.04	19,19,19,19	0
58	MG	2a	1783	1/1	0.97	0.06	46,46,46,46	0
58	MG	2A	3507	1/1	0.97	0.06	56,56,56,56	0
58	MG	1A	3389	1/1	0.97	0.18	39,39,39,39	0
58	MG	1A	3391	1/1	0.97	0.13	15,15,15,15	0
58	MG	1A	3308	1/1	0.97	0.04	18,18,18,18	0
58	MG	1A	3393	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3814	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3157	1/1	0.97	0.12	39,39,39,39	0
58	MG	1A	3049	1/1	0.97	0.03	11,11,11,11	0
58	MG	1A	3311	1/1	0.97	0.08	35,35,35,35	0
58	MG	1A	3930	1/1	0.97	0.05	38,38,38,38	0
58	MG	2A	3257	1/1	0.97	0.09	40,40,40,40	0
58	MG	2A	3820	1/1	0.97	0.05	41,41,41,41	0
58	MG	1a	1632	1/1	0.97	0.11	43,43,43,43	0
58	MG	2A	3822	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3160	1/1	0.97	0.16	25,25,25,25	0
58	MG	1a	1634	1/1	0.97	0.14	21,21,21,21	0
58	MG	2a	1802	1/1	0.97	0.16	52,52,52,52	0
58	MG	2A	3261	1/1	0.97	0.17	52,52,52,52	0
58	MG	1A	3161	1/1	0.97	0.06	28,28,28,28	0
58	MG	1A	3635	1/1	0.97	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1806	1/1	0.97	0.17	38,38,38,38	0
58	MG	2a	1807	1/1	0.97	0.12	44,44,44,44	0
58	MG	2A	3264	1/1	0.97	0.17	45,45,45,45	0
58	MG	1A	3036	1/1	0.97	0.06	30,30,30,30	0
58	MG	2A	3014	1/1	0.97	0.09	29,29,29,29	0
58	MG	2A	3831	1/1	0.97	0.05	32,32,32,32	0
58	MG	1A	3166	1/1	0.97	0.15	23,23,23,23	0
58	MG	1A	3640	1/1	0.97	0.04	14,14,14,14	0
58	MG	2A	3530	1/1	0.97	0.06	25,25,25,25	0
58	MG	2a	1815	1/1	0.97	0.09	59,59,59,59	0
58	MG	1A	3234	1/1	0.97	0.15	37,37,37,37	0
58	MG	2A	3018	1/1	0.97	0.07	37,37,37,37	0
58	MG	2A	3840	1/1	0.97	0.09	21,21,21,21	0
58	MG	2A	3271	1/1	0.97	0.16	54,54,54,54	0
58	MG	1A	3511	1/1	0.97	0.07	40,40,40,40	0
58	MG	2A	3273	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3781	1/1	0.97	0.05	20,20,20,20	0
58	MG	2A	3846	1/1	0.97	0.04	28,28,28,28	0
58	MG	1a	1644	1/1	0.97	0.09	52,52,52,52	0
58	MG	2A	3848	1/1	0.97	0.07	53,53,53,53	0
58	MG	2A	3849	1/1	0.97	0.12	42,42,42,42	0
58	MG	1A	3052	1/1	0.97	0.12	19,19,19,19	0
58	MG	1A	3944	1/1	0.97	0.05	33,33,33,33	0
58	MG	1A	3119	1/1	0.97	0.11	22,22,22,22	0
58	MG	1A	3645	1/1	0.97	0.06	37,37,37,37	0
58	MG	2A	3028	1/1	0.97	0.08	43,43,43,43	0
58	MG	2A	3544	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3786	1/1	0.97	0.02	14,14,14,14	0
58	MG	1A	3011	1/1	0.97	0.07	28,28,28,28	0
58	MG	1a	1654	1/1	0.97	0.13	55,55,55,55	0
58	MG	2A	3284	1/1	0.97	0.09	40,40,40,40	0
58	MG	1A	3239	1/1	0.97	0.27	27,27,27,27	0
58	MG	1A	3790	1/1	0.97	0.07	18,18,18,18	0
58	MG	2A	3864	1/1	0.97	0.06	45,45,45,45	0
58	MG	1B	216	1/1	0.97	0.04	52,52,52,52	0
58	MG	1a	1659	1/1	0.97	0.05	44,44,44,44	0
58	MG	1B	218	1/1	0.97	0.05	27,27,27,27	0
58	MG	2A	3556	1/1	0.97	0.10	25,25,25,25	0
58	MG	2l	202	1/1	0.97	0.13	53,53,53,53	0
58	MG	2l	203	1/1	0.97	0.08	54,54,54,54	0
58	MG	1A	3086	1/1	0.97	0.10	27,27,27,27	0
58	MG	2A	3038	1/1	0.97	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3561	1/1	0.97	0.07	27,27,27,27	0
58	MG	1A	3649	1/1	0.97	0.07	10,10,10,10	0
58	MG	2A	3563	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3955	1/1	0.97	0.05	59,59,59,59	0
58	MG	2B	204	1/1	0.97	0.06	55,55,55,55	0
58	MG	1A	3650	1/1	0.97	0.08	34,34,34,34	0
58	MG	1a	1665	1/1	0.97	0.14	48,48,48,48	0
58	MG	1a	1666	1/1	0.97	0.11	44,44,44,44	0
58	MG	1A	3241	1/1	0.97	0.05	31,31,31,31	0
58	MG	2A	3570	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3958	1/1	0.97	0.04	30,30,30,30	0
58	MG	2A	3048	1/1	0.97	0.17	49,49,49,49	0
58	MG	1A	3653	1/1	0.97	0.06	25,25,25,25	0
58	MG	2A	3574	1/1	0.97	0.06	30,30,30,30	0
58	MG	2x	102	1/1	0.97	0.10	46,46,46,46	0
58	MG	1a	1670	1/1	0.97	0.18	55,55,55,55	0
58	MG	2A	3576	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3088	1/1	0.97	0.12	25,25,25,25	0
58	MG	2x	106	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3797	1/1	0.97	0.03	14,14,14,14	0
58	MG	1A	3523	1/1	0.97	0.07	23,23,23,23	0
60	ZN	2Y	202	1/1	0.97	0.05	81,81,81,81	0
60	ZN	24	501	1/1	0.97	0.09	89,89,89,89	0
58	MG	1A	3245	1/1	0.97	0.11	34,34,34,34	0
58	MG	1A	3127	1/1	0.98	0.14	19,19,19,19	0
58	MG	1A	3782	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3182	1/1	0.98	0.05	21,21,21,21	0
58	MG	18	104	1/1	0.98	0.11	31,31,31,31	0
58	MG	1A	3652	1/1	0.98	0.07	17,17,17,17	0
58	MG	1A	3128	1/1	0.98	0.18	25,25,25,25	0
58	MG	1A	3059	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3060	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3935	1/1	0.98	0.03	25,25,25,25	0
58	MG	19	101	1/1	0.98	0.23	55,55,55,55	0
58	MG	1A	3788	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3937	1/1	0.98	0.03	10,10,10,10	0
58	MG	1A	3656	1/1	0.98	0.05	27,27,27,27	0
58	MG	1A	3022	1/1	0.98	0.06	31,31,31,31	0
58	MG	1A	3094	1/1	0.98	0.06	20,20,20,20	0
58	MG	1A	3426	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3255	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3188	1/1	0.98	0.03	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3945	1/1	0.98	0.06	45,45,45,45	0
58	MG	1A	3039	1/1	0.98	0.13	24,24,24,24	0
58	MG	2A	3444	1/1	0.98	0.09	37,37,37,37	0
58	MG	1a	1611	1/1	0.98	0.07	16,16,16,16	0
58	MG	1A	3018	1/1	0.98	0.12	20,20,20,20	0
58	MG	2A	3447	1/1	0.98	0.08	42,42,42,42	0
58	MG	1A	3432	1/1	0.98	0.04	35,35,35,35	0
58	MG	1B	205	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3041	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3799	1/1	0.98	0.07	41,41,41,41	0
58	MG	1A	3136	1/1	0.98	0.18	21,21,21,21	0
58	MG	1a	1618	1/1	0.98	0.06	27,27,27,27	0
58	MG	1B	209	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3801	1/1	0.98	0.07	40,40,40,40	0
58	MG	1A	3953	1/1	0.98	0.03	42,42,42,42	0
58	MG	1A	3194	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3137	1/1	0.98	0.03	32,32,32,32	0
58	MG	1A	3098	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3025	1/1	0.98	0.10	22,22,22,22	0
58	MG	1A	3672	1/1	0.98	0.08	35,35,35,35	0
58	MG	1B	217	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3545	1/1	0.98	0.08	19,19,19,19	0
58	MG	1A	3014	1/1	0.98	0.04	19,19,19,19	0
58	MG	2A	3466	1/1	0.98	0.08	15,15,15,15	0
58	MG	1B	220	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3547	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3008	1/1	0.98	0.06	21,21,21,21	0
58	MG	2A	3233	1/1	0.98	0.16	34,34,34,34	0
58	MG	1A	3071	1/1	0.98	0.03	9,9,9,9	0
58	MG	1A	3812	1/1	0.98	0.05	14,14,14,14	0
58	MG	1A	3813	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3814	1/1	0.98	0.04	18,18,18,18	0
58	MG	1a	1637	1/1	0.98	0.07	38,38,38,38	0
58	MG	2A	3735	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3679	1/1	0.98	0.05	13,13,13,13	0
58	MG	1A	3028	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3270	1/1	0.98	0.14	27,27,27,27	0
58	MG	2A	3009	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3243	1/1	0.98	0.06	39,39,39,39	0
58	MG	2A	3010	1/1	0.98	0.09	38,38,38,38	0
58	MG	1A	3202	1/1	0.98	0.09	21,21,21,21	0
58	MG	1A	3351	1/1	0.98	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3744	1/1	0.98	0.08	23,23,23,23	0
58	MG	1B	232	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3104	1/1	0.98	0.09	23,23,23,23	0
58	MG	1A	3075	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3823	1/1	0.98	0.04	15,15,15,15	0
58	MG	1A	3975	1/1	0.98	0.08	36,36,36,36	0
58	MG	1A	3448	1/1	0.98	0.16	21,21,21,21	0
58	MG	1D	301	1/1	0.98	0.06	20,20,20,20	0
58	MG	1A	3825	1/1	0.98	0.14	24,24,24,24	0
58	MG	2A	3021	1/1	0.98	0.05	16,16,16,16	0
58	MG	1a	1652	1/1	0.98	0.08	33,33,33,33	0
58	MG	1a	1653	1/1	0.98	0.04	39,39,39,39	0
58	MG	1D	303	1/1	0.98	0.05	32,32,32,32	0
58	MG	1a	1655	1/1	0.98	0.05	38,38,38,38	0
58	MG	2A	3026	1/1	0.98	0.06	33,33,33,33	0
58	MG	1D	304	1/1	0.98	0.06	14,14,14,14	0
58	MG	1D	305	1/1	0.98	0.05	25,25,25,25	0
58	MG	1D	307	1/1	0.98	0.08	26,26,26,26	0
58	MG	1D	309	1/1	0.98	0.04	31,31,31,31	0
58	MG	2A	3503	1/1	0.98	0.14	42,42,42,42	0
58	MG	1D	310	1/1	0.98	0.12	20,20,20,20	0
58	MG	2A	3505	1/1	0.98	0.06	55,55,55,55	0
58	MG	1A	3449	1/1	0.98	0.12	27,27,27,27	0
58	MG	1A	3021	1/1	0.98	0.07	12,12,12,12	0
58	MG	1A	3828	1/1	0.98	0.03	14,14,14,14	0
58	MG	1E	302	1/1	0.98	0.08	32,32,32,32	0
58	MG	1E	304	1/1	0.98	0.05	20,20,20,20	0
58	MG	1A	3830	1/1	0.98	0.06	21,21,21,21	0
58	MG	1A	3206	1/1	0.98	0.10	12,12,12,12	0
58	MG	1E	307	1/1	0.98	0.04	25,25,25,25	0
58	MG	2A	3041	1/1	0.98	0.08	48,48,48,48	0
58	MG	1E	308	1/1	0.98	0.06	35,35,35,35	0
58	MG	1A	3148	1/1	0.98	0.07	24,24,24,24	0
58	MG	2A	3777	1/1	0.98	0.11	38,38,38,38	0
58	MG	1A	3453	1/1	0.98	0.07	25,25,25,25	0
58	MG	2A	3779	1/1	0.98	0.03	38,38,38,38	0
58	MG	1A	3834	1/1	0.98	0.04	20,20,20,20	0
58	MG	2a	1693	1/1	0.98	0.09	44,44,44,44	0
58	MG	1a	1673	1/1	0.98	0.07	39,39,39,39	0
58	MG	1A	3149	1/1	0.98	0.15	20,20,20,20	0
58	MG	2a	1696	1/1	0.98	0.09	40,40,40,40	0
58	MG	2A	3521	1/1	0.98	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1F	301	1/1	0.98	0.05	25,25,25,25	0
58	MG	1A	3358	1/1	0.98	0.05	34,34,34,34	0
58	MG	2a	1700	1/1	0.98	0.11	26,26,26,26	0
58	MG	1F	304	1/1	0.98	0.09	22,22,22,22	0
58	MG	1A	3107	1/1	0.98	0.07	29,29,29,29	0
58	MG	1A	3109	1/1	0.98	0.09	28,28,28,28	0
58	MG	1A	3030	1/1	0.98	0.20	18,18,18,18	0
58	MG	2A	3528	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3281	1/1	0.98	0.06	14,14,14,14	0
58	MG	1A	3574	1/1	0.98	0.13	24,24,24,24	0
58	MG	1A	3283	1/1	0.98	0.24	28,28,28,28	0
58	MG	1A	3994	1/1	0.98	0.05	24,24,24,24	0
58	MG	1A	3213	1/1	0.98	0.09	33,33,33,33	0
58	MG	1A	3286	1/1	0.98	0.20	26,26,26,26	0
58	MG	2A	3061	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3366	1/1	0.98	0.16	24,24,24,24	0
58	MG	1A	3579	1/1	0.98	0.15	40,40,40,40	0
58	MG	2A	3538	1/1	0.98	0.08	38,38,38,38	0
58	MG	1A	3287	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3288	1/1	0.98	0.07	25,25,25,25	0
58	MG	1G	205	1/1	0.98	0.09	41,41,41,41	0
58	MG	1A	3583	1/1	0.98	0.40	32,32,32,32	0
58	MG	1A	3289	1/1	0.98	0.07	31,31,31,31	0
58	MG	1A	3371	1/1	0.98	0.04	28,28,28,28	0
58	MG	2A	3545	1/1	0.98	0.05	36,36,36,36	0
58	MG	1N	203	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3852	1/1	0.98	0.06	41,41,41,41	0
58	MG	1A	3468	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3290	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3291	1/1	0.98	0.07	41,41,41,41	0
58	MG	2A	3075	1/1	0.98	0.09	38,38,38,38	0
58	MG	1A	3714	1/1	0.98	0.04	26,26,26,26	0
58	MG	2A	3553	1/1	0.98	0.08	39,39,39,39	0
58	MG	1A	3214	1/1	0.98	0.12	22,22,22,22	0
58	MG	1A	3153	1/1	0.98	0.10	27,27,27,27	0
58	MG	1A	3717	1/1	0.98	0.03	28,28,28,28	0
58	MG	2A	3557	1/1	0.98	0.09	29,29,29,29	0
58	MG	2A	3558	1/1	0.98	0.10	44,44,44,44	0
58	MG	1P	202	1/1	0.98	0.06	20,20,20,20	0
58	MG	1P	203	1/1	0.98	0.14	24,24,24,24	0
58	MG	1A	3111	1/1	0.98	0.20	21,21,21,21	0
58	MG	2A	3084	1/1	0.98	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
58	MG	1Q	201	1/1	0.98	0.22	33,33,33,33	0
58	MG	1A	3377	1/1	0.98	0.11	34,34,34,34	0
58	MG	2A	3087	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3155	1/1	0.98	0.07	24,24,24,24	0
58	MG	1Q	204	1/1	0.98	0.06	35,35,35,35	0
58	MG	1A	3219	1/1	0.98	0.11	25,25,25,25	0
58	MG	1A	3112	1/1	0.98	0.04	29,29,29,29	0
58	MG	2A	3324	1/1	0.98	0.05	33,33,33,33	0
58	MG	2A	3093	1/1	0.98	0.09	37,37,37,37	0
58	MG	1A	3598	1/1	0.98	0.11	17,17,17,17	0
58	MG	1A	3724	1/1	0.98	0.04	18,18,18,18	0
58	MG	2A	3837	1/1	0.98	0.05	41,41,41,41	0
58	MG	2A	3838	1/1	0.98	0.05	53,53,53,53	0
58	MG	1A	3032	1/1	0.98	0.07	17,17,17,17	0
58	MG	1A	3081	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3870	1/1	0.98	0.09	43,43,43,43	0
58	MG	2A	3842	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3383	1/1	0.98	0.07	19,19,19,19	0
58	MG	2A	3332	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3159	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3482	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3874	1/1	0.98	0.08	20,20,20,20	0
58	MG	1A	3484	1/1	0.98	0.05	27,27,27,27	0
58	MG	2a	1764	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3485	1/1	0.98	0.13	40,40,40,40	0
58	MG	2A	3850	1/1	0.98	0.07	37,37,37,37	0
58	MG	1A	3033	1/1	0.98	0.19	25,25,25,25	0
58	MG	1A	3386	1/1	0.98	0.07	28,28,28,28	0
58	MG	2A	3853	1/1	0.98	0.04	47,47,47,47	0
58	MG	1A	3387	1/1	0.98	0.06	46,46,46,46	0
58	MG	2a	1771	1/1	0.98	0.11	45,45,45,45	0
58	MG	1A	3736	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3225	1/1	0.98	0.08	27,27,27,27	0
58	MG	2a	1774	1/1	0.98	0.05	53,53,53,53	0
58	MG	1A	4034	1/1	0.98	0.03	13,13,13,13	0
58	MG	2a	1776	1/1	0.98	0.04	39,39,39,39	0
58	MG	2A	3111	1/1	0.98	0.10	35,35,35,35	0
58	MG	2A	3592	1/1	0.98	0.07	32,32,32,32	0
58	MG	1U	206	1/1	0.98	0.18	30,30,30,30	0
58	MG	1U	207	1/1	0.98	0.16	27,27,27,27	0
58	MG	1U	208	1/1	0.98	0.11	28,28,28,28	0
58	MG	1a	1735	1/1	0.98	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3053	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3883	1/1	0.98	0.09	26,26,26,26	0
58	MG	2a	1785	1/1	0.98	0.09	42,42,42,42	0
58	MG	2A	3119	1/1	0.98	0.04	26,26,26,26	0
58	MG	2A	3601	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	4037	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3390	1/1	0.98	0.14	21,21,21,21	0
58	MG	1A	3054	1/1	0.98	0.08	41,41,41,41	0
58	MG	1A	3307	1/1	0.98	0.06	27,27,27,27	0
58	MG	1A	3163	1/1	0.98	0.11	25,25,25,25	0
58	MG	1A	3743	1/1	0.98	0.04	45,45,45,45	0
58	MG	1A	3230	1/1	0.98	0.08	25,25,25,25	0
58	MG	1A	3085	1/1	0.98	0.17	25,25,25,25	0
58	MG	1W	204	1/1	0.98	0.07	22,22,22,22	0
58	MG	1A	3121	1/1	0.98	0.09	27,27,27,27	0
58	MG	2A	3362	1/1	0.98	0.09	48,48,48,48	0
58	MG	2a	1799	1/1	0.98	0.07	46,46,46,46	0
58	MG	1A	3397	1/1	0.98	0.06	45,45,45,45	0
58	MG	2A	3614	1/1	0.98	0.07	49,49,49,49	0
58	MG	1A	3893	1/1	0.98	0.06	26,26,26,26	0
58	MG	1X	101	1/1	0.98	0.16	28,28,28,28	0
58	MG	1a	1751	1/1	0.98	0.17	34,34,34,34	0
58	MG	1a	1752	1/1	0.98	0.04	41,41,41,41	0
58	MG	1A	3619	1/1	0.98	0.09	35,35,35,35	0
58	MG	1A	3055	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3169	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3138	1/1	0.98	0.04	29,29,29,29	0
58	MG	1X	105	1/1	0.98	0.07	35,35,35,35	0
58	MG	1A	3400	1/1	0.98	0.08	22,22,22,22	0
58	MG	1A	3402	1/1	0.98	0.19	25,25,25,25	0
58	MG	1A	3503	1/1	0.98	0.15	26,26,26,26	0
58	MG	2A	3376	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3625	1/1	0.98	0.09	27,27,27,27	0
58	MG	1Y	204	1/1	0.98	0.17	38,38,38,38	0
58	MG	2D	305	1/1	0.98	0.03	21,21,21,21	0
58	MG	1A	3504	1/1	0.98	0.07	24,24,24,24	0
58	MG	1a	1765	1/1	0.98	0.05	44,44,44,44	0
58	MG	1A	3170	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3171	1/1	0.98	0.04	22,22,22,22	0
58	MG	1A	3237	1/1	0.98	0.16	33,33,33,33	0
58	MG	1A	3087	1/1	0.98	0.07	20,20,20,20	0
58	MG	2E	304	1/1	0.98	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3034	1/1	0.98	0.13	21,21,21,21	0
58	MG	10	106	1/1	0.98	0.05	31,31,31,31	0
58	MG	2A	3153	1/1	0.98	0.08	37,37,37,37	0
58	MG	1A	3408	1/1	0.98	0.05	36,36,36,36	0
58	MG	1A	3409	1/1	0.98	0.06	35,35,35,35	0
58	MG	1A	4063	1/1	0.98	0.03	14,14,14,14	0
58	MG	2A	3157	1/1	0.98	0.06	46,46,46,46	0
58	MG	1A	3035	1/1	0.98	0.04	35,35,35,35	0
58	MG	1A	3636	1/1	0.98	0.04	23,23,23,23	0
58	MG	1A	4066	1/1	0.98	0.06	32,32,32,32	0
58	MG	1a	1778	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3090	1/1	0.98	0.12	34,34,34,34	0
58	MG	2d	302	1/1	0.98	0.04	52,52,52,52	0
58	MG	1A	3321	1/1	0.98	0.19	22,22,22,22	0
58	MG	2f	201	1/1	0.98	0.11	39,39,39,39	0
58	MG	1A	3515	1/1	0.98	0.03	37,37,37,37	0
58	MG	1A	4070	1/1	0.98	0.05	19,19,19,19	0
58	MG	1a	1783	1/1	0.98	0.04	54,54,54,54	0
58	MG	1A	3516	1/1	0.98	0.09	44,44,44,44	0
58	MG	2A	3654	1/1	0.98	0.16	35,35,35,35	0
58	MG	1A	3242	1/1	0.98	0.07	16,16,16,16	0
58	MG	13	101	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3657	1/1	0.98	0.13	53,53,53,53	0
58	MG	1A	3177	1/1	0.98	0.20	24,24,24,24	0
58	MG	1a	1790	1/1	0.98	0.04	43,43,43,43	0
58	MG	13	103	1/1	0.98	0.06	35,35,35,35	0
58	MG	1A	3519	1/1	0.98	0.11	21,21,21,21	0
58	MG	1A	4075	1/1	0.98	0.06	24,24,24,24	0
58	MG	2W	202	1/1	0.98	0.12	31,31,31,31	0
58	MG	2r	101	1/1	0.98	0.05	44,44,44,44	0
58	MG	1A	3921	1/1	0.98	0.03	22,22,22,22	0
58	MG	2A	3664	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3244	1/1	0.98	0.10	21,21,21,21	0
58	MG	2X	102	1/1	0.98	0.03	47,47,47,47	0
58	MG	2X	103	1/1	0.98	0.10	40,40,40,40	0
58	MG	15	104	1/1	0.98	0.16	24,24,24,24	0
58	MG	1A	3521	1/1	0.98	0.14	19,19,19,19	0
58	MG	15	106	1/1	0.98	0.15	39,39,39,39	0
58	MG	1A	3416	1/1	0.98	0.15	29,29,29,29	0
58	MG	1A	3925	1/1	0.98	0.07	40,40,40,40	0
58	MG	2A	3184	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3179	1/1	0.98	0.03	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3674	1/1	0.98	0.04	36,36,36,36	0
58	MG	17	102	1/1	0.98	0.07	17,17,17,17	0
58	MG	1A	4082	1/1	0.98	0.06	18,18,18,18	0
58	MG	25	104	1/1	0.98	0.05	49,49,49,49	0
58	MG	2A	3188	1/1	0.98	0.04	32,32,32,32	0
59	K	1A	3568	1/1	0.98	0.09	37,37,37,37	0
59	K	2A	3465	1/1	0.98	0.05	50,50,50,50	0
60	ZN	14	102	1/1	0.98	0.06	81,81,81,81	0
60	ZN	1n	103	1/1	0.98	0.03	51,51,51,51	0
58	MG	1a	1804	1/1	0.98	0.05	58,58,58,58	0
58	MG	2A	3422	1/1	0.98	0.07	32,32,32,32	0
60	ZN	25	106	1/1	0.98	0.04	73,73,73,73	0
60	ZN	29	102	1/1	0.98	0.04	56,56,56,56	0
58	MG	1A	3180	1/1	0.98	0.03	20,20,20,20	0
58	MG	1A	3114	1/1	0.99	0.09	20,20,20,20	0
58	MG	1A	3299	1/1	0.99	0.07	27,27,27,27	0
58	MG	2A	3640	1/1	0.99	0.12	33,33,33,33	0
58	MG	1A	3207	1/1	0.99	0.04	24,24,24,24	0
58	MG	1A	3079	1/1	0.99	0.08	19,19,19,19	0
58	MG	1A	3675	1/1	0.99	0.02	15,15,15,15	0
58	MG	1A	3729	1/1	0.99	0.08	15,15,15,15	0
58	MG	1F	309	1/1	0.99	0.11	19,19,19,19	0
58	MG	1A	3031	1/1	0.99	0.13	21,21,21,21	0
58	MG	1A	3303	1/1	0.99	0.04	18,18,18,18	0
58	MG	1A	3580	1/1	0.99	0.07	30,30,30,30	0
58	MG	1A	3269	1/1	0.99	0.10	24,24,24,24	0
58	MG	1A	3680	1/1	0.99	0.05	20,20,20,20	0
58	MG	1Y	205	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3038	1/1	0.99	0.09	16,16,16,16	0
58	MG	1a	1789	1/1	0.99	0.02	34,34,34,34	0
58	MG	1A	3630	1/1	0.99	0.05	20,20,20,20	0
58	MG	1A	3683	1/1	0.99	0.08	20,20,20,20	0
58	MG	2A	3471	1/1	0.99	0.12	30,30,30,30	0
58	MG	1A	3916	1/1	0.99	0.05	30,30,30,30	0
58	MG	1A	3065	1/1	0.99	0.10	30,30,30,30	0
58	MG	10	104	1/1	0.99	0.10	29,29,29,29	0
58	MG	1A	3046	1/1	0.99	0.05	23,23,23,23	0
58	MG	2A	3567	1/1	0.99	0.06	36,36,36,36	0
58	MG	2A	3116	1/1	0.99	0.10	41,41,41,41	0
58	MG	1A	3120	1/1	0.99	0.09	28,28,28,28	0
58	MG	1A	3920	1/1	0.99	0.04	18,18,18,18	0
58	MG	1A	3056	1/1	0.99	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3068	1/1	0.99	0.04	22,22,22,22	0
58	MG	1a	1718	1/1	0.99	0.08	28,28,28,28	0
58	MG	1A	3588	1/1	0.99	0.05	21,21,21,21	0
58	MG	1A	3164	1/1	0.99	0.03	17,17,17,17	0
58	MG	1A	3190	1/1	0.99	0.12	27,27,27,27	0
58	MG	2A	3671	1/1	0.99	0.03	41,41,41,41	0
58	MG	2A	3303	1/1	0.99	0.15	34,34,34,34	0
58	MG	1A	3639	1/1	0.99	0.03	21,21,21,21	0
58	MG	2A	3039	1/1	0.99	0.03	16,16,16,16	0
58	MG	1A	3348	1/1	0.99	0.20	26,26,26,26	0
58	MG	1A	3865	1/1	0.99	0.07	31,31,31,31	0
58	MG	1A	3748	1/1	0.99	0.04	41,41,41,41	0
58	MG	2A	3678	1/1	0.99	0.05	37,37,37,37	0
58	MG	1P	201	1/1	0.99	0.05	19,19,19,19	0
58	MG	1a	1809	1/1	0.99	0.10	34,34,34,34	0
58	MG	1A	3592	1/1	0.99	0.05	37,37,37,37	0
58	MG	1A	3750	1/1	0.99	0.03	13,13,13,13	0
58	MG	1a	1651	1/1	0.99	0.06	36,36,36,36	0
58	MG	1A	3218	1/1	0.99	0.11	28,28,28,28	0
58	MG	1A	3165	1/1	0.99	0.06	14,14,14,14	0
58	MG	1A	3023	1/1	0.99	0.04	9,9,9,9	0
58	MG	1A	3070	1/1	0.99	0.09	18,18,18,18	0
58	MG	1A	3428	1/1	0.99	0.07	21,21,21,21	0
58	MG	1A	3282	1/1	0.99	0.09	22,22,22,22	0
58	MG	2a	1731	1/1	0.99	0.07	52,52,52,52	0
58	MG	1A	3251	1/1	0.99	0.08	25,25,25,25	0
58	MG	1A	3003	1/1	0.99	0.08	19,19,19,19	0
58	MG	1A	3940	1/1	0.99	0.03	23,23,23,23	0
58	MG	2A	3057	1/1	0.99	0.09	45,45,45,45	0
58	MG	2A	3598	1/1	0.99	0.08	32,32,32,32	0
58	MG	2A	3695	1/1	0.99	0.06	49,49,49,49	0
58	MG	1A	3285	1/1	0.99	0.14	23,23,23,23	0
58	MG	1A	3818	1/1	0.99	0.05	23,23,23,23	0
58	MG	1R	203	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3072	1/1	0.99	0.13	27,27,27,27	0
58	MG	1A	3147	1/1	0.99	0.04	29,29,29,29	0
58	MG	1A	3073	1/1	0.99	0.04	15,15,15,15	0
58	MG	1A	3108	1/1	0.99	0.03	19,19,19,19	0
58	MG	1A	3009	1/1	0.99	0.05	15,15,15,15	0
58	MG	1A	3558	1/1	0.99	0.05	18,18,18,18	0
58	MG	1D	306	1/1	0.99	0.04	24,24,24,24	0
58	MG	1A	3228	1/1	0.99	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1D	308	1/1	0.99	0.07	34,34,34,34	0
58	MG	1A	3768	1/1	0.99	0.04	29,29,29,29	0
58	MG	1A	3560	1/1	0.99	0.08	23,23,23,23	0
58	MG	1A	3174	1/1	0.99	0.11	9,9,9,9	0
58	MG	2E	309	1/1	0.99	0.06	23,23,23,23	0
58	MG	1A	3829	1/1	0.99	0.03	25,25,25,25	0
58	MG	1A	3401	1/1	0.99	0.05	19,19,19,19	0
58	MG	1a	1756	1/1	0.99	0.08	45,45,45,45	0
58	MG	2A	3714	1/1	0.99	0.05	20,20,20,20	0
58	MG	2A	3076	1/1	0.99	0.12	29,29,29,29	0
58	MG	1A	3010	1/1	0.99	0.07	25,25,25,25	0
58	MG	1E	303	1/1	0.99	0.13	21,21,21,21	0
58	MG	1A	3051	1/1	0.99	0.08	17,17,17,17	0
58	MG	1A	3043	1/1	0.99	0.13	24,24,24,24	0
58	MG	1A	3664	1/1	0.99	0.05	32,32,32,32	0
58	MG	1a	1762	1/1	0.99	0.03	34,34,34,34	0
58	MG	1V	203	1/1	0.99	0.08	24,24,24,24	0
58	MG	1A	3483	1/1	0.99	0.04	32,32,32,32	0
58	MG	1A	3896	1/1	0.99	0.04	37,37,37,37	0
58	MG	1A	3178	1/1	0.99	0.13	18,18,18,18	0
58	MG	1E	310	1/1	0.99	0.08	18,18,18,18	0
58	MG	1a	1688	1/1	0.99	0.15	31,31,31,31	0
58	MG	1A	3078	1/1	0.99	0.03	23,23,23,23	0
58	MG	2A	3177	1/1	0.99	0.05	28,28,28,28	0
60	ZN	1Y	206	1/1	0.99	0.02	52,52,52,52	0
58	MG	1A	3571	1/1	0.99	0.07	19,19,19,19	0
60	ZN	15	108	1/1	0.99	0.04	60,60,60,60	0
60	ZN	16	102	1/1	0.99	0.03	37,37,37,37	0
58	MG	1A	3572	1/1	0.99	0.03	11,11,11,11	0
58	MG	2A	3180	1/1	0.99	0.06	45,45,45,45	0
58	MG	2A	3092	1/1	0.99	0.03	27,27,27,27	0
58	MG	1A	3369	1/1	0.99	0.12	28,28,28,28	0
60	ZN	26	102	1/1	0.99	0.04	52,52,52,52	0
58	MG	1F	302	1/1	0.99	0.12	20,20,20,20	0
58	MG	2A	3834	1/1	0.99	0.04	25,25,25,25	0
61	SF4	1d	302	8/8	0.99	0.05	51,52,59,61	0
61	SF4	2d	303	8/8	0.99	0.04	52,61,73,73	0
58	MG	1A	3037	1/1	1.00	0.07	16,16,16,16	0
58	MG	1a	1788	1/1	1.00	0.01	37,37,37,37	0
58	MG	1A	3561	1/1	1.00	0.12	25,25,25,25	0
58	MG	1A	3007	1/1	1.00	0.06	30,30,30,30	0
58	MG	1A	3535	1/1	1.00	0.06	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4006	1/1	1.00	0.03	25,25,25,25	0
60	ZN	19	102	1/1	1.00	0.04	36,36,36,36	0
58	MG	1A	3761	1/1	1.00	0.08	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.