



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 01:30 AM UTC

PDB ID : 9O3H / pdb_00009o3h
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with macrolide erythromycin, mRNA, aminoacylated A-site Lys-tRNA^{Lys}, P-site fMRC-peptidyl-tRNA^{Met}, and deacylated E-site tRNA^{Lys} at 2.65Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Kruglov, A.A.; Paranjpe, M.N.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2025-04-07
Resolution : 2.65 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

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

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

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

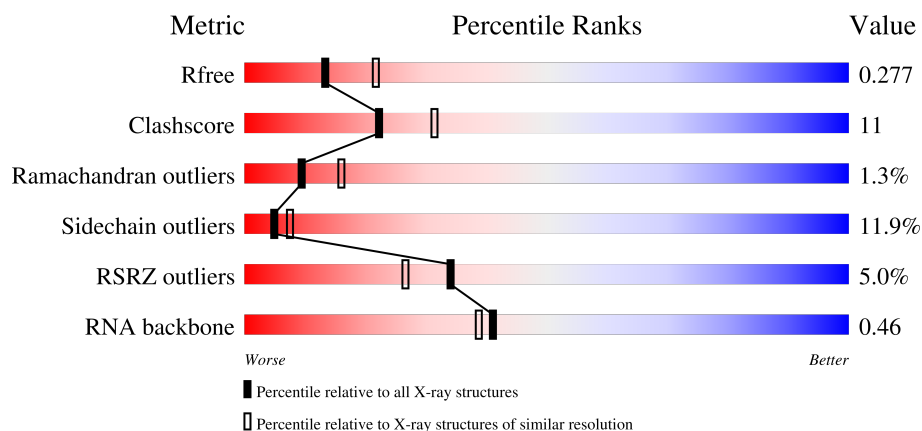
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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	3% 59% 32% 7% •
1	2A	2915	3% 53% 36% 8% •

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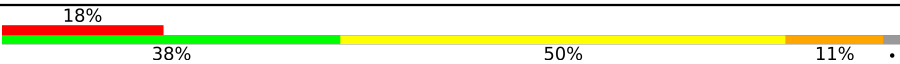
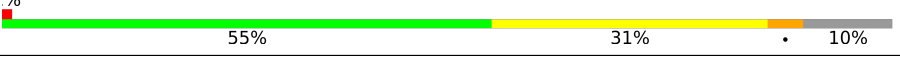
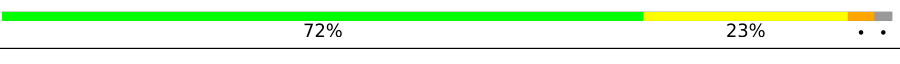
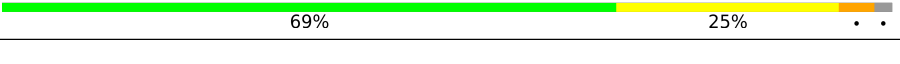
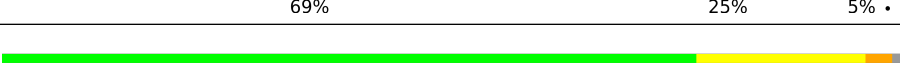
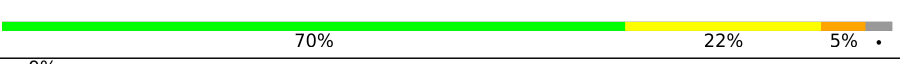
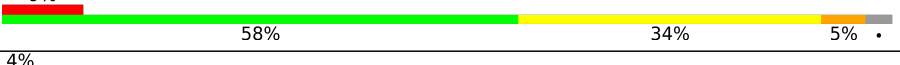
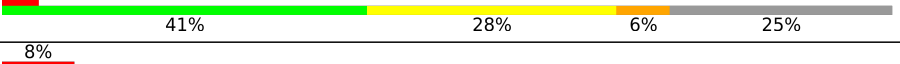
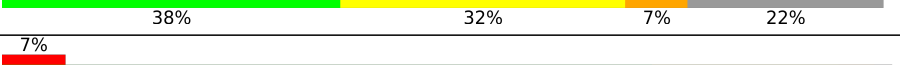
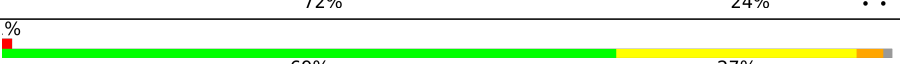
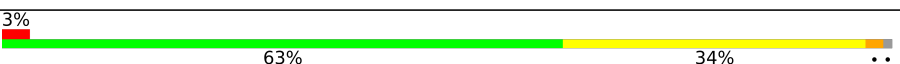
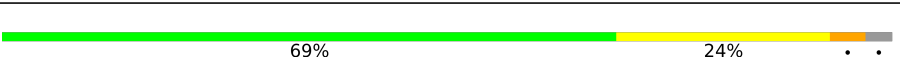
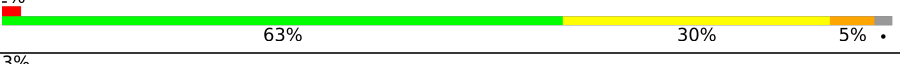
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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

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

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

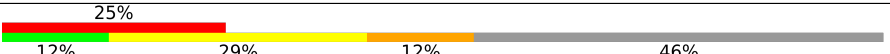
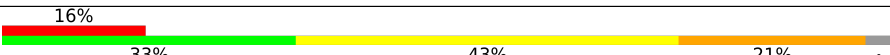
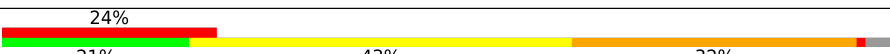
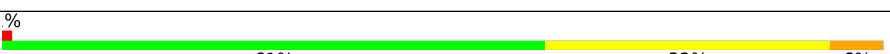
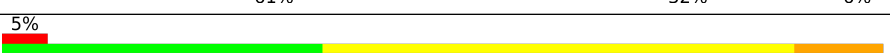
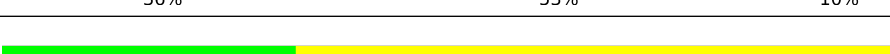
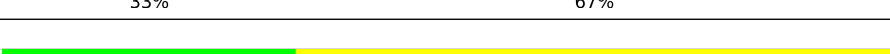
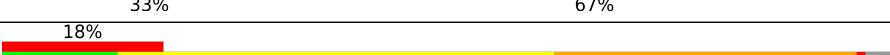
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Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49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

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
62	SF4	2d	303	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 299863 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-LYS-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			283	128	59	83	13			
53	2v	13	Total	C	N	O	P	0	0	0
			283	128	59	83	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Lys-tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			
54	2w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			

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

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

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

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

- Molecule 57 is a RNA chain called E-site Deacylated tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			
57	2y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1102	Total	Mg	0	0
			1102	1102		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	36	Total 36	Mg 36	0	0
58	1D	14	Total 14	Mg 14	0	0
58	1E	14	Total 14	Mg 14	0	0
58	1F	12	Total 12	Mg 12	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	4	Total 4	Mg 4	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	3	Total 3	Mg 3	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	11	Total 11	Mg 11	0	0
58	1V	7	Total 7	Mg 7	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	5	Total 5	Mg 5	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	3	Total 3	Mg 3	0	0
58	10	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	6	Total 6	Mg 6	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	6	Total 6	Mg 6	0	0
58	15	10	Total 10	Mg 10	0	0
58	16	1	Total 1	Mg 1	0	0
58	17	5	Total 5	Mg 5	0	0
58	18	7	Total 7	Mg 7	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	215	Total 215	Mg 215	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	1	Total 1	Mg 1	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	2	Total 2	Mg 2	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1s	1	Total 1	Mg 1	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1v	1	Total 1	Mg 1	0	0
58	1w	6	Total 6	Mg 6	0	0
58	1x	11	Total 11	Mg 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2A	858	Total 858	Mg 858	0	0
58	2B	20	Total 20	Mg 20	0	0
58	2D	9	Total 9	Mg 9	0	0
58	2E	7	Total 7	Mg 7	0	0
58	2F	6	Total 6	Mg 6	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2O	2	Total 2	Mg 2	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	2	Total 2	Mg 2	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	2	Total 2	Mg 2	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	3	Total 3	Mg 3	0	0
58	23	4	Total 4	Mg 4	0	0
58	25	6	Total 6	Mg 6	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	4	Total 4 Mg 4	0	0
58	2a	230	Total 230 Mg 230	0	0
58	2d	2	Total 2 Mg 2	0	0
58	2e	2	Total 2 Mg 2	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	2	Total 2 Mg 2	0	0
58	2k	1	Total 1 Mg 1	0	0
58	2l	6	Total 6 Mg 6	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	2v	5	Total 5 Mg 5	0	0
58	2w	2	Total 2 Mg 2	0	0
58	2x	5	Total 5 Mg 5	0	0
58	2y	1	Total 1 Mg 1	0	0

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

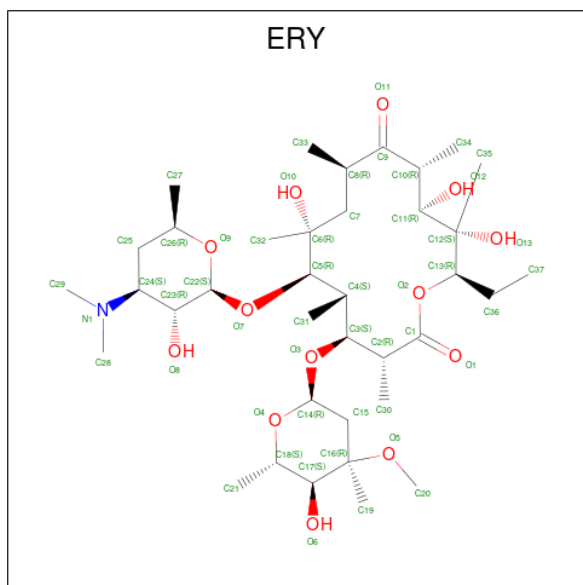
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total 1 K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2x	1	Total K 1 1	0	0

- Molecule 60 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1	Total C N O 51 37 1 13	0	0
60	2A	1	Total C N O 51 37 1 13	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

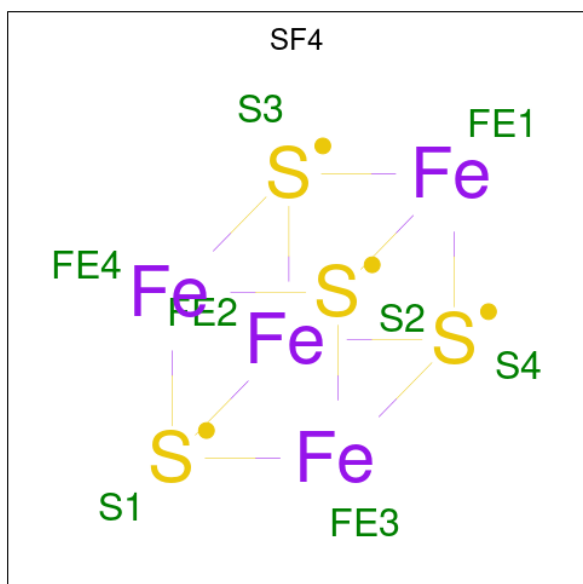
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Y	1	Total Zn 1 1	0	0
61	14	1	Total Zn 1 1	0	0
61	15	1	Total Zn 1 1	0	0
61	16	1	Total Zn 1 1	0	0
61	19	1	Total Zn 1 1	0	0
61	1n	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2Y	1	Total	Zn	0	0
			1	1		
61	24	1	Total	Zn	0	0
			1	1		
61	25	1	Total	Zn	0	0
			1	1		
61	26	1	Total	Zn	0	0
			1	1		
61	29	1	Total	Zn	0	0
			1	1		
61	2n	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	1d	1	Total	Fe	S	0	0
			8	4	4		
62	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1896	Total	O	0	0
			1896	1896		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1B	61	Total 61	O 61	0	0
63	1D	25	Total 25	O 25	0	0
63	1E	30	Total 30	O 30	0	0
63	1F	17	Total 17	O 17	0	0
63	1G	3	Total 3	O 3	0	0
63	1H	2	Total 2	O 2	0	0
63	1N	4	Total 4	O 4	0	0
63	1O	5	Total 5	O 5	0	0
63	1P	25	Total 25	O 25	0	0
63	1Q	7	Total 7	O 7	0	0
63	1R	16	Total 16	O 16	0	0
63	1S	3	Total 3	O 3	0	0
63	1T	5	Total 5	O 5	0	0
63	1U	14	Total 14	O 14	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	6	Total 6	O 6	0	0
63	1X	8	Total 8	O 8	0	0
63	1Y	5	Total 5	O 5	0	0
63	1Z	1	Total 1	O 1	0	0
63	10	13	Total 13	O 13	0	0
63	11	9	Total 9	O 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	12	3	Total 3	O 3	0	0
63	13	6	Total 6	O 6	0	0
63	14	1	Total 1	O 1	0	0
63	15	5	Total 5	O 5	0	0
63	16	3	Total 3	O 3	0	0
63	17	8	Total 8	O 8	0	0
63	18	10	Total 10	O 10	0	0
63	1a	305	Total 305	O 305	0	0
63	1b	1	Total 1	O 1	0	0
63	1e	1	Total 1	O 1	0	0
63	1f	1	Total 1	O 1	0	0
63	1i	1	Total 1	O 1	0	0
63	1l	4	Total 4	O 4	0	0
63	1q	2	Total 2	O 2	0	0
63	1u	1	Total 1	O 1	0	0
63	1v	5	Total 5	O 5	0	0
63	1w	6	Total 6	O 6	0	0
63	1x	5	Total 5	O 5	0	0
63	1y	1	Total 1	O 1	0	0
63	2A	992	Total 992	O 992	0	0
63	2B	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2D	20	Total 20	O 20	0	0
63	2E	13	Total 13	O 13	0	0
63	2F	14	Total 14	O 14	0	0
63	2N	1	Total 1	O 1	0	0
63	2O	2	Total 2	O 2	0	0
63	2P	7	Total 7	O 7	0	0
63	2Q	1	Total 1	O 1	0	0
63	2R	3	Total 3	O 3	0	0
63	2T	5	Total 5	O 5	0	0
63	2U	3	Total 3	O 3	0	0
63	2W	2	Total 2	O 2	0	0
63	2X	2	Total 2	O 2	0	0
63	2Y	1	Total 1	O 1	0	0
63	2Z	1	Total 1	O 1	0	0
63	20	2	Total 2	O 2	0	0
63	21	6	Total 6	O 6	0	0
63	25	1	Total 1	O 1	0	0
63	27	3	Total 3	O 3	0	0
63	28	2	Total 2	O 2	0	0
63	29	1	Total 1	O 1	0	0
63	2a	172	Total 172	O 172	0	0

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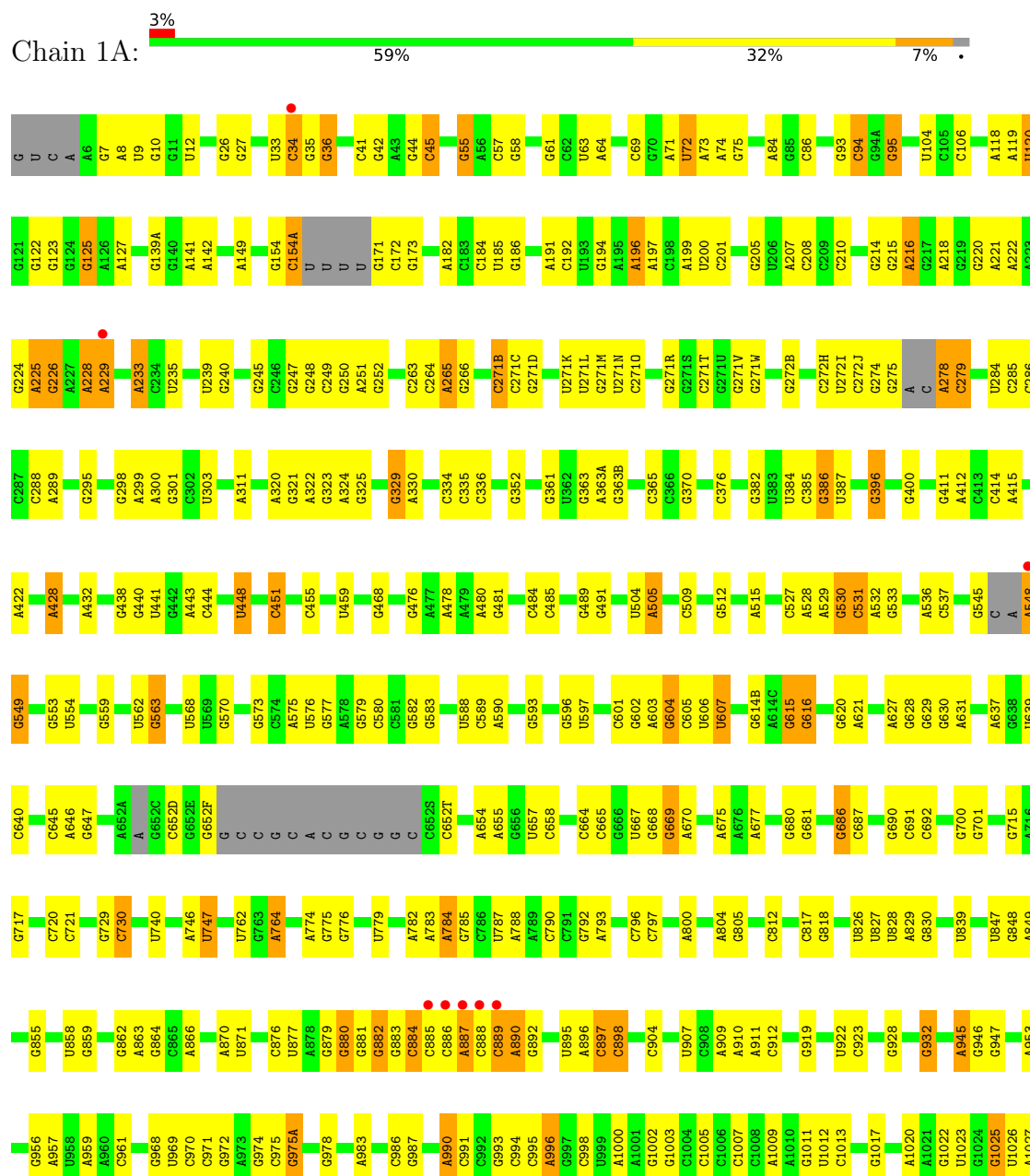
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2e	1	Total	O	0	0
			1	1		
63	2g	1	Total	O	0	0
			1	1		
63	2j	2	Total	O	0	0
			2	2		
63	2l	3	Total	O	0	0
			3	3		
63	2p	3	Total	O	0	0
			3	3		
63	2r	1	Total	O	0	0
			1	1		
63	2t	1	Total	O	0	0
			1	1		
63	2v	2	Total	O	0	0
			2	2		
63	2w	1	Total	O	0	0
			1	1		
63	2x	2	Total	O	0	0
			2	2		

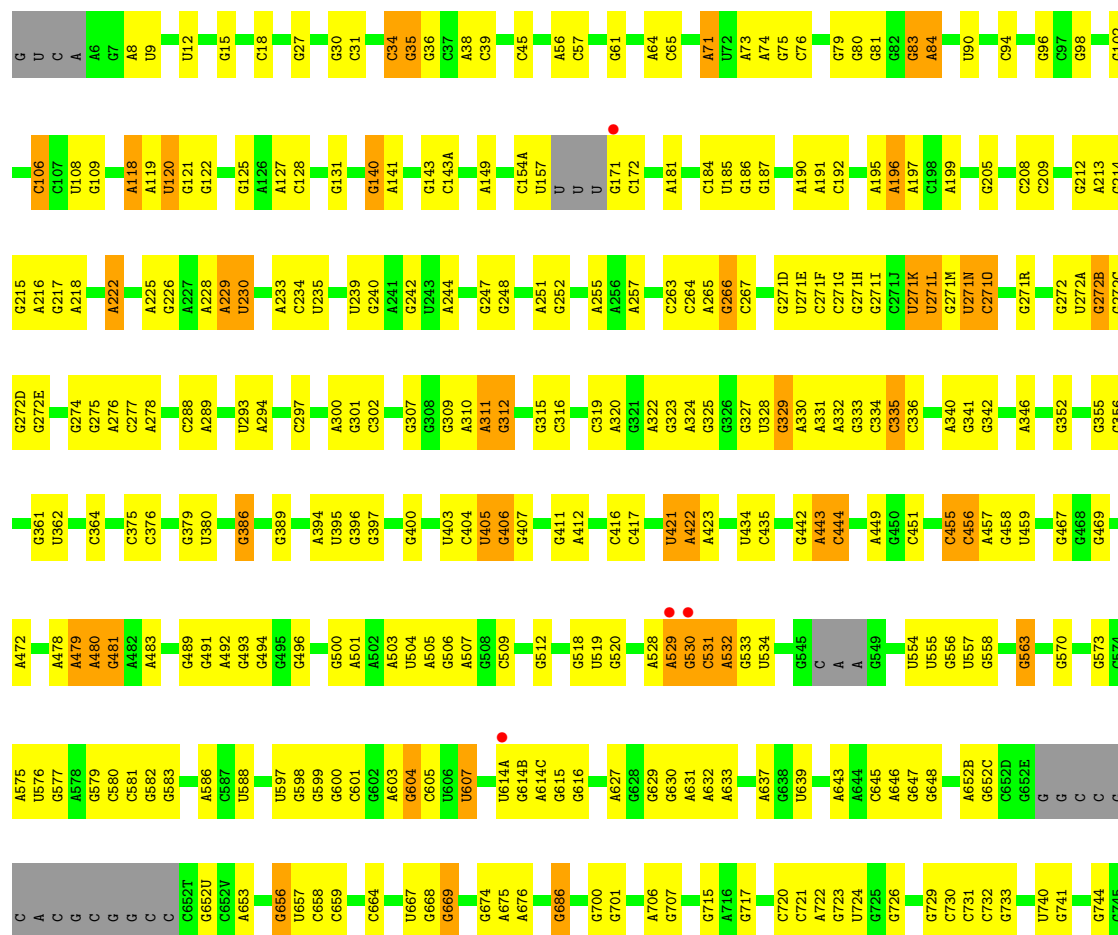
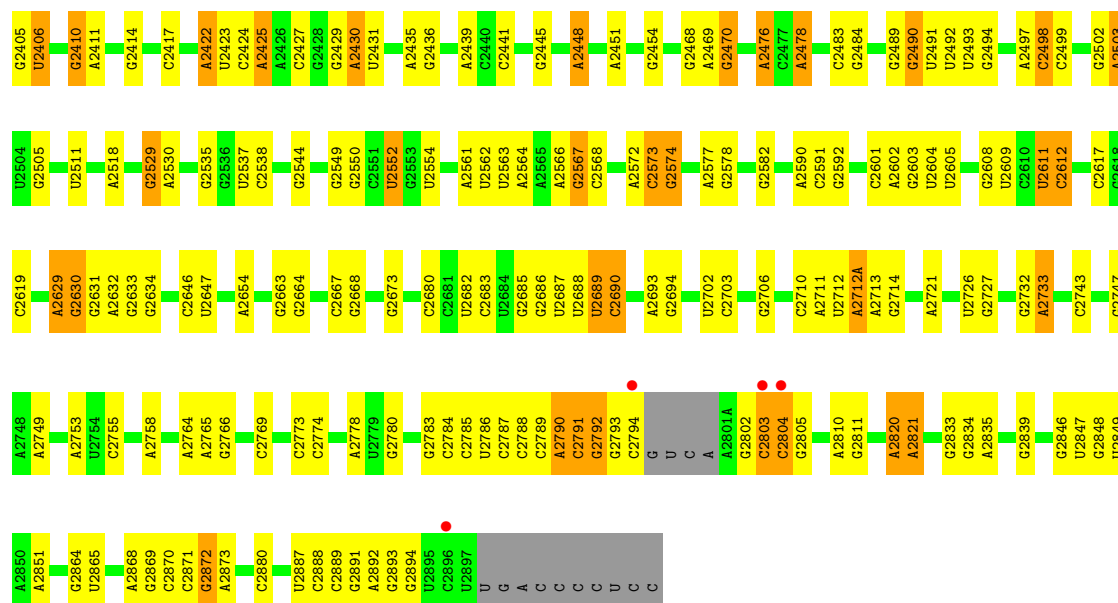
3 Residue-property plots

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

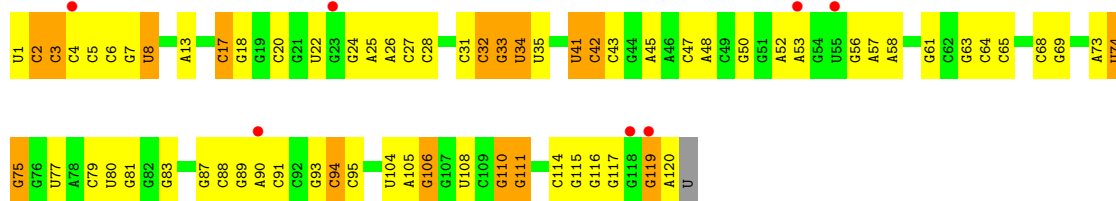
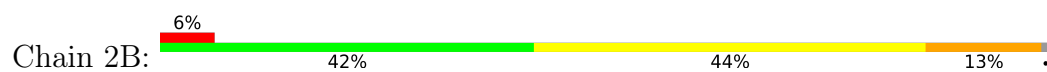
• Molecule 1: 23S Ribosomal RNA



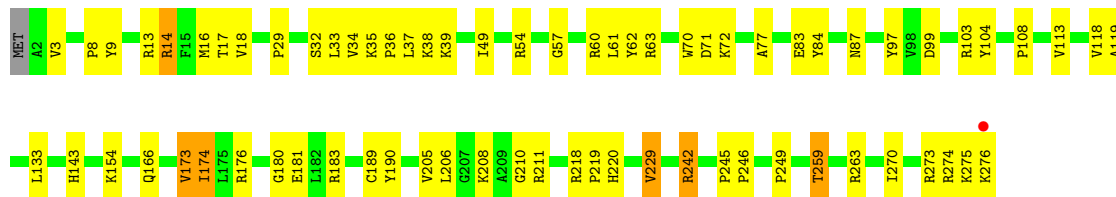
C2294	C2295	U2296	G2194	G2133	G2061	G1948	A1825	U1720	A1614	G1510	U1420	A1301	U1175	G1089	A1028
C2296	A2198	G2196	A2198	A2134	A2062	U1955	G1826	G1721	G1627	C1511	U1421	A1302	G1176	U1090	A1029
G2304	G2207	G2067	C2065	A2136	C2065	U1963	G1827	U1739	G1627	U1512	G1421	G1303	C1178	C1091	G1030
A2305	G2206	G2067	C2066	C2137	C2067	U1963	A1829	G1740	A1633	G1515	G1425	G1311	C1179	G1093	U1034
G2308	A2208	U2068	U2068	C2139	U2068	G1964	A1837	G1742	A1634	U1518	G1426	U1312	C1180	U1094	G1035
U2312	G2219	G2070	G2069	C2140	G2069	U1965	G1839	G1746	G1635	G1519	C1428	C1315	C1185	A1095	U1036
G2312	G2219	A2071	G2070	G2141	G2070	C1966	G1839	G1746	A1636	G1520	G1429	U1316	G1186	U1097	G1037
G2319	G2222	C2143	G2072	C2142	G2072	C1967	A1847	G1753	A1637	G1526	C1430	U1317	G1187	A1098	C1038
A2320	A2225	C2144	G2073	C2145	G2073	U1969	A1848	G1753	A1641	G1527	C1432	G1318	U1188	G1099	C1039
G2325	G2228	C2146	U2074	C2147	U2074	A1970	A1851	G1766	G1642	C1532	U1433	C1320	G1191	U1101	C1040
C2326	C2228	G2148	U2086	G2147	U2086	A1972	C1852	A1769	G1647	G	A1439	A1321	C1201	C1102	G1042
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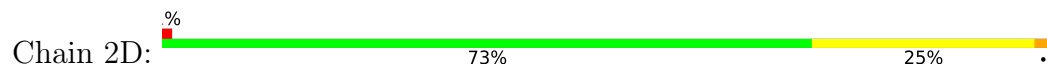
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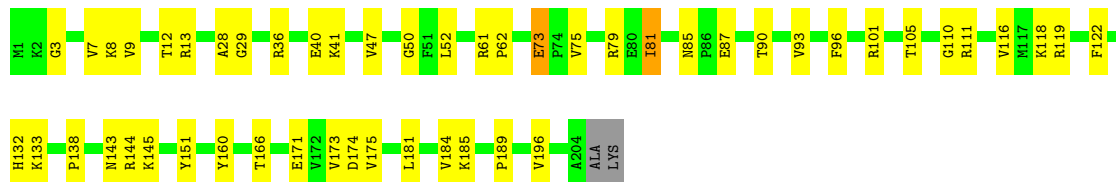
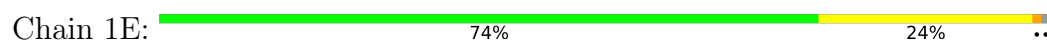
• Molecule 3: 50S ribosomal protein L2



• Molecule 3: 50S ribosomal protein L2

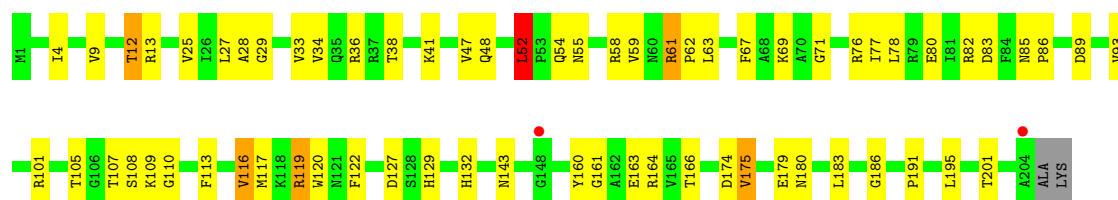


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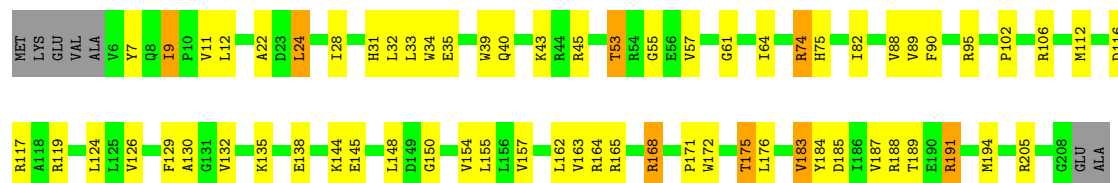
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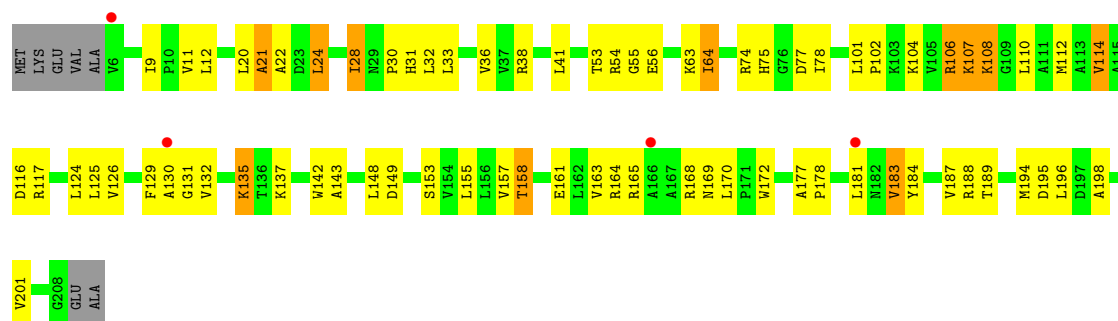
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 65% 28%



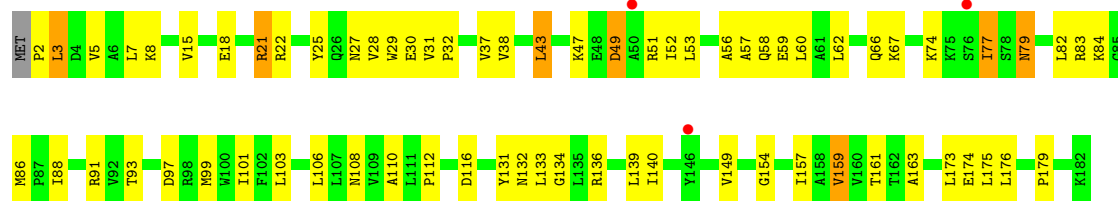
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 2% 61% 30% 5%



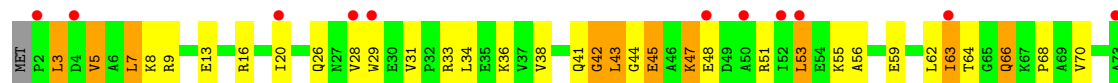
• Molecule 6: 50S ribosomal protein L5

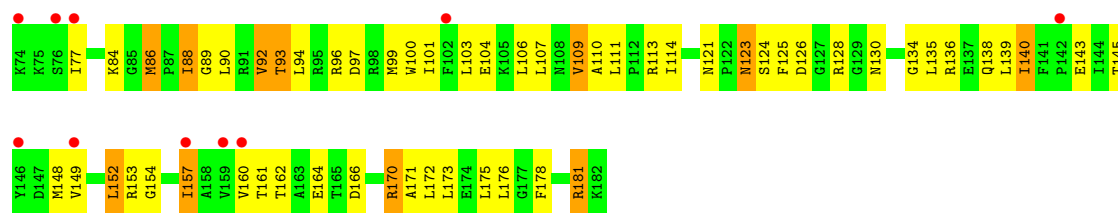
Chain 1G: 2% 62% 34%



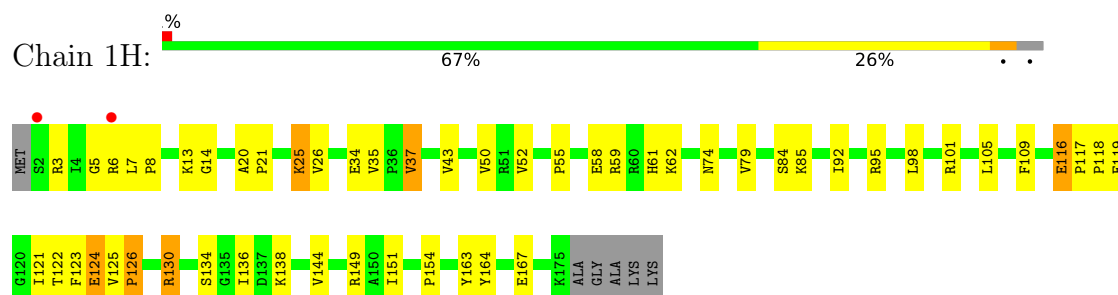
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 12% 49% 38% 12%

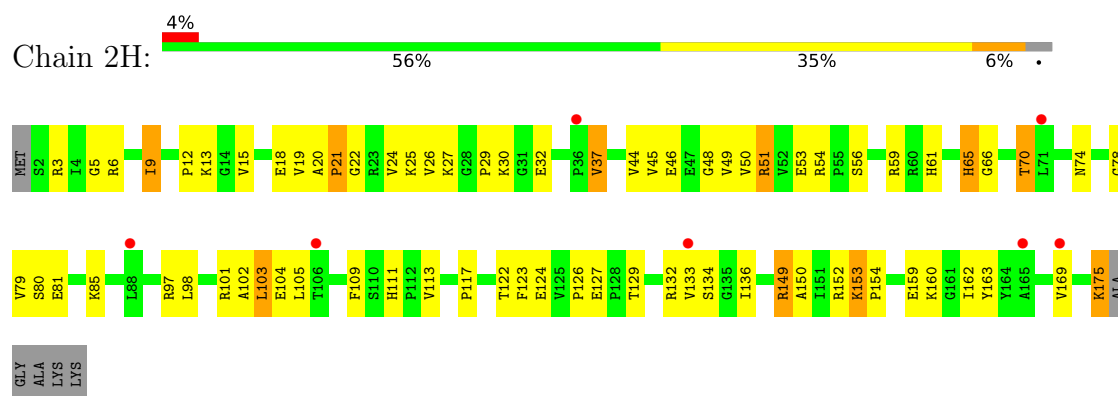




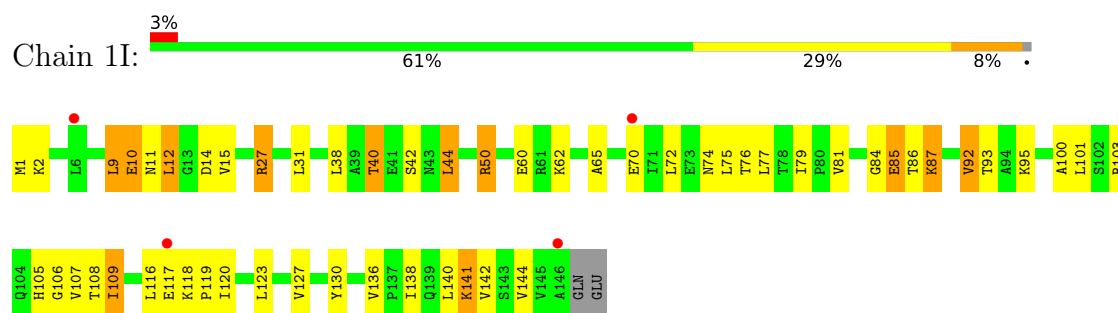
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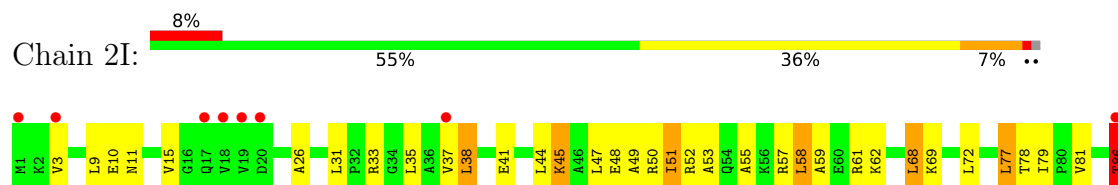
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9

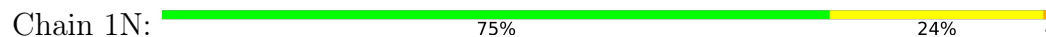


• Molecule 8: 50S ribosomal protein L9

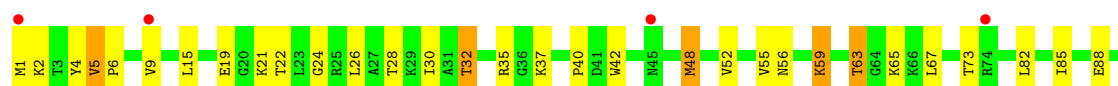




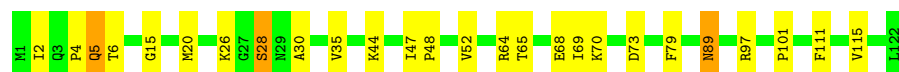
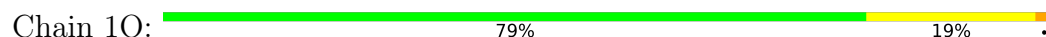
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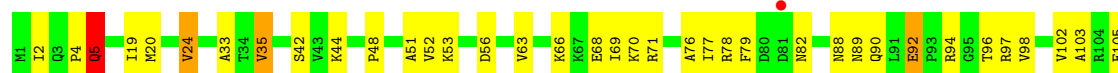
• Molecule 9: 50S ribosomal protein L13



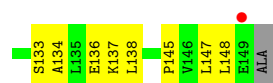
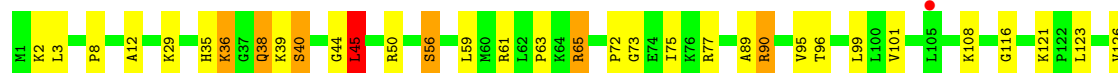
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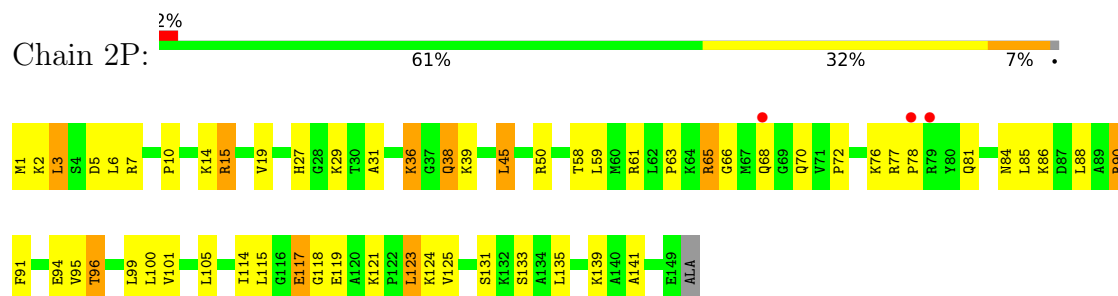
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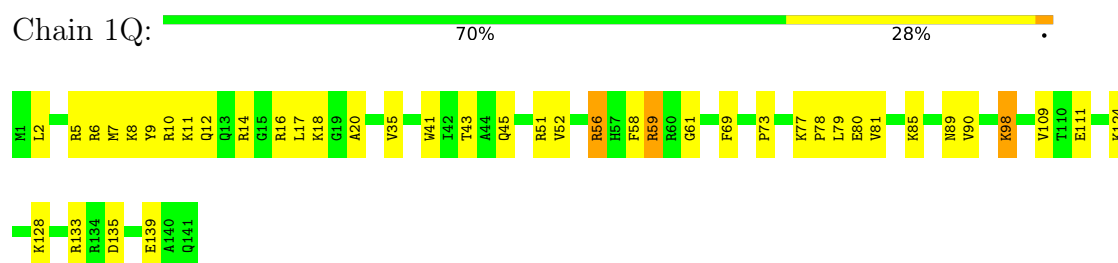
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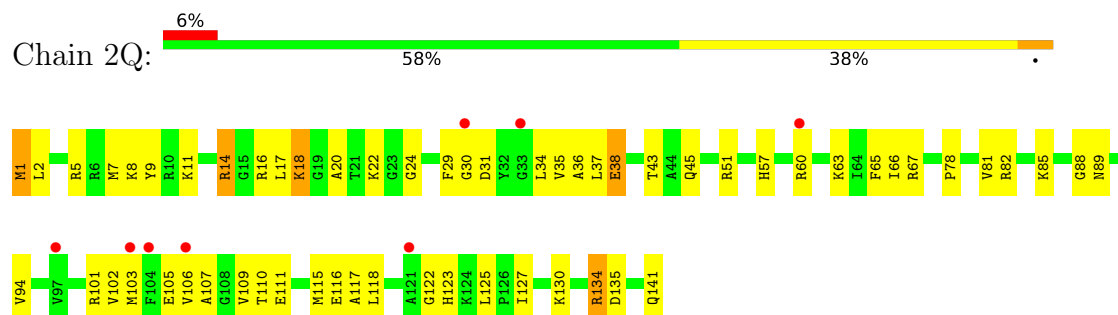
- Molecule 11: 50S ribosomal protein L15



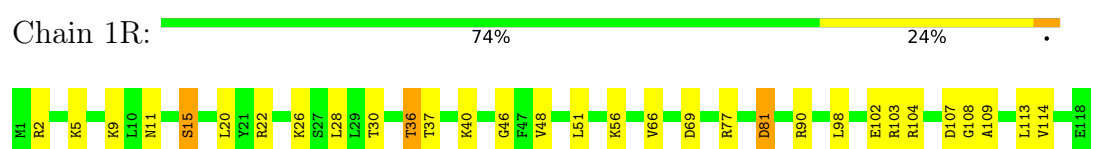
- Molecule 12: 50S ribosomal protein L16



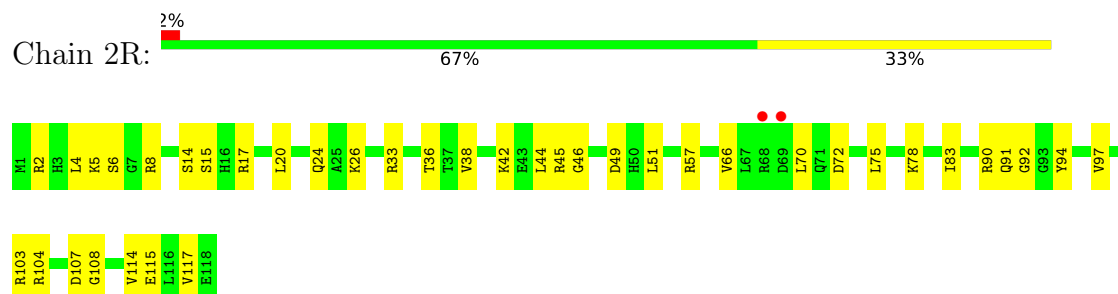
- Molecule 12: 50S ribosomal protein L16



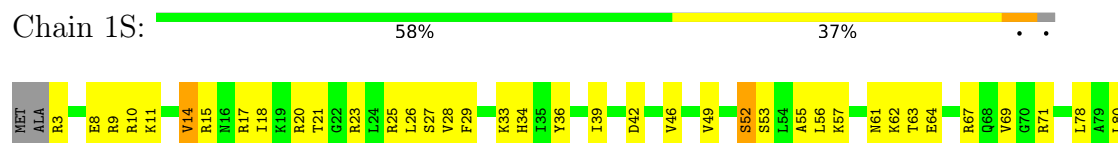
- Molecule 13: 50S ribosomal protein L17



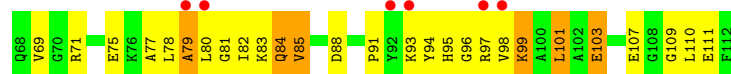
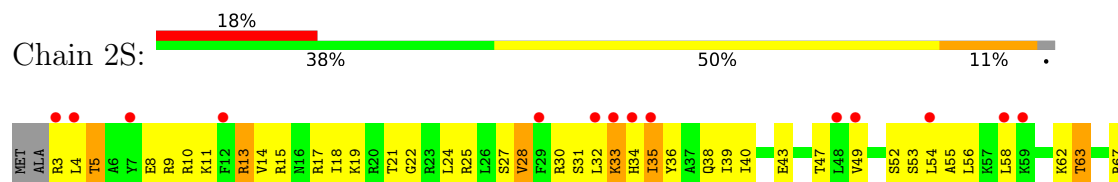
- Molecule 13: 50S ribosomal protein L17



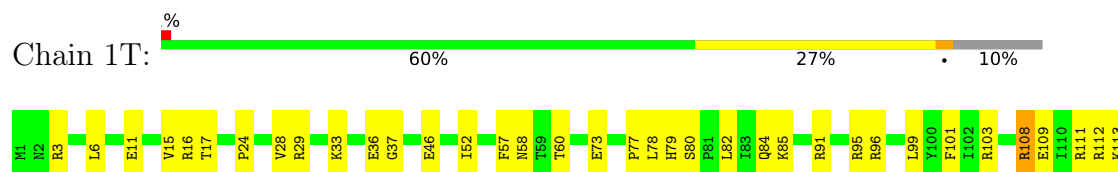
- Molecule 14: 50S ribosomal protein L18



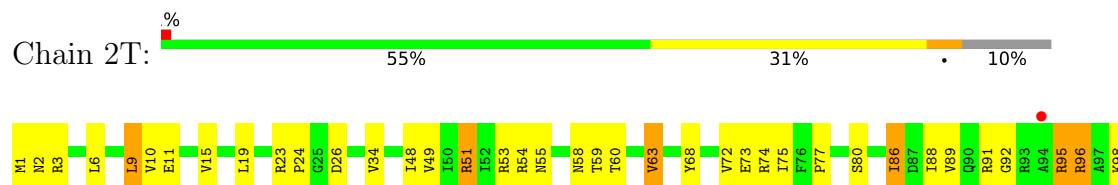
• Molecule 14: 50S ribosomal protein L18



• Molecule 15: 50S ribosomal protein L19



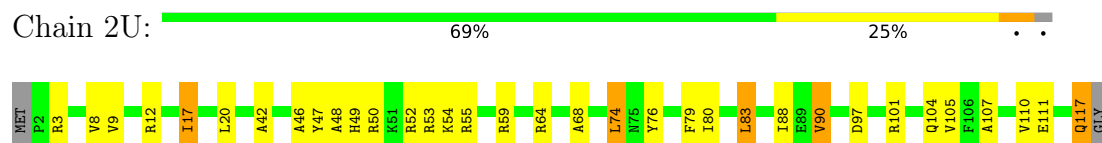
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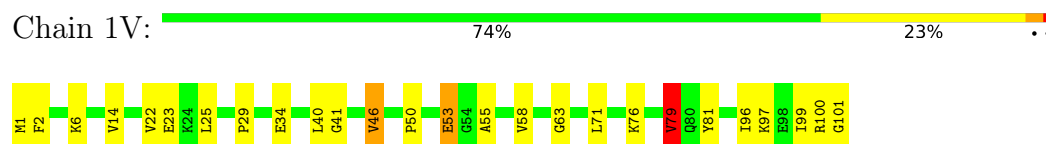
• Molecule 16: 50S ribosomal protein L20



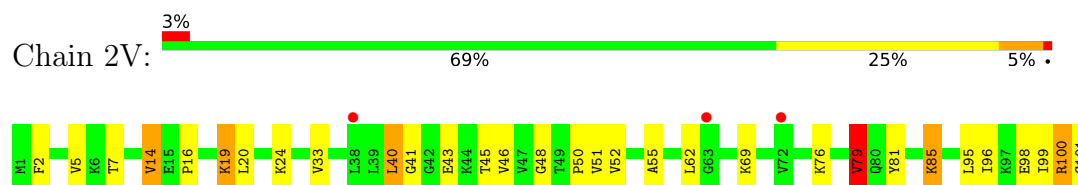
• Molecule 16: 50S ribosomal protein L20



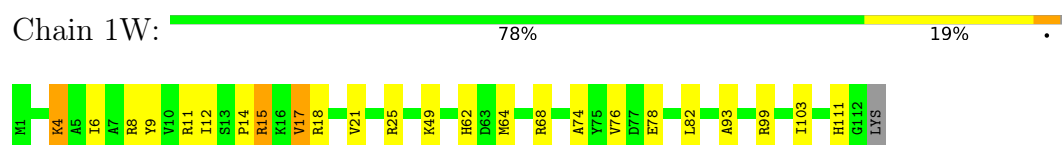
- Molecule 17: 50S ribosomal protein L21



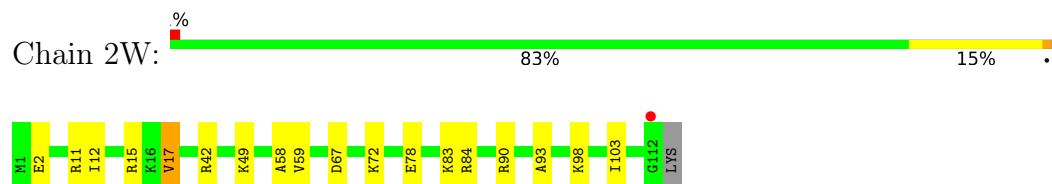
- Molecule 17: 50S ribosomal protein L21



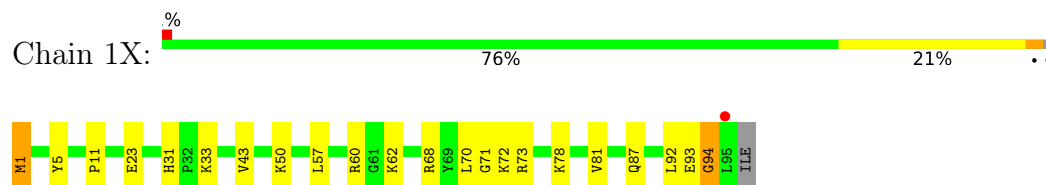
- Molecule 18: 50S ribosomal protein L22



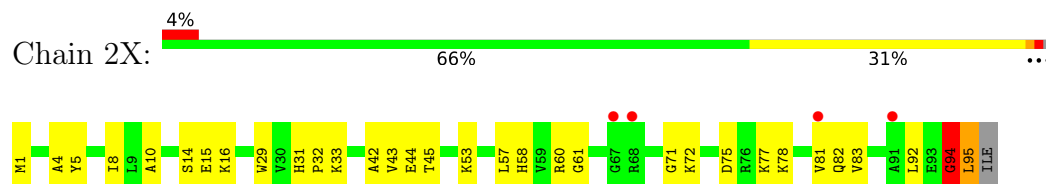
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L23



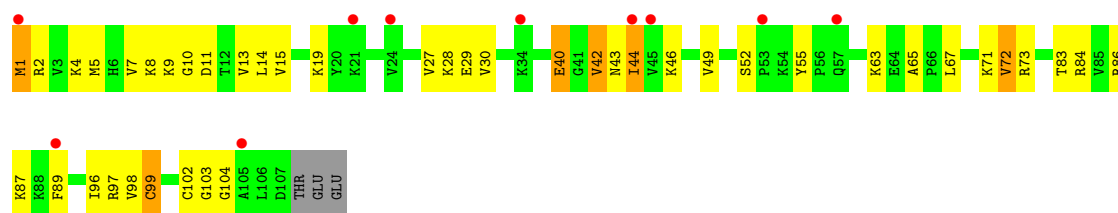
- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 



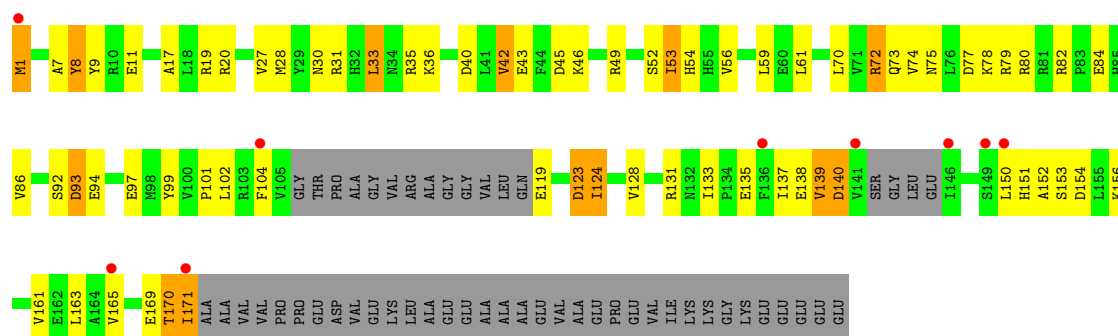
- Molecule 20: 50S ribosomal protein L24

Chain 2Y: 

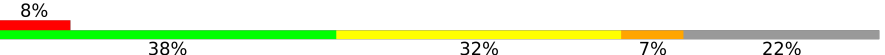


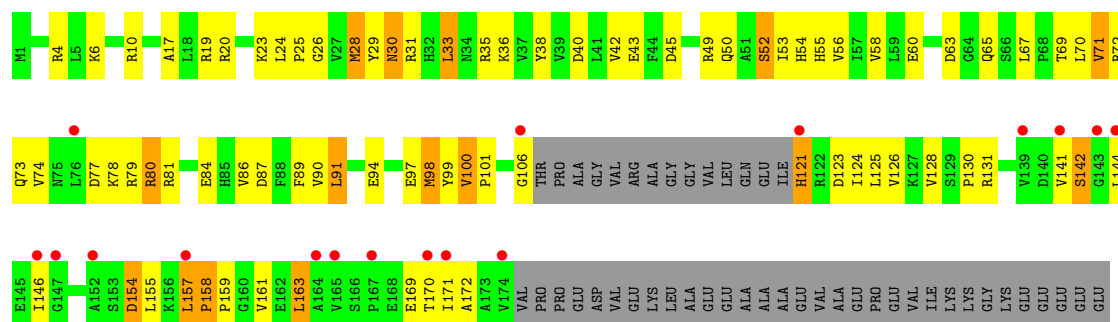
- Molecule 21: 50S ribosomal protein L25

Chain 1Z: 



- Molecule 21: 50S ribosomal protein L25

Chain 2Z: 



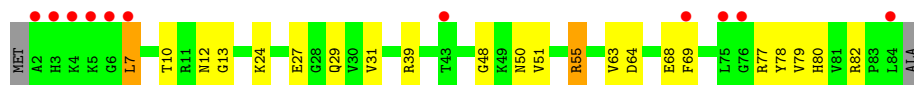
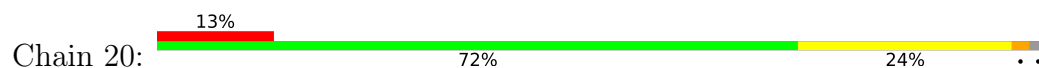
- Molecule 22: 50S ribosomal protein L27

Chain 10: 





- Molecule 22: 50S ribosomal protein L27



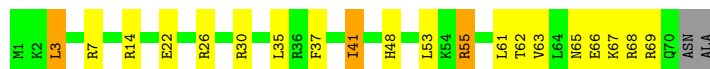
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



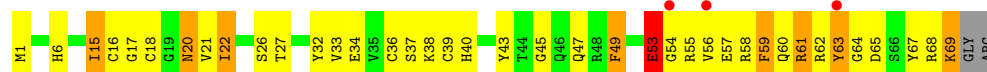
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



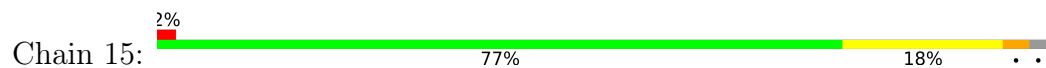
- Molecule 26: 50S ribosomal protein L31



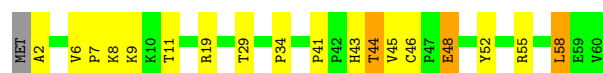
- Molecule 26: 50S ribosomal protein L31



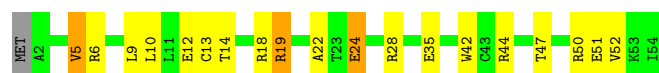
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

Chain 17:  71% 27% .



• Molecule 29: 50S ribosomal protein L34

Chain 27:  65% 33% .



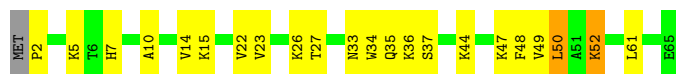
• Molecule 30: 50S ribosomal protein L35

Chain 18:  71% 28% .



• Molecule 30: 50S ribosomal protein L35

Chain 28:  65% 31% . .



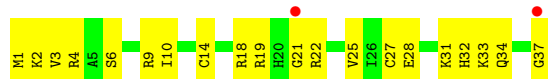
• Molecule 31: 50S ribosomal protein L36

Chain 19:  81% 19% .



• Molecule 31: 50S ribosomal protein L36

Chain 29:  46% 54% .

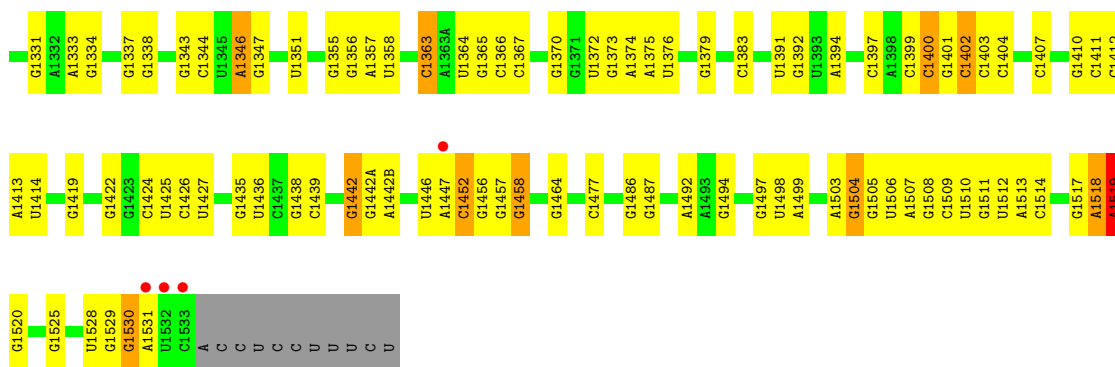


• Molecule 32: 16S Ribosomal RNA

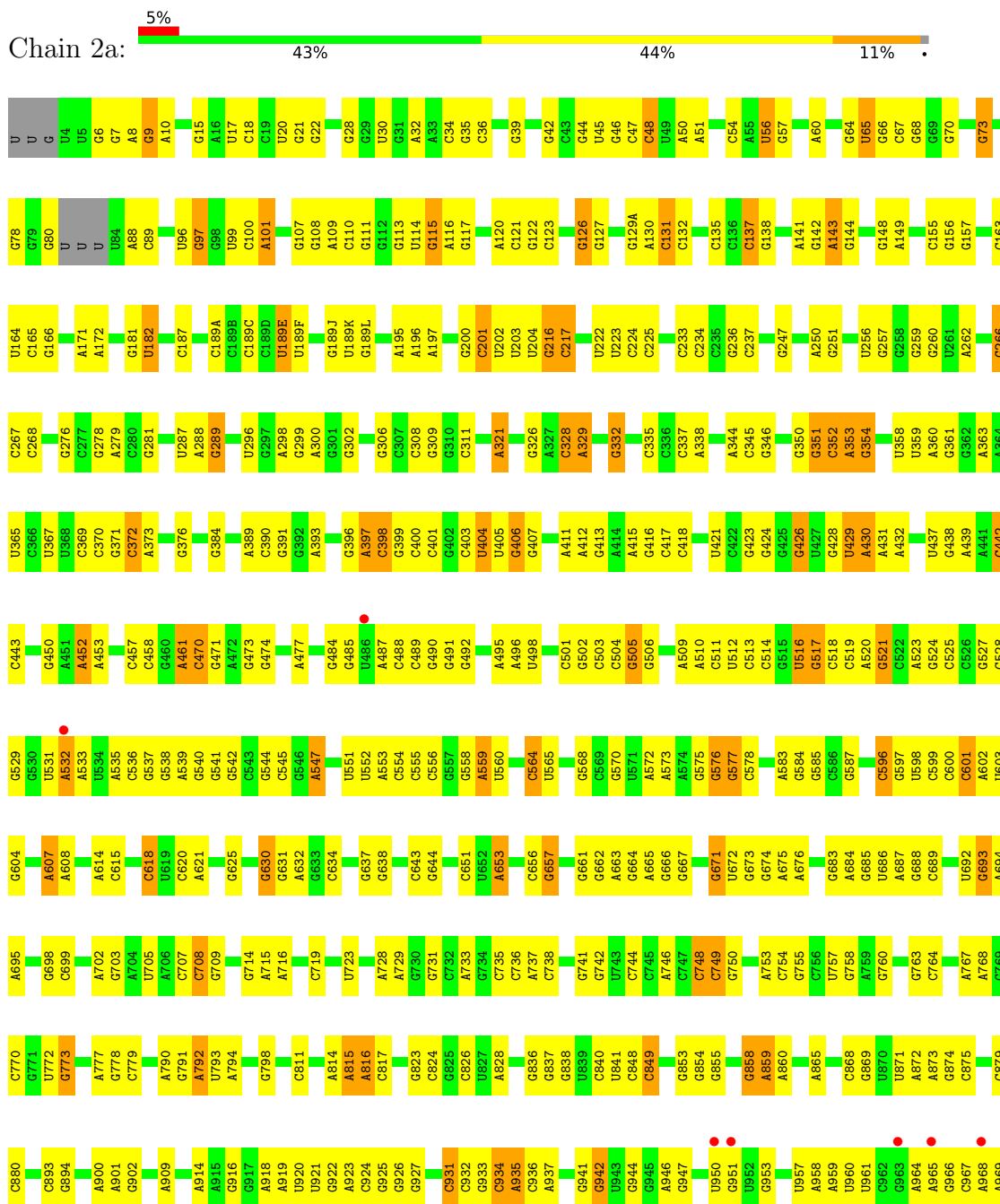
Chain 1a:  52% 40% 6% .



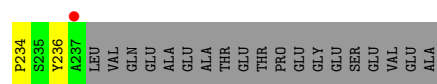




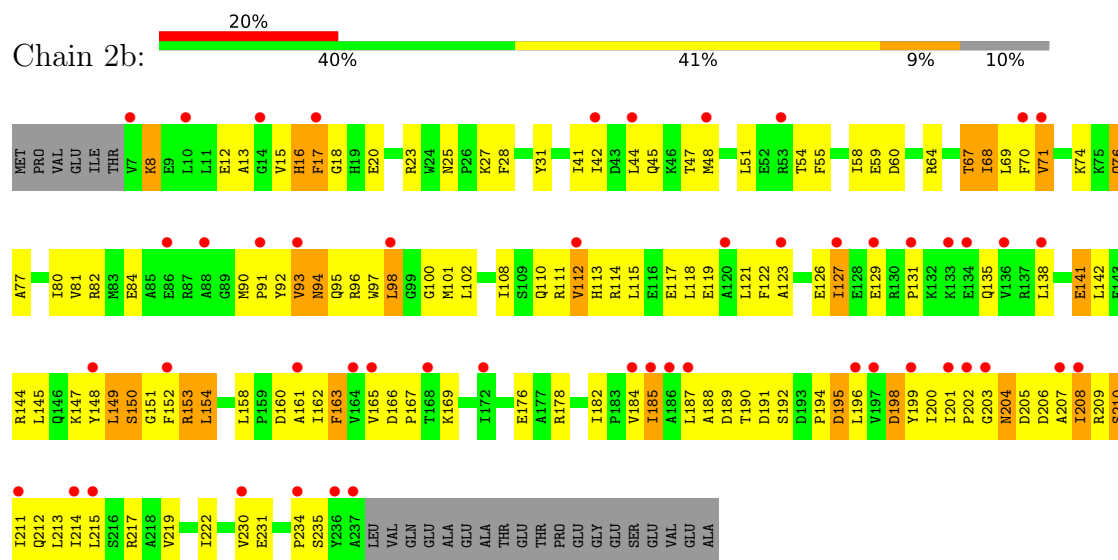
• Molecule 32: 16S Ribosomal RNA



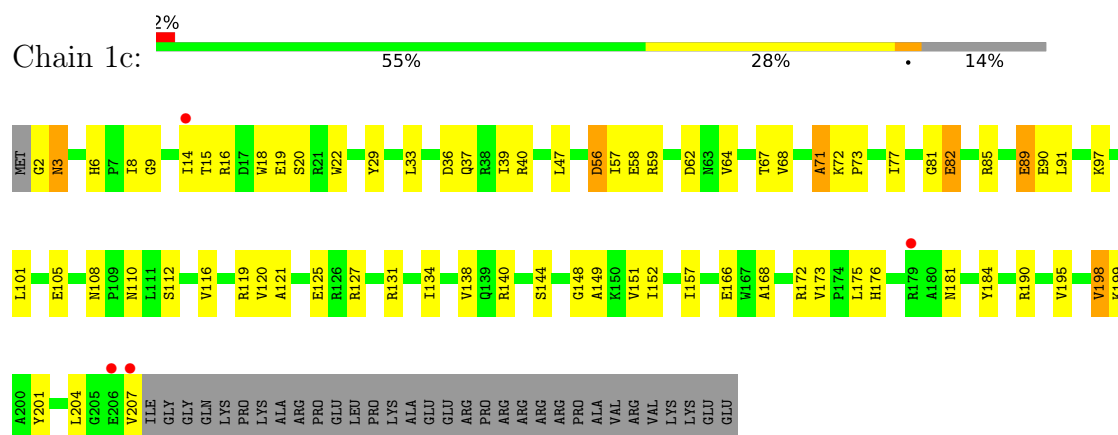




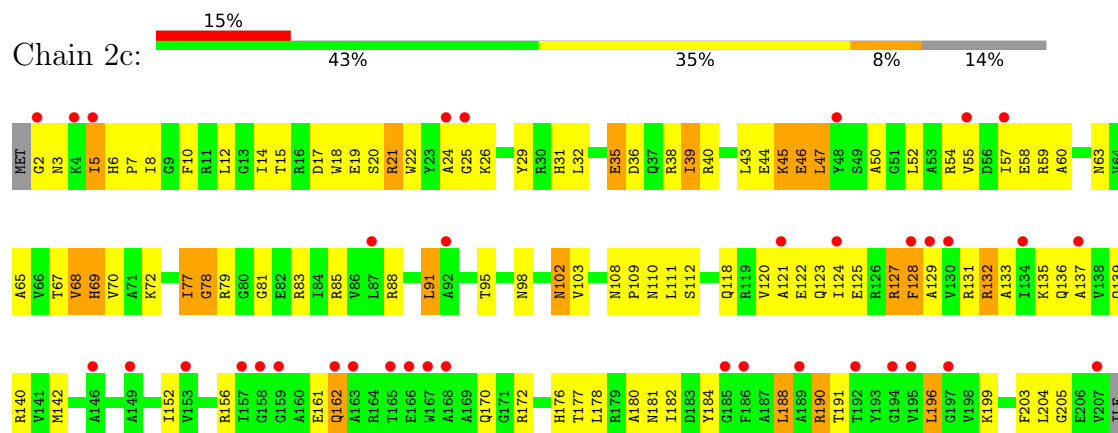
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3



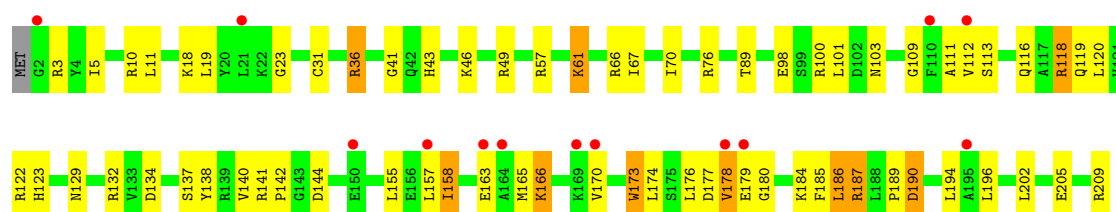
• Molecule 34: 30S ribosomal protein S3



GLY
GLY
GLN
LYS
PRO
LYS
PRO
ALA
ARG
PRO
GLU
LEU
LYS
LYS
ALA
GLU
GLU
ARG
PRO
PRO
ARG
ARG
ARG
ARG
PRO
ALA
VAL
ARG
VAL
LYS
LYS
GLU
GLU

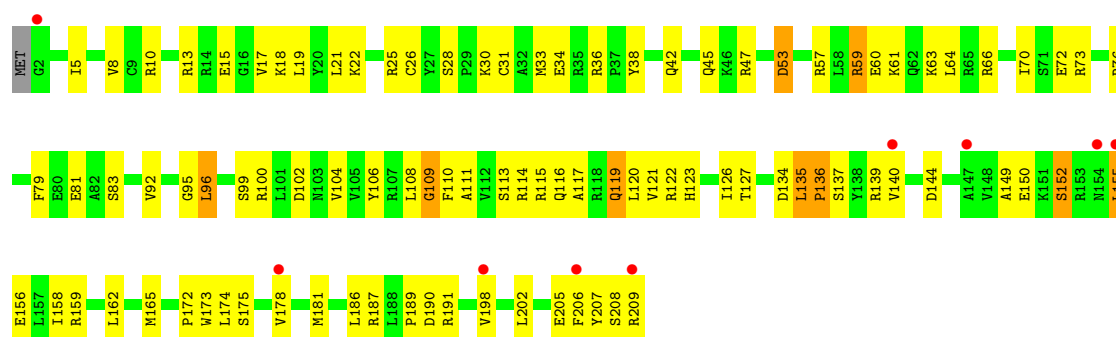
• Molecule 35: 30S ribosomal protein S4

Chain 1d: 6% 67% 28% 5%



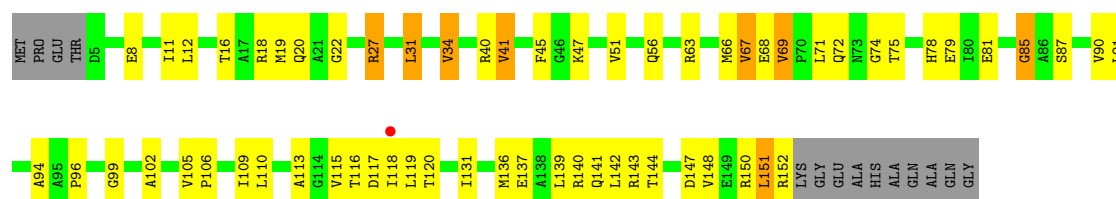
• Molecule 35: 30S ribosomal protein S4

Chain 2d: 4% 54% 41% .



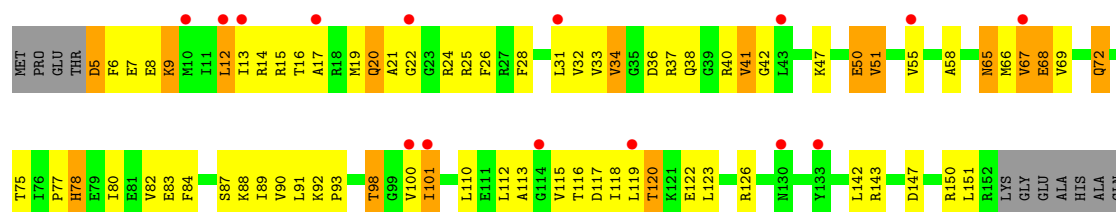
• Molecule 36: 30S ribosomal protein S5

Chain 1e: % 53% 33% 5% 9%



• Molecule 36: 30S ribosomal protein S5

Chain 2e: 9% 46% 36% 10% 9%



ALA
GLN
GLY

• Molecule 37: 30S ribosomal protein S6



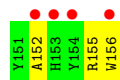
• Molecule 37: 30S ribosomal protein S6



• Molecule 38: 30S ribosomal protein S7

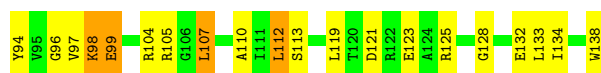


• Molecule 38: 30S ribosomal protein S7

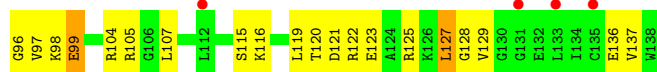
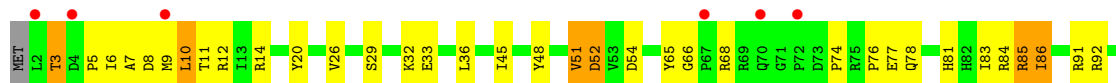


• Molecule 39: 30S ribosomal protein S8

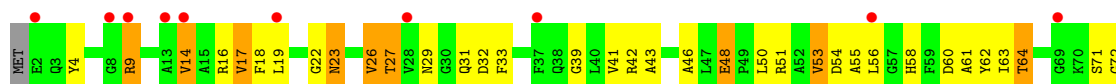




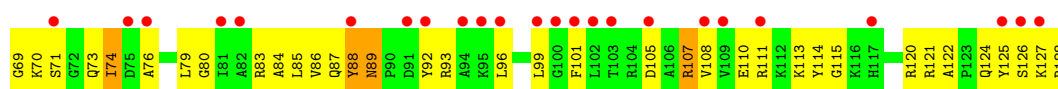
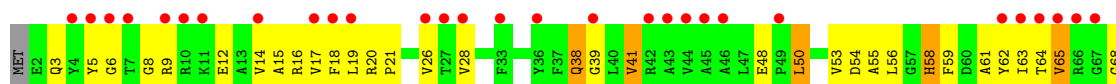
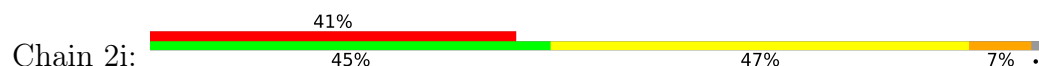
- Molecule 39: 30S ribosomal protein S8



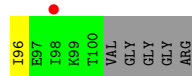
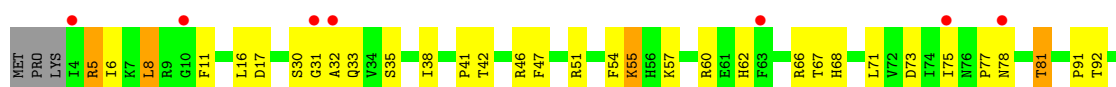
- Molecule 40: 30S ribosomal protein S9



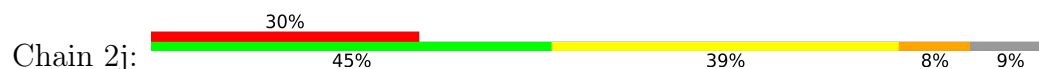
- Molecule 40: 30S ribosomal protein S9

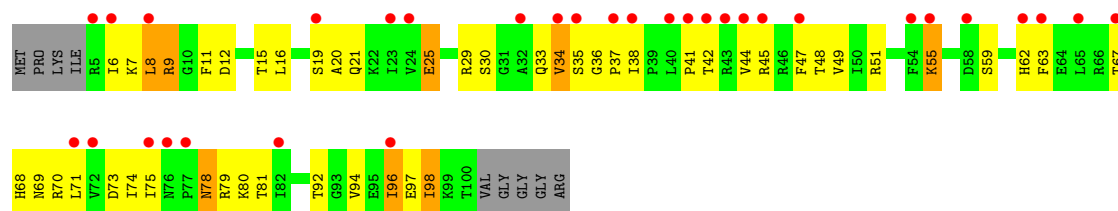


- Molecule 41: 30S ribosomal protein S10

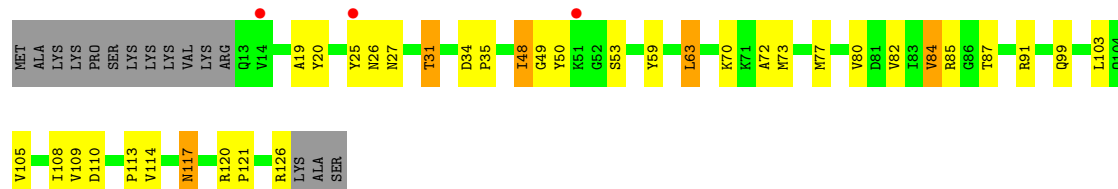


- Molecule 41: 30S ribosomal protein S10

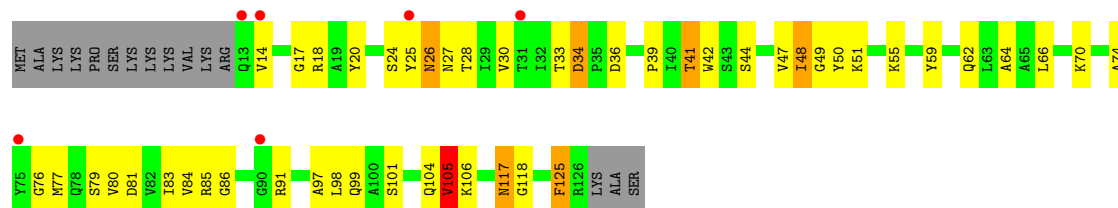




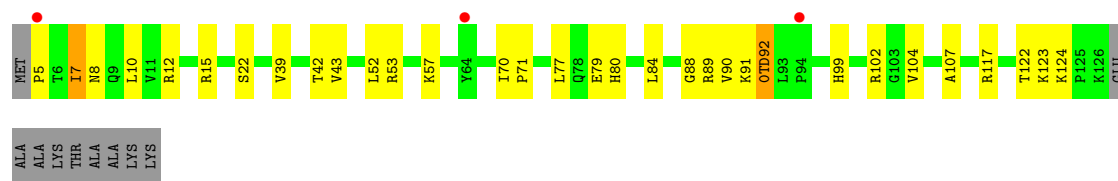
• Molecule 42: 30S ribosomal protein S11



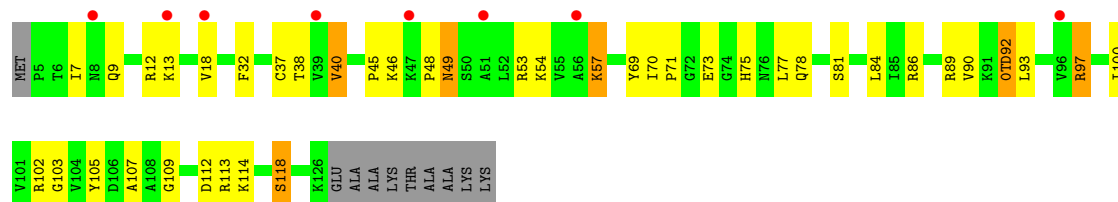
• Molecule 42: 30S ribosomal protein S11



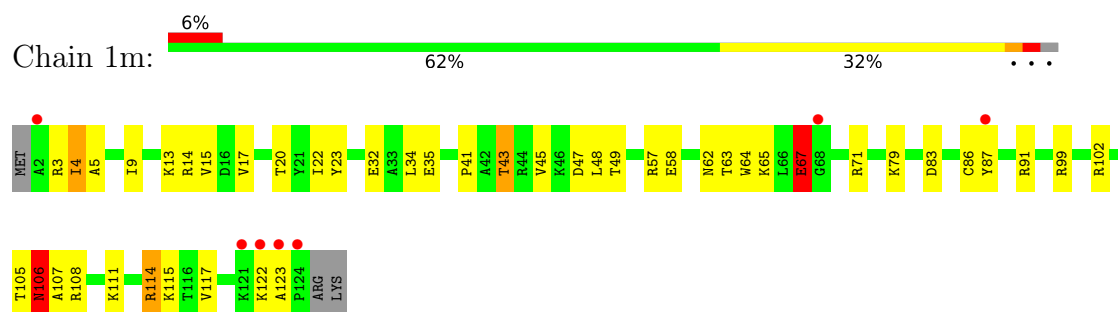
• Molecule 43: 30S ribosomal protein S12



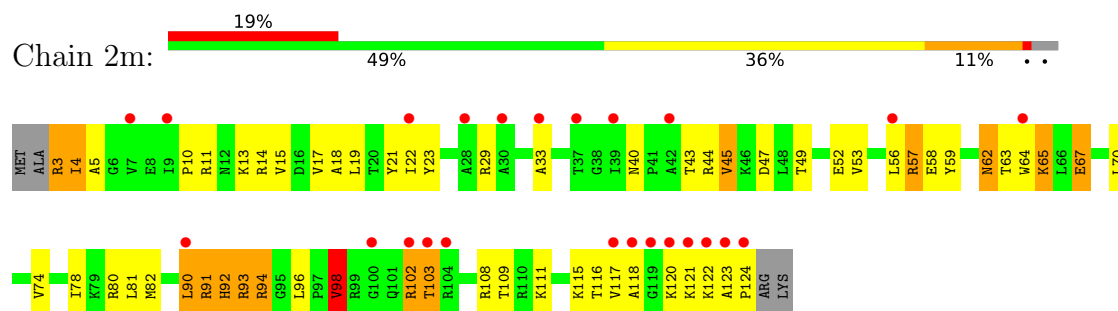
• Molecule 43: 30S ribosomal protein S12



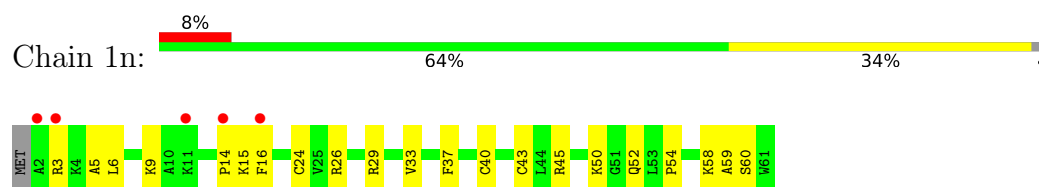
• Molecule 44: 30S ribosomal protein S13



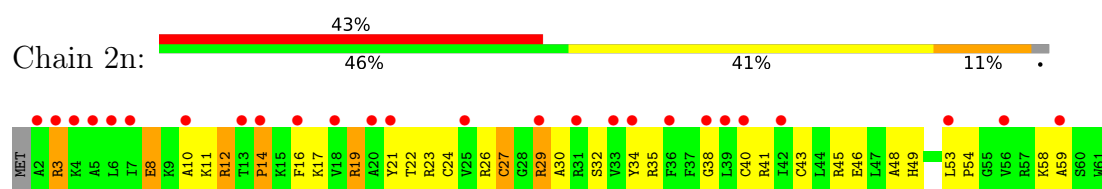
- Molecule 44: 30S ribosomal protein S13



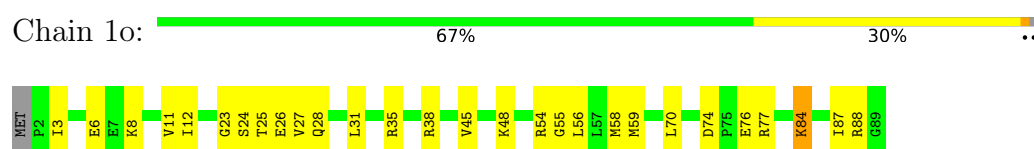
- Molecule 45: 30S ribosomal protein S14 type Z



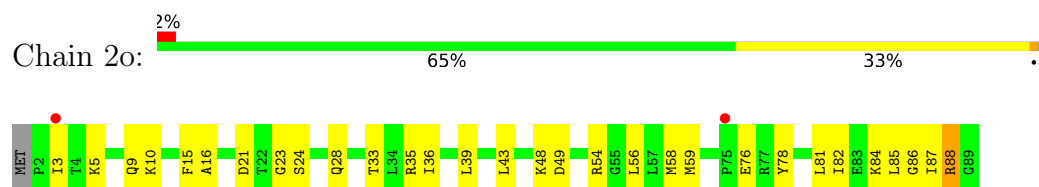
- Molecule 45: 30S ribosomal protein S14 type Z



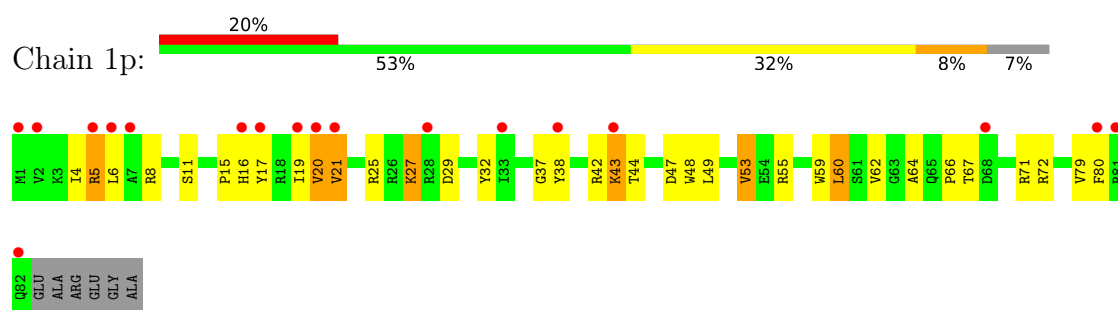
- Molecule 46: 30S ribosomal protein S15



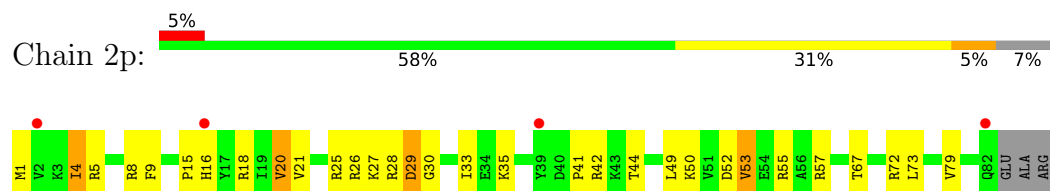
- Molecule 46: 30S ribosomal protein S15



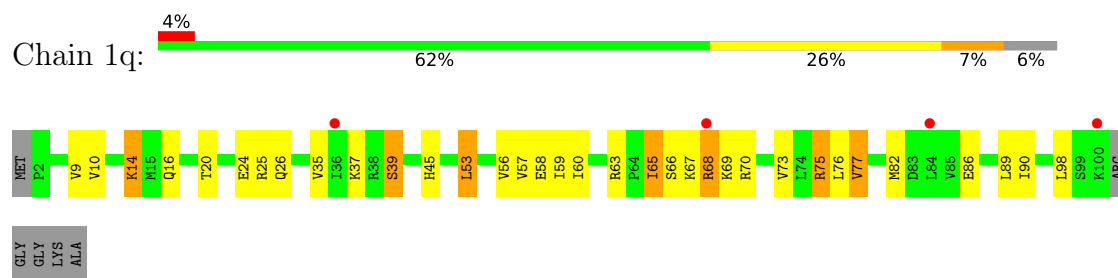
- Molecule 47: 30S ribosomal protein S16



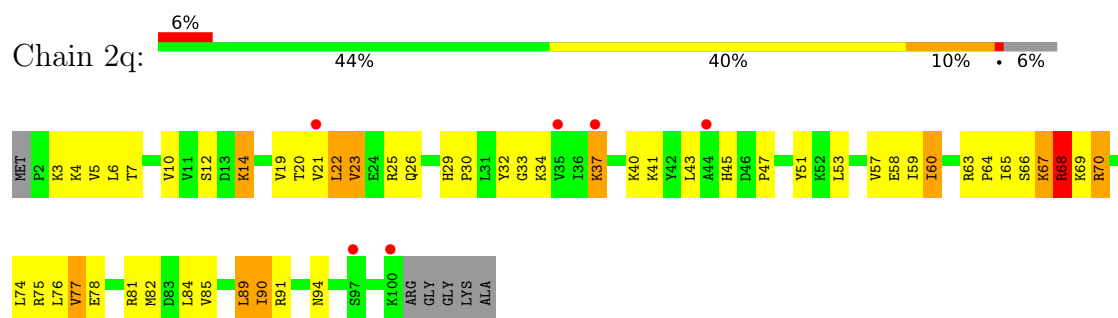
- Molecule 47: 30S ribosomal protein S16



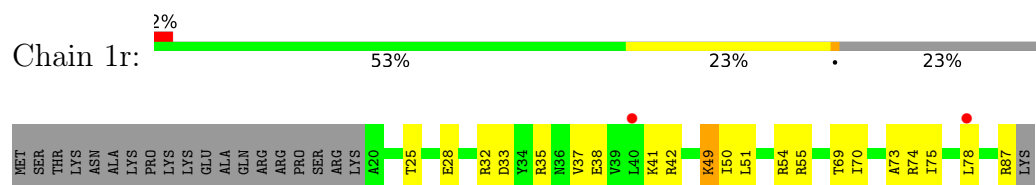
- Molecule 48: 30S ribosomal protein S17



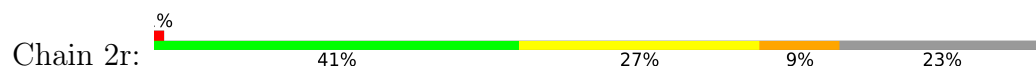
- Molecule 48: 30S ribosomal protein S17

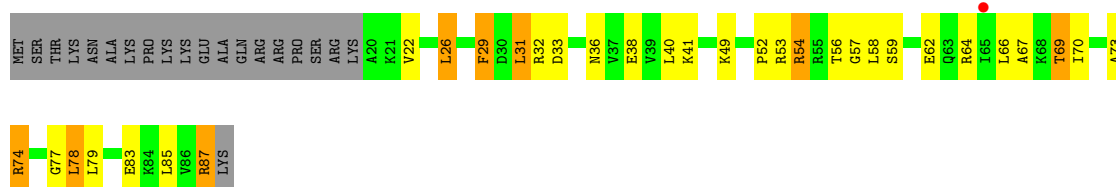


- Molecule 49: 30S ribosomal protein S18

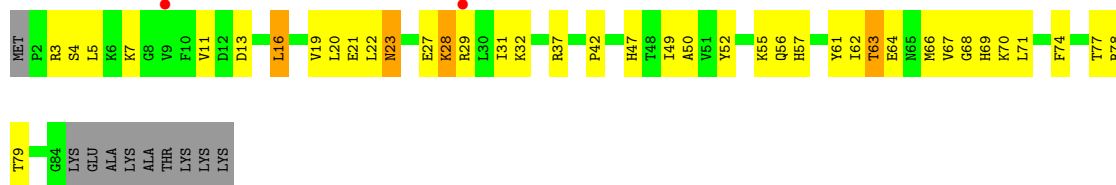


- Molecule 49: 30S ribosomal protein S18

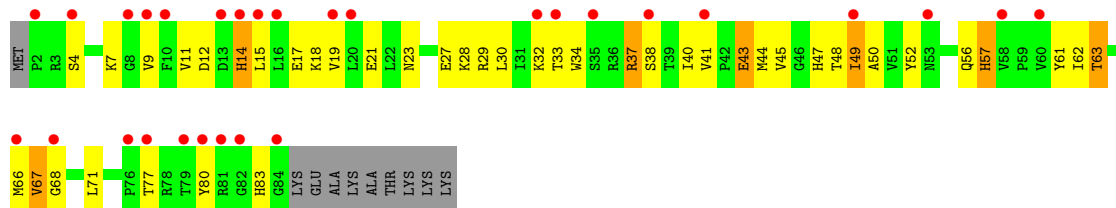
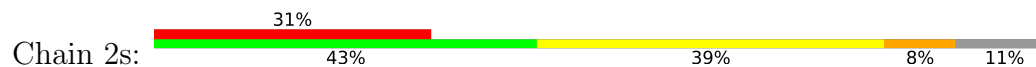




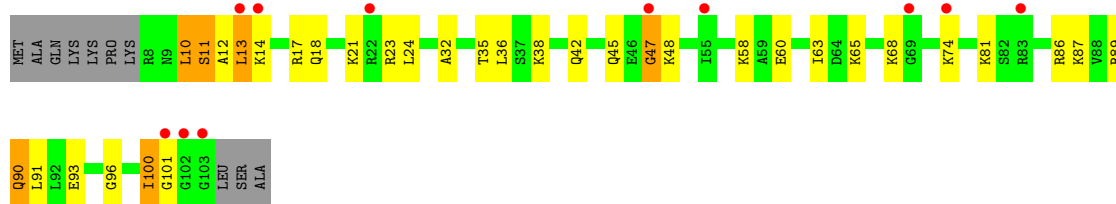
- Molecule 50: 30S ribosomal protein S19



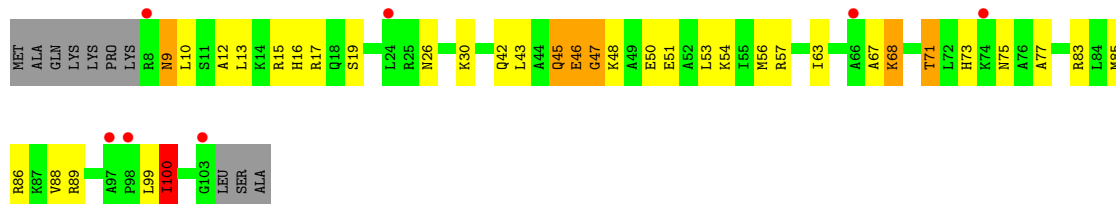
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20



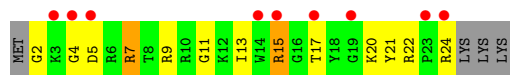
- Molecule 52: 30S ribosomal protein Thx

Chain 1u: 

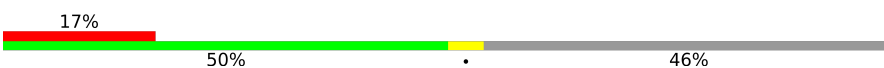


- Molecule 52: 30S ribosomal protein Thx

Chain 2u: 

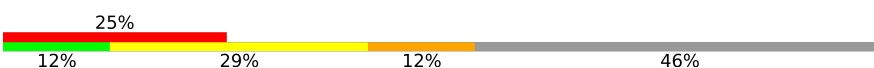


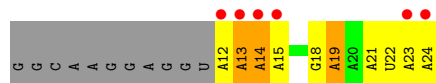
- Molecule 53: MET-LYS-mRNA

Chain 1v: 



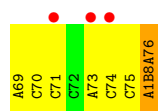
- Molecule 53: MET-LYS-mRNA

Chain 2v: 



- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA_{Lys}

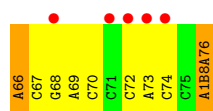
Chain 1w: 



- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNA_{Lys}

Chain 2w: 

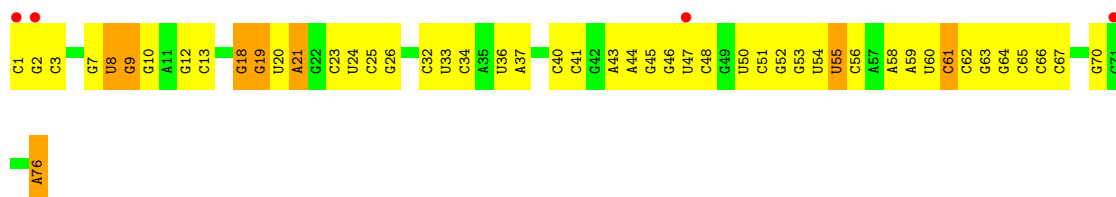




- Molecule 55: P-site Peptidyl-tRNA fMRC-tRNAcys RNA-part



- Molecule 55: P-site Peptidyl-tRNA fMRC-tRNAcys RNA-part



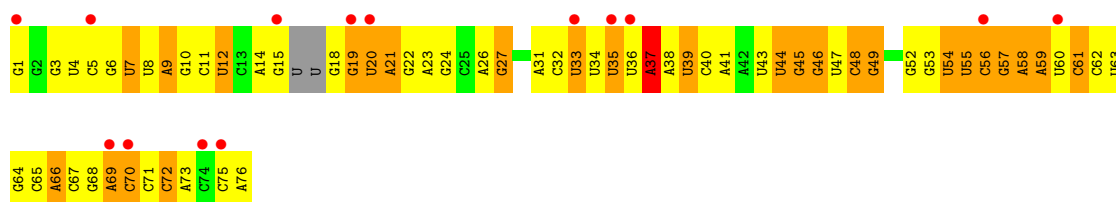
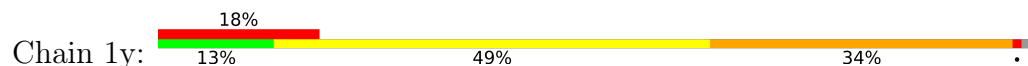
- Molecule 56: P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part



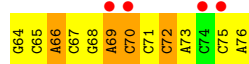
- Molecule 56: P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part

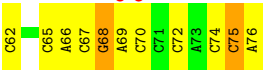


- Molecule 57: E-site Deacylated tRNAlys



- Molecule 57: E-site Deacylated tRNAlys





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.26Å 449.45Å 619.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	124.44 – 2.65 124.44 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (124.44-2.65) 99.3 (124.44-2.65)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.225 , 0.276 0.226 , 0.277	Depositor DCC
R_{free} test set	82975 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299863	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: OMG, 2MG, M2G, U8U, MA6, K, 2MA, T6A, A1B8A, FME, 4OC, MG, PSU, 4SU, ERY, 0TD, OMU, OMC, UR3, G7M, SF4, ZN, 5MU, 8AN, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.29	1/69011 (0.0%)	0.47	1/107720 (0.0%)
1	2A	0.21	0/67295	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.41	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.27	0/2186	0.49	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.42	0/2149
5	1F	0.26	0/1619	0.47	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.22	0/1448	0.47	1/1957 (0.1%)
6	2G	0.21	0/1453	0.47	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.42	0/1834
8	1I	0.20	0/1112	0.43	0/1514
8	2I	0.20	0/1079	0.45	1/1475 (0.1%)
9	1N	0.25	0/1144	0.48	0/1543
9	2N	0.20	0/1144	0.41	0/1543
10	1O	0.28	0/943	0.47	0/1269
10	2O	0.23	0/943	0.48	0/1269
11	1P	0.26	0/1152	0.55	0/1533
11	2P	0.22	0/1152	0.50	0/1533
12	1Q	0.27	0/1143	0.51	0/1527
12	2Q	0.19	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.49	0/1312
13	2R	0.21	0/982	0.47	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.20	0/880	0.45	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.20	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.22	0/977	0.45	0/1301
17	1V	0.25	0/782	0.49	0/1049
17	2V	0.20	0/782	0.43	0/1049
18	1W	0.28	0/897	0.47	0/1205
18	2W	0.21	0/897	0.42	0/1205
19	1X	0.28	0/764	0.56	2/1025 (0.2%)
19	2X	0.27	0/764	0.59	2/1025 (0.2%)
20	1Y	0.23	0/819	0.50	0/1095
20	2Y	0.21	0/819	0.45	0/1095
21	1Z	0.24	0/1267	0.49	0/1717
21	2Z	0.22	0/1299	0.42	0/1763
22	10	0.27	0/662	0.52	0/881
22	20	0.21	0/662	0.43	0/881
23	11	0.27	0/762	0.45	0/1014
23	21	0.23	0/762	0.41	0/1014
24	12	0.25	0/590	0.49	0/781
24	22	0.20	0/590	0.38	0/781
25	13	0.24	0/474	0.43	0/635
25	23	0.18	0/469	0.39	0/630
26	14	0.24	0/565	0.56	0/761
26	24	0.26	0/545	0.54	0/737
27	15	0.34	0/469	0.58	0/635
27	25	0.21	0/469	0.44	0/635
28	16	0.26	0/460	0.48	0/613
28	26	0.20	0/456	0.44	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.26	0/525	0.50	0/691
30	28	0.22	0/525	0.41	0/691
31	19	0.29	0/310	0.54	0/407
31	29	0.20	0/310	0.42	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.20	0/35886	0.38	0/56005
33	1b	0.22	0/1881	0.49	0/2542
33	2b	0.24	0/1860	0.52	0/2518
34	1c	0.19	0/1572	0.40	0/2126
34	2c	0.25	0/1566	0.55	1/2119 (0.0%)
35	1d	0.21	0/1685	0.45	0/2262
35	2d	0.20	0/1704	0.45	0/2284
36	1e	0.22	0/1145	0.45	0/1543
36	2e	0.24	0/1149	0.54	2/1548 (0.1%)
37	1f	0.19	0/823	0.39	0/1115
37	2f	0.20	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1250	0.43	0/1679
38	2g	0.22	0/1254	0.42	0/1683
39	1h	0.21	0/1108	0.44	0/1494
39	2h	0.21	0/1108	0.44	0/1494
40	1i	0.26	0/1002	0.55	1/1346 (0.1%)
40	2i	0.24	0/997	0.52	0/1343
41	1j	0.20	0/722	0.44	0/982
41	2j	0.23	0/727	0.47	0/988
42	1k	0.18	0/844	0.39	0/1145
42	2k	0.20	0/848	0.47	1/1149 (0.1%)
43	1l	0.21	0/937	0.44	0/1260
43	2l	0.21	0/937	0.46	0/1260
44	1m	0.20	0/969	0.52	0/1302
44	2m	0.22	0/961	0.47	0/1291
45	1n	0.19	0/501	0.42	0/664
45	2n	0.20	0/501	0.43	0/664
46	1o	0.19	0/739	0.42	0/985
46	2o	0.20	0/739	0.43	0/985
47	1p	0.22	0/697	0.51	0/939
47	2p	0.20	0/693	0.51	0/935
48	1q	0.20	0/836	0.51	1/1117 (0.1%)
48	2q	0.20	0/836	0.45	0/1117
49	1r	0.20	0/560	0.45	0/746
49	2r	0.19	0/560	0.40	0/746
50	1s	0.21	0/667	0.49	0/900
50	2s	0.25	0/661	0.58	0/893
51	1t	0.21	0/730	0.48	0/965
51	2t	0.21	0/729	0.47	0/965
52	1u	0.20	0/203	0.47	0/266
52	2u	0.22	0/203	0.46	0/266
53	1v	0.20	0/319	0.35	0/495
53	2v	0.24	0/319	0.43	0/495
54	1w	0.31	2/1593 (0.1%)	0.40	0/2474
54	2w	0.33	2/1593 (0.1%)	0.45	0/2474
55	1x	0.25	0/1723	0.40	0/2684
55	2x	0.24	0/1723	0.39	0/2684
56	1z	0.70	0/16	0.46	0/19
56	2z	0.41	0/16	0.72	0/19
57	1y	0.31	0/1618	0.45	0/2513
57	2y	0.33	2/1618 (0.1%)	0.51	0/2513
All	All	0.24	7/316807 (0.0%)	0.43	16/474290 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O3'-P	5.68	1.61	1.56
57	2y	46	G7M	O3'-P	5.54	1.61	1.56
54	2w	37	T6A	O3'-P	5.53	1.61	1.56
54	2w	46	G7M	O3'-P	5.48	1.61	1.56
57	2y	37	T6A	O3'-P	5.44	1.61	1.56

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1i	88	TYR	N-CA-C	-8.51	104.92	114.62
34	2c	78	GLY	N-CA-C	7.53	120.39	111.35
19	2X	94	GLY	CA-C-N	7.35	134.93	121.70
19	2X	94	GLY	C-N-CA	7.35	134.93	121.70
48	1q	77	VAL	N-CA-C	-7.03	105.93	112.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	20	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	711	0
1	2A	60322	0	30427	806	0
2	1B	2577	0	1305	29	0
2	2B	2575	0	1303	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	59	0
3	2D	2136	0	2218	48	0
4	1E	1559	0	1617	31	0
4	2E	1559	0	1618	44	0
5	1F	1584	0	1625	50	0
5	2F	1580	0	1619	51	0
6	1G	1423	0	1436	41	0
6	2G	1428	0	1438	65	0
7	1H	1330	0	1407	33	0
7	2H	1330	0	1407	45	0
8	1I	1097	0	1140	33	0
8	2I	1064	0	1082	36	0
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	31	0
10	1O	933	0	996	17	0
10	2O	933	0	996	31	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	46	0
12	1Q	1122	0	1179	33	0
12	2Q	1122	0	1179	45	0
13	1R	968	0	1033	22	0
13	2R	968	0	1033	23	0
14	1S	873	0	927	31	0
14	2S	870	0	923	58	0
15	1T	1091	0	1151	29	0
15	2T	1083	0	1136	39	0
16	1U	959	0	1018	22	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	13	0
17	2V	771	0	829	20	0
18	1W	886	0	940	13	0
18	2W	886	0	940	12	0
19	1X	750	0	814	14	0
19	2X	750	0	814	23	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	24	0
21	1Z	1240	0	1240	43	0
21	2Z	1271	0	1273	59	0
22	10	653	0	674	19	0
22	20	653	0	674	18	0
23	11	755	0	826	20	0
23	21	755	0	826	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	13	0
24	22	588	0	643	18	0
25	13	469	0	518	11	0
25	23	464	0	514	16	0
26	14	552	0	533	30	0
26	24	532	0	503	36	0
27	15	455	0	465	8	0
27	25	455	0	465	12	0
28	16	453	0	473	10	0
28	26	449	0	469	9	0
29	17	418	0	467	11	0
29	27	418	0	467	10	0
30	18	517	0	582	16	0
30	28	517	0	582	17	0
31	19	307	0	335	5	0
31	29	307	0	335	12	0
32	1a	32246	0	16293	427	0
32	2a	32327	0	16338	623	0
33	1b	1846	0	1867	69	0
33	2b	1825	0	1828	95	0
34	1c	1548	0	1535	46	0
34	2c	1542	0	1517	76	0
35	1d	1655	0	1672	46	0
35	2d	1674	0	1714	68	0
36	1e	1129	0	1185	44	0
36	2e	1133	0	1191	52	0
37	1f	810	0	804	15	0
37	2f	816	0	808	25	0
38	1g	1231	0	1238	32	0
38	2g	1235	0	1249	48	0
39	1h	1088	0	1126	43	0
39	2h	1088	0	1126	38	0
40	1i	983	0	986	45	0
40	2i	978	0	966	52	0
41	1j	709	0	650	27	0
41	2j	714	0	672	39	0
42	1k	829	0	825	22	0
42	2k	833	0	834	30	0
43	1l	932	0	981	20	0
43	2l	932	0	981	24	0
44	1m	958	0	1002	23	0
44	2m	950	0	988	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	17	0
45	2n	492	0	529	26	0
46	1o	728	0	760	14	0
46	2o	728	0	760	21	0
47	1p	681	0	697	24	0
47	2p	677	0	686	22	0
48	1q	823	0	891	22	0
48	2q	823	0	891	39	0
49	1r	555	0	618	14	0
49	2r	555	0	618	24	0
50	1s	652	0	662	27	0
50	2s	646	0	644	28	0
51	1t	728	0	798	28	0
51	2t	727	0	796	23	0
52	1u	199	0	208	13	0
52	2u	199	0	208	12	0
53	1v	283	0	141	0	0
53	2v	283	0	142	9	0
54	1w	1599	0	800	29	0
54	2w	1599	0	801	49	0
55	1x	1646	0	839	16	0
55	2x	1646	0	837	34	0
56	1z	27	0	28	3	0
56	2z	27	0	28	3	0
57	1y	1577	0	799	45	0
57	2y	1577	0	798	34	0
58	10	8	0	0	0	0
58	11	6	0	0	0	0
58	12	2	0	0	0	0
58	13	6	0	0	0	0
58	15	10	0	0	0	0
58	16	1	0	0	0	0
58	17	5	0	0	0	0
58	18	7	0	0	0	0
58	19	1	0	0	0	0
58	1A	1102	0	0	0	0
58	1B	36	0	0	0	0
58	1D	14	0	0	0	0
58	1E	14	0	0	0	0
58	1F	12	0	0	0	0
58	1G	5	0	0	0	0
58	1H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1I	1	0	0	0	0
58	1N	4	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	3	0	0	0	0
58	1S	3	0	0	0	0
58	1T	2	0	0	0	0
58	1U	11	0	0	0	0
58	1V	7	0	0	0	0
58	1W	7	0	0	0	0
58	1X	5	0	0	0	0
58	1Y	3	0	0	0	0
58	1Z	3	0	0	0	0
58	1a	215	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	1	0	0	0	0
58	1f	2	0	0	0	0
58	1l	2	0	0	0	0
58	1m	2	0	0	0	0
58	1n	2	0	0	0	0
58	1s	1	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	6	0	0	0	0
58	1x	11	0	0	0	0
58	20	3	0	0	0	0
58	23	4	0	0	0	0
58	25	6	0	0	0	0
58	26	1	0	0	0	0
58	27	3	0	0	0	0
58	28	4	0	0	0	0
58	2A	858	0	0	0	0
58	2B	20	0	0	0	0
58	2D	9	0	0	0	0
58	2E	7	0	0	0	0
58	2F	6	0	0	0	0
58	2G	1	0	0	0	0
58	2O	2	0	0	0	0
58	2P	2	0	0	0	0
58	2Q	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2R	1	0	0	0	0
58	2T	2	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	2	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	230	0	0	0	0
58	2d	2	0	0	0	0
58	2e	2	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2i	1	0	0	0	0
58	2j	2	0	0	0	0
58	2k	1	0	0	0	0
58	2l	6	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	2v	5	0	0	0	0
58	2w	2	0	0	0	0
58	2x	5	0	0	0	0
58	2y	1	0	0	0	0
59	1A	1	0	0	0	0
59	2x	1	0	0	0	0
60	1A	51	0	67	4	0
60	2A	51	0	67	2	0
61	14	1	0	0	0	0
61	15	1	0	0	0	0
61	16	1	0	0	0	0
61	19	1	0	0	0	0
61	1Y	1	0	0	0	0
61	1n	1	0	0	0	0
61	24	1	0	0	0	0
61	25	1	0	0	0	0
61	26	1	0	0	0	0
61	29	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2n	1	0	0	0	0
62	1d	8	0	0	1	0
62	2d	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	10	13	0	0	2	0
63	11	9	0	0	0	0
63	12	3	0	0	1	0
63	13	6	0	0	1	0
63	14	1	0	0	0	0
63	15	5	0	0	0	0
63	16	3	0	0	0	0
63	17	8	0	0	0	0
63	18	10	0	0	1	0
63	1A	1896	0	0	95	0
63	1B	61	0	0	4	0
63	1D	25	0	0	2	0
63	1E	30	0	0	3	0
63	1F	17	0	0	2	0
63	1G	3	0	0	0	0
63	1H	2	0	0	0	0
63	1N	4	0	0	0	0
63	1O	5	0	0	0	0
63	1P	25	0	0	1	0
63	1Q	7	0	0	0	0
63	1R	16	0	0	4	0
63	1S	3	0	0	0	0
63	1T	5	0	0	0	0
63	1U	14	0	0	0	0
63	1V	9	0	0	0	0
63	1W	6	0	0	0	0
63	1X	8	0	0	0	0
63	1Y	5	0	0	0	0
63	1Z	1	0	0	0	0
63	1a	305	0	0	21	0
63	1b	1	0	0	0	0
63	1e	1	0	0	0	0
63	1f	1	0	0	0	0
63	1i	1	0	0	0	0
63	1l	4	0	0	0	0
63	1q	2	0	0	0	0
63	1u	1	0	0	0	0
63	1v	5	0	0	0	0
63	1w	6	0	0	0	0
63	1x	5	0	0	0	0
63	1y	1	0	0	0	0
63	20	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	21	6	0	0	1	0
63	25	1	0	0	1	0
63	27	3	0	0	0	0
63	28	2	0	0	0	0
63	29	1	0	0	0	0
63	2A	992	0	0	91	0
63	2B	19	0	0	0	0
63	2D	20	0	0	1	0
63	2E	13	0	0	2	0
63	2F	14	0	0	0	0
63	2N	1	0	0	0	0
63	2O	2	0	0	0	0
63	2P	7	0	0	0	0
63	2Q	1	0	0	0	0
63	2R	3	0	0	0	0
63	2T	5	0	0	0	0
63	2U	3	0	0	0	0
63	2W	2	0	0	0	0
63	2X	2	0	0	2	0
63	2Y	1	0	0	0	0
63	2Z	1	0	0	0	0
63	2a	172	0	0	23	0
63	2e	1	0	0	0	0
63	2g	1	0	0	0	0
63	2j	2	0	0	1	0
63	2l	3	0	0	0	0
63	2p	3	0	0	0	0
63	2r	1	0	0	0	0
63	2t	1	0	0	0	0
63	2v	2	0	0	0	0
63	2w	1	0	0	0	0
63	2x	2	0	0	0	0
All	All	299863	0	196891	5069	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 11.

The worst 5 of 5069 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	1.21	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:51:A:N6	54:2w:63:U:C4	2.23	1.05
1:1A:1082:U:O4	1:1A:1086:A:N1	1.94	1.00
54:2w:51:A:N6	54:2w:63:U:N3	2.12	0.98
57:1y:4:U:H3	57:1y:69:A:N6	1.64	0.96

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%)	250 (92%)	20 (7%)	3 (1%)	11	19
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	39
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24	39
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	39
5	2F	201/210 (96%)	183 (91%)	17 (8%)	1 (0%)	24	39
6	1G	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	21	34
6	2G	179/182 (98%)	150 (84%)	24 (13%)	5 (3%)	4	6
7	1H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	21	34
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	7	12
8	1I	144/148 (97%)	129 (90%)	13 (9%)	2 (1%)	9	14
8	2I	144/148 (97%)	123 (85%)	20 (14%)	1 (1%)	18	30
9	1N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	30
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	30
10	1O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	27
10	2O	120/122 (98%)	105 (88%)	14 (12%)	1 (1%)	16	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	6
11	2P	147/150 (98%)	127 (86%)	17 (12%)	3 (2%)	6	10
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	95 (88%)	7 (6%)	6 (6%)	1	1
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7	12
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	3	5
17	2V	99/101 (98%)	91 (92%)	5 (5%)	3 (3%)	3	5
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	14	24
19	1X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	19
19	2X	93/96 (97%)	81 (87%)	10 (11%)	2 (2%)	5	9
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	10
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	14
21	2Z	156/206 (76%)	123 (79%)	28 (18%)	5 (3%)	3	4
22	10	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	19
23	21	95/98 (97%)	88 (93%)	7 (7%)	0	100	100
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	46 (69%)	15 (22%)	6 (9%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	46 (69%)	18 (27%)	3 (4%)	2	2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	50 (88%)	7 (12%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	3	5
33	1b	229/256 (90%)	196 (86%)	24 (10%)	9 (4%)	2	3
33	2b	229/256 (90%)	183 (80%)	39 (17%)	7 (3%)	3	5
34	1c	204/239 (85%)	177 (87%)	25 (12%)	2 (1%)	12	20
34	2c	204/239 (85%)	159 (78%)	39 (19%)	6 (3%)	3	5
35	1d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	12	20
35	2d	206/209 (99%)	176 (85%)	27 (13%)	3 (2%)	8	13
36	1e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	9
36	2e	146/162 (90%)	122 (84%)	21 (14%)	3 (2%)	5	9
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	130 (85%)	21 (14%)	2 (1%)	9	16
38	2g	153/156 (98%)	124 (81%)	26 (17%)	3 (2%)	6	10
39	1h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	18	30
39	2h	135/138 (98%)	120 (89%)	15 (11%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	27
40	2i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	7	12
41	1j	95/105 (90%)	76 (80%)	16 (17%)	3 (3%)	3	4
41	2j	94/105 (90%)	77 (82%)	13 (14%)	4 (4%)	2	2
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14	24
42	2k	112/129 (87%)	94 (84%)	14 (12%)	4 (4%)	2	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	16	27
43	2l	119/132 (90%)	101 (85%)	16 (13%)	2 (2%)	7	12
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	7	12
44	2m	120/126 (95%)	100 (83%)	19 (16%)	1 (1%)	16	27
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	4
46	1o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	17
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12	20
48	2q	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	2	3
49	1r	66/88 (75%)	56 (85%)	9 (14%)	1 (2%)	8	13
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	13
50	1s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	63 (78%)	16 (20%)	2 (2%)	4	7
51	1t	94/106 (89%)	84 (89%)	7 (7%)	3 (3%)	3	4
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	2
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	4 (19%)	0	100	100
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	0	1 (100%)	0	100	100
All	All	11372/12134 (94%)	10153 (89%)	1069 (9%)	150 (1%)	9	16

5 of 150 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	126	PRO
8	1I	85	GLU
11	1P	36	LYS
19	1X	93	GLU
21	1Z	53	ILE

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%)	204 (95%)	11 (5%)	21	36
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	24
4	1E	164/166 (99%)	152 (93%)	12 (7%)	13	22
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	25
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9	15
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	9
6	1G	143/156 (92%)	123 (86%)	20 (14%)	3	5
6	2G	143/156 (92%)	111 (78%)	32 (22%)	1	1
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	14
7	2H	144/148 (97%)	126 (88%)	18 (12%)	4	6
8	1I	113/124 (91%)	92 (81%)	21 (19%)	1	2
8	2I	105/124 (85%)	84 (80%)	21 (20%)	1	1
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	21
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	9
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	47
10	2O	100/100 (100%)	88 (88%)	12 (12%)	5	7
11	1P	115/116 (99%)	101 (88%)	14 (12%)	5	7
11	2P	115/116 (99%)	97 (84%)	18 (16%)	2	3
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	14
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	11
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	24
13	2R	101/101 (100%)	93 (92%)	8 (8%)	11	19
14	1S	86/88 (98%)	74 (86%)	12 (14%)	3	5
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	2
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	24
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	16
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	16
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	21
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	6
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	25
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	32
19	1X	77/78 (99%)	69 (90%)	8 (10%)	7	10
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	48
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	6
20	2Y	85/91 (93%)	70 (82%)	15 (18%)	2	2
21	1Z	135/179 (75%)	112 (83%)	23 (17%)	2	2
21	2Z	137/179 (76%)	111 (81%)	26 (19%)	1	2
22	10	65/67 (97%)	58 (89%)	7 (11%)	6	9
22	20	65/67 (97%)	62 (95%)	3 (5%)	24	41
23	11	80/83 (96%)	72 (90%)	8 (10%)	7	11
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	11
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	14
24	22	65/67 (97%)	60 (92%)	5 (8%)	12	20
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	7
25	23	50/52 (96%)	44 (88%)	6 (12%)	5	7
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	1
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	4
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	7
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	11
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	11
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	3
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	38
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	11
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	50
30	28	54/55 (98%)	49 (91%)	5 (9%)	8	13
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	30
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	3
33	2b	187/220 (85%)	150 (80%)	37 (20%)	1	1
34	1c	142/188 (76%)	125 (88%)	17 (12%)	5	7
34	2c	140/188 (74%)	115 (82%)	25 (18%)	2	2
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	8
35	2d	173/181 (96%)	152 (88%)	21 (12%)	5	7
36	1e	113/123 (92%)	97 (86%)	16 (14%)	3	5
36	2e	114/123 (93%)	90 (79%)	24 (21%)	1	1
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	13
37	2f	85/90 (94%)	74 (87%)	11 (13%)	4	6
38	1g	119/127 (94%)	100 (84%)	19 (16%)	2	3
38	2g	120/127 (94%)	103 (86%)	17 (14%)	3	5
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	19
39	2h	114/119 (96%)	97 (85%)	17 (15%)	3	4
40	1i	90/99 (91%)	75 (83%)	15 (17%)	2	3
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	3
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	7
41	2j	69/92 (75%)	56 (81%)	13 (19%)	1	2
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	9
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	36
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5	8
44	1m	93/101 (92%)	78 (84%)	15 (16%)	2	3
44	2m	92/101 (91%)	71 (77%)	21 (23%)	1	1
45	1n	49/50 (98%)	47 (96%)	2 (4%)	27	46
45	2n	49/50 (98%)	41 (84%)	8 (16%)	2	3
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	10
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	36
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2	2
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	82 (87%)	12 (13%)	4	6
48	2q	94/97 (97%)	81 (86%)	13 (14%)	3	5
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	36
49	2r	59/77 (77%)	50 (85%)	9 (15%)	3	4
50	1s	69/80 (86%)	58 (84%)	11 (16%)	2	3
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	2
51	1t	70/82 (85%)	63 (90%)	7 (10%)	7	11
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	6
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	3
52	2u	18/22 (82%)	13 (72%)	5 (28%)	0	0
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%)	8196 (88%)	1111 (12%)	5	7

5 of 1111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	2e	101	ILE
38	2g	78	ARG
36	2e	100	VAL
44	2m	115	LYS
39	1h	99	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 164 such sidechains are listed below:

Mol	Chain	Res	Type
21	2Z	75	ASN
37	2f	73	ASN
24	22	65	ASN
33	2b	212	GLN
41	2j	21	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	482 (16%)	21 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2791/2915 (95%)	519 (18%)	26 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	32 (27%)	1 (0%)
32	1a	1497/1521 (98%)	271 (18%)	0
32	2a	1501/1521 (98%)	354 (23%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	28 (39%)	0
54	2w	71/76 (93%)	30 (42%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	14 (18%)	0
57	1y	72/76 (94%)	33 (45%)	0
57	2y	72/76 (94%)	34 (47%)	0
All	All	9350/9620 (97%)	1824 (19%)	48 (0%)

5 of 1824 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	33	U
1	1A	34	C
1	1A	36	G

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	479	A
1	2A	1420	U
1	2A	528	A
1	2A	856	C
1	2A	1530	C

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	5MU	2y	54	57	19,22,23	1.43	5 (26%)	27,32,35	1.85	5 (18%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	2.05	9 (27%)
1	5MU	1A	1939	58,1	19,22,23	1.41	5 (26%)	27,32,35	2.24	6 (22%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.04	4 (19%)
57	PSU	1y	39	57	18,21,22	1.33	3 (16%)	21,30,33	2.20	4 (19%)
54	PSU	1w	55	54	18,21,22	1.33	2 (11%)	21,30,33	1.96	4 (19%)
55	8AN	1x	76	58,55	21,24,25	1.40	3 (14%)	26,35,38	2.60	10 (38%)
57	5MU	1y	54	57	19,22,23	1.40	5 (26%)	27,32,35	2.03	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.43	3 (16%)	21,30,33	2.06	4 (19%)
54	T6A	2w	37	54	31,34,35	1.40	4 (12%)	43,49,52	2.07	10 (23%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.24	8 (24%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.14	3 (11%)
1	2MA	2A	2503	58,1	22,25,26	1.43	4 (18%)	32,37,40	2.20	9 (28%)
55	8AN	2x	76	58,55,59	21,24,25	1.44	4 (19%)	26,35,38	3.80	11 (42%)
32	4OC	2a	1402	32,58	20,23,24	0.76	0	25,32,35	1.10	3 (12%)
32	PSU	2a	516	32	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
54	PSU	2w	39	54	18,21,22	1.32	2 (11%)	21,30,33	2.07	3 (14%)
1	PSU	1A	2605	58,1	18,21,22	1.37	3 (16%)	21,30,33	2.18	4 (19%)
32	5MC	1a	967	32	19,22,23	1.52	3 (15%)	26,32,35	1.10	2 (7%)
1	5MC	1A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.17	2 (7%)
57	PSU	2y	39	57	18,21,22	1.31	2 (11%)	21,30,33	2.08	4 (19%)
54	G7M	2w	46	54	23,26,27	1.53	3 (13%)	34,39,42	1.77	5 (14%)
1	5MC	2A	1962	58,1	19,22,23	1.59	3 (15%)	26,32,35	1.15	2 (7%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.15	3 (14%)
1	OMG	2A	2251	58,55,1	23,26,27	1.24	3 (13%)	32,38,41	1.85	6 (18%)
32	M2G	2a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.94	6 (18%)
55	5MU	2x	54	55	19,22,23	1.36	5 (26%)	27,32,35	2.04	6 (22%)
1	OMU	2A	2552	58,1	19,22,23	1.20	2 (10%)	25,31,34	1.81	5 (20%)
32	UR3	1a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.78	3 (11%)
32	PSU	1a	516	32,58	18,21,22	1.39	2 (11%)	21,30,33	2.02	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.11	2 (7%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	1.97	2 (33%)
32	MA6	1a	1519	32	23,26,27	0.41	0	33,38,41	2.04	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.90	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.85	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.05	9 (27%)
1	5MU	2A	1939	1	19,22,23	1.38	4 (21%)	27,32,35	2.20	6 (22%)
1	2MA	1A	2503	58,1	22,25,26	1.47	5 (22%)	32,37,40	2.35	8 (25%)
32	2MG	2a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.11	7 (21%)
32	G7M	2a	527	32,58	23,26,27	1.49	3 (13%)	34,39,42	1.71	5 (14%)
43	0TD	2l	92	43	8,9,10	4.54	1 (12%)	6,11,13	2.44	1 (16%)
55	4SU	1x	8	55	18,21,22	2.26	5 (27%)	25,30,33	1.42	5 (20%)
55	5MC	2x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.26	4 (15%)
1	OMU	1A	2552	58,1	19,22,23	1.21	3 (15%)	25,31,34	1.77	5 (20%)
54	5MU	2w	54	54	19,22,23	1.47	5 (26%)	27,32,35	1.59	5 (18%)
54	PSU	2w	55	58,54	18,21,22	1.33	2 (11%)	21,30,33	2.01	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.85	0	25,31,34	0.99	1 (4%)
1	5MU	1A	1915	1	19,22,23	1.34	3 (15%)	27,32,35	2.06	7 (25%)
55	5MC	1x	32	55	19,22,23	1.62	3 (15%)	26,32,35	1.21	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.16	3 (11%)
32	M2G	1a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.83	5 (15%)
32	G7M	1a	527	32,58	23,26,27	1.53	4 (17%)	34,39,42	1.68	5 (14%)
54	5MU	1w	54	54	19,22,23	1.36	4 (21%)	27,32,35	2.14	6 (22%)
54	U8U	1w	34	53,54	20,24,25	1.39	3 (15%)	22,34,37	0.97	2 (9%)
56	FME	2z	1	56	8,9,10	0.98	0	8,9,11	0.76	0
32	UR3	2a	1498	32,58	19,22,23	0.97	1 (5%)	26,32,35	1.75	3 (11%)
57	T6A	2y	37	57	21,24,35	1.58	4 (19%)	30,35,52	2.06	8 (26%)
57	G7M	2y	46	57	23,26,27	1.55	3 (13%)	34,39,42	1.77	5 (14%)
54	A1B8A	1w	76	54	30,33,34	1.27	4 (13%)	36,46,49	1.92	9 (25%)
32	5MC	1a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
32	5MC	2a	967	32	19,22,23	1.80	3 (15%)	26,32,35	1.18	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.79	3 (15%)	26,32,35	1.20	4 (15%)
55	5MU	1x	54	55	19,22,23	1.43	5 (26%)	27,32,35	1.94	6 (22%)
57	U8U	1y	34	57	17,21,25	1.57	3 (17%)	21,30,37	1.46	3 (14%)
32	5MC	2a	1407	32	19,22,23	1.62	3 (15%)	26,32,35	1.21	3 (11%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	21,30,33	1.97	5 (23%)
54	U8U	2w	34	53,54	20,24,25	1.34	3 (15%)	22,34,37	1.09	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	FME	1z	1	56	8,9,10	1.06	0	8,9,11	0.74	0
1	5MU	2A	1915	1	19,22,23	1.47	5 (26%)	27,32,35	2.04	6 (22%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	1.04	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	1.87	3 (14%)
54	T6A	1w	37	54	31,34,35	1.40	4 (12%)	43,49,52	1.86	9 (20%)
57	T6A	1y	37	57	21,24,35	1.57	4 (19%)	30,35,52	1.98	7 (23%)
1	OMG	1A	2251	58,55,1	23,26,27	1.21	3 (13%)	32,38,41	1.99	7 (21%)
54	G7M	1w	46	54	23,26,27	1.52	4 (17%)	34,39,42	1.77	5 (14%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.13	10 (30%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
57	PSU	2y	55	57	18,21,22	1.42	2 (11%)	21,30,33	2.09	3 (14%)
54	A1B8A	2w	76	54	30,33,34	1.25	3 (10%)	36,46,49	1.91	9 (25%)
55	4SU	2x	8	55	18,21,22	2.06	5 (27%)	25,30,33	1.35	3 (12%)
57	U8U	2y	34	57,53	17,21,25	1.65	4 (23%)	21,30,37	1.51	3 (14%)
1	5MC	1A	1962	58,1	19,22,23	1.82	3 (15%)	26,32,35	1.22	3 (11%)
57	PSU	1y	55	57	18,21,22	1.38	2 (11%)	21,30,33	2.18	4 (19%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
57	G7M	1y	46	57	23,26,27	1.65	3 (13%)	34,39,42	1.86	3 (8%)

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
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	58,55	-	3/7/25/26	0/3/3/3
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	T6A	2w	37	54	-	4/23/41/42	0/3/3/3
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	8AN	2x	76	58,55,59	-	3/7/25/26	0/3/3/3
32	4OC	2a	1402	32,58	-	0/9/29/30	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57	-	1/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	58,55,1	-	1/9/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,58	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	2/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	G7M	2a	527	32,58	-	3/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
54	5MU	2w	54	54	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	58,54	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	32,58	-	2/7/25/26	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	U8U	1w	34	53,54	-	0/10/28/29	0/2/2/2
56	FME	2z	1	56	-	4/7/9/11	-
32	UR3	2a	1498	32,58	-	0/7/25/26	0/2/2/2
57	T6A	2y	37	57	-	0/7/25/42	0/3/3/3
57	G7M	2y	46	57	-	0/7/25/26	0/3/3/3
54	A1B8A	1w	76	54	-	3/20/38/39	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
57	U8U	1y	34	57	-	0/7/25/29	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	U8U	2w	34	53,54	-	2/10/28/29	0/2/2/2
56	FME	1z	1	56	-	7/7/9/11	-
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	2/7/25/26	0/2/2/2
54	T6A	1w	37	54	-	2/23/41/42	0/3/3/3
57	T6A	1y	37	57	-	2/7/25/42	0/3/3/3
1	OMG	1A	2251	58,55,1	-	0/9/27/28	0/3/3/3
54	G7M	1w	46	54	-	2/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	2/7/25/26	0/2/2/2
54	A1B8A	2w	76	54	-	3/20/38/39	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
57	U8U	2y	34	57,53	-	2/7/25/29	0/2/2/2
1	5MC	1A	1962	58,1	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	0/7/25/26	0/3/3/3

The worst 5 of 240 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.39	1.69	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.13	1.70	1.82
32	2a	967	5MC	C5-C4	6.76	1.49	1.44
1	1A	1962	5MC	C5-C4	6.75	1.49	1.44
32	2a	1400	5MC	C5-C4	6.69	1.49	1.44

The worst 5 of 402 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	76	8AN	O4'-C1'-N9	14.20	135.35	108.09
1	2A	2503	2MA	C5-C4-N3	-7.94	118.82	127.18
1	1A	2503	2MA	C5-C4-N3	-7.50	119.28	127.18
32	2a	1498	UR3	C4-N3-C2	-7.08	118.88	124.58
32	1a	1498	UR3	C4-N3-C2	-7.06	118.89	124.58

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
55	1x	76	8AN	C4'-C5'-O5'-P
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	1518	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

52 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1518	MA6	1	0
1	1A	1939	5MU	2	0
55	2x	55	PSU	1	0
57	1y	39	PSU	1	0
54	1w	55	PSU	1	0
55	1x	76	8AN	2	0
57	1y	54	5MU	3	0
54	2w	37	T6A	1	0
1	2A	2503	2MA	2	0
55	2x	76	8AN	1	0
32	2a	1402	4OC	2	0
32	2a	516	PSU	2	0
54	2w	39	PSU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	967	5MC	1	0
57	2y	39	PSU	1	0
54	2w	46	G7M	1	0
55	1x	55	PSU	1	0
1	2A	2251	OMG	1	0
1	2A	2552	OMU	1	0
43	1l	92	0TD	2	0
32	1a	1519	MA6	1	0
32	1a	1400	5MC	1	0
32	2a	1518	MA6	3	0
1	2A	1939	5MU	2	0
1	1A	2503	2MA	1	0
32	2a	1207	2MG	4	0
43	2l	92	0TD	1	0
55	1x	8	4SU	1	0
1	1A	2552	OMU	1	0
54	2w	54	5MU	2	0
54	2w	55	PSU	1	0
32	2a	1404	5MC	1	0
54	1w	54	5MU	3	0
54	1w	34	U8U	1	0
56	2z	1	FME	1	0
57	2y	37	T6A	2	0
57	2y	46	G7M	3	0
54	1w	76	A1B8A	4	0
32	2a	1400	5MC	4	0
55	1x	54	5MU	1	0
32	2a	1407	5MC	1	0
54	2w	34	U8U	1	0
56	1z	1	FME	1	0
1	2A	1915	5MU	1	0
32	1a	1402	4OC	2	0
57	1y	37	T6A	1	0
1	1A	2251	OMG	1	0
32	2a	1519	MA6	2	0
54	2w	76	A1B8A	2	0
55	2x	8	4SU	2	0
57	2y	34	U8U	1	0
57	1y	55	PSU	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2767 ligands modelled in this entry, 2763 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	SF4	1d	302	35	0,12,12	-	-	-		
60	ERY	2A	3859	-	53,53,53	0.91	1 (1%)	82,82,82	1.52	14 (17%)
60	ERY	1A	4104	-	53,53,53	0.97	2 (3%)	82,82,82	1.44	13 (15%)
62	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
62	SF4	1d	302	35	-	-	0/6/5/5
60	ERY	2A	3859	-	-	19/72/107/107	0/3/3/3
60	ERY	1A	4104	-	-	8/72/107/107	0/3/3/3
62	SF4	2d	303	35	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	2A	3859	ERY	O2-C1	5.21	1.46	1.34
60	1A	4104	ERY	O2-C1	5.15	1.46	1.34
60	1A	4104	ERY	O2-C13	-2.65	1.42	1.46

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	1A	4104	ERY	O3-C3-C4	5.39	114.59	108.23
60	2A	3859	ERY	O5-C16-C17	4.55	110.46	103.86
60	1A	4104	ERY	O7-C5-C6	4.33	111.57	106.40
60	1A	4104	ERY	C6-C5-C4	-3.92	108.20	113.89
60	2A	3859	ERY	O2-C1-C2	3.85	119.76	111.53

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	2A	3859	ERY	C11-C10-C9-C8
60	2A	3859	ERY	C11-C10-C9-O11
60	2A	3859	ERY	C11-C12-C13-O2
60	2A	3859	ERY	C11-C12-C13-C36
60	2A	3859	ERY	C35-C12-C13-O2

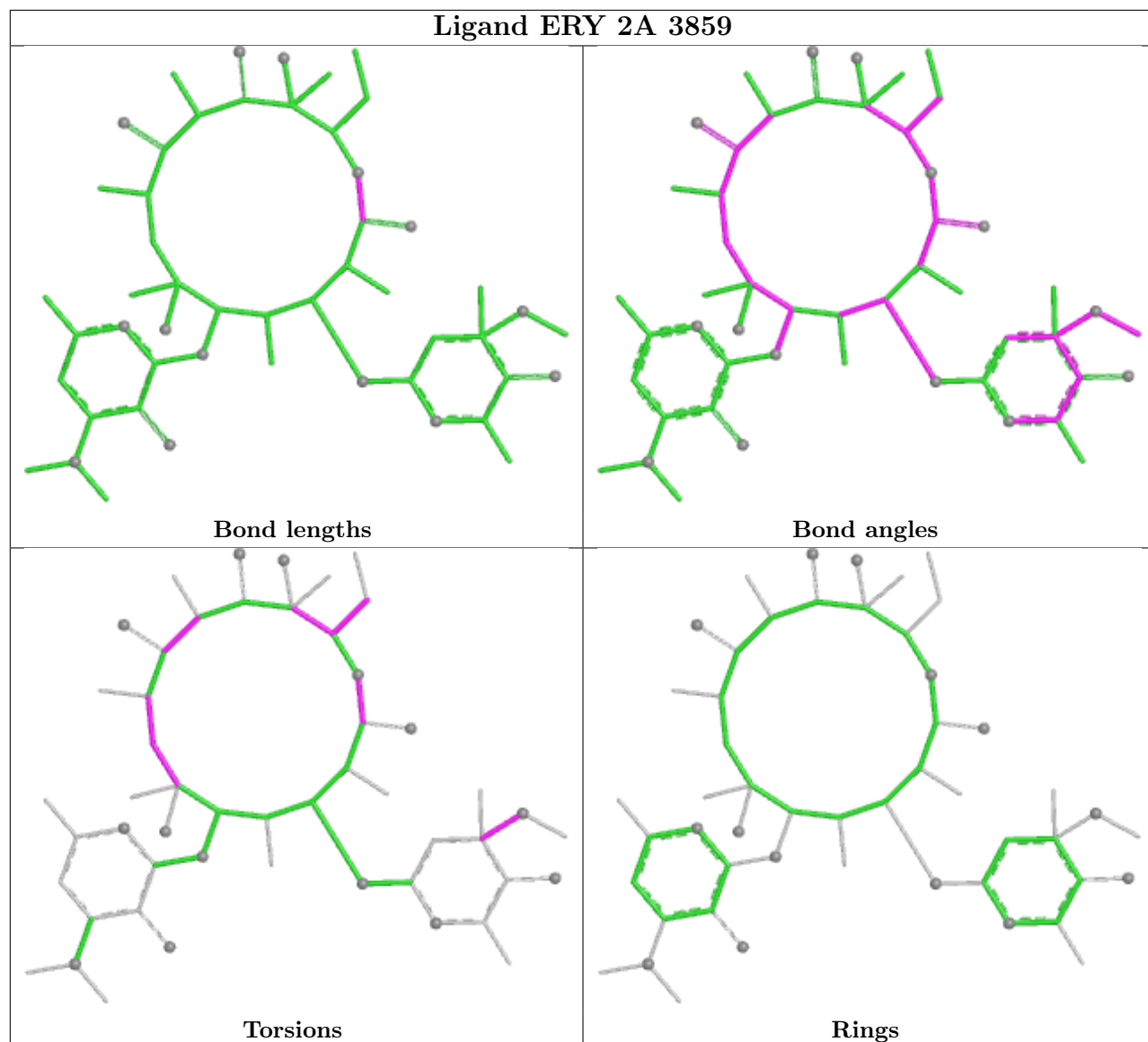
There are no ring outliers.

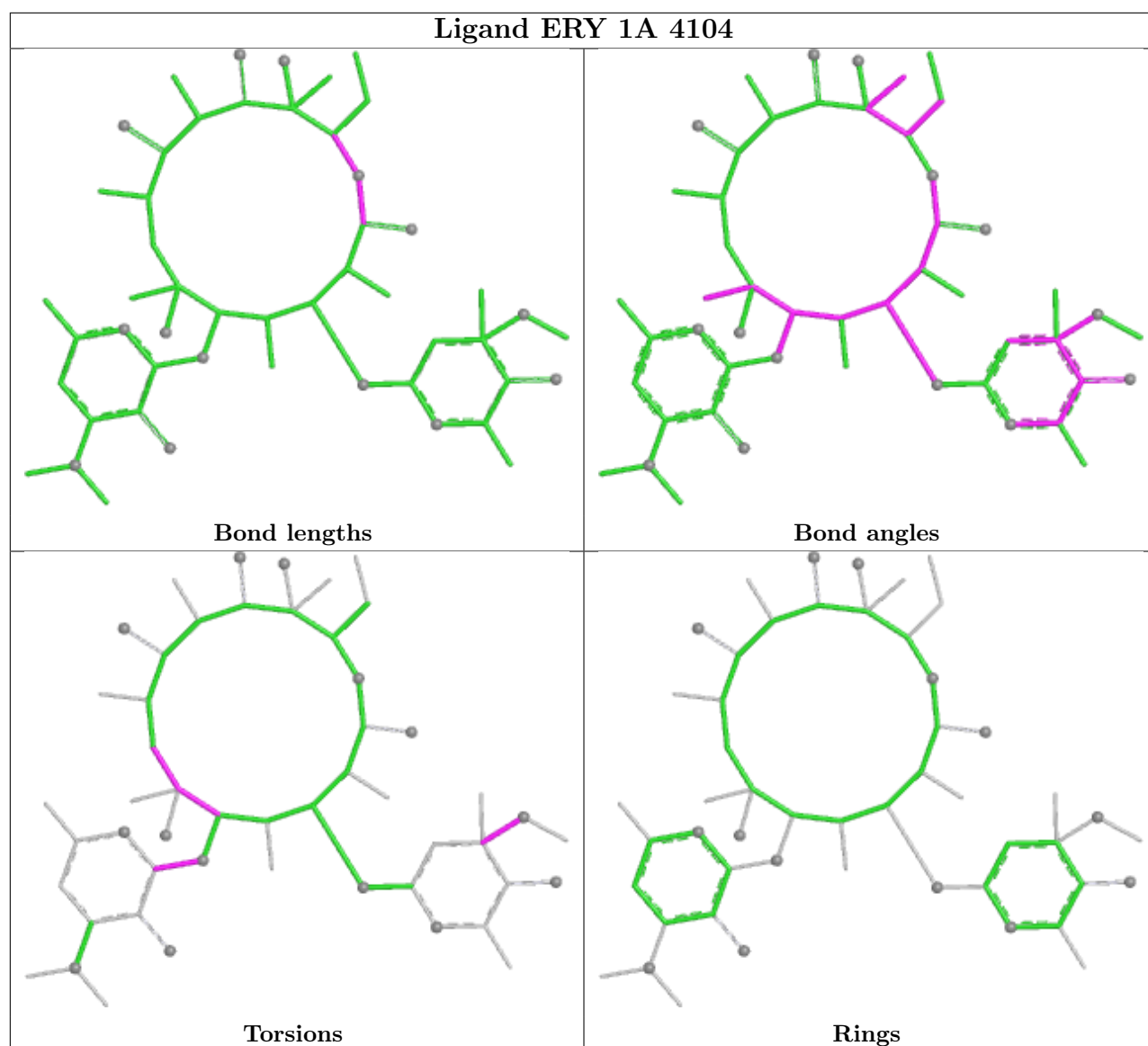
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	1d	302	SF4	1	0
60	2A	3859	ERY	2	0
60	1A	4104	ERY	4	0
62	2d	303	SF4	2	0

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

Ligand ERY 2A 3859





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%)	-0.57	101 (3%) 47 38	17, 35, 91, 102	0
1	2A	2789/2915 (95%)	-0.03	83 (2%) 52 45	30, 57, 88, 104	0
2	1B	120/121 (99%)	-0.46	1 (0%) 82 79	30, 49, 61, 81	0
2	2B	120/121 (99%)	0.77	7 (5%) 29 22	63, 78, 86, 92	0
3	1D	275/276 (99%)	-0.18	1 (0%) 88 87	18, 35, 49, 67	0
3	2D	275/276 (99%)	0.31	4 (1%) 72 67	32, 49, 62, 76	0
4	1E	204/206 (99%)	-0.18	0 100 100	18, 38, 59, 69	0
4	2E	204/206 (99%)	0.26	2 (0%) 79 76	36, 57, 68, 76	0
5	1F	203/210 (96%)	-0.18	0 100 100	18, 41, 65, 83	0
5	2F	203/210 (96%)	0.45	4 (1%) 65 59	35, 65, 77, 82	0
6	1G	181/182 (99%)	0.28	3 (1%) 69 64	39, 57, 68, 78	0
6	2G	181/182 (99%)	1.14	21 (11%) 9 8	68, 77, 82, 89	0
7	1H	174/180 (96%)	0.08	2 (1%) 78 75	35, 52, 62, 67	0
7	2H	174/180 (96%)	0.83	7 (4%) 42 34	64, 77, 82, 88	0
8	1I	146/148 (98%)	0.63	4 (2%) 56 49	41, 68, 76, 80	0
8	2I	146/148 (98%)	0.94	12 (8%) 17 13	54, 70, 79, 82	0
9	1N	140/140 (100%)	-0.10	0 100 100	23, 39, 56, 75	0
9	2N	140/140 (100%)	0.55	4 (2%) 53 46	44, 61, 73, 80	0
10	1O	122/122 (100%)	-0.10	0 100 100	25, 38, 54, 60	0
10	2O	122/122 (100%)	0.42	1 (0%) 82 79	44, 55, 66, 68	0
11	1P	149/150 (99%)	-0.02	2 (1%) 75 71	19, 42, 64, 70	0
11	2P	149/150 (99%)	0.48	3 (2%) 65 59	35, 65, 76, 80	0
12	1Q	141/141 (100%)	-0.09	0 100 100	27, 41, 54, 65	0
12	2Q	141/141 (100%)	0.89	8 (5%) 29 23	48, 65, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.24	0 100 100	25, 35, 46, 58	0
13	2R	118/118 (100%)	0.29	2 (1%) 69 64	38, 51, 59, 66	0
14	1S	110/112 (98%)	0.01	0 100 100	36, 47, 58, 63	0
14	2S	110/112 (98%)	1.20	20 (18%) 3 2	63, 72, 78, 84	0
15	1T	131/146 (89%)	0.01	2 (1%) 72 67	30, 43, 64, 74	0
15	2T	131/146 (89%)	0.37	1 (0%) 82 79	47, 59, 71, 74	0
16	1U	116/118 (98%)	-0.31	0 100 100	22, 31, 48, 60	0
16	2U	116/118 (98%)	0.42	0 100 100	43, 60, 71, 74	0
17	1V	101/101 (100%)	-0.20	0 100 100	21, 41, 56, 67	0
17	2V	101/101 (100%)	0.59	3 (2%) 52 45	43, 68, 74, 80	0
18	1W	112/113 (99%)	-0.39	0 100 100	22, 31, 46, 71	0
18	2W	112/113 (99%)	0.28	1 (0%) 81 78	37, 49, 64, 85	0
19	1X	95/96 (98%)	-0.12	1 (1%) 78 75	23, 36, 55, 68	0
19	2X	95/96 (98%)	0.72	4 (4%) 40 32	42, 58, 69, 75	0
20	1Y	107/110 (97%)	0.08	0 100 100	30, 46, 66, 76	0
20	2Y	107/110 (97%)	0.95	10 (9%) 14 11	57, 67, 76, 82	0
21	1Z	154/206 (74%)	0.52	9 (5%) 29 22	43, 61, 77, 87	0
21	2Z	160/206 (77%)	1.05	17 (10%) 11 9	57, 77, 85, 89	0
22	10	83/85 (97%)	0.08	6 (7%) 21 16	26, 38, 61, 71	0
22	20	83/85 (97%)	1.08	11 (13%) 7 6	46, 63, 73, 83	0
23	11	97/98 (98%)	-0.05	1 (1%) 79 76	26, 43, 62, 67	0
23	21	97/98 (98%)	0.43	3 (3%) 51 43	38, 54, 70, 72	0
24	12	70/72 (97%)	0.01	0 100 100	34, 46, 56, 62	0
24	22	70/72 (97%)	0.47	0 100 100	56, 68, 74, 77	0
25	13	59/60 (98%)	-0.15	1 (1%) 69 64	26, 38, 59, 68	0
25	23	59/60 (98%)	0.62	2 (3%) 48 40	55, 63, 71, 78	0
26	14	69/71 (97%)	0.55	3 (4%) 40 32	51, 72, 84, 89	0
26	24	69/71 (97%)	1.08	8 (11%) 9 8	72, 81, 89, 90	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 64	18, 33, 54, 63	0
27	25	59/60 (98%)	0.18	0 100 100	36, 50, 63, 73	0
28	16	53/54 (98%)	-0.11	0 100 100	30, 41, 53, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.82	2 (3%) 44 36	53, 61, 67, 72	0
29	17	48/49 (97%)	-0.40	0 100 100	21, 26, 50, 57	0
29	27	48/49 (97%)	0.08	1 (2%) 63 57	32, 42, 62, 70	0
30	18	64/65 (98%)	-0.15	1 (1%) 70 66	26, 32, 41, 51	0
30	28	64/65 (98%)	0.59	0 100 100	45, 54, 63, 67	0
31	19	37/37 (100%)	-0.14	1 (2%) 56 49	27, 40, 57, 62	0
31	29	37/37 (100%)	1.11	2 (5%) 31 25	59, 65, 75, 81	0
32	1a	1488/1521 (97%)	0.13	26 (1%) 69 64	32, 65, 88, 100	0
32	2a	1491/1521 (98%)	0.54	69 (4%) 37 29	53, 76, 91, 102	0
33	1b	231/256 (90%)	0.79	21 (9%) 15 11	62, 74, 81, 88	0
33	2b	231/256 (90%)	1.41	51 (22%) 2 1	68, 80, 85, 90	0
34	1c	206/239 (86%)	0.57	4 (1%) 66 61	56, 68, 77, 81	0
34	2c	206/239 (86%)	1.31	37 (17%) 3 2	69, 80, 84, 90	0
35	1d	208/209 (99%)	0.78	13 (6%) 26 19	51, 65, 74, 76	0
35	2d	208/209 (99%)	0.74	9 (4%) 40 32	58, 69, 77, 82	0
36	1e	148/162 (91%)	0.39	1 (0%) 84 82	49, 61, 68, 77	0
36	2e	148/162 (91%)	1.08	15 (10%) 12 10	65, 73, 79, 86	0
37	1f	100/101 (99%)	0.38	1 (1%) 79 76	52, 64, 71, 74	0
37	2f	100/101 (99%)	0.52	1 (1%) 79 76	58, 68, 75, 77	0
38	1g	155/156 (99%)	0.72	14 (9%) 15 12	52, 67, 79, 84	0
38	2g	155/156 (99%)	1.08	23 (14%) 5 4	67, 77, 84, 89	0
39	1h	137/138 (99%)	0.44	1 (0%) 84 82	55, 64, 69, 75	0
39	2h	137/138 (99%)	0.97	10 (7%) 21 15	64, 73, 78, 81	0
40	1i	127/128 (99%)	0.99	15 (11%) 9 7	49, 73, 78, 80	0
40	2i	127/128 (99%)	1.80	53 (41%) 0 0	70, 80, 85, 88	0
41	1j	97/105 (92%)	1.01	8 (8%) 17 13	55, 73, 81, 84	0
41	2j	96/105 (91%)	1.72	32 (33%) 1 0	68, 81, 86, 87	0
42	1k	114/129 (88%)	0.47	3 (2%) 57 51	42, 64, 74, 82	0
42	2k	114/129 (88%)	0.96	6 (5%) 32 25	57, 71, 78, 80	0
43	1l	121/132 (91%)	0.35	3 (2%) 58 52	44, 55, 64, 71	0
43	2l	121/132 (91%)	0.91	8 (6%) 24 18	56, 69, 75, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.60	7 (5%) 29 23	54, 67, 77, 86	0
44	2m	122/126 (96%)	1.50	24 (19%) 3 2	70, 80, 85, 90	0
45	1n	60/61 (98%)	0.88	5 (8%) 17 12	55, 63, 72, 74	0
45	2n	60/61 (98%)	1.95	26 (43%) 0 0	69, 80, 84, 87	0
46	1o	88/89 (98%)	0.59	0 100 100	46, 62, 71, 74	0
46	2o	88/89 (98%)	0.73	2 (2%) 61 54	58, 70, 75, 78	0
47	1p	82/88 (93%)	1.22	18 (21%) 2 1	57, 67, 74, 82	0
47	2p	82/88 (93%)	0.83	4 (4%) 35 27	53, 66, 74, 78	0
48	1q	99/105 (94%)	0.81	4 (4%) 42 34	53, 65, 71, 74	0
48	2q	99/105 (94%)	0.88	6 (6%) 27 20	60, 69, 76, 79	0
49	1r	68/88 (77%)	0.50	2 (2%) 53 46	54, 64, 72, 76	0
49	2r	68/88 (77%)	0.44	1 (1%) 72 67	60, 70, 76, 82	0
50	1s	83/93 (89%)	0.73	2 (2%) 59 53	61, 70, 77, 80	0
50	2s	83/93 (89%)	1.74	29 (34%) 1 0	76, 83, 88, 89	0
51	1t	96/106 (90%)	0.93	11 (11%) 9 8	58, 67, 74, 80	0
51	2t	96/106 (90%)	0.77	7 (7%) 21 15	54, 68, 76, 79	0
52	1u	23/27 (85%)	0.85	0 100 100	59, 65, 70, 72	0
52	2u	23/27 (85%)	1.79	9 (39%) 1 0	73, 77, 81, 82	0
53	1v	13/24 (54%)	1.28	4 (30%) 1 0	44, 71, 85, 87	0
53	2v	13/24 (54%)	1.81	6 (46%) 0 0	72, 85, 91, 94	0
54	1w	67/76 (88%)	1.23	12 (17%) 3 2	52, 91, 97, 101	0
54	2w	67/76 (88%)	1.63	18 (26%) 1 1	74, 95, 99, 102	0
55	1x	72/77 (93%)	0.22	1 (1%) 73 69	36, 65, 80, 82	0
55	2x	72/77 (93%)	0.63	4 (5%) 30 24	52, 78, 86, 91	0
56	1z	2/3 (66%)	0.85	0 100 100	40, 40, 40, 45	0
56	2z	2/3 (66%)	1.15	0 100 100	58, 58, 58, 63	0
57	1y	68/76 (89%)	1.53	14 (20%) 2 1	52, 95, 100, 101	0
57	2y	68/76 (89%)	1.61	16 (23%) 2 1	68, 97, 101, 104	0
All	All	20884/21754 (96%)	0.30	1039 (4%) 34 26	17, 62, 86, 104	0

The worst 5 of 1039 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	11.1
44	2m	123	ALA	7.2
44	2m	102	ARG	6.9
44	1m	123	ALA	6.2
45	1n	2	ALA	6.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	2w	55	20/21	0.42	0.16	92,99,108,115	0
57	G7M	2y	46	24/25	0.49	0.16	85,98,103,121	0
54	5MU	2w	54	21/22	0.50	0.17	85,93,98,107	0
54	G7M	2w	46	24/25	0.52	0.14	89,95,108,118	0
54	G7M	1w	46	24/25	0.54	0.14	82,90,102,113	0
57	U8U	2y	34	20/24	0.55	0.21	95,100,108,118	0
57	5MU	2y	54	21/22	0.58	0.15	89,97,108,119	0
54	PSU	1w	55	20/21	0.60	0.16	78,94,102,102	0
57	PSU	1y	39	20/21	0.60	0.14	88,94,102,113	0
57	U8U	1y	34	20/24	0.62	0.20	88,94,102,103	0
57	G7M	1y	46	24/25	0.62	0.14	85,94,97,110	0
57	T6A	2y	37	22/33	0.65	0.17	83,93,100,108	0
57	PSU	2y	55	20/21	0.67	0.12	90,97,110,117	0
57	T6A	1y	37	22/33	0.67	0.15	79,87,92,101	0
57	PSU	2y	39	20/21	0.67	0.15	85,90,97,100	0
57	PSU	1y	55	20/21	0.68	0.12	88,94,102,112	0
54	T6A	2w	37	32/33	0.71	0.16	69,87,96,98	0
57	5MU	1y	54	21/22	0.76	0.12	83,89,97,107	0
54	5MU	1w	54	21/22	0.79	0.11	71,87,91,93	0
1	5MU	2A	1915	21/22	0.80	0.14	76,79,82,96	0
54	U8U	2w	34	23/24	0.82	0.17	73,84,89,95	0
54	U8U	1w	34	23/24	0.82	0.16	72,77,85,89	0
54	T6A	1w	37	32/33	0.84	0.15	66,77,83,86	0
32	2MG	2a	1207	24/25	0.85	0.13	78,85,92,100	0
55	4SU	2x	8	20/21	0.85	0.12	70,80,85,89	0
54	PSU	2w	39	20/21	0.85	0.14	79,86,92,95	0
32	5MC	2a	967	21/22	0.86	0.16	63,70,80,85	0
43	0TD	1l	92	10/11	0.87	0.14	45,50,56,69	0
55	5MU	2x	54	21/22	0.87	0.11	75,81,87,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	PSU	2x	55	20/21	0.87	0.10	73,78,81,91	0
32	M2G	2a	966	25/26	0.87	0.17	55,66,85,90	0
32	5MC	2a	1400	21/22	0.88	0.17	68,75,79,81	0
32	PSU	2a	516	20/21	0.88	0.11	73,79,88,88	0
1	PSU	2A	1917	20/21	0.88	0.11	64,74,84,84	0
55	PSU	1x	55	20/21	0.89	0.10	54,64,73,76	0
1	PSU	2A	1911	20/21	0.90	0.10	63,70,79,79	0
32	G7M	2a	527	24/25	0.91	0.14	60,65,70,76	0
54	PSU	1w	39	20/21	0.91	0.10	68,77,83,84	0
32	5MC	2a	1404	21/22	0.91	0.10	55,60,65,68	0
54	A1B8A	2w	76	31/32	0.91	0.14	46,62,66,76	0
43	0TD	2l	92	10/11	0.92	0.12	64,69,77,83	0
55	5MU	1x	54	21/22	0.92	0.10	60,68,72,76	0
55	5MC	2x	32	21/22	0.92	0.12	65,74,77,81	0
1	OMC	2A	1920	21/22	0.92	0.11	58,67,73,76	0
32	4OC	2a	1402	22/23	0.92	0.12	58,64,67,71	0
55	4SU	1x	8	20/21	0.92	0.10	59,64,76,76	0
32	PSU	1a	516	20/21	0.93	0.08	58,64,72,75	0
55	8AN	2x	76	22/23	0.93	0.11	45,53,63,65	0
32	MA6	2a	1518	24/25	0.93	0.11	47,64,69,70	0
56	FME	1z	1	10/11	0.93	0.17	38,49,57,58	0
56	FME	2z	1	10/11	0.93	0.18	57,64,70,70	0
32	5MC	2a	1407	21/22	0.94	0.10	52,59,65,66	0
1	5MC	2A	1962	21/22	0.94	0.11	43,52,62,64	0
54	A1B8A	1w	76	31/32	0.94	0.11	33,45,52,53	0
1	5MC	2A	1942	21/22	0.95	0.10	49,63,66,72	0
32	G7M	1a	527	24/25	0.95	0.09	39,45,52,54	0
55	5MC	1x	32	21/22	0.95	0.11	46,49,51,59	0
32	2MG	1a	1207	24/25	0.95	0.09	51,67,70,73	0
1	5MU	1A	1915	21/22	0.95	0.09	49,55,61,66	0
32	UR3	2a	1498	21/22	0.95	0.11	47,61,67,67	0
55	8AN	1x	76	22/23	0.95	0.09	26,40,52,55	0
32	5MC	1a	1404	21/22	0.96	0.09	36,44,49,50	0
32	MA6	1a	1519	24/25	0.96	0.10	32,42,45,46	0
1	OMG	2A	2251	24/25	0.96	0.09	33,41,48,54	0
1	2MA	2A	2503	23/24	0.96	0.10	31,37,44,46	0
1	5MC	1A	1942	21/22	0.96	0.09	32,43,48,60	0
32	M2G	1a	966	25/26	0.96	0.09	46,55,60,62	0
32	5MC	1a	967	21/22	0.96	0.10	54,58,61,65	0
32	MA6	2a	1519	24/25	0.96	0.13	53,63,70,71	0
1	PSU	1A	1917	20/21	0.96	0.07	41,50,59,64	0
1	OMC	1A	1920	21/22	0.97	0.08	34,40,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	1400	21/22	0.97	0.09	41,48,53,56	0
32	4OC	1a	1402	22/23	0.97	0.09	42,48,51,55	0
1	OMU	2A	2552	21/22	0.97	0.09	32,42,46,51	0
1	PSU	2A	2605	20/21	0.97	0.07	31,39,42,43	0
1	PSU	1A	1911	20/21	0.97	0.07	42,46,50,50	0
32	5MC	1a	1407	21/22	0.97	0.08	29,37,42,42	0
1	5MU	2A	1939	21/22	0.97	0.08	33,40,45,47	0
32	MA6	1a	1518	24/25	0.97	0.10	31,41,46,47	0
1	2MA	1A	2503	23/24	0.98	0.06	14,18,23,24	0
1	OMU	1A	2552	21/22	0.98	0.06	15,27,29,33	0
1	PSU	1A	2605	20/21	0.98	0.06	18,24,31,32	0
1	5MU	1A	1939	21/22	0.98	0.06	20,27,33,33	0
32	UR3	1a	1498	21/22	0.98	0.07	32,42,45,47	0
1	5MC	1A	1962	21/22	0.99	0.06	19,28,34,42	0
1	OMG	1A	2251	24/25	0.99	0.05	18,23,27,30	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	2A	3750	1/1	0.60	0.24	59,59,59,59	0
58	MG	2A	3646	1/1	0.64	0.18	79,79,79,79	0
58	MG	2a	1803	1/1	0.65	0.18	74,74,74,74	0
58	MG	2A	3495	1/1	0.66	0.18	66,66,66,66	0
58	MG	2A	3193	1/1	0.66	0.28	74,74,74,74	0
58	MG	2A	3733	1/1	0.67	0.20	54,54,54,54	0
58	MG	1A	3813	1/1	0.68	0.18	54,54,54,54	0
58	MG	2A	3383	1/1	0.70	0.17	82,82,82,82	0
58	MG	1A	3512	1/1	0.70	0.20	58,58,58,58	0
58	MG	2a	1807	1/1	0.70	0.27	71,71,71,71	0
58	MG	1A	4080	1/1	0.71	0.25	39,39,39,39	0
58	MG	2a	1610	1/1	0.71	0.38	81,81,81,81	0
58	MG	2A	3692	1/1	0.71	0.23	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3305	1/1	0.71	0.20	71,71,71,71	0
58	MG	1B	230	1/1	0.72	0.14	74,74,74,74	0
58	MG	2a	1819	1/1	0.72	0.13	84,84,84,84	0
58	MG	2A	3171	1/1	0.73	0.18	70,70,70,70	0
58	MG	2A	3519	1/1	0.73	0.21	71,71,71,71	0
58	MG	1A	3878	1/1	0.74	0.35	57,57,57,57	0
58	MG	2A	3375	1/1	0.74	0.17	66,66,66,66	0
58	MG	2a	1641	1/1	0.74	0.29	72,72,72,72	0
58	MG	2A	3663	1/1	0.75	0.18	65,65,65,65	0
58	MG	2w	101	1/1	0.75	0.22	80,80,80,80	0
58	MG	1f	202	1/1	0.76	0.21	76,76,76,76	0
58	MG	1w	105	1/1	0.76	0.12	77,77,77,77	0
58	MG	1A	3413	1/1	0.76	0.15	64,64,64,64	0
58	MG	1A	3885	1/1	0.76	0.15	27,27,27,27	0
58	MG	1a	1633	1/1	0.76	0.25	68,68,68,68	0
58	MG	2A	3744	1/1	0.77	0.16	65,65,65,65	0
58	MG	2A	3606	1/1	0.77	0.22	75,75,75,75	0
58	MG	2B	213	1/1	0.77	0.21	71,71,71,71	0
58	MG	2a	1605	1/1	0.77	0.19	71,71,71,71	0
58	MG	1a	1765	1/1	0.77	0.13	76,76,76,76	0
58	MG	1A	4039	1/1	0.77	0.13	55,55,55,55	0
58	MG	2a	1755	1/1	0.77	0.36	80,80,80,80	0
58	MG	2A	3204	1/1	0.77	0.16	67,67,67,67	0
58	MG	2A	3723	1/1	0.77	0.19	62,62,62,62	0
58	MG	2A	3730	1/1	0.77	0.17	74,74,74,74	0
58	MG	1A	3504	1/1	0.77	0.23	67,67,67,67	0
58	MG	2A	3828	1/1	0.78	0.17	52,52,52,52	0
58	MG	1a	1780	1/1	0.78	0.19	44,44,44,44	0
58	MG	2E	301	1/1	0.78	0.13	62,62,62,62	0
58	MG	1A	3598	1/1	0.78	0.15	67,67,67,67	0
58	MG	2A	3721	1/1	0.78	0.12	56,56,56,56	0
58	MG	1B	228	1/1	0.78	0.13	77,77,77,77	0
58	MG	2A	3726	1/1	0.78	0.18	64,64,64,64	0
58	MG	2A	3106	1/1	0.78	0.26	73,73,73,73	0
58	MG	1A	3647	1/1	0.78	0.20	63,63,63,63	0
58	MG	1A	3955	1/1	0.78	0.23	67,67,67,67	0
58	MG	1A	3540	1/1	0.78	0.21	67,67,67,67	0
58	MG	2A	3323	1/1	0.79	0.27	73,73,73,73	0
58	MG	2A	3329	1/1	0.79	0.19	74,74,74,74	0
58	MG	2A	3365	1/1	0.79	0.21	68,68,68,68	0
58	MG	1A	3837	1/1	0.79	0.14	59,59,59,59	0
58	MG	2A	3112	1/1	0.79	0.12	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1800	1/1	0.79	0.15	82,82,82,82	0
58	MG	2A	3664	1/1	0.79	0.16	65,65,65,65	0
58	MG	2A	3478	1/1	0.79	0.29	67,67,67,67	0
58	MG	2A	3845	1/1	0.79	0.13	71,71,71,71	0
58	MG	2j	202	1/1	0.79	0.17	76,76,76,76	0
58	MG	2A	3494	1/1	0.79	0.20	70,70,70,70	0
58	MG	1a	1774	1/1	0.80	0.18	74,74,74,74	0
58	MG	1A	3396	1/1	0.80	0.14	67,67,67,67	0
58	MG	1a	1811	1/1	0.80	0.23	70,70,70,70	0
58	MG	2a	1607	1/1	0.80	0.36	72,72,72,72	0
58	MG	2A	3346	1/1	0.80	0.26	64,64,64,64	0
58	MG	2a	1625	1/1	0.80	0.19	70,70,70,70	0
58	MG	2A	3185	1/1	0.80	0.17	69,69,69,69	0
58	MG	2a	1736	1/1	0.80	0.30	78,78,78,78	0
58	MG	1a	1673	1/1	0.80	0.24	68,68,68,68	0
58	MG	2a	1763	1/1	0.80	0.12	81,81,81,81	0
58	MG	1A	3329	1/1	0.80	0.15	70,70,70,70	0
58	MG	2A	3818	1/1	0.80	0.16	46,46,46,46	0
58	MG	2A	3667	1/1	0.80	0.18	74,74,74,74	0
58	MG	2A	3297	1/1	0.80	0.35	68,68,68,68	0
58	MG	2A	3856	1/1	0.80	0.20	66,66,66,66	0
58	MG	2l	206	1/1	0.80	0.10	75,75,75,75	0
58	MG	2B	206	1/1	0.80	0.24	76,76,76,76	0
58	MG	2w	102	1/1	0.80	0.16	85,85,85,85	0
58	MG	2B	216	1/1	0.81	0.21	78,78,78,78	0
58	MG	2A	3665	1/1	0.81	0.12	75,75,75,75	0
58	MG	2A	3089	1/1	0.81	0.26	65,65,65,65	0
58	MG	2A	3091	1/1	0.81	0.17	74,74,74,74	0
58	MG	2a	1609	1/1	0.81	0.13	49,49,49,49	0
58	MG	2A	3102	1/1	0.81	0.29	71,71,71,71	0
58	MG	2a	1613	1/1	0.81	0.39	77,77,77,77	0
58	MG	2a	1618	1/1	0.81	0.15	68,68,68,68	0
58	MG	1a	1621	1/1	0.81	0.21	58,58,58,58	0
58	MG	2a	1632	1/1	0.81	0.32	74,74,74,74	0
58	MG	1A	3961	1/1	0.81	0.10	57,57,57,57	0
58	MG	2a	1735	1/1	0.81	0.21	72,72,72,72	0
58	MG	1a	1779	1/1	0.81	0.13	62,62,62,62	0
58	MG	2a	1739	1/1	0.81	0.17	76,76,76,76	0
58	MG	1a	1660	1/1	0.81	0.10	70,70,70,70	0
58	MG	2A	3734	1/1	0.81	0.14	75,75,75,75	0
58	MG	2a	1793	1/1	0.81	0.18	72,72,72,72	0
58	MG	1a	1803	1/1	0.81	0.15	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	1A	4089	1/1	0.81	0.15	74,74,74,74	0
58	MG	2a	1805	1/1	0.81	0.16	74,74,74,74	0
58	MG	2A	3264	1/1	0.81	0.15	70,70,70,70	0
58	MG	2A	3626	1/1	0.81	0.15	39,39,39,39	0
58	MG	1a	1724	1/1	0.81	0.18	77,77,77,77	0
58	MG	2l	205	1/1	0.81	0.19	54,54,54,54	0
58	MG	2A	3658	1/1	0.81	0.20	72,72,72,72	0
58	MG	2v	103	1/1	0.81	0.42	76,76,76,76	0
58	MG	1a	1740	1/1	0.81	0.16	82,82,82,82	0
58	MG	2A	3075	1/1	0.81	0.12	70,70,70,70	0
58	MG	1a	1781	1/1	0.82	0.13	54,54,54,54	0
58	MG	2A	3369	1/1	0.82	0.21	63,63,63,63	0
58	MG	2A	3114	1/1	0.82	0.27	67,67,67,67	0
58	MG	2A	3121	1/1	0.82	0.18	64,64,64,64	0
58	MG	2A	3442	1/1	0.82	0.11	54,54,54,54	0
58	MG	2a	1701	1/1	0.82	0.18	74,74,74,74	0
58	MG	2a	1722	1/1	0.82	0.15	58,58,58,58	0
58	MG	2A	3466	1/1	0.82	0.21	66,66,66,66	0
58	MG	1A	3975	1/1	0.82	0.16	73,73,73,73	0
58	MG	1A	3514	1/1	0.82	0.27	65,65,65,65	0
58	MG	2A	3772	1/1	0.82	0.14	65,65,65,65	0
58	MG	2A	3802	1/1	0.82	0.15	41,41,41,41	0
58	MG	2a	1775	1/1	0.82	0.14	67,67,67,67	0
58	MG	1A	3881	1/1	0.82	0.13	54,54,54,54	0
58	MG	1A	3205	1/1	0.82	0.23	61,61,61,61	0
58	MG	2A	3238	1/1	0.82	0.13	66,66,66,66	0
58	MG	1w	106	1/1	0.82	0.15	79,79,79,79	0
58	MG	2A	3284	1/1	0.82	0.15	66,66,66,66	0
58	MG	1A	3927	1/1	0.82	0.13	33,33,33,33	0
58	MG	2a	1820	1/1	0.82	0.33	71,71,71,71	0
58	MG	2a	1826	1/1	0.82	0.14	60,60,60,60	0
58	MG	1B	229	1/1	0.82	0.15	61,61,61,61	0
58	MG	2l	201	1/1	0.82	0.30	68,68,68,68	0
58	MG	1A	3334	1/1	0.82	0.10	52,52,52,52	0
58	MG	15	110	1/1	0.82	0.12	50,50,50,50	0
58	MG	2A	3332	1/1	0.82	0.14	74,74,74,74	0
58	MG	1A	3850	1/1	0.82	0.19	71,71,71,71	0
58	MG	2A	3705	1/1	0.82	0.17	62,62,62,62	0
58	MG	2A	3410	1/1	0.83	0.16	52,52,52,52	0
58	MG	2A	3431	1/1	0.83	0.20	50,50,50,50	0
58	MG	1A	3943	1/1	0.83	0.10	30,30,30,30	0
58	MG	2A	3327	1/1	0.83	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3471	1/1	0.83	0.24	49,49,49,49	0
58	MG	2A	3687	1/1	0.83	0.11	62,62,62,62	0
58	MG	1a	1698	1/1	0.83	0.22	57,57,57,57	0
58	MG	1U	203	1/1	0.83	0.10	60,60,60,60	0
58	MG	2A	3843	1/1	0.83	0.15	73,73,73,73	0
58	MG	2A	3713	1/1	0.83	0.18	72,72,72,72	0
58	MG	2A	3718	1/1	0.83	0.17	56,56,56,56	0
58	MG	1A	4086	1/1	0.83	0.19	74,74,74,74	0
58	MG	1A	3909	1/1	0.83	0.12	37,37,37,37	0
58	MG	1A	3310	1/1	0.83	0.22	55,55,55,55	0
58	MG	2B	220	1/1	0.83	0.16	76,76,76,76	0
58	MG	1a	1641	1/1	0.83	0.14	60,60,60,60	0
58	MG	2x	104	1/1	0.83	0.22	78,78,78,78	0
58	MG	2F	303	1/1	0.84	0.09	48,48,48,48	0
58	MG	1A	3131	1/1	0.84	0.10	68,68,68,68	0
58	MG	2A	3684	1/1	0.84	0.20	73,73,73,73	0
58	MG	1A	4019	1/1	0.84	0.17	58,58,58,58	0
58	MG	2A	3688	1/1	0.84	0.26	61,61,61,61	0
58	MG	1A	3684	1/1	0.84	0.13	47,47,47,47	0
58	MG	2A	3700	1/1	0.84	0.14	54,54,54,54	0
58	MG	2a	1620	1/1	0.84	0.14	58,58,58,58	0
58	MG	2A	3129	1/1	0.84	0.12	56,56,56,56	0
58	MG	1A	3741	1/1	0.84	0.15	63,63,63,63	0
58	MG	1A	3895	1/1	0.84	0.11	40,40,40,40	0
58	MG	2A	3429	1/1	0.84	0.24	56,56,56,56	0
58	MG	2a	1706	1/1	0.84	0.11	74,74,74,74	0
58	MG	2a	1716	1/1	0.84	0.23	61,61,61,61	0
58	MG	2A	3190	1/1	0.84	0.15	61,61,61,61	0
58	MG	1A	3776	1/1	0.84	0.09	18,18,18,18	0
58	MG	1l	201	1/1	0.84	0.14	74,74,74,74	0
58	MG	1t	201	1/1	0.84	0.17	58,58,58,58	0
58	MG	2A	3489	1/1	0.84	0.16	67,67,67,67	0
58	MG	2A	3251	1/1	0.84	0.23	65,65,65,65	0
58	MG	1A	3262	1/1	0.84	0.26	74,74,74,74	0
58	MG	2A	3757	1/1	0.84	0.20	81,81,81,81	0
58	MG	2a	1795	1/1	0.84	0.19	73,73,73,73	0
58	MG	2A	3770	1/1	0.84	0.10	69,69,69,69	0
58	MG	2A	3277	1/1	0.84	0.22	79,79,79,79	0
58	MG	2A	3553	1/1	0.84	0.12	37,37,37,37	0
58	MG	2A	3577	1/1	0.84	0.10	66,66,66,66	0
58	MG	2A	3599	1/1	0.84	0.21	64,64,64,64	0
58	MG	2A	3841	1/1	0.84	0.29	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1705	1/1	0.84	0.18	69,69,69,69	0
58	MG	1x	109	1/1	0.84	0.25	66,66,66,66	0
58	MG	1A	3270	1/1	0.84	0.17	47,47,47,47	0
58	MG	2B	203	1/1	0.84	0.18	80,80,80,80	0
58	MG	2A	3650	1/1	0.84	0.12	54,54,54,54	0
58	MG	1A	3846	1/1	0.84	0.10	54,54,54,54	0
58	MG	1a	1760	1/1	0.84	0.16	69,69,69,69	0
58	MG	1E	309	1/1	0.84	0.13	25,25,25,25	0
58	MG	1A	3385	1/1	0.84	0.15	58,58,58,58	0
58	MG	1A	3753	1/1	0.85	0.12	61,61,61,61	0
58	MG	2A	3533	1/1	0.85	0.12	46,46,46,46	0
58	MG	2a	1623	1/1	0.85	0.19	73,73,73,73	0
58	MG	1b	301	1/1	0.85	0.16	81,81,81,81	0
58	MG	2A	3574	1/1	0.85	0.11	73,73,73,73	0
58	MG	1A	3552	1/1	0.85	0.23	66,66,66,66	0
58	MG	2a	1646	1/1	0.85	0.12	66,66,66,66	0
58	MG	2A	3334	1/1	0.85	0.13	61,61,61,61	0
58	MG	2A	3336	1/1	0.85	0.10	64,64,64,64	0
58	MG	2a	1709	1/1	0.85	0.12	76,76,76,76	0
58	MG	2A	3616	1/1	0.85	0.09	62,62,62,62	0
58	MG	1B	234	1/1	0.85	0.12	61,61,61,61	0
58	MG	2A	3363	1/1	0.85	0.20	61,61,61,61	0
58	MG	1A	3461	1/1	0.85	0.11	55,55,55,55	0
58	MG	2A	3367	1/1	0.85	0.28	65,65,65,65	0
58	MG	2a	1740	1/1	0.85	0.18	67,67,67,67	0
58	MG	2A	3829	1/1	0.85	0.13	66,66,66,66	0
58	MG	2A	3835	1/1	0.85	0.19	68,68,68,68	0
58	MG	2a	1773	1/1	0.85	0.11	84,84,84,84	0
58	MG	1a	1737	1/1	0.85	0.13	58,58,58,58	0
58	MG	2a	1788	1/1	0.85	0.20	65,65,65,65	0
58	MG	2a	1792	1/1	0.85	0.14	72,72,72,72	0
58	MG	1A	4034	1/1	0.85	0.12	60,60,60,60	0
58	MG	2A	3211	1/1	0.85	0.34	72,72,72,72	0
58	MG	1a	1750	1/1	0.85	0.19	71,71,71,71	0
58	MG	2A	3412	1/1	0.85	0.20	64,64,64,64	0
58	MG	1l	105	1/1	0.85	0.09	58,58,58,58	0
58	MG	1A	3644	1/1	0.85	0.18	59,59,59,59	0
58	MG	2a	1810	1/1	0.85	0.19	81,81,81,81	0
58	MG	1A	3513	1/1	0.85	0.18	60,60,60,60	0
58	MG	2A	3699	1/1	0.85	0.16	64,64,64,64	0
58	MG	2a	1825	1/1	0.85	0.19	63,63,63,63	0
58	MG	2D	302	1/1	0.85	0.34	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	3280	1/1	0.85	0.22	65,65,65,65	0
58	MG	2A	3701	1/1	0.85	0.17	57,57,57,57	0
58	MG	2I	204	1/1	0.85	0.13	63,63,63,63	0
58	MG	20	103	1/1	0.85	0.18	70,70,70,70	0
58	MG	1A	3382	1/1	0.85	0.12	67,67,67,67	0
58	MG	2A	3479	1/1	0.85	0.17	61,61,61,61	0
58	MG	1a	1634	1/1	0.85	0.21	53,53,53,53	0
58	MG	1A	3953	1/1	0.85	0.09	66,66,66,66	0
58	MG	1A	3372	1/1	0.85	0.14	43,43,43,43	0
58	MG	1a	1624	1/1	0.86	0.17	67,67,67,67	0
58	MG	1a	1630	1/1	0.86	0.11	50,50,50,50	0
58	MG	2A	3285	1/1	0.86	0.16	56,56,56,56	0
58	MG	1A	3202	1/1	0.86	0.13	51,51,51,51	0
58	MG	2A	3480	1/1	0.86	0.14	68,68,68,68	0
58	MG	1A	3829	1/1	0.86	0.10	38,38,38,38	0
58	MG	2A	3308	1/1	0.86	0.12	47,47,47,47	0
58	MG	2a	1656	1/1	0.86	0.15	72,72,72,72	0
58	MG	2A	3312	1/1	0.86	0.10	62,62,62,62	0
58	MG	2A	3512	1/1	0.86	0.14	65,65,65,65	0
58	MG	2A	3513	1/1	0.86	0.12	40,40,40,40	0
58	MG	2a	1713	1/1	0.86	0.10	69,69,69,69	0
58	MG	2A	3748	1/1	0.86	0.10	33,33,33,33	0
58	MG	2A	3321	1/1	0.86	0.15	67,67,67,67	0
58	MG	2A	3532	1/1	0.86	0.12	49,49,49,49	0
58	MG	2A	3767	1/1	0.86	0.13	42,42,42,42	0
58	MG	2A	3322	1/1	0.86	0.12	56,56,56,56	0
58	MG	1A	3122	1/1	0.86	0.18	43,43,43,43	0
58	MG	2a	1751	1/1	0.86	0.13	86,86,86,86	0
58	MG	1A	3944	1/1	0.86	0.11	26,26,26,26	0
58	MG	1A	3711	1/1	0.86	0.12	31,31,31,31	0
58	MG	2A	3820	1/1	0.86	0.17	63,63,63,63	0
58	MG	2A	3586	1/1	0.86	0.12	35,35,35,35	0
58	MG	2A	3331	1/1	0.86	0.22	70,70,70,70	0
58	MG	1A	3732	1/1	0.86	0.20	56,56,56,56	0
58	MG	1A	3861	1/1	0.86	0.29	43,43,43,43	0
58	MG	2A	3842	1/1	0.86	0.16	67,67,67,67	0
58	MG	1a	1721	1/1	0.86	0.14	69,69,69,69	0
58	MG	2A	3344	1/1	0.86	0.16	71,71,71,71	0
58	MG	2A	3345	1/1	0.86	0.19	51,51,51,51	0
58	MG	2A	3651	1/1	0.86	0.12	58,58,58,58	0
58	MG	1A	3965	1/1	0.86	0.07	38,38,38,38	0
58	MG	1A	3254	1/1	0.86	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3207	1/1	0.86	0.19	66,66,66,66	0
58	MG	1a	1738	1/1	0.86	0.17	69,69,69,69	0
58	MG	2A	3215	1/1	0.86	0.15	62,62,62,62	0
58	MG	2A	3674	1/1	0.86	0.12	62,62,62,62	0
58	MG	2A	3370	1/1	0.86	0.09	61,61,61,61	0
58	MG	2l	203	1/1	0.86	0.21	68,68,68,68	0
58	MG	1A	3643	1/1	0.86	0.13	47,47,47,47	0
58	MG	25	102	1/1	0.86	0.18	52,52,52,52	0
58	MG	2A	3241	1/1	0.86	0.20	67,67,67,67	0
58	MG	2A	3242	1/1	0.86	0.21	63,63,63,63	0
58	MG	2A	3001	1/1	0.86	0.21	53,53,53,53	0
58	MG	1A	3771	1/1	0.86	0.10	24,24,24,24	0
58	MG	1A	3487	1/1	0.86	0.19	50,50,50,50	0
58	MG	2B	214	1/1	0.87	0.10	66,66,66,66	0
58	MG	2A	3604	1/1	0.87	0.19	72,72,72,72	0
58	MG	1B	223	1/1	0.87	0.12	61,61,61,61	0
58	MG	1A	3728	1/1	0.87	0.14	71,71,71,71	0
58	MG	1A	3358	1/1	0.87	0.11	71,71,71,71	0
58	MG	2A	3634	1/1	0.87	0.09	49,49,49,49	0
58	MG	2W	201	1/1	0.87	0.27	54,54,54,54	0
58	MG	2A	3110	1/1	0.87	0.14	57,57,57,57	0
58	MG	2A	3330	1/1	0.87	0.17	67,67,67,67	0
58	MG	1A	3360	1/1	0.87	0.10	45,45,45,45	0
58	MG	1A	3858	1/1	0.87	0.10	27,27,27,27	0
58	MG	2A	3333	1/1	0.87	0.10	75,75,75,75	0
58	MG	1A	3333	1/1	0.87	0.20	43,43,43,43	0
58	MG	1A	3330	1/1	0.87	0.16	53,53,53,53	0
58	MG	2a	1614	1/1	0.87	0.24	65,65,65,65	0
58	MG	2A	3340	1/1	0.87	0.25	76,76,76,76	0
58	MG	2A	3131	1/1	0.87	0.10	63,63,63,63	0
58	MG	2A	3681	1/1	0.87	0.22	67,67,67,67	0
58	MG	1Y	202	1/1	0.87	0.13	61,61,61,61	0
58	MG	2a	1627	1/1	0.87	0.13	61,61,61,61	0
58	MG	1A	3967	1/1	0.87	0.14	47,47,47,47	0
58	MG	2a	1637	1/1	0.87	0.23	55,55,55,55	0
58	MG	2a	1639	1/1	0.87	0.19	61,61,61,61	0
58	MG	2A	3347	1/1	0.87	0.14	65,65,65,65	0
58	MG	2A	3188	1/1	0.87	0.21	61,61,61,61	0
58	MG	2a	1650	1/1	0.87	0.11	61,61,61,61	0
58	MG	2A	3694	1/1	0.87	0.14	66,66,66,66	0
58	MG	2a	1666	1/1	0.87	0.25	66,66,66,66	0
58	MG	2a	1672	1/1	0.87	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1778	1/1	0.87	0.11	72,72,72,72	0
58	MG	1A	3880	1/1	0.87	0.16	28,28,28,28	0
58	MG	1A	3986	1/1	0.87	0.10	35,35,35,35	0
58	MG	1A	3772	1/1	0.87	0.11	32,32,32,32	0
58	MG	2A	3706	1/1	0.87	0.12	58,58,58,58	0
58	MG	1a	1787	1/1	0.87	0.17	59,59,59,59	0
58	MG	1A	3533	1/1	0.87	0.10	57,57,57,57	0
58	MG	2A	3231	1/1	0.87	0.11	61,61,61,61	0
58	MG	1A	3803	1/1	0.87	0.10	18,18,18,18	0
58	MG	2A	3240	1/1	0.87	0.22	63,63,63,63	0
58	MG	1A	4075	1/1	0.87	0.13	48,48,48,48	0
58	MG	1A	3898	1/1	0.87	0.11	61,61,61,61	0
58	MG	2A	3245	1/1	0.87	0.23	65,65,65,65	0
58	MG	2A	3469	1/1	0.87	0.16	65,65,65,65	0
58	MG	1A	3536	1/1	0.87	0.19	46,46,46,46	0
58	MG	2A	3257	1/1	0.87	0.15	58,58,58,58	0
58	MG	2A	3260	1/1	0.87	0.08	73,73,73,73	0
58	MG	1a	1665	1/1	0.87	0.15	59,59,59,59	0
58	MG	2A	3267	1/1	0.87	0.13	56,56,56,56	0
58	MG	1a	1671	1/1	0.87	0.29	69,69,69,69	0
58	MG	2A	3776	1/1	0.87	0.23	86,86,86,86	0
58	MG	2A	3796	1/1	0.87	0.15	50,50,50,50	0
58	MG	2A	3502	1/1	0.87	0.16	33,33,33,33	0
58	MG	2a	1808	1/1	0.87	0.22	58,58,58,58	0
58	MG	1A	4088	1/1	0.87	0.12	49,49,49,49	0
58	MG	2a	1814	1/1	0.87	0.18	65,65,65,65	0
58	MG	2a	1816	1/1	0.87	0.11	59,59,59,59	0
58	MG	1x	106	1/1	0.87	0.20	68,68,68,68	0
58	MG	2A	3824	1/1	0.87	0.12	59,59,59,59	0
58	MG	1x	107	1/1	0.87	0.12	38,38,38,38	0
58	MG	2A	3288	1/1	0.87	0.20	76,76,76,76	0
58	MG	1a	1683	1/1	0.87	0.24	65,65,65,65	0
58	MG	2A	3536	1/1	0.87	0.12	40,40,40,40	0
58	MG	2A	3298	1/1	0.87	0.17	63,63,63,63	0
58	MG	2A	3560	1/1	0.87	0.11	47,47,47,47	0
58	MG	2A	3565	1/1	0.87	0.14	57,57,57,57	0
58	MG	1A	3343	1/1	0.87	0.17	49,49,49,49	0
58	MG	2A	3065	1/1	0.87	0.17	58,58,58,58	0
58	MG	1B	211	1/1	0.87	0.09	59,59,59,59	0
58	MG	2B	208	1/1	0.87	0.14	70,70,70,70	0
58	MG	1a	1714	1/1	0.87	0.12	48,48,48,48	0
58	MG	2y	101	1/1	0.87	0.09	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3558	1/1	0.88	0.25	39,39,39,39	0
58	MG	25	104	1/1	0.88	0.17	55,55,55,55	0
58	MG	1a	1775	1/1	0.88	0.12	67,67,67,67	0
58	MG	1B	212	1/1	0.88	0.17	55,55,55,55	0
58	MG	1A	3981	1/1	0.88	0.14	71,71,71,71	0
58	MG	1A	3984	1/1	0.88	0.14	25,25,25,25	0
58	MG	2A	3191	1/1	0.88	0.19	65,65,65,65	0
58	MG	2A	3672	1/1	0.88	0.20	61,61,61,61	0
58	MG	1a	1644	1/1	0.88	0.15	72,72,72,72	0
58	MG	2A	3355	1/1	0.88	0.11	53,53,53,53	0
58	MG	2A	3198	1/1	0.88	0.21	59,59,59,59	0
58	MG	2A	3199	1/1	0.88	0.17	65,65,65,65	0
58	MG	2A	3202	1/1	0.88	0.13	66,66,66,66	0
58	MG	2a	1630	1/1	0.88	0.24	65,65,65,65	0
58	MG	1a	1784	1/1	0.88	0.13	45,45,45,45	0
58	MG	1A	3773	1/1	0.88	0.14	43,43,43,43	0
58	MG	1A	3930	1/1	0.88	0.14	48,48,48,48	0
58	MG	1a	1669	1/1	0.88	0.27	64,64,64,64	0
58	MG	2A	3387	1/1	0.88	0.13	61,61,61,61	0
58	MG	2A	3389	1/1	0.88	0.12	69,69,69,69	0
58	MG	2a	1651	1/1	0.88	0.10	60,60,60,60	0
58	MG	1a	1814	1/1	0.88	0.28	64,64,64,64	0
58	MG	1A	3714	1/1	0.88	0.14	44,44,44,44	0
58	MG	2A	3413	1/1	0.88	0.25	51,51,51,51	0
58	MG	2a	1677	1/1	0.88	0.34	70,70,70,70	0
58	MG	2a	1686	1/1	0.88	0.22	77,77,77,77	0
58	MG	1A	4036	1/1	0.88	0.09	36,36,36,36	0
58	MG	1a	1675	1/1	0.88	0.23	73,73,73,73	0
58	MG	2a	1708	1/1	0.88	0.17	71,71,71,71	0
58	MG	1E	311	1/1	0.88	0.12	65,65,65,65	0
58	MG	1w	102	1/1	0.88	0.10	83,83,83,83	0
58	MG	1a	1694	1/1	0.88	0.20	65,65,65,65	0
58	MG	2a	1720	1/1	0.88	0.16	69,69,69,69	0
58	MG	1E	312	1/1	0.88	0.20	48,48,48,48	0
58	MG	2a	1726	1/1	0.88	0.13	57,57,57,57	0
58	MG	2a	1730	1/1	0.88	0.18	69,69,69,69	0
58	MG	2A	3259	1/1	0.88	0.26	70,70,70,70	0
58	MG	1x	105	1/1	0.88	0.20	65,65,65,65	0
58	MG	1a	1701	1/1	0.88	0.17	60,60,60,60	0
58	MG	1O	205	1/1	0.88	0.14	68,68,68,68	0
58	MG	2A	3764	1/1	0.88	0.17	67,67,67,67	0
58	MG	2A	3275	1/1	0.88	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1758	1/1	0.88	0.22	70,70,70,70	0
58	MG	1a	1710	1/1	0.88	0.11	55,55,55,55	0
58	MG	1A	3792	1/1	0.88	0.09	57,57,57,57	0
58	MG	2A	3283	1/1	0.88	0.22	58,58,58,58	0
58	MG	2a	1780	1/1	0.88	0.17	57,57,57,57	0
58	MG	2A	3790	1/1	0.88	0.13	52,52,52,52	0
58	MG	2A	3053	1/1	0.88	0.13	65,65,65,65	0
58	MG	1a	1719	1/1	0.88	0.14	65,65,65,65	0
58	MG	2A	3073	1/1	0.88	0.13	51,51,51,51	0
58	MG	1V	206	1/1	0.88	0.21	57,57,57,57	0
58	MG	2A	3546	1/1	0.88	0.15	51,51,51,51	0
58	MG	1a	1723	1/1	0.88	0.21	58,58,58,58	0
58	MG	2A	3300	1/1	0.88	0.13	56,56,56,56	0
58	MG	1A	3052	1/1	0.88	0.13	35,35,35,35	0
58	MG	2A	3566	1/1	0.88	0.22	68,68,68,68	0
58	MG	2A	3568	1/1	0.88	0.10	64,64,64,64	0
58	MG	2a	1815	1/1	0.88	0.12	65,65,65,65	0
58	MG	2A	3092	1/1	0.88	0.12	51,51,51,51	0
58	MG	2A	3576	1/1	0.88	0.15	62,62,62,62	0
58	MG	2A	3098	1/1	0.88	0.17	75,75,75,75	0
58	MG	2a	1824	1/1	0.88	0.17	70,70,70,70	0
58	MG	1A	3347	1/1	0.88	0.11	49,49,49,49	0
58	MG	2A	3590	1/1	0.88	0.14	56,56,56,56	0
58	MG	2a	1830	1/1	0.88	0.25	74,74,74,74	0
58	MG	2A	3592	1/1	0.88	0.14	51,51,51,51	0
58	MG	2B	212	1/1	0.88	0.27	69,69,69,69	0
58	MG	2A	3105	1/1	0.88	0.09	60,60,60,60	0
58	MG	1A	3040	1/1	0.88	0.17	61,61,61,61	0
58	MG	1a	1611	1/1	0.88	0.12	69,69,69,69	0
58	MG	1a	1746	1/1	0.88	0.18	67,67,67,67	0
58	MG	1A	3293	1/1	0.88	0.16	47,47,47,47	0
58	MG	2A	3118	1/1	0.88	0.30	62,62,62,62	0
58	MG	2A	3638	1/1	0.88	0.18	65,65,65,65	0
58	MG	1A	3255	1/1	0.88	0.09	54,54,54,54	0
58	MG	1a	1629	1/1	0.88	0.17	53,53,53,53	0
58	MG	1A	3438	1/1	0.89	0.09	58,58,58,58	0
58	MG	1S	202	1/1	0.89	0.13	49,49,49,49	0
58	MG	1A	3269	1/1	0.89	0.26	70,70,70,70	0
58	MG	2a	1601	1/1	0.89	0.09	60,60,60,60	0
58	MG	2A	3635	1/1	0.89	0.14	52,52,52,52	0
58	MG	1a	1744	1/1	0.89	0.13	60,60,60,60	0
58	MG	1U	211	1/1	0.89	0.29	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	3778	1/1	0.89	0.08	20,20,20,20	0
58	MG	2A	3335	1/1	0.89	0.13	51,51,51,51	0
58	MG	1A	3591	1/1	0.89	0.24	62,62,62,62	0
58	MG	2A	3157	1/1	0.89	0.19	62,62,62,62	0
58	MG	2A	3166	1/1	0.89	0.14	68,68,68,68	0
58	MG	2a	1622	1/1	0.89	0.29	74,74,74,74	0
58	MG	1A	3121	1/1	0.89	0.17	43,43,43,43	0
58	MG	2A	3177	1/1	0.89	0.13	53,53,53,53	0
58	MG	2A	3668	1/1	0.89	0.11	60,60,60,60	0
58	MG	1A	3630	1/1	0.89	0.14	52,52,52,52	0
58	MG	1A	3824	1/1	0.89	0.09	41,41,41,41	0
58	MG	1a	1613	1/1	0.89	0.13	61,61,61,61	0
58	MG	1A	3642	1/1	0.89	0.09	37,37,37,37	0
58	MG	1a	1623	1/1	0.89	0.11	71,71,71,71	0
58	MG	1A	3835	1/1	0.89	0.11	48,48,48,48	0
58	MG	1A	3836	1/1	0.89	0.10	43,43,43,43	0
58	MG	2A	3373	1/1	0.89	0.18	65,65,65,65	0
58	MG	2a	1653	1/1	0.89	0.11	62,62,62,62	0
58	MG	1A	3473	1/1	0.89	0.12	44,44,44,44	0
58	MG	2a	1665	1/1	0.89	0.09	65,65,65,65	0
58	MG	2A	3382	1/1	0.89	0.09	59,59,59,59	0
58	MG	2a	1670	1/1	0.89	0.28	64,64,64,64	0
58	MG	1a	1800	1/1	0.89	0.08	55,55,55,55	0
58	MG	2A	3205	1/1	0.89	0.14	64,64,64,64	0
58	MG	2a	1681	1/1	0.89	0.18	65,65,65,65	0
58	MG	2a	1685	1/1	0.89	0.23	68,68,68,68	0
58	MG	1A	3474	1/1	0.89	0.15	67,67,67,67	0
58	MG	2a	1695	1/1	0.89	0.10	76,76,76,76	0
58	MG	2A	3403	1/1	0.89	0.17	44,44,44,44	0
58	MG	1A	3483	1/1	0.89	0.11	57,57,57,57	0
58	MG	2a	1707	1/1	0.89	0.28	70,70,70,70	0
58	MG	1a	1637	1/1	0.89	0.13	72,72,72,72	0
58	MG	2A	3221	1/1	0.89	0.23	54,54,54,54	0
58	MG	1A	3379	1/1	0.89	0.13	57,57,57,57	0
58	MG	2A	3430	1/1	0.89	0.17	57,57,57,57	0
58	MG	2A	3235	1/1	0.89	0.09	56,56,56,56	0
58	MG	1A	3691	1/1	0.89	0.14	59,59,59,59	0
58	MG	2A	3239	1/1	0.89	0.09	51,51,51,51	0
58	MG	1a	1650	1/1	0.89	0.13	67,67,67,67	0
58	MG	2a	1732	1/1	0.89	0.11	82,82,82,82	0
58	MG	1A	3869	1/1	0.89	0.15	36,36,36,36	0
58	MG	1A	3208	1/1	0.89	0.08	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	1737	1/1	0.89	0.24	63,63,63,63	0
58	MG	1w	104	1/1	0.89	0.15	65,65,65,65	0
58	MG	2A	3487	1/1	0.89	0.14	57,57,57,57	0
58	MG	1A	3505	1/1	0.89	0.15	58,58,58,58	0
58	MG	2A	3255	1/1	0.89	0.16	62,62,62,62	0
58	MG	1A	3718	1/1	0.89	0.07	59,59,59,59	0
58	MG	2a	1761	1/1	0.89	0.13	65,65,65,65	0
58	MG	2A	3784	1/1	0.89	0.09	64,64,64,64	0
58	MG	2a	1764	1/1	0.89	0.06	86,86,86,86	0
58	MG	1A	3307	1/1	0.89	0.12	59,59,59,59	0
58	MG	1A	3256	1/1	0.89	0.10	58,58,58,58	0
58	MG	1a	1680	1/1	0.89	0.19	61,61,61,61	0
58	MG	2A	3804	1/1	0.89	0.14	57,57,57,57	0
58	MG	2A	3813	1/1	0.89	0.12	65,65,65,65	0
58	MG	1x	108	1/1	0.89	0.08	79,79,79,79	0
58	MG	1B	221	1/1	0.89	0.14	58,58,58,58	0
58	MG	1a	1688	1/1	0.89	0.10	63,63,63,63	0
58	MG	2A	3023	1/1	0.89	0.32	70,70,70,70	0
58	MG	2A	3031	1/1	0.89	0.14	62,62,62,62	0
58	MG	2a	1806	1/1	0.89	0.12	70,70,70,70	0
58	MG	2A	3041	1/1	0.89	0.18	60,60,60,60	0
58	MG	1A	3409	1/1	0.89	0.18	46,46,46,46	0
58	MG	2A	3564	1/1	0.89	0.15	51,51,51,51	0
58	MG	1a	1695	1/1	0.89	0.33	64,64,64,64	0
58	MG	2A	3296	1/1	0.89	0.09	52,52,52,52	0
58	MG	2A	3848	1/1	0.89	0.11	55,55,55,55	0
58	MG	1A	3907	1/1	0.89	0.24	27,27,27,27	0
58	MG	2A	3857	1/1	0.89	0.15	55,55,55,55	0
58	MG	2A	3074	1/1	0.89	0.06	52,52,52,52	0
58	MG	2B	205	1/1	0.89	0.11	59,59,59,59	0
58	MG	1A	3751	1/1	0.89	0.20	58,58,58,58	0
58	MG	1A	3232	1/1	0.89	0.16	57,57,57,57	0
58	MG	2d	302	1/1	0.89	0.16	71,71,71,71	0
58	MG	1B	232	1/1	0.89	0.12	54,54,54,54	0
58	MG	2A	3589	1/1	0.89	0.18	56,56,56,56	0
58	MG	1A	3428	1/1	0.89	0.10	54,54,54,54	0
58	MG	1A	3931	1/1	0.89	0.11	43,43,43,43	0
58	MG	1A	3933	1/1	0.89	0.15	47,47,47,47	0
58	MG	1A	3437	1/1	0.89	0.09	44,44,44,44	0
58	MG	2v	101	1/1	0.89	0.25	73,73,73,73	0
58	MG	1O	202	1/1	0.89	0.18	57,57,57,57	0
58	MG	2v	104	1/1	0.89	0.13	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2E	306	1/1	0.89	0.14	55,55,55,55	0
58	MG	2A	3609	1/1	0.89	0.20	74,74,74,74	0
58	MG	2G	201	1/1	0.89	0.21	67,67,67,67	0
58	MG	2A	3612	1/1	0.89	0.19	49,49,49,49	0
58	MG	1a	1815	1/1	0.90	0.33	69,69,69,69	0
58	MG	1A	4008	1/1	0.90	0.10	31,31,31,31	0
58	MG	2A	3508	1/1	0.90	0.16	65,65,65,65	0
58	MG	1A	3705	1/1	0.90	0.10	41,41,41,41	0
58	MG	1A	4022	1/1	0.90	0.13	57,57,57,57	0
58	MG	1A	3430	1/1	0.90	0.10	52,52,52,52	0
58	MG	1A	3865	1/1	0.90	0.13	48,48,48,48	0
58	MG	1a	1651	1/1	0.90	0.12	60,60,60,60	0
58	MG	1a	1659	1/1	0.90	0.11	65,65,65,65	0
58	MG	1A	3867	1/1	0.90	0.15	63,63,63,63	0
58	MG	1a	1661	1/1	0.90	0.16	54,54,54,54	0
58	MG	2E	304	1/1	0.90	0.10	33,33,33,33	0
58	MG	2A	3555	1/1	0.90	0.08	36,36,36,36	0
58	MG	2A	3556	1/1	0.90	0.17	61,61,61,61	0
58	MG	2A	3557	1/1	0.90	0.21	62,62,62,62	0
58	MG	2Q	202	1/1	0.90	0.18	49,49,49,49	0
58	MG	1a	1663	1/1	0.90	0.14	69,69,69,69	0
58	MG	1A	4067	1/1	0.90	0.18	52,52,52,52	0
58	MG	2A	3265	1/1	0.90	0.43	70,70,70,70	0
58	MG	1a	1668	1/1	0.90	0.21	56,56,56,56	0
58	MG	25	106	1/1	0.90	0.10	44,44,44,44	0
58	MG	2A	3272	1/1	0.90	0.13	57,57,57,57	0
58	MG	1A	4074	1/1	0.90	0.16	46,46,46,46	0
58	MG	1A	3431	1/1	0.90	0.12	55,55,55,55	0
58	MG	2A	3279	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3004	1/1	0.90	0.25	52,52,52,52	0
58	MG	2a	1612	1/1	0.90	0.16	62,62,62,62	0
58	MG	2A	3005	1/1	0.90	0.22	69,69,69,69	0
58	MG	1A	3871	1/1	0.90	0.21	42,42,42,42	0
58	MG	1A	3872	1/1	0.90	0.17	33,33,33,33	0
58	MG	2A	3032	1/1	0.90	0.23	59,59,59,59	0
58	MG	2A	3034	1/1	0.90	0.15	51,51,51,51	0
58	MG	1A	3184	1/1	0.90	0.12	74,74,74,74	0
58	MG	2A	3049	1/1	0.90	0.10	56,56,56,56	0
58	MG	1A	3117	1/1	0.90	0.22	31,31,31,31	0
58	MG	1A	3439	1/1	0.90	0.21	41,41,41,41	0
58	MG	2A	3619	1/1	0.90	0.14	40,40,40,40	0
58	MG	2a	1634	1/1	0.90	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1635	1/1	0.90	0.17	57,57,57,57	0
58	MG	2A	3306	1/1	0.90	0.15	64,64,64,64	0
58	MG	2A	3627	1/1	0.90	0.12	49,49,49,49	0
58	MG	2A	3629	1/1	0.90	0.09	48,48,48,48	0
58	MG	2A	3630	1/1	0.90	0.13	57,57,57,57	0
58	MG	2A	3068	1/1	0.90	0.24	67,67,67,67	0
58	MG	1a	1692	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3636	1/1	0.90	0.30	61,61,61,61	0
58	MG	2a	1654	1/1	0.90	0.09	64,64,64,64	0
58	MG	2a	1655	1/1	0.90	0.17	69,69,69,69	0
58	MG	1A	3132	1/1	0.90	0.10	44,44,44,44	0
58	MG	2a	1660	1/1	0.90	0.09	41,41,41,41	0
58	MG	2a	1662	1/1	0.90	0.17	80,80,80,80	0
58	MG	2A	3642	1/1	0.90	0.16	77,77,77,77	0
58	MG	2A	3643	1/1	0.90	0.14	60,60,60,60	0
58	MG	1A	3889	1/1	0.90	0.10	36,36,36,36	0
58	MG	1A	3551	1/1	0.90	0.08	57,57,57,57	0
58	MG	2a	1674	1/1	0.90	0.14	60,60,60,60	0
58	MG	1a	1700	1/1	0.90	0.29	62,62,62,62	0
58	MG	2a	1678	1/1	0.90	0.18	59,59,59,59	0
58	MG	2a	1679	1/1	0.90	0.15	76,76,76,76	0
58	MG	2A	3656	1/1	0.90	0.10	48,48,48,48	0
58	MG	1A	3470	1/1	0.90	0.11	57,57,57,57	0
58	MG	2A	3095	1/1	0.90	0.11	53,53,53,53	0
58	MG	2a	1687	1/1	0.90	0.14	71,71,71,71	0
58	MG	1A	3904	1/1	0.90	0.14	43,43,43,43	0
58	MG	1A	3761	1/1	0.90	0.14	59,59,59,59	0
58	MG	1A	3148	1/1	0.90	0.16	42,42,42,42	0
58	MG	1A	3913	1/1	0.90	0.20	43,43,43,43	0
58	MG	2A	3670	1/1	0.90	0.10	57,57,57,57	0
58	MG	1D	313	1/1	0.90	0.12	39,39,39,39	0
58	MG	1A	3562	1/1	0.90	0.30	60,60,60,60	0
58	MG	1A	3928	1/1	0.90	0.08	37,37,37,37	0
58	MG	2a	1717	1/1	0.90	0.12	67,67,67,67	0
58	MG	2A	3682	1/1	0.90	0.13	47,47,47,47	0
58	MG	2A	3117	1/1	0.90	0.16	53,53,53,53	0
58	MG	1a	1725	1/1	0.90	0.33	73,73,73,73	0
58	MG	1A	3582	1/1	0.90	0.06	36,36,36,36	0
58	MG	1A	3587	1/1	0.90	0.06	23,23,23,23	0
58	MG	2A	3353	1/1	0.90	0.16	63,63,63,63	0
58	MG	1A	3392	1/1	0.90	0.29	42,42,42,42	0
58	MG	1A	3785	1/1	0.90	0.12	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	3158	1/1	0.90	0.12	67,67,67,67	0
58	MG	1A	3314	1/1	0.90	0.28	54,54,54,54	0
58	MG	2a	1748	1/1	0.90	0.18	63,63,63,63	0
58	MG	2A	3168	1/1	0.90	0.09	73,73,73,73	0
58	MG	1a	1748	1/1	0.90	0.08	56,56,56,56	0
58	MG	2A	3176	1/1	0.90	0.14	52,52,52,52	0
58	MG	1A	3600	1/1	0.90	0.14	48,48,48,48	0
58	MG	2A	3722	1/1	0.90	0.13	58,58,58,58	0
58	MG	2A	3378	1/1	0.90	0.17	62,62,62,62	0
58	MG	2A	3184	1/1	0.90	0.20	65,65,65,65	0
58	MG	1A	3404	1/1	0.90	0.15	50,50,50,50	0
58	MG	2a	1777	1/1	0.90	0.11	74,74,74,74	0
58	MG	2a	1779	1/1	0.90	0.14	70,70,70,70	0
58	MG	2A	3731	1/1	0.90	0.10	66,66,66,66	0
58	MG	2a	1784	1/1	0.90	0.13	50,50,50,50	0
58	MG	1A	3960	1/1	0.90	0.10	34,34,34,34	0
58	MG	2A	3388	1/1	0.90	0.14	61,61,61,61	0
58	MG	1a	1766	1/1	0.90	0.12	61,61,61,61	0
58	MG	1a	1771	1/1	0.90	0.07	51,51,51,51	0
58	MG	1A	3484	1/1	0.90	0.24	47,47,47,47	0
58	MG	2A	3197	1/1	0.90	0.17	61,61,61,61	0
58	MG	1A	3962	1/1	0.90	0.07	19,19,19,19	0
58	MG	2A	3422	1/1	0.90	0.15	54,54,54,54	0
58	MG	2A	3425	1/1	0.90	0.13	40,40,40,40	0
58	MG	1A	3353	1/1	0.90	0.16	59,59,59,59	0
58	MG	2A	3200	1/1	0.90	0.14	57,57,57,57	0
58	MG	1A	3495	1/1	0.90	0.13	39,39,39,39	0
58	MG	2A	3786	1/1	0.90	0.15	76,76,76,76	0
58	MG	2A	3434	1/1	0.90	0.23	63,63,63,63	0
58	MG	2A	3436	1/1	0.90	0.24	59,59,59,59	0
58	MG	2A	3438	1/1	0.90	0.21	49,49,49,49	0
58	MG	2A	3441	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	3502	1/1	0.90	0.09	57,57,57,57	0
58	MG	2A	3456	1/1	0.90	0.16	56,56,56,56	0
58	MG	2A	3461	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3465	1/1	0.90	0.08	57,57,57,57	0
58	MG	2e	201	1/1	0.90	0.13	73,73,73,73	0
58	MG	1A	3323	1/1	0.90	0.18	49,49,49,49	0
58	MG	2k	201	1/1	0.90	0.14	67,67,67,67	0
58	MG	1A	3689	1/1	0.90	0.08	38,38,38,38	0
58	MG	1a	1628	1/1	0.90	0.18	61,61,61,61	0
58	MG	2A	3836	1/1	0.90	0.14	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	3837	1/1	0.90	0.13	60,60,60,60	0
58	MG	1A	3158	1/1	0.90	0.14	70,70,70,70	0
58	MG	1A	3991	1/1	0.90	0.09	45,45,45,45	0
58	MG	2A	3229	1/1	0.90	0.20	64,64,64,64	0
58	MG	1a	1632	1/1	0.90	0.36	63,63,63,63	0
58	MG	2A	3491	1/1	0.90	0.13	59,59,59,59	0
58	MG	2A	3849	1/1	0.90	0.14	54,54,54,54	0
58	MG	2A	3492	1/1	0.90	0.17	73,73,73,73	0
58	MG	1A	4001	1/1	0.90	0.15	80,80,80,80	0
58	MG	1a	1642	1/1	0.91	0.16	57,57,57,57	0
58	MG	1A	4068	1/1	0.91	0.10	44,44,44,44	0
58	MG	2A	3852	1/1	0.91	0.07	67,67,67,67	0
58	MG	2A	3855	1/1	0.91	0.17	61,61,61,61	0
58	MG	2A	3232	1/1	0.91	0.14	52,52,52,52	0
58	MG	2A	3234	1/1	0.91	0.14	55,55,55,55	0
58	MG	1a	1646	1/1	0.91	0.15	52,52,52,52	0
58	MG	1m	3002	1/1	0.91	0.20	55,55,55,55	0
58	MG	2A	3500	1/1	0.91	0.13	36,36,36,36	0
58	MG	1A	3472	1/1	0.91	0.13	52,52,52,52	0
58	MG	1A	3407	1/1	0.91	0.18	37,37,37,37	0
58	MG	1w	103	1/1	0.91	0.15	69,69,69,69	0
58	MG	1A	4077	1/1	0.91	0.10	49,49,49,49	0
58	MG	1A	3882	1/1	0.91	0.07	26,26,26,26	0
58	MG	2A	3524	1/1	0.91	0.13	43,43,43,43	0
58	MG	2A	3525	1/1	0.91	0.18	58,58,58,58	0
58	MG	1A	3884	1/1	0.91	0.15	60,60,60,60	0
58	MG	2A	3252	1/1	0.91	0.10	63,63,63,63	0
58	MG	1A	3747	1/1	0.91	0.09	13,13,13,13	0
58	MG	2A	3543	1/1	0.91	0.15	36,36,36,36	0
58	MG	1A	3408	1/1	0.91	0.17	49,49,49,49	0
58	MG	2P	202	1/1	0.91	0.12	48,48,48,48	0
58	MG	1B	202	1/1	0.91	0.12	50,50,50,50	0
58	MG	2T	201	1/1	0.91	0.10	64,64,64,64	0
58	MG	2V	202	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3144	1/1	0.91	0.07	36,36,36,36	0
58	MG	2A	3261	1/1	0.91	0.12	59,59,59,59	0
58	MG	23	102	1/1	0.91	0.10	62,62,62,62	0
58	MG	2A	3262	1/1	0.91	0.09	66,66,66,66	0
58	MG	2A	3559	1/1	0.91	0.13	64,64,64,64	0
58	MG	1A	3756	1/1	0.91	0.07	62,62,62,62	0
58	MG	1A	3411	1/1	0.91	0.10	40,40,40,40	0
58	MG	2a	1604	1/1	0.91	0.21	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	3251	1/1	0.91	0.07	63,63,63,63	0
58	MG	2A	3269	1/1	0.91	0.07	53,53,53,53	0
58	MG	1a	1676	1/1	0.91	0.10	57,57,57,57	0
58	MG	2A	3008	1/1	0.91	0.27	63,63,63,63	0
58	MG	2A	3276	1/1	0.91	0.12	57,57,57,57	0
58	MG	2A	3013	1/1	0.91	0.11	51,51,51,51	0
58	MG	2A	3581	1/1	0.91	0.14	56,56,56,56	0
58	MG	2a	1617	1/1	0.91	0.15	64,64,64,64	0
58	MG	2A	3584	1/1	0.91	0.19	61,61,61,61	0
58	MG	2A	3016	1/1	0.91	0.21	60,60,60,60	0
58	MG	2A	3020	1/1	0.91	0.18	60,60,60,60	0
58	MG	1A	3326	1/1	0.91	0.17	48,48,48,48	0
58	MG	1a	1682	1/1	0.91	0.09	58,58,58,58	0
58	MG	1A	3604	1/1	0.91	0.13	36,36,36,36	0
58	MG	2A	3603	1/1	0.91	0.13	36,36,36,36	0
58	MG	2A	3287	1/1	0.91	0.08	72,72,72,72	0
58	MG	1a	1685	1/1	0.91	0.14	54,54,54,54	0
58	MG	1a	1687	1/1	0.91	0.15	70,70,70,70	0
58	MG	2A	3044	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3609	1/1	0.91	0.08	46,46,46,46	0
58	MG	2a	1640	1/1	0.91	0.17	70,70,70,70	0
58	MG	1A	3614	1/1	0.91	0.08	27,27,27,27	0
58	MG	2a	1642	1/1	0.91	0.24	65,65,65,65	0
58	MG	2A	3056	1/1	0.91	0.28	71,71,71,71	0
58	MG	2a	1648	1/1	0.91	0.12	60,60,60,60	0
58	MG	2a	1649	1/1	0.91	0.12	74,74,74,74	0
58	MG	1A	3062	1/1	0.91	0.16	60,60,60,60	0
58	MG	2A	3628	1/1	0.91	0.15	61,61,61,61	0
58	MG	2a	1652	1/1	0.91	0.27	64,64,64,64	0
58	MG	1A	3635	1/1	0.91	0.06	21,21,21,21	0
58	MG	2A	3309	1/1	0.91	0.09	45,45,45,45	0
58	MG	2A	3072	1/1	0.91	0.10	53,53,53,53	0
58	MG	2A	3318	1/1	0.91	0.14	54,54,54,54	0
58	MG	2a	1659	1/1	0.91	0.15	59,59,59,59	0
58	MG	1a	1697	1/1	0.91	0.19	51,51,51,51	0
58	MG	1E	305	1/1	0.91	0.23	50,50,50,50	0
58	MG	1A	3287	1/1	0.91	0.18	46,46,46,46	0
58	MG	2A	3086	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	3804	1/1	0.91	0.08	32,32,32,32	0
58	MG	1A	3332	1/1	0.91	0.12	45,45,45,45	0
58	MG	2a	1673	1/1	0.91	0.09	69,69,69,69	0
58	MG	1A	3815	1/1	0.91	0.07	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	3653	1/1	0.91	0.12	67,67,67,67	0
58	MG	2A	3655	1/1	0.91	0.20	62,62,62,62	0
58	MG	1a	1712	1/1	0.91	0.25	58,58,58,58	0
58	MG	2A	3097	1/1	0.91	0.09	59,59,59,59	0
58	MG	1A	3157	1/1	0.91	0.10	35,35,35,35	0
58	MG	1a	1715	1/1	0.91	0.18	55,55,55,55	0
58	MG	1A	3388	1/1	0.91	0.20	29,29,29,29	0
58	MG	2a	1688	1/1	0.91	0.15	61,61,61,61	0
58	MG	2A	3666	1/1	0.91	0.11	45,45,45,45	0
58	MG	1A	3830	1/1	0.91	0.07	42,42,42,42	0
58	MG	2a	1702	1/1	0.91	0.22	54,54,54,54	0
58	MG	1A	3660	1/1	0.91	0.12	41,41,41,41	0
58	MG	1A	3671	1/1	0.91	0.11	27,27,27,27	0
58	MG	1A	3448	1/1	0.91	0.22	48,48,48,48	0
58	MG	1Z	301	1/1	0.91	0.08	50,50,50,50	0
58	MG	2A	3349	1/1	0.91	0.18	54,54,54,54	0
58	MG	2A	3352	1/1	0.91	0.12	58,58,58,58	0
58	MG	2A	3683	1/1	0.91	0.18	56,56,56,56	0
58	MG	1Z	302	1/1	0.91	0.08	61,61,61,61	0
58	MG	10	107	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3123	1/1	0.91	0.23	69,69,69,69	0
58	MG	2A	3364	1/1	0.91	0.15	54,54,54,54	0
58	MG	11	101	1/1	0.91	0.32	41,41,41,41	0
58	MG	2A	3698	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3839	1/1	0.91	0.08	40,40,40,40	0
58	MG	2A	3144	1/1	0.91	0.26	65,65,65,65	0
58	MG	2A	3148	1/1	0.91	0.11	60,60,60,60	0
58	MG	1A	3687	1/1	0.91	0.13	56,56,56,56	0
58	MG	16	101	1/1	0.91	0.11	59,59,59,59	0
58	MG	2A	3163	1/1	0.91	0.36	63,63,63,63	0
58	MG	2a	1753	1/1	0.91	0.17	77,77,77,77	0
58	MG	2A	3379	1/1	0.91	0.12	55,55,55,55	0
58	MG	1a	1754	1/1	0.91	0.08	52,52,52,52	0
58	MG	1a	1602	1/1	0.91	0.40	68,68,68,68	0
58	MG	1a	1763	1/1	0.91	0.19	60,60,60,60	0
58	MG	2A	3173	1/1	0.91	0.13	57,57,57,57	0
58	MG	2a	1765	1/1	0.91	0.11	55,55,55,55	0
58	MG	2a	1767	1/1	0.91	0.18	69,69,69,69	0
58	MG	2a	1769	1/1	0.91	0.08	36,36,36,36	0
58	MG	1a	1604	1/1	0.91	0.11	64,64,64,64	0
58	MG	2A	3392	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3522	1/1	0.91	0.10	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	2A	3409	1/1	0.91	0.17	51,51,51,51	0
58	MG	1a	1768	1/1	0.91	0.08	52,52,52,52	0
58	MG	2a	1783	1/1	0.91	0.10	71,71,71,71	0
58	MG	2A	3746	1/1	0.91	0.12	51,51,51,51	0
58	MG	1A	3026	1/1	0.91	0.14	51,51,51,51	0
58	MG	2A	3187	1/1	0.91	0.10	70,70,70,70	0
58	MG	2A	3419	1/1	0.91	0.12	63,63,63,63	0
58	MG	2a	1794	1/1	0.91	0.20	60,60,60,60	0
58	MG	1A	3702	1/1	0.91	0.10	31,31,31,31	0
58	MG	1A	3468	1/1	0.91	0.09	49,49,49,49	0
58	MG	1A	3469	1/1	0.91	0.21	51,51,51,51	0
58	MG	2A	3771	1/1	0.91	0.12	45,45,45,45	0
58	MG	1a	1625	1/1	0.91	0.09	39,39,39,39	0
58	MG	2A	3774	1/1	0.91	0.12	59,59,59,59	0
58	MG	2A	3775	1/1	0.91	0.13	72,72,72,72	0
58	MG	1A	3544	1/1	0.91	0.29	66,66,66,66	0
58	MG	2a	1811	1/1	0.91	0.16	69,69,69,69	0
58	MG	2a	1812	1/1	0.91	0.26	54,54,54,54	0
58	MG	2A	3780	1/1	0.91	0.12	55,55,55,55	0
58	MG	2A	3432	1/1	0.91	0.24	52,52,52,52	0
58	MG	1A	3309	1/1	0.91	0.11	55,55,55,55	0
58	MG	2A	3789	1/1	0.91	0.08	45,45,45,45	0
58	MG	1a	1783	1/1	0.91	0.12	68,68,68,68	0
58	MG	2a	1821	1/1	0.91	0.20	67,67,67,67	0
58	MG	2A	3795	1/1	0.91	0.12	70,70,70,70	0
58	MG	1A	4033	1/1	0.91	0.11	60,60,60,60	0
58	MG	1A	3721	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3873	1/1	0.91	0.07	30,30,30,30	0
58	MG	2A	3446	1/1	0.91	0.15	53,53,53,53	0
58	MG	2A	3452	1/1	0.91	0.12	57,57,57,57	0
58	MG	2e	202	1/1	0.91	0.21	59,59,59,59	0
58	MG	2g	201	1/1	0.91	0.17	68,68,68,68	0
58	MG	1A	3875	1/1	0.91	0.35	45,45,45,45	0
58	MG	2A	3821	1/1	0.91	0.08	56,56,56,56	0
58	MG	1a	1804	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3827	1/1	0.91	0.10	57,57,57,57	0
58	MG	2A	3463	1/1	0.91	0.13	70,70,70,70	0
58	MG	2A	3464	1/1	0.91	0.13	41,41,41,41	0
58	MG	2A	3209	1/1	0.91	0.12	59,59,59,59	0
58	MG	2q	202	1/1	0.91	0.10	73,73,73,73	0
58	MG	1A	4047	1/1	0.91	0.12	48,48,48,48	0
58	MG	2A	3212	1/1	0.91	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3838	1/1	0.91	0.09	50,50,50,50	0
58	MG	1a	1638	1/1	0.91	0.13	39,39,39,39	0
58	MG	2A	3219	1/1	0.91	0.12	46,46,46,46	0
58	MG	2x	103	1/1	0.91	0.10	69,69,69,69	0
58	MG	1A	3261	1/1	0.91	0.21	64,64,64,64	0
58	MG	2A	3483	1/1	0.91	0.24	66,66,66,66	0
60	ERY	2A	3859	51/51	0.91	0.16	44,61,72,79	0
58	MG	2A	3529	1/1	0.92	0.10	33,33,33,33	0
58	MG	1A	3539	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3266	1/1	0.92	0.07	54,54,54,54	0
58	MG	2B	217	1/1	0.92	0.06	49,49,49,49	0
58	MG	2A	3534	1/1	0.92	0.13	36,36,36,36	0
58	MG	1A	4079	1/1	0.92	0.10	42,42,42,42	0
58	MG	2D	304	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3874	1/1	0.92	0.22	37,37,37,37	0
58	MG	1A	4083	1/1	0.92	0.15	47,47,47,47	0
58	MG	1A	3356	1/1	0.92	0.10	60,60,60,60	0
58	MG	1A	3168	1/1	0.92	0.11	32,32,32,32	0
58	MG	1a	1679	1/1	0.92	0.17	49,49,49,49	0
58	MG	2O	202	1/1	0.92	0.18	58,58,58,58	0
58	MG	1A	3719	1/1	0.92	0.17	56,56,56,56	0
58	MG	1A	4099	1/1	0.92	0.21	60,60,60,60	0
58	MG	2A	3282	1/1	0.92	0.17	62,62,62,62	0
58	MG	2A	3561	1/1	0.92	0.13	46,46,46,46	0
58	MG	1A	3549	1/1	0.92	0.12	65,65,65,65	0
58	MG	20	101	1/1	0.92	0.13	53,53,53,53	0
58	MG	20	102	1/1	0.92	0.12	59,59,59,59	0
58	MG	1B	203	1/1	0.92	0.07	29,29,29,29	0
58	MG	2A	3052	1/1	0.92	0.17	62,62,62,62	0
58	MG	1a	1686	1/1	0.92	0.22	64,64,64,64	0
58	MG	1B	208	1/1	0.92	0.14	50,50,50,50	0
58	MG	2A	3295	1/1	0.92	0.14	49,49,49,49	0
58	MG	28	103	1/1	0.92	0.08	60,60,60,60	0
58	MG	2A	3060	1/1	0.92	0.20	59,59,59,59	0
58	MG	2a	1602	1/1	0.92	0.16	68,68,68,68	0
58	MG	2A	3062	1/1	0.92	0.12	62,62,62,62	0
58	MG	2A	3064	1/1	0.92	0.10	43,43,43,43	0
58	MG	2a	1606	1/1	0.92	0.18	53,53,53,53	0
58	MG	1B	209	1/1	0.92	0.14	66,66,66,66	0
58	MG	2A	3587	1/1	0.92	0.17	64,64,64,64	0
58	MG	2A	3588	1/1	0.92	0.12	48,48,48,48	0
58	MG	2A	3301	1/1	0.92	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3304	1/1	0.92	0.22	63,63,63,63	0
58	MG	2A	3066	1/1	0.92	0.15	56,56,56,56	0
58	MG	2a	1616	1/1	0.92	0.13	62,62,62,62	0
58	MG	2A	3596	1/1	0.92	0.13	59,59,59,59	0
58	MG	2A	3597	1/1	0.92	0.07	29,29,29,29	0
58	MG	1A	3723	1/1	0.92	0.10	56,56,56,56	0
58	MG	2A	3600	1/1	0.92	0.10	53,53,53,53	0
58	MG	2A	3602	1/1	0.92	0.09	39,39,39,39	0
58	MG	2a	1624	1/1	0.92	0.14	60,60,60,60	0
58	MG	2A	3307	1/1	0.92	0.08	39,39,39,39	0
58	MG	2A	3069	1/1	0.92	0.08	48,48,48,48	0
58	MG	1A	3550	1/1	0.92	0.07	61,61,61,61	0
58	MG	2a	1631	1/1	0.92	0.06	74,74,74,74	0
58	MG	1A	3137	1/1	0.92	0.23	39,39,39,39	0
58	MG	2A	3314	1/1	0.92	0.29	61,61,61,61	0
58	MG	2A	3317	1/1	0.92	0.09	47,47,47,47	0
58	MG	2a	1636	1/1	0.92	0.33	63,63,63,63	0
58	MG	1A	3311	1/1	0.92	0.23	51,51,51,51	0
58	MG	1A	3455	1/1	0.92	0.17	64,64,64,64	0
58	MG	1a	1699	1/1	0.92	0.15	51,51,51,51	0
58	MG	2A	3088	1/1	0.92	0.15	63,63,63,63	0
58	MG	1A	3896	1/1	0.92	0.09	23,23,23,23	0
58	MG	1A	3897	1/1	0.92	0.10	68,68,68,68	0
58	MG	2a	1647	1/1	0.92	0.27	64,64,64,64	0
58	MG	1A	3196	1/1	0.92	0.27	54,54,54,54	0
58	MG	1A	3899	1/1	0.92	0.18	36,36,36,36	0
58	MG	1A	3197	1/1	0.92	0.10	40,40,40,40	0
58	MG	1A	3199	1/1	0.92	0.10	38,38,38,38	0
58	MG	2A	3639	1/1	0.92	0.22	67,67,67,67	0
58	MG	2A	3101	1/1	0.92	0.23	60,60,60,60	0
58	MG	1A	3589	1/1	0.92	0.12	43,43,43,43	0
58	MG	1a	1718	1/1	0.92	0.10	58,58,58,58	0
58	MG	1A	3762	1/1	0.92	0.12	50,50,50,50	0
58	MG	2A	3341	1/1	0.92	0.17	59,59,59,59	0
58	MG	2A	3342	1/1	0.92	0.24	55,55,55,55	0
58	MG	2A	3343	1/1	0.92	0.10	62,62,62,62	0
58	MG	1A	3917	1/1	0.92	0.09	24,24,24,24	0
58	MG	1a	1722	1/1	0.92	0.12	47,47,47,47	0
58	MG	1F	312	1/1	0.92	0.09	50,50,50,50	0
58	MG	1G	203	1/1	0.92	0.06	64,64,64,64	0
58	MG	1N	201	1/1	0.92	0.07	43,43,43,43	0
58	MG	2A	3351	1/1	0.92	0.11	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1732	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	3918	1/1	0.92	0.10	37,37,37,37	0
58	MG	1A	3765	1/1	0.92	0.15	45,45,45,45	0
58	MG	2A	3360	1/1	0.92	0.14	60,60,60,60	0
58	MG	2A	3361	1/1	0.92	0.17	62,62,62,62	0
58	MG	1Q	201	1/1	0.92	0.30	40,40,40,40	0
58	MG	2A	3138	1/1	0.92	0.20	62,62,62,62	0
58	MG	1Q	208	1/1	0.92	0.11	35,35,35,35	0
58	MG	1a	1745	1/1	0.92	0.13	69,69,69,69	0
58	MG	1A	3018	1/1	0.92	0.14	24,24,24,24	0
58	MG	1A	3593	1/1	0.92	0.20	64,64,64,64	0
58	MG	2A	3160	1/1	0.92	0.20	68,68,68,68	0
58	MG	1U	204	1/1	0.92	0.18	39,39,39,39	0
58	MG	1A	3597	1/1	0.92	0.23	61,61,61,61	0
58	MG	1A	3774	1/1	0.92	0.14	39,39,39,39	0
58	MG	1a	1762	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	3938	1/1	0.92	0.09	50,50,50,50	0
58	MG	2A	3386	1/1	0.92	0.10	64,64,64,64	0
58	MG	1A	3066	1/1	0.92	0.15	52,52,52,52	0
58	MG	1A	3207	1/1	0.92	0.07	52,52,52,52	0
58	MG	2a	1725	1/1	0.92	0.15	67,67,67,67	0
58	MG	2A	3715	1/1	0.92	0.20	62,62,62,62	0
58	MG	2A	3179	1/1	0.92	0.15	50,50,50,50	0
58	MG	2A	3390	1/1	0.92	0.18	62,62,62,62	0
58	MG	1A	3401	1/1	0.92	0.12	57,57,57,57	0
58	MG	2A	3397	1/1	0.92	0.15	55,55,55,55	0
58	MG	2A	3399	1/1	0.92	0.10	34,34,34,34	0
58	MG	1A	3403	1/1	0.92	0.10	39,39,39,39	0
58	MG	2A	3406	1/1	0.92	0.21	46,46,46,46	0
58	MG	2a	1743	1/1	0.92	0.26	58,58,58,58	0
58	MG	1A	3956	1/1	0.92	0.08	60,60,60,60	0
58	MG	2a	1749	1/1	0.92	0.14	60,60,60,60	0
58	MG	2a	1750	1/1	0.92	0.12	60,60,60,60	0
58	MG	1A	3957	1/1	0.92	0.09	44,44,44,44	0
58	MG	2A	3736	1/1	0.92	0.07	41,41,41,41	0
58	MG	2A	3742	1/1	0.92	0.13	65,65,65,65	0
58	MG	2a	1757	1/1	0.92	0.14	68,68,68,68	0
58	MG	1A	3799	1/1	0.92	0.17	53,53,53,53	0
58	MG	1A	3802	1/1	0.92	0.07	26,26,26,26	0
58	MG	1A	3613	1/1	0.92	0.08	40,40,40,40	0
58	MG	2A	3420	1/1	0.92	0.12	50,50,50,50	0
58	MG	2A	3752	1/1	0.92	0.09	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	2A	3194	1/1	0.92	0.20	62,62,62,62	0
58	MG	2A	3423	1/1	0.92	0.12	60,60,60,60	0
58	MG	2A	3766	1/1	0.92	0.16	55,55,55,55	0
58	MG	2A	3196	1/1	0.92	0.35	61,61,61,61	0
58	MG	1a	1607	1/1	0.92	0.21	58,58,58,58	0
58	MG	1A	3286	1/1	0.92	0.08	47,47,47,47	0
58	MG	1A	3069	1/1	0.92	0.12	50,50,50,50	0
58	MG	2a	1782	1/1	0.92	0.17	72,72,72,72	0
58	MG	1A	3972	1/1	0.92	0.11	71,71,71,71	0
58	MG	1a	1792	1/1	0.92	0.10	63,63,63,63	0
58	MG	1a	1793	1/1	0.92	0.09	66,66,66,66	0
58	MG	2A	3779	1/1	0.92	0.13	56,56,56,56	0
58	MG	1a	1799	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3335	1/1	0.92	0.17	52,52,52,52	0
58	MG	1A	3336	1/1	0.92	0.07	44,44,44,44	0
58	MG	2A	3788	1/1	0.92	0.10	72,72,72,72	0
58	MG	2A	3210	1/1	0.92	0.20	69,69,69,69	0
58	MG	2A	3448	1/1	0.92	0.11	51,51,51,51	0
58	MG	1A	3341	1/1	0.92	0.12	41,41,41,41	0
58	MG	1a	1626	1/1	0.92	0.21	46,46,46,46	0
58	MG	2A	3457	1/1	0.92	0.12	48,48,48,48	0
58	MG	2A	3458	1/1	0.92	0.14	59,59,59,59	0
58	MG	2A	3214	1/1	0.92	0.21	48,48,48,48	0
58	MG	2A	3814	1/1	0.92	0.10	45,45,45,45	0
58	MG	2A	3462	1/1	0.92	0.23	56,56,56,56	0
58	MG	1A	3009	1/1	0.92	0.08	24,24,24,24	0
58	MG	1A	3419	1/1	0.92	0.18	59,59,59,59	0
58	MG	2a	1818	1/1	0.92	0.20	66,66,66,66	0
58	MG	1A	3654	1/1	0.92	0.07	59,59,59,59	0
58	MG	1a	1631	1/1	0.92	0.27	62,62,62,62	0
58	MG	1A	4003	1/1	0.92	0.07	70,70,70,70	0
58	MG	2a	1823	1/1	0.92	0.15	57,57,57,57	0
58	MG	1A	3423	1/1	0.92	0.19	43,43,43,43	0
58	MG	1A	4016	1/1	0.92	0.08	69,69,69,69	0
58	MG	1A	3665	1/1	0.92	0.07	21,21,21,21	0
58	MG	1A	3667	1/1	0.92	0.06	24,24,24,24	0
58	MG	1A	4027	1/1	0.92	0.13	51,51,51,51	0
58	MG	1A	3848	1/1	0.92	0.20	46,46,46,46	0
58	MG	1A	3427	1/1	0.92	0.13	48,48,48,48	0
58	MG	1x	101	1/1	0.92	0.28	62,62,62,62	0
58	MG	2j	201	1/1	0.92	0.10	63,63,63,63	0
58	MG	1x	103	1/1	0.92	0.16	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	1A	3295	1/1	0.92	0.16	41,41,41,41	0
58	MG	2A	3496	1/1	0.92	0.08	52,52,52,52	0
58	MG	1A	3429	1/1	0.92	0.13	57,57,57,57	0
58	MG	1A	4043	1/1	0.92	0.14	36,36,36,36	0
58	MG	1A	3524	1/1	0.92	0.11	65,65,65,65	0
58	MG	1A	3527	1/1	0.92	0.11	61,61,61,61	0
58	MG	2A	3858	1/1	0.92	0.12	61,61,61,61	0
58	MG	2t	201	1/1	0.92	0.13	37,37,37,37	0
58	MG	2B	202	1/1	0.92	0.09	67,67,67,67	0
58	MG	1x	111	1/1	0.92	0.21	58,58,58,58	0
58	MG	2B	204	1/1	0.92	0.11	64,64,64,64	0
58	MG	1A	3696	1/1	0.92	0.06	15,15,15,15	0
58	MG	2A	3521	1/1	0.92	0.09	57,57,57,57	0
58	MG	2x	102	1/1	0.92	0.18	62,62,62,62	0
58	MG	2B	207	1/1	0.92	0.09	65,65,65,65	0
58	MG	1A	3350	1/1	0.92	0.16	41,41,41,41	0
58	MG	2B	209	1/1	0.92	0.17	61,61,61,61	0
58	MG	1A	3247	1/1	0.92	0.20	59,59,59,59	0
58	MG	1B	204	1/1	0.93	0.14	55,55,55,55	0
58	MG	1A	3906	1/1	0.93	0.10	42,42,42,42	0
58	MG	1a	1672	1/1	0.93	0.08	48,48,48,48	0
58	MG	1A	3362	1/1	0.93	0.07	38,38,38,38	0
58	MG	2A	3024	1/1	0.93	0.16	57,57,57,57	0
58	MG	2A	3028	1/1	0.93	0.09	49,49,49,49	0
58	MG	2F	301	1/1	0.93	0.13	56,56,56,56	0
58	MG	1a	1674	1/1	0.93	0.34	58,58,58,58	0
58	MG	1A	3908	1/1	0.93	0.15	57,57,57,57	0
58	MG	1A	3364	1/1	0.93	0.12	41,41,41,41	0
58	MG	2P	201	1/1	0.93	0.09	50,50,50,50	0
58	MG	1A	3602	1/1	0.93	0.06	32,32,32,32	0
58	MG	1A	3084	1/1	0.93	0.18	36,36,36,36	0
58	MG	2A	3045	1/1	0.93	0.08	47,47,47,47	0
58	MG	2V	201	1/1	0.93	0.29	52,52,52,52	0
58	MG	2A	3046	1/1	0.93	0.08	72,72,72,72	0
58	MG	2A	3048	1/1	0.93	0.15	57,57,57,57	0
58	MG	2W	203	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3302	1/1	0.93	0.14	56,56,56,56	0
58	MG	2A	3303	1/1	0.93	0.15	56,56,56,56	0
58	MG	1a	1681	1/1	0.93	0.25	50,50,50,50	0
58	MG	1A	3605	1/1	0.93	0.13	50,50,50,50	0
58	MG	1A	3145	1/1	0.93	0.11	32,32,32,32	0
58	MG	2A	3054	1/1	0.93	0.17	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	2A	3591	1/1	0.93	0.11	61,61,61,61	0
58	MG	28	102	1/1	0.93	0.11	49,49,49,49	0
58	MG	1a	1684	1/1	0.93	0.06	43,43,43,43	0
58	MG	1A	3610	1/1	0.93	0.10	18,18,18,18	0
58	MG	1A	3507	1/1	0.93	0.11	40,40,40,40	0
58	MG	2A	3313	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3381	1/1	0.93	0.22	44,44,44,44	0
58	MG	2A	3316	1/1	0.93	0.10	63,63,63,63	0
58	MG	1A	3302	1/1	0.93	0.06	27,27,27,27	0
58	MG	1A	3433	1/1	0.93	0.10	35,35,35,35	0
58	MG	1A	3636	1/1	0.93	0.07	30,30,30,30	0
58	MG	1E	310	1/1	0.93	0.10	26,26,26,26	0
58	MG	1a	1696	1/1	0.93	0.18	41,41,41,41	0
58	MG	2A	3326	1/1	0.93	0.17	70,70,70,70	0
58	MG	2a	1615	1/1	0.93	0.16	52,52,52,52	0
58	MG	1A	3795	1/1	0.93	0.06	24,24,24,24	0
58	MG	2A	3624	1/1	0.93	0.17	61,61,61,61	0
58	MG	2A	3328	1/1	0.93	0.11	53,53,53,53	0
58	MG	2a	1619	1/1	0.93	0.14	70,70,70,70	0
58	MG	1A	3950	1/1	0.93	0.07	77,77,77,77	0
58	MG	1A	3384	1/1	0.93	0.06	40,40,40,40	0
58	MG	1A	3053	1/1	0.93	0.07	40,40,40,40	0
58	MG	1I	201	1/1	0.93	0.18	65,65,65,65	0
58	MG	2A	3632	1/1	0.93	0.20	63,63,63,63	0
58	MG	1a	1702	1/1	0.93	0.23	49,49,49,49	0
58	MG	2a	1629	1/1	0.93	0.18	65,65,65,65	0
58	MG	1a	1704	1/1	0.93	0.11	46,46,46,46	0
58	MG	1A	3525	1/1	0.93	0.07	57,57,57,57	0
58	MG	2A	3093	1/1	0.93	0.07	37,37,37,37	0
58	MG	1a	1708	1/1	0.93	0.15	62,62,62,62	0
58	MG	1O	201	1/1	0.93	0.07	59,59,59,59	0
58	MG	1a	1711	1/1	0.93	0.16	62,62,62,62	0
58	MG	1A	3526	1/1	0.93	0.07	55,55,55,55	0
58	MG	1O	203	1/1	0.93	0.09	53,53,53,53	0
58	MG	2A	3104	1/1	0.93	0.14	36,36,36,36	0
58	MG	1A	3652	1/1	0.93	0.06	25,25,25,25	0
58	MG	1A	3204	1/1	0.93	0.06	28,28,28,28	0
58	MG	2a	1644	1/1	0.93	0.19	52,52,52,52	0
58	MG	1A	3821	1/1	0.93	0.13	44,44,44,44	0
58	MG	2A	3657	1/1	0.93	0.08	58,58,58,58	0
58	MG	1R	203	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3661	1/1	0.93	0.11	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	3662	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3657	1/1	0.93	0.11	45,45,45,45	0
58	MG	1S	203	1/1	0.93	0.08	66,66,66,66	0
58	MG	1A	3966	1/1	0.93	0.07	21,21,21,21	0
58	MG	2A	3358	1/1	0.93	0.14	62,62,62,62	0
58	MG	2A	3120	1/1	0.93	0.15	40,40,40,40	0
58	MG	1A	3532	1/1	0.93	0.16	45,45,45,45	0
58	MG	2a	1657	1/1	0.93	0.10	61,61,61,61	0
58	MG	2A	3122	1/1	0.93	0.12	43,43,43,43	0
58	MG	1U	206	1/1	0.93	0.18	29,29,29,29	0
58	MG	2a	1661	1/1	0.93	0.12	66,66,66,66	0
58	MG	2A	3128	1/1	0.93	0.10	58,58,58,58	0
58	MG	2A	3675	1/1	0.93	0.10	52,52,52,52	0
58	MG	1a	1733	1/1	0.93	0.08	40,40,40,40	0
58	MG	2a	1668	1/1	0.93	0.10	71,71,71,71	0
58	MG	1A	3663	1/1	0.93	0.16	41,41,41,41	0
58	MG	2A	3132	1/1	0.93	0.15	67,67,67,67	0
58	MG	2A	3135	1/1	0.93	0.07	45,45,45,45	0
58	MG	2A	3686	1/1	0.93	0.08	70,70,70,70	0
58	MG	2a	1676	1/1	0.93	0.12	50,50,50,50	0
58	MG	1A	3446	1/1	0.93	0.11	33,33,33,33	0
58	MG	2A	3376	1/1	0.93	0.11	57,57,57,57	0
58	MG	2A	3377	1/1	0.93	0.18	49,49,49,49	0
58	MG	2a	1680	1/1	0.93	0.14	45,45,45,45	0
58	MG	2A	3693	1/1	0.93	0.25	64,64,64,64	0
58	MG	2a	1682	1/1	0.93	0.10	65,65,65,65	0
58	MG	2A	3140	1/1	0.93	0.12	53,53,53,53	0
58	MG	1W	207	1/1	0.93	0.11	19,19,19,19	0
58	MG	1X	104	1/1	0.93	0.09	39,39,39,39	0
58	MG	1A	3980	1/1	0.93	0.12	55,55,55,55	0
58	MG	1Y	203	1/1	0.93	0.28	41,41,41,41	0
58	MG	2a	1697	1/1	0.93	0.16	41,41,41,41	0
58	MG	2a	1699	1/1	0.93	0.13	56,56,56,56	0
58	MG	2a	1700	1/1	0.93	0.16	68,68,68,68	0
58	MG	1A	3535	1/1	0.93	0.14	39,39,39,39	0
58	MG	1A	3054	1/1	0.93	0.10	33,33,33,33	0
58	MG	1a	1753	1/1	0.93	0.15	48,48,48,48	0
58	MG	2A	3714	1/1	0.93	0.13	52,52,52,52	0
58	MG	10	103	1/1	0.93	0.08	38,38,38,38	0
58	MG	2A	3717	1/1	0.93	0.14	47,47,47,47	0
58	MG	2a	1710	1/1	0.93	0.09	65,65,65,65	0
58	MG	10	104	1/1	0.93	0.13	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	3720	1/1	0.93	0.16	48,48,48,48	0
58	MG	1a	1761	1/1	0.93	0.08	52,52,52,52	0
58	MG	2a	1718	1/1	0.93	0.07	50,50,50,50	0
58	MG	2a	1719	1/1	0.93	0.08	63,63,63,63	0
58	MG	10	105	1/1	0.93	0.20	71,71,71,71	0
58	MG	1A	3838	1/1	0.93	0.09	39,39,39,39	0
58	MG	2a	1724	1/1	0.93	0.25	67,67,67,67	0
58	MG	2A	3724	1/1	0.93	0.12	47,47,47,47	0
58	MG	2A	3404	1/1	0.93	0.17	51,51,51,51	0
58	MG	2A	3178	1/1	0.93	0.07	58,58,58,58	0
58	MG	2a	1731	1/1	0.93	0.22	54,54,54,54	0
58	MG	1A	3989	1/1	0.93	0.08	30,30,30,30	0
58	MG	2a	1733	1/1	0.93	0.13	44,44,44,44	0
58	MG	2a	1734	1/1	0.93	0.26	57,57,57,57	0
58	MG	2A	3732	1/1	0.93	0.10	51,51,51,51	0
58	MG	11	103	1/1	0.93	0.09	47,47,47,47	0
58	MG	11	104	1/1	0.93	0.11	39,39,39,39	0
58	MG	1a	1770	1/1	0.93	0.06	66,66,66,66	0
58	MG	1A	3680	1/1	0.93	0.13	17,17,17,17	0
58	MG	2a	1741	1/1	0.93	0.30	55,55,55,55	0
58	MG	2A	3743	1/1	0.93	0.15	45,45,45,45	0
58	MG	2a	1744	1/1	0.93	0.13	50,50,50,50	0
58	MG	2a	1745	1/1	0.93	0.34	71,71,71,71	0
58	MG	2a	1747	1/1	0.93	0.22	60,60,60,60	0
58	MG	11	106	1/1	0.93	0.09	43,43,43,43	0
58	MG	13	105	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3192	1/1	0.93	0.07	45,45,45,45	0
58	MG	1A	3996	1/1	0.93	0.08	27,27,27,27	0
58	MG	1A	3999	1/1	0.93	0.10	21,21,21,21	0
58	MG	2A	3753	1/1	0.93	0.09	66,66,66,66	0
58	MG	2A	3195	1/1	0.93	0.21	58,58,58,58	0
58	MG	2A	3762	1/1	0.93	0.08	50,50,50,50	0
58	MG	2a	1760	1/1	0.93	0.17	54,54,54,54	0
58	MG	19	101	1/1	0.93	0.10	38,38,38,38	0
58	MG	1A	3682	1/1	0.93	0.05	23,23,23,23	0
58	MG	1A	3454	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3435	1/1	0.93	0.23	47,47,47,47	0
58	MG	2a	1766	1/1	0.93	0.22	73,73,73,73	0
58	MG	1a	1606	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3393	1/1	0.93	0.10	58,58,58,58	0
58	MG	2a	1771	1/1	0.93	0.17	54,54,54,54	0
58	MG	2a	1772	1/1	0.93	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3773	1/1	0.93	0.12	58,58,58,58	0
58	MG	1a	1790	1/1	0.93	0.08	68,68,68,68	0
58	MG	1A	3339	1/1	0.93	0.06	49,49,49,49	0
58	MG	2A	3444	1/1	0.93	0.10	52,52,52,52	0
58	MG	1A	3860	1/1	0.93	0.10	56,56,56,56	0
58	MG	1a	1798	1/1	0.93	0.07	82,82,82,82	0
58	MG	2A	3783	1/1	0.93	0.10	53,53,53,53	0
58	MG	1A	4020	1/1	0.93	0.07	64,64,64,64	0
58	MG	2a	1786	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3547	1/1	0.93	0.16	49,49,49,49	0
58	MG	1A	3206	1/1	0.93	0.10	34,34,34,34	0
58	MG	1A	4031	1/1	0.93	0.08	40,40,40,40	0
58	MG	1a	1805	1/1	0.93	0.09	56,56,56,56	0
58	MG	1a	1806	1/1	0.93	0.07	58,58,58,58	0
58	MG	2a	1799	1/1	0.93	0.19	74,74,74,74	0
58	MG	2A	3216	1/1	0.93	0.24	52,52,52,52	0
58	MG	2a	1802	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	3006	1/1	0.93	0.07	40,40,40,40	0
58	MG	2A	3803	1/1	0.93	0.07	33,33,33,33	0
58	MG	1A	3704	1/1	0.93	0.06	28,28,28,28	0
58	MG	2A	3805	1/1	0.93	0.07	37,37,37,37	0
58	MG	1A	3315	1/1	0.93	0.06	31,31,31,31	0
58	MG	2A	3468	1/1	0.93	0.06	49,49,49,49	0
58	MG	1A	3319	1/1	0.93	0.16	31,31,31,31	0
58	MG	2A	3476	1/1	0.93	0.13	43,43,43,43	0
58	MG	1A	3322	1/1	0.93	0.08	47,47,47,47	0
58	MG	1A	3717	1/1	0.93	0.12	49,49,49,49	0
58	MG	1A	3046	1/1	0.93	0.07	25,25,25,25	0
58	MG	1n	101	1/1	0.93	0.07	49,49,49,49	0
58	MG	2A	3486	1/1	0.93	0.19	57,57,57,57	0
58	MG	2A	3833	1/1	0.93	0.08	55,55,55,55	0
58	MG	1s	101	1/1	0.93	0.16	62,62,62,62	0
58	MG	1A	3572	1/1	0.93	0.14	48,48,48,48	0
58	MG	1v	101	1/1	0.93	0.13	78,78,78,78	0
58	MG	1a	1636	1/1	0.93	0.24	52,52,52,52	0
58	MG	1A	3016	1/1	0.93	0.15	52,52,52,52	0
58	MG	2a	1828	1/1	0.93	0.14	72,72,72,72	0
58	MG	1A	3586	1/1	0.93	0.10	57,57,57,57	0
58	MG	1A	3477	1/1	0.93	0.07	36,36,36,36	0
58	MG	2A	3497	1/1	0.93	0.12	32,32,32,32	0
58	MG	2A	3499	1/1	0.93	0.06	56,56,56,56	0
58	MG	2f	202	1/1	0.93	0.08	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3731	1/1	0.93	0.09	68,68,68,68	0
58	MG	2i	201	1/1	0.93	0.06	55,55,55,55	0
58	MG	1A	3481	1/1	0.93	0.11	44,44,44,44	0
58	MG	2A	3507	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3075	1/1	0.93	0.23	55,55,55,55	0
58	MG	1A	3743	1/1	0.93	0.09	45,45,45,45	0
58	MG	1A	3361	1/1	0.93	0.06	49,49,49,49	0
58	MG	2B	201	1/1	0.93	0.16	66,66,66,66	0
58	MG	2A	3518	1/1	0.93	0.11	56,56,56,56	0
58	MG	1a	1658	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3750	1/1	0.93	0.07	14,14,14,14	0
58	MG	1A	4094	1/1	0.93	0.07	52,52,52,52	0
58	MG	1A	4098	1/1	0.93	0.14	60,60,60,60	0
58	MG	2v	102	1/1	0.93	0.27	66,66,66,66	0
58	MG	1A	3595	1/1	0.93	0.19	51,51,51,51	0
58	MG	2A	3003	1/1	0.93	0.24	51,51,51,51	0
58	MG	1a	1664	1/1	0.93	0.17	60,60,60,60	0
58	MG	2A	3273	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3752	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3006	1/1	0.93	0.14	56,56,56,56	0
58	MG	1A	3420	1/1	0.93	0.13	54,54,54,54	0
58	MG	2x	106	1/1	0.93	0.16	67,67,67,67	0
58	MG	2A	3278	1/1	0.93	0.12	44,44,44,44	0
60	ERY	1A	4104	51/51	0.93	0.13	25,44,56,62	0
58	MG	2B	219	1/1	0.93	0.19	81,81,81,81	0
58	MG	2A	3449	1/1	0.94	0.10	58,58,58,58	0
58	MG	2A	3161	1/1	0.94	0.08	59,59,59,59	0
58	MG	2A	3162	1/1	0.94	0.10	38,38,38,38	0
58	MG	2A	3851	1/1	0.94	0.08	68,68,68,68	0
58	MG	1A	3399	1/1	0.94	0.09	42,42,42,42	0
58	MG	2A	3164	1/1	0.94	0.23	54,54,54,54	0
58	MG	2A	3460	1/1	0.94	0.21	57,57,57,57	0
58	MG	1A	3320	1/1	0.94	0.08	49,49,49,49	0
58	MG	1D	303	1/1	0.94	0.23	43,43,43,43	0
58	MG	1D	305	1/1	0.94	0.09	37,37,37,37	0
58	MG	1A	3695	1/1	0.94	0.08	21,21,21,21	0
58	MG	2A	3174	1/1	0.94	0.10	48,48,48,48	0
58	MG	1D	314	1/1	0.94	0.09	35,35,35,35	0
58	MG	1E	301	1/1	0.94	0.14	44,44,44,44	0
58	MG	1E	304	1/1	0.94	0.10	40,40,40,40	0
58	MG	1A	3249	1/1	0.94	0.11	48,48,48,48	0
58	MG	2A	3183	1/1	0.94	0.06	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	1731	1/1	0.94	0.12	60,60,60,60	0
58	MG	1E	308	1/1	0.94	0.10	55,55,55,55	0
58	MG	2A	3482	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3002	1/1	0.94	0.11	48,48,48,48	0
58	MG	1A	3405	1/1	0.94	0.19	54,54,54,54	0
58	MG	2A	3189	1/1	0.94	0.12	59,59,59,59	0
58	MG	1A	3325	1/1	0.94	0.11	46,46,46,46	0
58	MG	1A	3710	1/1	0.94	0.08	29,29,29,29	0
58	MG	2D	301	1/1	0.94	0.13	45,45,45,45	0
58	MG	1E	313	1/1	0.94	0.05	51,51,51,51	0
58	MG	1A	3528	1/1	0.94	0.08	44,44,44,44	0
58	MG	2D	306	1/1	0.94	0.18	58,58,58,58	0
58	MG	1A	3055	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3136	1/1	0.94	0.13	24,24,24,24	0
58	MG	1A	3059	1/1	0.94	0.07	37,37,37,37	0
58	MG	2E	307	1/1	0.94	0.11	53,53,53,53	0
58	MG	1N	204	1/1	0.94	0.11	44,44,44,44	0
58	MG	1A	3085	1/1	0.94	0.06	34,34,34,34	0
58	MG	2F	306	1/1	0.94	0.08	56,56,56,56	0
58	MG	2A	3501	1/1	0.94	0.11	45,45,45,45	0
58	MG	2O	201	1/1	0.94	0.13	64,64,64,64	0
58	MG	1a	1755	1/1	0.94	0.08	54,54,54,54	0
58	MG	2A	3503	1/1	0.94	0.14	56,56,56,56	0
58	MG	1a	1757	1/1	0.94	0.12	37,37,37,37	0
58	MG	1A	3416	1/1	0.94	0.09	48,48,48,48	0
58	MG	2A	3509	1/1	0.94	0.08	34,34,34,34	0
58	MG	2T	202	1/1	0.94	0.12	66,66,66,66	0
58	MG	1A	3418	1/1	0.94	0.26	49,49,49,49	0
58	MG	1A	3726	1/1	0.94	0.11	40,40,40,40	0
58	MG	2A	3517	1/1	0.94	0.11	35,35,35,35	0
58	MG	2A	3206	1/1	0.94	0.18	59,59,59,59	0
58	MG	1P	204	1/1	0.94	0.11	51,51,51,51	0
58	MG	1A	3542	1/1	0.94	0.10	39,39,39,39	0
58	MG	2A	3522	1/1	0.94	0.20	64,64,64,64	0
58	MG	23	101	1/1	0.94	0.17	59,59,59,59	0
58	MG	1Q	207	1/1	0.94	0.09	43,43,43,43	0
58	MG	1A	3919	1/1	0.94	0.12	43,43,43,43	0
58	MG	2A	3526	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	3730	1/1	0.94	0.27	58,58,58,58	0
58	MG	27	102	1/1	0.94	0.08	44,44,44,44	0
58	MG	27	103	1/1	0.94	0.10	45,45,45,45	0
58	MG	28	101	1/1	0.94	0.10	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1S	201	1/1	0.94	0.13	45,45,45,45	0
58	MG	1A	3095	1/1	0.94	0.10	41,41,41,41	0
58	MG	1A	3929	1/1	0.94	0.09	46,46,46,46	0
58	MG	1T	202	1/1	0.94	0.11	43,43,43,43	0
58	MG	1A	3546	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3738	1/1	0.94	0.10	60,60,60,60	0
58	MG	2A	3548	1/1	0.94	0.14	49,49,49,49	0
58	MG	2A	3550	1/1	0.94	0.08	57,57,57,57	0
58	MG	2A	3551	1/1	0.94	0.20	38,38,38,38	0
58	MG	2A	3230	1/1	0.94	0.27	52,52,52,52	0
58	MG	2a	1611	1/1	0.94	0.12	71,71,71,71	0
58	MG	2A	3554	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3739	1/1	0.94	0.10	53,53,53,53	0
58	MG	1A	3263	1/1	0.94	0.08	43,43,43,43	0
58	MG	1V	204	1/1	0.94	0.18	48,48,48,48	0
58	MG	2A	3558	1/1	0.94	0.07	44,44,44,44	0
58	MG	1A	3422	1/1	0.94	0.08	43,43,43,43	0
58	MG	1W	201	1/1	0.94	0.07	36,36,36,36	0
58	MG	1W	202	1/1	0.94	0.21	51,51,51,51	0
58	MG	1A	3745	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3268	1/1	0.94	0.23	45,45,45,45	0
58	MG	1A	3424	1/1	0.94	0.09	38,38,38,38	0
58	MG	1A	3110	1/1	0.94	0.28	32,32,32,32	0
58	MG	2A	3246	1/1	0.94	0.06	44,44,44,44	0
58	MG	2A	3247	1/1	0.94	0.08	62,62,62,62	0
58	MG	1A	3061	1/1	0.94	0.09	35,35,35,35	0
58	MG	1A	3278	1/1	0.94	0.12	30,30,30,30	0
58	MG	10	101	1/1	0.94	0.09	38,38,38,38	0
58	MG	1A	3034	1/1	0.94	0.16	31,31,31,31	0
58	MG	1a	1808	1/1	0.94	0.19	58,58,58,58	0
58	MG	1A	3344	1/1	0.94	0.12	38,38,38,38	0
58	MG	1a	1813	1/1	0.94	0.08	55,55,55,55	0
58	MG	1A	3432	1/1	0.94	0.10	39,39,39,39	0
58	MG	1A	3763	1/1	0.94	0.08	36,36,36,36	0
58	MG	10	108	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3595	1/1	0.94	0.11	63,63,63,63	0
58	MG	1d	301	1/1	0.94	0.25	55,55,55,55	0
58	MG	1A	3345	1/1	0.94	0.17	36,36,36,36	0
58	MG	2a	1645	1/1	0.94	0.10	67,67,67,67	0
58	MG	1A	3767	1/1	0.94	0.08	15,15,15,15	0
58	MG	1A	3588	1/1	0.94	0.11	33,33,33,33	0
58	MG	1A	3436	1/1	0.94	0.17	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	2A	3274	1/1	0.94	0.28	74,74,74,74	0
58	MG	1A	3976	1/1	0.94	0.09	49,49,49,49	0
58	MG	12	101	1/1	0.94	0.12	54,54,54,54	0
58	MG	13	101	1/1	0.94	0.07	56,56,56,56	0
58	MG	2A	3611	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3978	1/1	0.94	0.10	67,67,67,67	0
58	MG	2A	3615	1/1	0.94	0.12	30,30,30,30	0
58	MG	15	101	1/1	0.94	0.12	41,41,41,41	0
58	MG	2A	3618	1/1	0.94	0.08	34,34,34,34	0
58	MG	15	107	1/1	0.94	0.21	27,27,27,27	0
58	MG	1A	3024	1/1	0.94	0.11	46,46,46,46	0
58	MG	1A	3290	1/1	0.94	0.14	49,49,49,49	0
58	MG	17	105	1/1	0.94	0.06	41,41,41,41	0
58	MG	2a	1663	1/1	0.94	0.09	79,79,79,79	0
58	MG	2a	1664	1/1	0.94	0.09	57,57,57,57	0
58	MG	1x	102	1/1	0.94	0.14	55,55,55,55	0
58	MG	18	101	1/1	0.94	0.12	50,50,50,50	0
58	MG	2a	1667	1/1	0.94	0.10	61,61,61,61	0
58	MG	1A	3594	1/1	0.94	0.21	56,56,56,56	0
58	MG	2A	3290	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3292	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3985	1/1	0.94	0.06	29,29,29,29	0
58	MG	1A	3351	1/1	0.94	0.12	51,51,51,51	0
58	MG	2a	1675	1/1	0.94	0.24	61,61,61,61	0
58	MG	2A	3637	1/1	0.94	0.19	54,54,54,54	0
58	MG	1A	3596	1/1	0.94	0.16	44,44,44,44	0
58	MG	1A	3990	1/1	0.94	0.12	41,41,41,41	0
58	MG	1a	1608	1/1	0.94	0.16	64,64,64,64	0
58	MG	1A	3789	1/1	0.94	0.07	68,68,68,68	0
58	MG	2A	3645	1/1	0.94	0.09	79,79,79,79	0
58	MG	1A	3992	1/1	0.94	0.09	57,57,57,57	0
58	MG	2A	3647	1/1	0.94	0.12	71,71,71,71	0
58	MG	2A	3649	1/1	0.94	0.07	41,41,41,41	0
58	MG	1a	1619	1/1	0.94	0.11	56,56,56,56	0
58	MG	1A	3292	1/1	0.94	0.09	41,41,41,41	0
58	MG	2a	1690	1/1	0.94	0.12	59,59,59,59	0
58	MG	2a	1691	1/1	0.94	0.27	60,60,60,60	0
58	MG	1A	3997	1/1	0.94	0.09	16,16,16,16	0
58	MG	2a	1696	1/1	0.94	0.25	55,55,55,55	0
58	MG	2A	3007	1/1	0.94	0.16	60,60,60,60	0
58	MG	1A	3998	1/1	0.94	0.13	36,36,36,36	0
58	MG	1A	3355	1/1	0.94	0.13	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	3796	1/1	0.94	0.15	66,66,66,66	0
58	MG	2A	3660	1/1	0.94	0.17	51,51,51,51	0
58	MG	2a	1703	1/1	0.94	0.12	61,61,61,61	0
58	MG	2a	1704	1/1	0.94	0.07	45,45,45,45	0
58	MG	2A	3310	1/1	0.94	0.14	44,44,44,44	0
58	MG	1A	4002	1/1	0.94	0.12	83,83,83,83	0
58	MG	1A	3209	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3357	1/1	0.94	0.12	41,41,41,41	0
58	MG	2A	3315	1/1	0.94	0.22	59,59,59,59	0
58	MG	1A	3214	1/1	0.94	0.14	52,52,52,52	0
58	MG	2a	1715	1/1	0.94	0.15	56,56,56,56	0
58	MG	1A	3296	1/1	0.94	0.06	43,43,43,43	0
58	MG	1A	3299	1/1	0.94	0.34	58,58,58,58	0
58	MG	1A	3300	1/1	0.94	0.21	47,47,47,47	0
58	MG	2A	3671	1/1	0.94	0.12	63,63,63,63	0
58	MG	2A	3039	1/1	0.94	0.14	31,31,31,31	0
58	MG	2A	3040	1/1	0.94	0.15	60,60,60,60	0
58	MG	1A	3817	1/1	0.94	0.07	44,44,44,44	0
58	MG	2A	3677	1/1	0.94	0.07	75,75,75,75	0
58	MG	2A	3680	1/1	0.94	0.09	52,52,52,52	0
58	MG	2a	1728	1/1	0.94	0.28	64,64,64,64	0
58	MG	2a	1729	1/1	0.94	0.13	65,65,65,65	0
58	MG	1A	4028	1/1	0.94	0.08	36,36,36,36	0
58	MG	1A	3820	1/1	0.94	0.06	27,27,27,27	0
58	MG	1a	1640	1/1	0.94	0.22	49,49,49,49	0
58	MG	1A	3363	1/1	0.94	0.09	58,58,58,58	0
58	MG	1A	3219	1/1	0.94	0.13	46,46,46,46	0
58	MG	2A	3050	1/1	0.94	0.09	26,26,26,26	0
58	MG	1A	4035	1/1	0.94	0.09	37,37,37,37	0
58	MG	1a	1645	1/1	0.94	0.12	63,63,63,63	0
58	MG	1A	3615	1/1	0.94	0.15	57,57,57,57	0
58	MG	1A	3366	1/1	0.94	0.13	39,39,39,39	0
58	MG	2A	3695	1/1	0.94	0.10	47,47,47,47	0
58	MG	2a	1742	1/1	0.94	0.13	58,58,58,58	0
58	MG	2A	3697	1/1	0.94	0.10	37,37,37,37	0
58	MG	2A	3337	1/1	0.94	0.12	49,49,49,49	0
58	MG	1A	3832	1/1	0.94	0.15	40,40,40,40	0
58	MG	1a	1655	1/1	0.94	0.14	61,61,61,61	0
58	MG	1A	3303	1/1	0.94	0.15	50,50,50,50	0
58	MG	2A	3702	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	4050	1/1	0.94	0.12	66,66,66,66	0
58	MG	1A	4057	1/1	0.94	0.22	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1752	1/1	0.94	0.18	48,48,48,48	0
58	MG	2A	3711	1/1	0.94	0.15	56,56,56,56	0
58	MG	2A	3067	1/1	0.94	0.13	43,43,43,43	0
58	MG	1A	4060	1/1	0.94	0.09	51,51,51,51	0
58	MG	1a	1662	1/1	0.94	0.27	66,66,66,66	0
58	MG	1A	4061	1/1	0.94	0.13	54,54,54,54	0
58	MG	1A	3306	1/1	0.94	0.07	31,31,31,31	0
58	MG	2a	1762	1/1	0.94	0.11	56,56,56,56	0
58	MG	1A	3640	1/1	0.94	0.06	23,23,23,23	0
58	MG	1a	1667	1/1	0.94	0.14	49,49,49,49	0
58	MG	2A	3354	1/1	0.94	0.22	50,50,50,50	0
58	MG	2A	3080	1/1	0.94	0.07	52,52,52,52	0
58	MG	2A	3082	1/1	0.94	0.15	50,50,50,50	0
58	MG	2A	3725	1/1	0.94	0.06	73,73,73,73	0
58	MG	2A	3083	1/1	0.94	0.24	60,60,60,60	0
58	MG	1A	4069	1/1	0.94	0.11	19,19,19,19	0
58	MG	1A	3223	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3308	1/1	0.94	0.18	46,46,46,46	0
58	MG	2a	1776	1/1	0.94	0.09	61,61,61,61	0
58	MG	2A	3090	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3840	1/1	0.94	0.05	47,47,47,47	0
58	MG	2A	3368	1/1	0.94	0.17	53,53,53,53	0
58	MG	2A	3739	1/1	0.94	0.07	41,41,41,41	0
58	MG	2A	3741	1/1	0.94	0.15	54,54,54,54	0
58	MG	1A	3841	1/1	0.94	0.15	57,57,57,57	0
58	MG	1A	3842	1/1	0.94	0.12	57,57,57,57	0
58	MG	2A	3371	1/1	0.94	0.06	65,65,65,65	0
58	MG	2a	1789	1/1	0.94	0.11	68,68,68,68	0
58	MG	2A	3372	1/1	0.94	0.20	63,63,63,63	0
58	MG	2A	3094	1/1	0.94	0.26	45,45,45,45	0
58	MG	1A	3843	1/1	0.94	0.07	39,39,39,39	0
58	MG	1A	3383	1/1	0.94	0.12	57,57,57,57	0
58	MG	2a	1796	1/1	0.94	0.19	70,70,70,70	0
58	MG	1A	4087	1/1	0.94	0.16	58,58,58,58	0
58	MG	1A	3169	1/1	0.94	0.17	54,54,54,54	0
58	MG	2a	1801	1/1	0.94	0.14	49,49,49,49	0
58	MG	1A	3648	1/1	0.94	0.17	67,67,67,67	0
58	MG	1A	4093	1/1	0.94	0.11	55,55,55,55	0
58	MG	2A	3765	1/1	0.94	0.07	76,76,76,76	0
58	MG	1A	3857	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3385	1/1	0.94	0.12	52,52,52,52	0
58	MG	1A	4097	1/1	0.94	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	2a	1809	1/1	0.94	0.27	56,56,56,56	0
58	MG	2A	3107	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3108	1/1	0.94	0.10	41,41,41,41	0
58	MG	1A	3489	1/1	0.94	0.17	48,48,48,48	0
58	MG	1A	3653	1/1	0.94	0.06	32,32,32,32	0
58	MG	2A	3113	1/1	0.94	0.26	66,66,66,66	0
58	MG	2A	3393	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	4101	1/1	0.94	0.07	39,39,39,39	0
58	MG	2A	3115	1/1	0.94	0.19	57,57,57,57	0
58	MG	2A	3782	1/1	0.94	0.09	70,70,70,70	0
58	MG	2A	3116	1/1	0.94	0.23	49,49,49,49	0
58	MG	1A	3494	1/1	0.94	0.09	44,44,44,44	0
58	MG	2A	3785	1/1	0.94	0.14	71,71,71,71	0
58	MG	1A	3233	1/1	0.94	0.06	49,49,49,49	0
58	MG	2A	3407	1/1	0.94	0.27	56,56,56,56	0
58	MG	2A	3119	1/1	0.94	0.10	39,39,39,39	0
58	MG	2a	1829	1/1	0.94	0.08	60,60,60,60	0
58	MG	1A	3497	1/1	0.94	0.20	50,50,50,50	0
58	MG	2d	301	1/1	0.94	0.21	44,44,44,44	0
58	MG	1A	3239	1/1	0.94	0.10	36,36,36,36	0
58	MG	1A	3390	1/1	0.94	0.07	47,47,47,47	0
58	MG	2A	3798	1/1	0.94	0.09	59,59,59,59	0
58	MG	2f	201	1/1	0.94	0.13	56,56,56,56	0
58	MG	2A	3414	1/1	0.94	0.16	53,53,53,53	0
58	MG	2A	3415	1/1	0.94	0.21	54,54,54,54	0
58	MG	2A	3418	1/1	0.94	0.17	48,48,48,48	0
58	MG	1A	3391	1/1	0.94	0.34	43,43,43,43	0
58	MG	2A	3809	1/1	0.94	0.09	49,49,49,49	0
58	MG	2A	3124	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3668	1/1	0.94	0.07	41,41,41,41	0
58	MG	1B	220	1/1	0.94	0.11	62,62,62,62	0
58	MG	1A	3506	1/1	0.94	0.09	39,39,39,39	0
58	MG	1B	222	1/1	0.94	0.13	53,53,53,53	0
58	MG	2A	3822	1/1	0.94	0.13	67,67,67,67	0
58	MG	1A	3242	1/1	0.94	0.17	36,36,36,36	0
58	MG	2r	101	1/1	0.94	0.06	54,54,54,54	0
58	MG	1a	1703	1/1	0.94	0.15	59,59,59,59	0
58	MG	1B	224	1/1	0.94	0.06	54,54,54,54	0
58	MG	1B	225	1/1	0.94	0.07	48,48,48,48	0
58	MG	2A	3830	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3832	1/1	0.94	0.12	59,59,59,59	0
58	MG	2A	3146	1/1	0.94	0.17	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	3511	1/1	0.94	0.07	52,52,52,52	0
58	MG	2A	3150	1/1	0.94	0.17	57,57,57,57	0
58	MG	2A	3153	1/1	0.94	0.10	46,46,46,46	0
58	MG	2A	3154	1/1	0.94	0.13	52,52,52,52	0
58	MG	2A	3840	1/1	0.94	0.11	54,54,54,54	0
58	MG	1A	3244	1/1	0.94	0.12	47,47,47,47	0
59	K	1A	3564	1/1	0.94	0.12	69,69,69,69	0
58	MG	1A	3183	1/1	0.94	0.05	45,45,45,45	0
58	MG	1B	231	1/1	0.94	0.20	59,59,59,59	0
58	MG	2B	211	1/1	0.95	0.21	69,69,69,69	0
58	MG	2A	3222	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3225	1/1	0.95	0.22	48,48,48,48	0
58	MG	10	102	1/1	0.95	0.20	40,40,40,40	0
58	MG	2B	215	1/1	0.95	0.14	75,75,75,75	0
58	MG	2A	3520	1/1	0.95	0.10	38,38,38,38	0
58	MG	1A	3982	1/1	0.95	0.09	53,53,53,53	0
58	MG	2B	218	1/1	0.95	0.11	64,64,64,64	0
58	MG	1A	3007	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	3781	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3782	1/1	0.95	0.06	34,34,34,34	0
58	MG	1a	1810	1/1	0.95	0.12	47,47,47,47	0
58	MG	2D	303	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3237	1/1	0.95	0.08	51,51,51,51	0
58	MG	2A	3531	1/1	0.95	0.14	48,48,48,48	0
58	MG	2D	309	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3324	1/1	0.95	0.06	41,41,41,41	0
58	MG	2E	302	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3786	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3787	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	3607	1/1	0.95	0.08	21,21,21,21	0
58	MG	2A	3541	1/1	0.95	0.09	36,36,36,36	0
58	MG	2F	302	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3542	1/1	0.95	0.11	36,36,36,36	0
58	MG	2F	304	1/1	0.95	0.14	58,58,58,58	0
58	MG	1A	3608	1/1	0.95	0.06	35,35,35,35	0
58	MG	1A	3188	1/1	0.95	0.07	37,37,37,37	0
58	MG	1e	201	1/1	0.95	0.07	49,49,49,49	0
58	MG	2A	3549	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3259	1/1	0.95	0.12	43,43,43,43	0
58	MG	2A	3248	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3552	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3249	1/1	0.95	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3612	1/1	0.95	0.09	20,20,20,20	0
58	MG	13	104	1/1	0.95	0.10	38,38,38,38	0
58	MG	1A	3800	1/1	0.95	0.08	21,21,21,21	0
58	MG	1n	102	1/1	0.95	0.19	54,54,54,54	0
58	MG	1A	3485	1/1	0.95	0.07	41,41,41,41	0
58	MG	2Z	301	1/1	0.95	0.11	78,78,78,78	0
58	MG	1A	3327	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	4004	1/1	0.95	0.15	42,42,42,42	0
58	MG	1A	4006	1/1	0.95	0.08	22,22,22,22	0
58	MG	1A	3195	1/1	0.95	0.19	30,30,30,30	0
58	MG	1A	4014	1/1	0.95	0.07	28,28,28,28	0
58	MG	18	104	1/1	0.95	0.10	32,32,32,32	0
58	MG	2A	3567	1/1	0.95	0.05	23,23,23,23	0
58	MG	25	105	1/1	0.95	0.07	52,52,52,52	0
58	MG	18	105	1/1	0.95	0.12	30,30,30,30	0
58	MG	26	101	1/1	0.95	0.14	59,59,59,59	0
58	MG	2A	3569	1/1	0.95	0.14	50,50,50,50	0
58	MG	2A	3570	1/1	0.95	0.13	54,54,54,54	0
58	MG	18	106	1/1	0.95	0.12	47,47,47,47	0
58	MG	2A	3575	1/1	0.95	0.09	55,55,55,55	0
58	MG	2A	3271	1/1	0.95	0.06	44,44,44,44	0
58	MG	18	107	1/1	0.95	0.13	44,44,44,44	0
58	MG	1A	4015	1/1	0.95	0.06	60,60,60,60	0
58	MG	1a	1601	1/1	0.95	0.11	55,55,55,55	0
58	MG	1A	3812	1/1	0.95	0.34	33,33,33,33	0
58	MG	1A	3616	1/1	0.95	0.07	32,32,32,32	0
58	MG	1A	3814	1/1	0.95	0.09	38,38,38,38	0
58	MG	1A	4021	1/1	0.95	0.06	55,55,55,55	0
58	MG	1A	3490	1/1	0.95	0.17	53,53,53,53	0
58	MG	1a	1610	1/1	0.95	0.15	46,46,46,46	0
58	MG	1A	4024	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3593	1/1	0.95	0.12	60,60,60,60	0
58	MG	2A	3594	1/1	0.95	0.09	51,51,51,51	0
58	MG	1A	4025	1/1	0.95	0.09	40,40,40,40	0
58	MG	1a	1614	1/1	0.95	0.05	59,59,59,59	0
58	MG	1a	1616	1/1	0.95	0.07	57,57,57,57	0
58	MG	2A	3598	1/1	0.95	0.08	25,25,25,25	0
58	MG	1A	3080	1/1	0.95	0.17	31,31,31,31	0
58	MG	1a	1620	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3601	1/1	0.95	0.13	48,48,48,48	0
58	MG	2A	3289	1/1	0.95	0.05	53,53,53,53	0
58	MG	2A	3010	1/1	0.95	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3818	1/1	0.95	0.12	46,46,46,46	0
58	MG	2A	3294	1/1	0.95	0.10	60,60,60,60	0
58	MG	2A	3015	1/1	0.95	0.09	43,43,43,43	0
58	MG	1a	1622	1/1	0.95	0.06	37,37,37,37	0
58	MG	1A	3126	1/1	0.95	0.26	36,36,36,36	0
58	MG	2A	3613	1/1	0.95	0.13	39,39,39,39	0
58	MG	1A	3267	1/1	0.95	0.21	60,60,60,60	0
58	MG	2A	3299	1/1	0.95	0.08	50,50,50,50	0
58	MG	1A	3822	1/1	0.95	0.30	31,31,31,31	0
58	MG	1A	3500	1/1	0.95	0.06	40,40,40,40	0
58	MG	2a	1638	1/1	0.95	0.04	73,73,73,73	0
58	MG	1a	1627	1/1	0.95	0.19	53,53,53,53	0
58	MG	1A	3825	1/1	0.95	0.05	21,21,21,21	0
58	MG	2A	3033	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	4037	1/1	0.95	0.06	22,22,22,22	0
58	MG	2A	3037	1/1	0.95	0.14	65,65,65,65	0
58	MG	1A	3406	1/1	0.95	0.09	43,43,43,43	0
58	MG	1A	4041	1/1	0.95	0.13	32,32,32,32	0
58	MG	1A	3503	1/1	0.95	0.19	46,46,46,46	0
58	MG	2A	3043	1/1	0.95	0.16	53,53,53,53	0
58	MG	1A	4046	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3646	1/1	0.95	0.06	13,13,13,13	0
58	MG	1A	3081	1/1	0.95	0.09	55,55,55,55	0
58	MG	1A	4052	1/1	0.95	0.07	61,61,61,61	0
58	MG	2A	3641	1/1	0.95	0.12	63,63,63,63	0
58	MG	1A	3083	1/1	0.95	0.10	31,31,31,31	0
58	MG	1A	3043	1/1	0.95	0.24	36,36,36,36	0
58	MG	1A	3271	1/1	0.95	0.11	36,36,36,36	0
58	MG	2A	3320	1/1	0.95	0.09	42,42,42,42	0
58	MG	1A	3508	1/1	0.95	0.09	41,41,41,41	0
58	MG	2A	3648	1/1	0.95	0.12	56,56,56,56	0
58	MG	1A	3655	1/1	0.95	0.09	46,46,46,46	0
58	MG	1A	3340	1/1	0.95	0.08	28,28,28,28	0
58	MG	2A	3059	1/1	0.95	0.13	51,51,51,51	0
58	MG	2A	3652	1/1	0.95	0.08	53,53,53,53	0
58	MG	1A	3272	1/1	0.95	0.16	30,30,30,30	0
58	MG	1a	1648	1/1	0.95	0.16	38,38,38,38	0
58	MG	2A	3063	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	3661	1/1	0.95	0.12	32,32,32,32	0
58	MG	1A	4076	1/1	0.95	0.10	23,23,23,23	0
58	MG	1a	1654	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3662	1/1	0.95	0.11	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	1656	1/1	0.95	0.06	49,49,49,49	0
58	MG	1A	3847	1/1	0.95	0.09	47,47,47,47	0
58	MG	1A	3273	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3013	1/1	0.95	0.19	29,29,29,29	0
58	MG	1A	3851	1/1	0.95	0.13	37,37,37,37	0
58	MG	1A	3853	1/1	0.95	0.09	47,47,47,47	0
58	MG	2A	3078	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3079	1/1	0.95	0.07	17,17,17,17	0
58	MG	1A	3517	1/1	0.95	0.35	39,39,39,39	0
58	MG	2a	1683	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3081	1/1	0.95	0.11	57,57,57,57	0
58	MG	1A	3282	1/1	0.95	0.24	38,38,38,38	0
58	MG	1A	3523	1/1	0.95	0.14	64,64,64,64	0
58	MG	2A	3085	1/1	0.95	0.06	47,47,47,47	0
58	MG	2a	1689	1/1	0.95	0.18	56,56,56,56	0
58	MG	2A	3678	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3679	1/1	0.95	0.23	71,71,71,71	0
58	MG	2a	1692	1/1	0.95	0.12	80,80,80,80	0
58	MG	1A	3675	1/1	0.95	0.07	41,41,41,41	0
58	MG	1A	3677	1/1	0.95	0.07	27,27,27,27	0
58	MG	1A	3421	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3090	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3870	1/1	0.95	0.07	28,28,28,28	0
58	MG	2A	3685	1/1	0.95	0.06	46,46,46,46	0
58	MG	2A	3356	1/1	0.95	0.07	63,63,63,63	0
58	MG	1A	4103	1/1	0.95	0.23	46,46,46,46	0
58	MG	1A	3349	1/1	0.95	0.07	35,35,35,35	0
58	MG	2A	3690	1/1	0.95	0.07	31,31,31,31	0
58	MG	1A	3029	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3426	1/1	0.95	0.14	39,39,39,39	0
58	MG	1a	1678	1/1	0.95	0.13	46,46,46,46	0
58	MG	1A	3100	1/1	0.95	0.07	35,35,35,35	0
58	MG	2a	1711	1/1	0.95	0.15	74,74,74,74	0
58	MG	1A	3152	1/1	0.95	0.12	45,45,45,45	0
58	MG	1B	210	1/1	0.95	0.09	50,50,50,50	0
58	MG	1A	3212	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3701	1/1	0.95	0.06	34,34,34,34	0
58	MG	1B	213	1/1	0.95	0.18	51,51,51,51	0
58	MG	1B	214	1/1	0.95	0.07	62,62,62,62	0
58	MG	2A	3703	1/1	0.95	0.14	56,56,56,56	0
58	MG	2a	1721	1/1	0.95	0.19	53,53,53,53	0
58	MG	1A	3156	1/1	0.95	0.22	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	3374	1/1	0.95	0.10	63,63,63,63	0
58	MG	2A	3707	1/1	0.95	0.10	54,54,54,54	0
58	MG	2A	3109	1/1	0.95	0.14	44,44,44,44	0
58	MG	1A	3217	1/1	0.95	0.06	43,43,43,43	0
58	MG	2A	3111	1/1	0.95	0.09	52,52,52,52	0
58	MG	1A	3218	1/1	0.95	0.14	44,44,44,44	0
58	MG	2A	3716	1/1	0.95	0.12	68,68,68,68	0
58	MG	1A	3707	1/1	0.95	0.09	21,21,21,21	0
58	MG	2A	3381	1/1	0.95	0.42	57,57,57,57	0
58	MG	2A	3719	1/1	0.95	0.06	46,46,46,46	0
58	MG	1A	3101	1/1	0.95	0.15	54,54,54,54	0
58	MG	1A	3892	1/1	0.95	0.08	25,25,25,25	0
58	MG	1A	3106	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3713	1/1	0.95	0.09	27,27,27,27	0
58	MG	1A	3545	1/1	0.95	0.18	44,44,44,44	0
58	MG	1A	3159	1/1	0.95	0.08	30,30,30,30	0
58	MG	1A	3304	1/1	0.95	0.30	53,53,53,53	0
58	MG	2A	3727	1/1	0.95	0.06	52,52,52,52	0
58	MG	2A	3729	1/1	0.95	0.10	46,46,46,46	0
58	MG	1B	233	1/1	0.95	0.08	60,60,60,60	0
58	MG	2a	1746	1/1	0.95	0.15	56,56,56,56	0
58	MG	2A	3391	1/1	0.95	0.08	49,49,49,49	0
58	MG	1A	3162	1/1	0.95	0.27	33,33,33,33	0
58	MG	1A	3441	1/1	0.95	0.13	40,40,40,40	0
58	MG	2A	3394	1/1	0.95	0.11	53,53,53,53	0
58	MG	1A	3722	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3738	1/1	0.95	0.12	46,46,46,46	0
58	MG	2A	3127	1/1	0.95	0.17	47,47,47,47	0
58	MG	2A	3400	1/1	0.95	0.17	47,47,47,47	0
58	MG	1D	308	1/1	0.95	0.11	34,34,34,34	0
58	MG	1A	3163	1/1	0.95	0.10	40,40,40,40	0
58	MG	1A	3164	1/1	0.95	0.20	46,46,46,46	0
58	MG	1A	3911	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3912	1/1	0.95	0.09	34,34,34,34	0
58	MG	2A	3749	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3136	1/1	0.95	0.13	40,40,40,40	0
58	MG	1a	1713	1/1	0.95	0.15	47,47,47,47	0
58	MG	1A	3553	1/1	0.95	0.22	30,30,30,30	0
58	MG	2A	3756	1/1	0.95	0.05	45,45,45,45	0
58	MG	2a	1768	1/1	0.95	0.11	64,64,64,64	0
58	MG	1A	3449	1/1	0.95	0.27	64,64,64,64	0
58	MG	1A	3561	1/1	0.95	0.11	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	2A	3416	1/1	0.95	0.06	43,43,43,43	0
58	MG	2A	3417	1/1	0.95	0.23	47,47,47,47	0
58	MG	2a	1774	1/1	0.95	0.07	61,61,61,61	0
58	MG	1A	3450	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3920	1/1	0.95	0.13	48,48,48,48	0
58	MG	2A	3769	1/1	0.95	0.09	58,58,58,58	0
58	MG	2A	3152	1/1	0.95	0.09	50,50,50,50	0
58	MG	1A	3921	1/1	0.95	0.05	38,38,38,38	0
58	MG	2a	1781	1/1	0.95	0.06	62,62,62,62	0
58	MG	1A	3563	1/1	0.95	0.17	42,42,42,42	0
58	MG	2A	3155	1/1	0.95	0.15	40,40,40,40	0
58	MG	2A	3428	1/1	0.95	0.05	42,42,42,42	0
58	MG	2a	1785	1/1	0.95	0.11	49,49,49,49	0
58	MG	1F	304	1/1	0.95	0.10	47,47,47,47	0
58	MG	2a	1787	1/1	0.95	0.14	48,48,48,48	0
58	MG	1F	309	1/1	0.95	0.06	48,48,48,48	0
58	MG	2A	3778	1/1	0.95	0.10	44,44,44,44	0
58	MG	2a	1790	1/1	0.95	0.10	62,62,62,62	0
58	MG	1a	1727	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3569	1/1	0.95	0.11	24,24,24,24	0
58	MG	2A	3781	1/1	0.95	0.07	59,59,59,59	0
58	MG	1A	3571	1/1	0.95	0.10	44,44,44,44	0
58	MG	1G	204	1/1	0.95	0.10	52,52,52,52	0
58	MG	1G	205	1/1	0.95	0.12	55,55,55,55	0
58	MG	1A	3451	1/1	0.95	0.14	35,35,35,35	0
58	MG	2A	3167	1/1	0.95	0.07	55,55,55,55	0
58	MG	1A	3574	1/1	0.95	0.31	34,34,34,34	0
58	MG	2A	3169	1/1	0.95	0.06	54,54,54,54	0
58	MG	2A	3170	1/1	0.95	0.10	57,57,57,57	0
58	MG	2A	3793	1/1	0.95	0.13	51,51,51,51	0
58	MG	1N	202	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3172	1/1	0.95	0.10	40,40,40,40	0
58	MG	1A	3577	1/1	0.95	0.11	41,41,41,41	0
58	MG	2A	3801	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3453	1/1	0.95	0.06	52,52,52,52	0
58	MG	2A	3455	1/1	0.95	0.10	62,62,62,62	0
58	MG	1A	3452	1/1	0.95	0.17	60,60,60,60	0
58	MG	1A	3378	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3806	1/1	0.95	0.06	47,47,47,47	0
58	MG	2A	3808	1/1	0.95	0.11	68,68,68,68	0
58	MG	1A	3243	1/1	0.95	0.14	56,56,56,56	0
58	MG	1O	204	1/1	0.95	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3946	1/1	0.95	0.11	66,66,66,66	0
58	MG	2a	1822	1/1	0.95	0.12	61,61,61,61	0
58	MG	2A	3817	1/1	0.95	0.12	57,57,57,57	0
58	MG	2A	3180	1/1	0.95	0.14	52,52,52,52	0
58	MG	1A	3949	1/1	0.95	0.09	48,48,48,48	0
58	MG	1A	3459	1/1	0.95	0.14	34,34,34,34	0
58	MG	2a	1827	1/1	0.95	0.15	54,54,54,54	0
58	MG	1A	3755	1/1	0.95	0.13	42,42,42,42	0
58	MG	2A	3823	1/1	0.95	0.08	70,70,70,70	0
58	MG	1A	3954	1/1	0.95	0.06	45,45,45,45	0
58	MG	2A	3467	1/1	0.95	0.06	47,47,47,47	0
58	MG	1A	3020	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3757	1/1	0.95	0.06	46,46,46,46	0
58	MG	1a	1764	1/1	0.95	0.09	62,62,62,62	0
58	MG	1A	3760	1/1	0.95	0.07	26,26,26,26	0
58	MG	1A	3462	1/1	0.95	0.23	54,54,54,54	0
58	MG	1a	1767	1/1	0.95	0.09	45,45,45,45	0
58	MG	1A	3463	1/1	0.95	0.10	35,35,35,35	0
58	MG	1A	3246	1/1	0.95	0.11	58,58,58,58	0
58	MG	2A	3484	1/1	0.95	0.06	57,57,57,57	0
58	MG	1A	3764	1/1	0.95	0.06	17,17,17,17	0
58	MG	1A	3113	1/1	0.95	0.13	38,38,38,38	0
58	MG	1A	3176	1/1	0.95	0.08	19,19,19,19	0
58	MG	1a	1776	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3969	1/1	0.95	0.22	55,55,55,55	0
58	MG	1A	3970	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3971	1/1	0.95	0.11	55,55,55,55	0
58	MG	1A	3178	1/1	0.95	0.07	22,22,22,22	0
58	MG	1W	205	1/1	0.95	0.08	31,31,31,31	0
58	MG	2A	3498	1/1	0.95	0.14	53,53,53,53	0
58	MG	1A	3974	1/1	0.95	0.08	56,56,56,56	0
58	MG	1X	103	1/1	0.95	0.08	34,34,34,34	0
58	MG	1A	3253	1/1	0.95	0.11	48,48,48,48	0
58	MG	2v	105	1/1	0.95	0.10	52,52,52,52	0
58	MG	1A	3389	1/1	0.95	0.24	27,27,27,27	0
58	MG	1A	3977	1/1	0.95	0.06	52,52,52,52	0
58	MG	1A	3601	1/1	0.95	0.08	40,40,40,40	0
58	MG	1A	3775	1/1	0.95	0.07	24,24,24,24	0
58	MG	1A	3035	1/1	0.95	0.12	38,38,38,38	0
58	MG	1a	1801	1/1	0.95	0.07	60,60,60,60	0
58	MG	1a	1802	1/1	0.95	0.11	69,69,69,69	0
58	MG	2A	3514	1/1	0.95	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3515	1/1	0.95	0.08	39,39,39,39	0
58	MG	2B	210	1/1	0.95	0.08	66,66,66,66	0
58	MG	1A	3768	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3165	1/1	0.96	0.10	36,36,36,36	0
58	MG	1R	202	1/1	0.96	0.08	26,26,26,26	0
58	MG	1A	3375	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3376	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3236	1/1	0.96	0.19	30,30,30,30	0
58	MG	1A	3077	1/1	0.96	0.06	30,30,30,30	0
58	MG	1T	201	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3973	1/1	0.96	0.04	54,54,54,54	0
58	MG	2A	3505	1/1	0.96	0.09	67,67,67,67	0
58	MG	2A	3506	1/1	0.96	0.12	54,54,54,54	0
58	MG	1U	202	1/1	0.96	0.28	42,42,42,42	0
58	MG	1a	1772	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3599	1/1	0.96	0.11	38,38,38,38	0
58	MG	1A	3091	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3171	1/1	0.96	0.06	36,36,36,36	0
58	MG	2A	3203	1/1	0.96	0.05	49,49,49,49	0
58	MG	1U	209	1/1	0.96	0.32	31,31,31,31	0
58	MG	1A	3172	1/1	0.96	0.06	34,34,34,34	0
58	MG	1V	203	1/1	0.96	0.22	35,35,35,35	0
58	MG	1A	3783	1/1	0.96	0.05	19,19,19,19	0
58	MG	2A	3208	1/1	0.96	0.09	51,51,51,51	0
58	MG	1A	3979	1/1	0.96	0.08	51,51,51,51	0
58	MG	1V	207	1/1	0.96	0.06	53,53,53,53	0
58	MG	1a	1785	1/1	0.96	0.07	46,46,46,46	0
58	MG	2D	305	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3093	1/1	0.96	0.13	53,53,53,53	0
58	MG	1a	1788	1/1	0.96	0.09	47,47,47,47	0
58	MG	2A	3528	1/1	0.96	0.11	54,54,54,54	0
58	MG	1A	3479	1/1	0.96	0.07	31,31,31,31	0
58	MG	1W	203	1/1	0.96	0.07	40,40,40,40	0
58	MG	2E	305	1/1	0.96	0.09	61,61,61,61	0
58	MG	1A	3606	1/1	0.96	0.05	40,40,40,40	0
58	MG	2A	3220	1/1	0.96	0.07	49,49,49,49	0
58	MG	1a	1796	1/1	0.96	0.05	67,67,67,67	0
58	MG	2A	3535	1/1	0.96	0.12	57,57,57,57	0
58	MG	1a	1797	1/1	0.96	0.06	67,67,67,67	0
58	MG	1A	3983	1/1	0.96	0.09	63,63,63,63	0
58	MG	2A	3227	1/1	0.96	0.18	30,30,30,30	0
58	MG	2A	3228	1/1	0.96	0.07	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	3545	1/1	0.96	0.05	25,25,25,25	0
58	MG	1A	3480	1/1	0.96	0.11	34,34,34,34	0
58	MG	2A	3547	1/1	0.96	0.08	55,55,55,55	0
58	MG	1A	3790	1/1	0.96	0.08	49,49,49,49	0
58	MG	1Y	201	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3312	1/1	0.96	0.13	41,41,41,41	0
58	MG	2A	3233	1/1	0.96	0.12	43,43,43,43	0
58	MG	2U	201	1/1	0.96	0.23	51,51,51,51	0
58	MG	1A	3794	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3482	1/1	0.96	0.10	39,39,39,39	0
58	MG	2A	3236	1/1	0.96	0.10	56,56,56,56	0
58	MG	2W	202	1/1	0.96	0.21	52,52,52,52	0
58	MG	1A	3313	1/1	0.96	0.07	49,49,49,49	0
58	MG	2X	102	1/1	0.96	0.07	59,59,59,59	0
58	MG	1Z	303	1/1	0.96	0.09	45,45,45,45	0
58	MG	1a	1807	1/1	0.96	0.05	59,59,59,59	0
58	MG	1A	3127	1/1	0.96	0.13	32,32,32,32	0
58	MG	1a	1809	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	3994	1/1	0.96	0.06	46,46,46,46	0
58	MG	2A	3243	1/1	0.96	0.32	55,55,55,55	0
58	MG	25	101	1/1	0.96	0.16	42,42,42,42	0
58	MG	2A	3563	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3078	1/1	0.96	0.11	39,39,39,39	0
58	MG	1a	1812	1/1	0.96	0.18	59,59,59,59	0
58	MG	1A	3486	1/1	0.96	0.07	29,29,29,29	0
58	MG	1A	3316	1/1	0.96	0.14	41,41,41,41	0
58	MG	10	106	1/1	0.96	0.12	65,65,65,65	0
58	MG	2A	3250	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3317	1/1	0.96	0.16	47,47,47,47	0
58	MG	1A	3808	1/1	0.96	0.04	22,22,22,22	0
58	MG	2A	3253	1/1	0.96	0.13	49,49,49,49	0
58	MG	2A	3254	1/1	0.96	0.24	61,61,61,61	0
58	MG	1A	3625	1/1	0.96	0.10	26,26,26,26	0
58	MG	2a	1603	1/1	0.96	0.11	60,60,60,60	0
58	MG	2A	3256	1/1	0.96	0.17	42,42,42,42	0
58	MG	1f	201	1/1	0.96	0.13	51,51,51,51	0
58	MG	2A	3585	1/1	0.96	0.05	62,62,62,62	0
58	MG	1A	3318	1/1	0.96	0.06	20,20,20,20	0
58	MG	2a	1608	1/1	0.96	0.11	52,52,52,52	0
58	MG	1A	3634	1/1	0.96	0.05	35,35,35,35	0
58	MG	1m	3001	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	4005	1/1	0.96	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3263	1/1	0.96	0.18	60,60,60,60	0
58	MG	1A	3492	1/1	0.96	0.08	43,43,43,43	0
58	MG	1A	3493	1/1	0.96	0.09	48,48,48,48	0
58	MG	1A	3637	1/1	0.96	0.06	21,21,21,21	0
58	MG	13	102	1/1	0.96	0.08	32,32,32,32	0
58	MG	1A	3819	1/1	0.96	0.13	52,52,52,52	0
58	MG	2A	3270	1/1	0.96	0.10	40,40,40,40	0
58	MG	1w	101	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3096	1/1	0.96	0.05	60,60,60,60	0
58	MG	2a	1621	1/1	0.96	0.08	60,60,60,60	0
58	MG	1A	4018	1/1	0.96	0.06	41,41,41,41	0
58	MG	15	105	1/1	0.96	0.18	20,20,20,20	0
58	MG	1A	3252	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3496	1/1	0.96	0.10	52,52,52,52	0
58	MG	1A	3823	1/1	0.96	0.06	40,40,40,40	0
58	MG	2a	1628	1/1	0.96	0.14	46,46,46,46	0
58	MG	1A	3321	1/1	0.96	0.10	29,29,29,29	0
58	MG	2A	3605	1/1	0.96	0.07	60,60,60,60	0
58	MG	1A	4023	1/1	0.96	0.10	73,73,73,73	0
58	MG	1x	104	1/1	0.96	0.15	55,55,55,55	0
58	MG	2a	1633	1/1	0.96	0.07	85,85,85,85	0
58	MG	18	103	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3185	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3827	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	4026	1/1	0.96	0.07	42,42,42,42	0
58	MG	1A	3186	1/1	0.96	0.05	39,39,39,39	0
58	MG	1A	3135	1/1	0.96	0.14	46,46,46,46	0
58	MG	1A	3649	1/1	0.96	0.13	23,23,23,23	0
58	MG	2A	3620	1/1	0.96	0.19	44,44,44,44	0
58	MG	2A	3622	1/1	0.96	0.07	47,47,47,47	0
58	MG	2a	1643	1/1	0.96	0.17	55,55,55,55	0
58	MG	2A	3623	1/1	0.96	0.09	32,32,32,32	0
58	MG	2A	3002	1/1	0.96	0.23	49,49,49,49	0
58	MG	2A	3291	1/1	0.96	0.12	52,52,52,52	0
58	MG	1A	3834	1/1	0.96	0.14	51,51,51,51	0
58	MG	2A	3293	1/1	0.96	0.12	45,45,45,45	0
58	MG	1a	1603	1/1	0.96	0.12	62,62,62,62	0
58	MG	1A	3097	1/1	0.96	0.13	41,41,41,41	0
58	MG	2A	3631	1/1	0.96	0.07	53,53,53,53	0
58	MG	1a	1605	1/1	0.96	0.08	48,48,48,48	0
58	MG	2A	3633	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3039	1/1	0.96	0.20	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3142	1/1	0.96	0.12	42,42,42,42	0
58	MG	1A	3198	1/1	0.96	0.17	32,32,32,32	0
58	MG	1A	4038	1/1	0.96	0.08	36,36,36,36	0
58	MG	2A	3014	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	3143	1/1	0.96	0.08	52,52,52,52	0
58	MG	1a	1612	1/1	0.96	0.12	29,29,29,29	0
58	MG	2A	3017	1/1	0.96	0.12	43,43,43,43	0
58	MG	1A	4040	1/1	0.96	0.10	38,38,38,38	0
58	MG	1A	3412	1/1	0.96	0.12	36,36,36,36	0
58	MG	1a	1615	1/1	0.96	0.17	47,47,47,47	0
58	MG	2A	3025	1/1	0.96	0.10	41,41,41,41	0
58	MG	2A	3026	1/1	0.96	0.18	44,44,44,44	0
58	MG	1A	4042	1/1	0.96	0.10	28,28,28,28	0
58	MG	2a	1669	1/1	0.96	0.06	57,57,57,57	0
58	MG	2A	3029	1/1	0.96	0.11	58,58,58,58	0
58	MG	1a	1618	1/1	0.96	0.04	47,47,47,47	0
58	MG	1A	3331	1/1	0.96	0.11	54,54,54,54	0
58	MG	1A	3415	1/1	0.96	0.05	45,45,45,45	0
58	MG	1A	3266	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	4048	1/1	0.96	0.06	22,22,22,22	0
58	MG	2A	3038	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3319	1/1	0.96	0.13	55,55,55,55	0
58	MG	2A	3659	1/1	0.96	0.11	34,34,34,34	0
58	MG	1A	3844	1/1	0.96	0.13	50,50,50,50	0
58	MG	1A	3845	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	4054	1/1	0.96	0.08	46,46,46,46	0
58	MG	2A	3042	1/1	0.96	0.12	48,48,48,48	0
58	MG	1A	4055	1/1	0.96	0.05	37,37,37,37	0
58	MG	1A	3515	1/1	0.96	0.11	24,24,24,24	0
58	MG	1A	3516	1/1	0.96	0.21	32,32,32,32	0
58	MG	1A	3063	1/1	0.96	0.24	42,42,42,42	0
58	MG	2A	3047	1/1	0.96	0.07	54,54,54,54	0
58	MG	2A	3669	1/1	0.96	0.19	49,49,49,49	0
58	MG	1A	3669	1/1	0.96	0.08	36,36,36,36	0
58	MG	1A	3520	1/1	0.96	0.08	43,43,43,43	0
58	MG	2a	1694	1/1	0.96	0.20	57,57,57,57	0
58	MG	1A	3673	1/1	0.96	0.04	20,20,20,20	0
58	MG	2A	3673	1/1	0.96	0.13	52,52,52,52	0
58	MG	1A	4073	1/1	0.96	0.14	55,55,55,55	0
58	MG	1A	3854	1/1	0.96	0.06	16,16,16,16	0
58	MG	1A	3521	1/1	0.96	0.08	51,51,51,51	0
58	MG	2A	3055	1/1	0.96	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3338	1/1	0.96	0.18	56,56,56,56	0
58	MG	2A	3339	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3102	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3058	1/1	0.96	0.10	57,57,57,57	0
58	MG	1A	3147	1/1	0.96	0.06	31,31,31,31	0
58	MG	1a	1639	1/1	0.96	0.18	52,52,52,52	0
58	MG	2A	3061	1/1	0.96	0.15	57,57,57,57	0
58	MG	1A	3103	1/1	0.96	0.11	47,47,47,47	0
58	MG	1A	3863	1/1	0.96	0.10	44,44,44,44	0
58	MG	1A	3337	1/1	0.96	0.06	37,37,37,37	0
58	MG	2a	1714	1/1	0.96	0.04	34,34,34,34	0
58	MG	1A	3104	1/1	0.96	0.11	29,29,29,29	0
58	MG	1A	3153	1/1	0.96	0.08	31,31,31,31	0
58	MG	1A	3155	1/1	0.96	0.17	42,42,42,42	0
58	MG	1A	3530	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	4090	1/1	0.96	0.07	53,53,53,53	0
58	MG	2A	3071	1/1	0.96	0.10	52,52,52,52	0
58	MG	1A	4091	1/1	0.96	0.20	40,40,40,40	0
58	MG	1A	3275	1/1	0.96	0.05	44,44,44,44	0
58	MG	2A	3359	1/1	0.96	0.08	66,66,66,66	0
58	MG	1A	3698	1/1	0.96	0.08	68,68,68,68	0
58	MG	1A	3699	1/1	0.96	0.09	23,23,23,23	0
58	MG	2a	1727	1/1	0.96	0.07	54,54,54,54	0
58	MG	2A	3077	1/1	0.96	0.10	36,36,36,36	0
58	MG	1a	1657	1/1	0.96	0.14	52,52,52,52	0
58	MG	1A	3276	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3210	1/1	0.96	0.08	42,42,42,42	0
58	MG	2A	3708	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3703	1/1	0.96	0.10	28,28,28,28	0
58	MG	1A	4102	1/1	0.96	0.12	43,43,43,43	0
58	MG	1A	3346	1/1	0.96	0.06	41,41,41,41	0
58	MG	1B	201	1/1	0.96	0.11	37,37,37,37	0
58	MG	1A	3537	1/1	0.96	0.17	26,26,26,26	0
58	MG	2a	1738	1/1	0.96	0.20	38,38,38,38	0
58	MG	1A	3279	1/1	0.96	0.17	35,35,35,35	0
58	MG	1A	3280	1/1	0.96	0.12	31,31,31,31	0
58	MG	1B	206	1/1	0.96	0.17	43,43,43,43	0
58	MG	1B	207	1/1	0.96	0.07	58,58,58,58	0
58	MG	1a	1670	1/1	0.96	0.21	53,53,53,53	0
58	MG	1A	3019	1/1	0.96	0.15	34,34,34,34	0
58	MG	1A	3543	1/1	0.96	0.17	49,49,49,49	0
58	MG	1A	3893	1/1	0.96	0.04	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	3434	1/1	0.96	0.08	39,39,39,39	0
58	MG	1A	3715	1/1	0.96	0.12	52,52,52,52	0
58	MG	2A	3100	1/1	0.96	0.11	52,52,52,52	0
58	MG	2A	3728	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3435	1/1	0.96	0.10	39,39,39,39	0
58	MG	1a	1677	1/1	0.96	0.15	45,45,45,45	0
58	MG	1A	3107	1/1	0.96	0.06	31,31,31,31	0
58	MG	1B	215	1/1	0.96	0.05	44,44,44,44	0
58	MG	1B	216	1/1	0.96	0.09	42,42,42,42	0
58	MG	1B	219	1/1	0.96	0.10	36,36,36,36	0
58	MG	2a	1759	1/1	0.96	0.07	59,59,59,59	0
58	MG	2A	3735	1/1	0.96	0.18	57,57,57,57	0
58	MG	1A	3352	1/1	0.96	0.16	47,47,47,47	0
58	MG	2A	3737	1/1	0.96	0.09	53,53,53,53	0
58	MG	1A	3900	1/1	0.96	0.08	46,46,46,46	0
58	MG	1A	3901	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3740	1/1	0.96	0.10	51,51,51,51	0
58	MG	2A	3396	1/1	0.96	0.14	37,37,37,37	0
58	MG	1A	3216	1/1	0.96	0.18	41,41,41,41	0
58	MG	2A	3398	1/1	0.96	0.20	46,46,46,46	0
58	MG	1A	3354	1/1	0.96	0.09	55,55,55,55	0
58	MG	1A	3440	1/1	0.96	0.16	31,31,31,31	0
58	MG	2A	3401	1/1	0.96	0.11	44,44,44,44	0
58	MG	2A	3402	1/1	0.96	0.21	46,46,46,46	0
58	MG	1A	3724	1/1	0.96	0.16	50,50,50,50	0
58	MG	1a	1690	1/1	0.96	0.12	37,37,37,37	0
58	MG	1A	3060	1/1	0.96	0.08	40,40,40,40	0
58	MG	1A	3442	1/1	0.96	0.09	33,33,33,33	0
58	MG	2a	1778	1/1	0.96	0.15	65,65,65,65	0
58	MG	2A	3408	1/1	0.96	0.12	34,34,34,34	0
58	MG	2A	3758	1/1	0.96	0.05	52,52,52,52	0
58	MG	2A	3759	1/1	0.96	0.19	59,59,59,59	0
58	MG	2A	3760	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3729	1/1	0.96	0.07	37,37,37,37	0
58	MG	1A	3557	1/1	0.96	0.21	33,33,33,33	0
58	MG	2A	3411	1/1	0.96	0.25	44,44,44,44	0
58	MG	1A	3444	1/1	0.96	0.24	33,33,33,33	0
58	MG	1A	3560	1/1	0.96	0.12	29,29,29,29	0
58	MG	1A	3112	1/1	0.96	0.05	32,32,32,32	0
58	MG	1D	304	1/1	0.96	0.11	34,34,34,34	0
58	MG	1A	3447	1/1	0.96	0.17	43,43,43,43	0
58	MG	2a	1791	1/1	0.96	0.14	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	1D	307	1/1	0.96	0.11	35,35,35,35	0
58	MG	1A	3740	1/1	0.96	0.06	35,35,35,35	0
58	MG	1D	311	1/1	0.96	0.05	32,32,32,32	0
58	MG	2A	3130	1/1	0.96	0.17	52,52,52,52	0
58	MG	2A	3421	1/1	0.96	0.20	47,47,47,47	0
58	MG	2a	1797	1/1	0.96	0.08	56,56,56,56	0
58	MG	2a	1798	1/1	0.96	0.06	56,56,56,56	0
58	MG	2A	3777	1/1	0.96	0.09	59,59,59,59	0
58	MG	1A	3923	1/1	0.96	0.10	33,33,33,33	0
58	MG	1A	3924	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3134	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3925	1/1	0.96	0.07	67,67,67,67	0
58	MG	1A	3926	1/1	0.96	0.09	55,55,55,55	0
58	MG	1A	3049	1/1	0.96	0.04	12,12,12,12	0
58	MG	1A	3565	1/1	0.96	0.13	35,35,35,35	0
58	MG	2A	3142	1/1	0.96	0.10	35,35,35,35	0
58	MG	2A	3143	1/1	0.96	0.16	39,39,39,39	0
58	MG	2A	3787	1/1	0.96	0.06	52,52,52,52	0
58	MG	1A	3220	1/1	0.96	0.18	44,44,44,44	0
58	MG	2A	3145	1/1	0.96	0.21	50,50,50,50	0
58	MG	2a	1813	1/1	0.96	0.15	47,47,47,47	0
58	MG	1A	3746	1/1	0.96	0.08	39,39,39,39	0
58	MG	2A	3439	1/1	0.96	0.08	57,57,57,57	0
58	MG	2A	3440	1/1	0.96	0.18	39,39,39,39	0
58	MG	2A	3147	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3797	1/1	0.96	0.06	42,42,42,42	0
58	MG	1a	1716	1/1	0.96	0.21	33,33,33,33	0
58	MG	2A	3443	1/1	0.96	0.08	47,47,47,47	0
58	MG	2A	3149	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3359	1/1	0.96	0.07	42,42,42,42	0
58	MG	2A	3447	1/1	0.96	0.08	41,41,41,41	0
58	MG	1A	3749	1/1	0.96	0.06	42,42,42,42	0
58	MG	1A	3088	1/1	0.96	0.16	27,27,27,27	0
58	MG	1F	301	1/1	0.96	0.15	39,39,39,39	0
58	MG	1A	3940	1/1	0.96	0.06	37,37,37,37	0
58	MG	1A	3298	1/1	0.96	0.17	35,35,35,35	0
58	MG	1A	3575	1/1	0.96	0.25	44,44,44,44	0
58	MG	2A	3816	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3159	1/1	0.96	0.14	51,51,51,51	0
58	MG	1a	1726	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3459	1/1	0.96	0.10	52,52,52,52	0
58	MG	1A	3224	1/1	0.96	0.08	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	3947	1/1	0.96	0.05	43,43,43,43	0
58	MG	1A	3579	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3580	1/1	0.96	0.23	43,43,43,43	0
58	MG	2A	3826	1/1	0.96	0.10	68,68,68,68	0
58	MG	2A	3165	1/1	0.96	0.13	37,37,37,37	0
58	MG	1a	1736	1/1	0.96	0.14	55,55,55,55	0
58	MG	1A	3951	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3226	1/1	0.96	0.06	49,49,49,49	0
58	MG	1a	1739	1/1	0.96	0.06	49,49,49,49	0
58	MG	1A	3758	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3834	1/1	0.96	0.13	53,53,53,53	0
58	MG	2q	201	1/1	0.96	0.06	73,73,73,73	0
58	MG	2A	3470	1/1	0.96	0.16	49,49,49,49	0
58	MG	2A	3473	1/1	0.96	0.17	43,43,43,43	0
58	MG	1A	3584	1/1	0.96	0.06	42,42,42,42	0
58	MG	2A	3477	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3456	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3457	1/1	0.96	0.15	40,40,40,40	0
58	MG	1A	3231	1/1	0.96	0.09	39,39,39,39	0
58	MG	1a	1749	1/1	0.96	0.09	55,55,55,55	0
58	MG	2A	3844	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3460	1/1	0.96	0.13	48,48,48,48	0
58	MG	1a	1751	1/1	0.96	0.17	36,36,36,36	0
58	MG	1A	3118	1/1	0.96	0.14	33,33,33,33	0
58	MG	1A	3367	1/1	0.96	0.16	35,35,35,35	0
58	MG	2x	105	1/1	0.96	0.22	59,59,59,59	0
58	MG	1Q	203	1/1	0.96	0.06	23,23,23,23	0
58	MG	2A	3854	1/1	0.96	0.09	66,66,66,66	0
58	MG	1Q	205	1/1	0.96	0.07	46,46,46,46	0
59	K	2x	101	1/1	0.96	0.09	68,68,68,68	0
58	MG	1a	1759	1/1	0.96	0.21	55,55,55,55	0
58	MG	1Q	206	1/1	0.96	0.06	39,39,39,39	0
58	MG	1a	1707	1/1	0.97	0.07	56,56,56,56	0
58	MG	2U	202	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3120	1/1	0.97	0.06	32,32,32,32	0
58	MG	2A	3096	1/1	0.97	0.06	33,33,33,33	0
58	MG	2A	3614	1/1	0.97	0.12	49,49,49,49	0
58	MG	1A	3089	1/1	0.97	0.16	36,36,36,36	0
58	MG	1A	3651	1/1	0.97	0.05	23,23,23,23	0
58	MG	2W	204	1/1	0.97	0.17	48,48,48,48	0
58	MG	2X	101	1/1	0.97	0.05	62,62,62,62	0
58	MG	2A	3617	1/1	0.97	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2Y	201	1/1	0.97	0.14	43,43,43,43	0
58	MG	1A	3810	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3811	1/1	0.97	0.08	16,16,16,16	0
58	MG	1A	3015	1/1	0.97	0.10	24,24,24,24	0
58	MG	1A	3166	1/1	0.97	0.09	33,33,33,33	0
58	MG	1A	3294	1/1	0.97	0.12	43,43,43,43	0
58	MG	1A	3167	1/1	0.97	0.07	32,32,32,32	0
58	MG	2A	3625	1/1	0.97	0.08	48,48,48,48	0
58	MG	1P	201	1/1	0.97	0.18	30,30,30,30	0
58	MG	25	103	1/1	0.97	0.12	45,45,45,45	0
58	MG	1P	202	1/1	0.97	0.17	23,23,23,23	0
58	MG	1A	3816	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3656	1/1	0.97	0.06	30,30,30,30	0
58	MG	1Q	202	1/1	0.97	0.31	35,35,35,35	0
58	MG	27	101	1/1	0.97	0.12	44,44,44,44	0
58	MG	2A	3348	1/1	0.97	0.12	70,70,70,70	0
58	MG	1A	3124	1/1	0.97	0.11	32,32,32,32	0
58	MG	2A	3350	1/1	0.97	0.08	65,65,65,65	0
58	MG	1A	3658	1/1	0.97	0.08	31,31,31,31	0
58	MG	1A	3297	1/1	0.97	0.07	31,31,31,31	0
58	MG	28	104	1/1	0.97	0.11	46,46,46,46	0
58	MG	1a	1728	1/1	0.97	0.10	61,61,61,61	0
58	MG	1a	1729	1/1	0.97	0.10	48,48,48,48	0
58	MG	1A	3987	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3988	1/1	0.97	0.09	32,32,32,32	0
58	MG	2A	3640	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3125	1/1	0.97	0.09	34,34,34,34	0
58	MG	1a	1734	1/1	0.97	0.12	31,31,31,31	0
58	MG	1A	3228	1/1	0.97	0.16	26,26,26,26	0
58	MG	2A	3644	1/1	0.97	0.08	56,56,56,56	0
58	MG	1A	3170	1/1	0.97	0.04	40,40,40,40	0
58	MG	1A	3008	1/1	0.97	0.05	20,20,20,20	0
58	MG	1A	3666	1/1	0.97	0.05	18,18,18,18	0
58	MG	2A	3125	1/1	0.97	0.05	56,56,56,56	0
58	MG	2A	3366	1/1	0.97	0.15	40,40,40,40	0
58	MG	2A	3126	1/1	0.97	0.11	52,52,52,52	0
58	MG	1A	3995	1/1	0.97	0.05	29,29,29,29	0
58	MG	1a	1741	1/1	0.97	0.16	44,44,44,44	0
58	MG	1A	3445	1/1	0.97	0.27	38,38,38,38	0
58	MG	2A	3654	1/1	0.97	0.05	35,35,35,35	0
58	MG	1U	201	1/1	0.97	0.10	33,33,33,33	0
58	MG	1A	3092	1/1	0.97	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1747	1/1	0.97	0.10	52,52,52,52	0
58	MG	2A	3133	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3365	1/1	0.97	0.12	27,27,27,27	0
58	MG	1A	3831	1/1	0.97	0.05	38,38,38,38	0
58	MG	1U	205	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3129	1/1	0.97	0.13	47,47,47,47	0
58	MG	2A	3139	1/1	0.97	0.13	38,38,38,38	0
58	MG	1a	1752	1/1	0.97	0.08	41,41,41,41	0
58	MG	2A	3141	1/1	0.97	0.18	46,46,46,46	0
58	MG	1U	207	1/1	0.97	0.17	30,30,30,30	0
58	MG	2A	3384	1/1	0.97	0.06	41,41,41,41	0
58	MG	1U	208	1/1	0.97	0.32	38,38,38,38	0
58	MG	1A	3238	1/1	0.97	0.15	24,24,24,24	0
58	MG	1A	3368	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3676	1/1	0.97	0.13	36,36,36,36	0
58	MG	1A	3369	1/1	0.97	0.18	29,29,29,29	0
58	MG	1V	205	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3370	1/1	0.97	0.07	50,50,50,50	0
58	MG	1A	3548	1/1	0.97	0.06	45,45,45,45	0
58	MG	2A	3676	1/1	0.97	0.11	43,43,43,43	0
58	MG	2A	3151	1/1	0.97	0.15	49,49,49,49	0
58	MG	1A	4009	1/1	0.97	0.07	21,21,21,21	0
58	MG	2A	3395	1/1	0.97	0.06	48,48,48,48	0
58	MG	1A	4010	1/1	0.97	0.04	32,32,32,32	0
58	MG	1A	3453	1/1	0.97	0.16	34,34,34,34	0
58	MG	1A	3685	1/1	0.97	0.05	46,46,46,46	0
58	MG	2A	3156	1/1	0.97	0.08	51,51,51,51	0
58	MG	1A	3177	1/1	0.97	0.09	29,29,29,29	0
58	MG	1X	101	1/1	0.97	0.05	38,38,38,38	0
58	MG	1X	102	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3374	1/1	0.97	0.23	47,47,47,47	0
58	MG	1A	3064	1/1	0.97	0.16	37,37,37,37	0
58	MG	2A	3405	1/1	0.97	0.28	48,48,48,48	0
58	MG	1A	3181	1/1	0.97	0.14	39,39,39,39	0
58	MG	1A	3555	1/1	0.97	0.08	50,50,50,50	0
58	MG	2a	1658	1/1	0.97	0.04	61,61,61,61	0
58	MG	1a	1777	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3697	1/1	0.97	0.04	20,20,20,20	0
58	MG	2A	3696	1/1	0.97	0.10	29,29,29,29	0
58	MG	1A	3556	1/1	0.97	0.16	29,29,29,29	0
58	MG	1A	3377	1/1	0.97	0.08	46,46,46,46	0
58	MG	1A	3182	1/1	0.97	0.12	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	3559	1/1	0.97	0.16	33,33,33,33	0
58	MG	1A	3245	1/1	0.97	0.13	51,51,51,51	0
58	MG	1A	3855	1/1	0.97	0.09	28,28,28,28	0
58	MG	1a	1786	1/1	0.97	0.18	60,60,60,60	0
58	MG	1A	3856	1/1	0.97	0.08	55,55,55,55	0
58	MG	1A	3047	1/1	0.97	0.09	29,29,29,29	0
58	MG	2a	1671	1/1	0.97	0.18	56,56,56,56	0
58	MG	1a	1789	1/1	0.97	0.05	60,60,60,60	0
58	MG	1A	3067	1/1	0.97	0.10	28,28,28,28	0
58	MG	2A	3709	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3464	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3708	1/1	0.97	0.04	14,14,14,14	0
58	MG	1a	1795	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3424	1/1	0.97	0.19	49,49,49,49	0
58	MG	2A	3181	1/1	0.97	0.11	50,50,50,50	0
58	MG	2A	3426	1/1	0.97	0.23	44,44,44,44	0
58	MG	1A	3862	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3467	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3864	1/1	0.97	0.04	30,30,30,30	0
58	MG	2a	1684	1/1	0.97	0.14	60,60,60,60	0
58	MG	1A	3568	1/1	0.97	0.26	36,36,36,36	0
58	MG	1A	3866	1/1	0.97	0.04	43,43,43,43	0
58	MG	2A	3433	1/1	0.97	0.25	57,57,57,57	0
58	MG	1A	3248	1/1	0.97	0.23	26,26,26,26	0
58	MG	1A	3868	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	4044	1/1	0.97	0.04	31,31,31,31	0
58	MG	2A	3437	1/1	0.97	0.07	43,43,43,43	0
58	MG	1A	3068	1/1	0.97	0.06	33,33,33,33	0
58	MG	1A	3027	1/1	0.97	0.16	60,60,60,60	0
58	MG	1A	3716	1/1	0.97	0.07	51,51,51,51	0
58	MG	15	102	1/1	0.97	0.18	32,32,32,32	0
58	MG	15	103	1/1	0.97	0.17	33,33,33,33	0
58	MG	2a	1698	1/1	0.97	0.15	46,46,46,46	0
58	MG	15	104	1/1	0.97	0.13	31,31,31,31	0
58	MG	1A	3573	1/1	0.97	0.14	34,34,34,34	0
58	MG	1A	4051	1/1	0.97	0.12	17,17,17,17	0
58	MG	1A	3051	1/1	0.97	0.06	24,24,24,24	0
58	MG	2A	3201	1/1	0.97	0.09	42,42,42,42	0
58	MG	1A	3192	1/1	0.97	0.10	53,53,53,53	0
58	MG	2A	3450	1/1	0.97	0.04	34,34,34,34	0
58	MG	2A	3451	1/1	0.97	0.33	35,35,35,35	0
58	MG	17	103	1/1	0.97	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3194	1/1	0.97	0.09	23,23,23,23	0
58	MG	2A	3454	1/1	0.97	0.07	53,53,53,53	0
58	MG	1A	4056	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3876	1/1	0.97	0.17	27,27,27,27	0
58	MG	1A	3578	1/1	0.97	0.17	41,41,41,41	0
58	MG	1A	3017	1/1	0.97	0.14	57,57,57,57	0
58	MG	1A	4064	1/1	0.97	0.07	11,11,11,11	0
58	MG	1A	3476	1/1	0.97	0.13	47,47,47,47	0
58	MG	1A	3581	1/1	0.97	0.28	34,34,34,34	0
58	MG	2A	3754	1/1	0.97	0.17	54,54,54,54	0
58	MG	1A	3001	1/1	0.97	0.06	33,33,33,33	0
58	MG	2A	3213	1/1	0.97	0.08	50,50,50,50	0
58	MG	1A	4070	1/1	0.97	0.05	41,41,41,41	0
58	MG	2a	1723	1/1	0.97	0.18	61,61,61,61	0
58	MG	1A	3583	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3886	1/1	0.97	0.05	28,28,28,28	0
58	MG	2A	3218	1/1	0.97	0.08	46,46,46,46	0
58	MG	2A	3763	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3887	1/1	0.97	0.07	22,22,22,22	0
58	MG	1A	3888	1/1	0.97	0.10	23,23,23,23	0
58	MG	1A	3478	1/1	0.97	0.16	52,52,52,52	0
58	MG	2A	3471	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3257	1/1	0.97	0.10	23,23,23,23	0
58	MG	2A	3474	1/1	0.97	0.07	51,51,51,51	0
58	MG	2A	3475	1/1	0.97	0.13	32,32,32,32	0
58	MG	2A	3223	1/1	0.97	0.05	38,38,38,38	0
58	MG	2A	3224	1/1	0.97	0.13	46,46,46,46	0
58	MG	1a	1609	1/1	0.97	0.07	50,50,50,50	0
58	MG	1A	3395	1/1	0.97	0.16	52,52,52,52	0
58	MG	1A	4081	1/1	0.97	0.12	56,56,56,56	0
58	MG	1A	4082	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3894	1/1	0.97	0.07	23,23,23,23	0
58	MG	1A	4084	1/1	0.97	0.09	32,32,32,32	0
58	MG	1A	4085	1/1	0.97	0.05	45,45,45,45	0
58	MG	1A	3733	1/1	0.97	0.07	46,46,46,46	0
58	MG	1a	1617	1/1	0.97	0.10	58,58,58,58	0
58	MG	1A	3735	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3736	1/1	0.97	0.06	20,20,20,20	0
58	MG	2A	3493	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3258	1/1	0.97	0.05	46,46,46,46	0
58	MG	1A	3398	1/1	0.97	0.19	28,28,28,28	0
58	MG	1x	110	1/1	0.97	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	3011	1/1	0.97	0.10	33,33,33,33	0
58	MG	1A	4092	1/1	0.97	0.11	43,43,43,43	0
58	MG	2a	1754	1/1	0.97	0.08	58,58,58,58	0
58	MG	2A	3791	1/1	0.97	0.07	53,53,53,53	0
58	MG	2a	1756	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3592	1/1	0.97	0.08	36,36,36,36	0
58	MG	1A	3902	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3903	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3400	1/1	0.97	0.13	31,31,31,31	0
58	MG	1A	3260	1/1	0.97	0.14	42,42,42,42	0
58	MG	1A	4100	1/1	0.97	0.16	51,51,51,51	0
58	MG	1A	3402	1/1	0.97	0.08	40,40,40,40	0
58	MG	2A	3009	1/1	0.97	0.05	49,49,49,49	0
58	MG	1A	3036	1/1	0.97	0.06	28,28,28,28	0
58	MG	2A	3011	1/1	0.97	0.10	39,39,39,39	0
58	MG	2A	3510	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3511	1/1	0.97	0.05	43,43,43,43	0
58	MG	2A	3012	1/1	0.97	0.06	36,36,36,36	0
58	MG	2A	3810	1/1	0.97	0.05	44,44,44,44	0
58	MG	2A	3811	1/1	0.97	0.06	56,56,56,56	0
58	MG	1A	3488	1/1	0.97	0.13	50,50,50,50	0
58	MG	1A	3057	1/1	0.97	0.20	37,37,37,37	0
58	MG	2A	3815	1/1	0.97	0.07	48,48,48,48	0
58	MG	1A	3328	1/1	0.97	0.17	43,43,43,43	0
58	MG	1A	3491	1/1	0.97	0.10	32,32,32,32	0
58	MG	2A	3258	1/1	0.97	0.05	46,46,46,46	0
58	MG	1A	3914	1/1	0.97	0.12	27,27,27,27	0
58	MG	2A	3018	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3915	1/1	0.97	0.06	23,23,23,23	0
58	MG	1A	3201	1/1	0.97	0.05	30,30,30,30	0
58	MG	1A	3264	1/1	0.97	0.04	44,44,44,44	0
58	MG	1A	3603	1/1	0.97	0.12	34,34,34,34	0
58	MG	1A	3265	1/1	0.97	0.23	38,38,38,38	0
58	MG	1A	3149	1/1	0.97	0.27	29,29,29,29	0
58	MG	1A	3203	1/1	0.97	0.13	23,23,23,23	0
58	MG	2A	3268	1/1	0.97	0.07	55,55,55,55	0
58	MG	2A	3831	1/1	0.97	0.08	41,41,41,41	0
58	MG	2A	3030	1/1	0.97	0.11	44,44,44,44	0
58	MG	1A	3150	1/1	0.97	0.24	28,28,28,28	0
58	MG	1a	1647	1/1	0.97	0.12	48,48,48,48	0
58	MG	1A	3151	1/1	0.97	0.36	37,37,37,37	0
58	MG	1a	1649	1/1	0.97	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3539	1/1	0.97	0.12	37,37,37,37	0
58	MG	1A	3108	1/1	0.97	0.05	20,20,20,20	0
58	MG	1A	3004	1/1	0.97	0.07	27,27,27,27	0
58	MG	1A	3611	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3417	1/1	0.97	0.06	42,42,42,42	0
58	MG	1A	3338	1/1	0.97	0.10	64,64,64,64	0
58	MG	1A	3111	1/1	0.97	0.20	28,28,28,28	0
58	MG	1A	3022	1/1	0.97	0.04	36,36,36,36	0
58	MG	2A	3846	1/1	0.97	0.10	57,57,57,57	0
58	MG	2a	1804	1/1	0.97	0.06	63,63,63,63	0
58	MG	2A	3281	1/1	0.97	0.09	55,55,55,55	0
58	MG	1A	3936	1/1	0.97	0.05	26,26,26,26	0
58	MG	1A	3086	1/1	0.97	0.10	33,33,33,33	0
58	MG	1B	226	1/1	0.97	0.05	37,37,37,37	0
58	MG	2A	3853	1/1	0.97	0.14	56,56,56,56	0
58	MG	1B	227	1/1	0.97	0.08	43,43,43,43	0
58	MG	2A	3286	1/1	0.97	0.21	46,46,46,46	0
58	MG	1A	3939	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3617	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	3941	1/1	0.97	0.09	47,47,47,47	0
58	MG	1A	3618	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3621	1/1	0.97	0.12	10,10,10,10	0
58	MG	2a	1817	1/1	0.97	0.06	64,64,64,64	0
58	MG	1A	3777	1/1	0.97	0.06	59,59,59,59	0
58	MG	1A	3624	1/1	0.97	0.07	43,43,43,43	0
58	MG	1B	235	1/1	0.97	0.05	35,35,35,35	0
58	MG	2A	3057	1/1	0.97	0.08	39,39,39,39	0
58	MG	1D	301	1/1	0.97	0.11	30,30,30,30	0
58	MG	1A	3510	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3342	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3633	1/1	0.97	0.06	24,24,24,24	0
58	MG	1A	3952	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3211	1/1	0.97	0.19	30,30,30,30	0
58	MG	2A	3571	1/1	0.97	0.13	48,48,48,48	0
58	MG	1A	3116	1/1	0.97	0.05	34,34,34,34	0
58	MG	1D	312	1/1	0.97	0.10	19,19,19,19	0
58	MG	1A	3425	1/1	0.97	0.05	32,32,32,32	0
58	MG	1A	3788	1/1	0.97	0.05	21,21,21,21	0
58	MG	2A	3578	1/1	0.97	0.11	38,38,38,38	0
58	MG	2A	3579	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3213	1/1	0.97	0.05	44,44,44,44	0
58	MG	1E	302	1/1	0.97	0.11	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	3070	1/1	0.97	0.05	37,37,37,37	0
58	MG	1A	3958	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3959	1/1	0.97	0.04	34,34,34,34	0
58	MG	1A	3639	1/1	0.97	0.09	26,26,26,26	0
58	MG	1A	3791	1/1	0.97	0.04	19,19,19,19	0
58	MG	2D	307	1/1	0.97	0.08	32,32,32,32	0
58	MG	2D	308	1/1	0.97	0.24	47,47,47,47	0
58	MG	1A	3087	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3963	1/1	0.97	0.09	47,47,47,47	0
58	MG	1a	1691	1/1	0.97	0.29	47,47,47,47	0
58	MG	2E	303	1/1	0.97	0.08	30,30,30,30	0
58	MG	1A	3964	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3215	1/1	0.97	0.12	35,35,35,35	0
58	MG	1A	3519	1/1	0.97	0.17	32,32,32,32	0
58	MG	1A	3284	1/1	0.97	0.12	36,36,36,36	0
58	MG	1F	305	1/1	0.97	0.05	27,27,27,27	0
58	MG	1F	307	1/1	0.97	0.10	24,24,24,24	0
58	MG	1A	3968	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3324	1/1	0.97	0.11	49,49,49,49	0
58	MG	2F	305	1/1	0.97	0.23	42,42,42,42	0
58	MG	2A	3325	1/1	0.97	0.09	47,47,47,47	0
58	MG	1F	311	1/1	0.97	0.15	35,35,35,35	0
58	MG	1A	3798	1/1	0.97	0.07	43,43,43,43	0
58	MG	1A	3645	1/1	0.97	0.06	18,18,18,18	0
58	MG	1A	3285	1/1	0.97	0.14	38,38,38,38	0
58	MG	1A	3041	1/1	0.97	0.04	30,30,30,30	0
58	MG	2Q	201	1/1	0.97	0.07	60,60,60,60	0
58	MG	2A	3607	1/1	0.97	0.09	41,41,41,41	0
58	MG	2R	201	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3608	1/1	0.97	0.05	32,32,32,32	0
58	MG	1H	201	1/1	0.97	0.08	34,34,34,34	0
61	ZN	24	501	1/1	0.97	0.10	119,119,119,119	0
58	MG	1A	3499	1/1	0.98	0.12	31,31,31,31	0
58	MG	1A	3709	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3590	1/1	0.98	0.19	22,22,22,22	0
58	MG	1A	3230	1/1	0.98	0.05	37,37,37,37	0
58	MG	2A	3019	1/1	0.98	0.03	31,31,31,31	0
58	MG	1A	3712	1/1	0.98	0.05	36,36,36,36	0
58	MG	2A	3021	1/1	0.98	0.04	34,34,34,34	0
58	MG	2A	3022	1/1	0.98	0.15	46,46,46,46	0
58	MG	1A	3501	1/1	0.98	0.16	42,42,42,42	0
58	MG	2A	3710	1/1	0.98	0.12	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	1E	314	1/1	0.98	0.04	34,34,34,34	0
58	MG	2a	1626	1/1	0.98	0.08	58,58,58,58	0
58	MG	2A	3712	1/1	0.98	0.05	28,28,28,28	0
58	MG	1A	3105	1/1	0.98	0.10	27,27,27,27	0
58	MG	1F	303	1/1	0.98	0.12	22,22,22,22	0
58	MG	2A	3244	1/1	0.98	0.14	57,57,57,57	0
58	MG	2A	3027	1/1	0.98	0.03	43,43,43,43	0
58	MG	1A	3849	1/1	0.98	0.07	45,45,45,45	0
58	MG	1a	1666	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3179	1/1	0.98	0.05	30,30,30,30	0
58	MG	1A	3180	1/1	0.98	0.04	25,25,25,25	0
58	MG	1F	308	1/1	0.98	0.23	27,27,27,27	0
58	MG	1A	3852	1/1	0.98	0.05	44,44,44,44	0
58	MG	1F	310	1/1	0.98	0.04	38,38,38,38	0
58	MG	2A	3035	1/1	0.98	0.04	41,41,41,41	0
58	MG	1A	4000	1/1	0.98	0.03	38,38,38,38	0
58	MG	1A	3235	1/1	0.98	0.04	63,63,63,63	0
58	MG	1G	201	1/1	0.98	0.07	34,34,34,34	0
58	MG	1G	202	1/1	0.98	0.11	45,45,45,45	0
58	MG	2A	3481	1/1	0.98	0.10	38,38,38,38	0
58	MG	1A	3056	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3237	1/1	0.98	0.10	24,24,24,24	0
58	MG	1A	3720	1/1	0.98	0.03	14,14,14,14	0
58	MG	2A	3485	1/1	0.98	0.22	60,60,60,60	0
58	MG	1A	3138	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3509	1/1	0.98	0.03	33,33,33,33	0
58	MG	1A	4007	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3859	1/1	0.98	0.10	24,24,24,24	0
58	MG	1N	203	1/1	0.98	0.10	47,47,47,47	0
58	MG	1A	3139	1/1	0.98	0.14	32,32,32,32	0
58	MG	1A	3301	1/1	0.98	0.12	24,24,24,24	0
58	MG	2A	3051	1/1	0.98	0.06	47,47,47,47	0
58	MG	1A	3725	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	3240	1/1	0.98	0.13	22,22,22,22	0
58	MG	1A	3241	1/1	0.98	0.09	25,25,25,25	0
58	MG	2A	3745	1/1	0.98	0.10	42,42,42,42	0
58	MG	1a	1689	1/1	0.98	0.15	44,44,44,44	0
58	MG	2A	3747	1/1	0.98	0.09	51,51,51,51	0
58	MG	1A	4017	1/1	0.98	0.04	65,65,65,65	0
58	MG	1A	3140	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3014	1/1	0.98	0.05	27,27,27,27	0
58	MG	2A	3751	1/1	0.98	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1693	1/1	0.98	0.22	44,44,44,44	0
58	MG	1P	203	1/1	0.98	0.11	32,32,32,32	0
58	MG	1A	3021	1/1	0.98	0.05	20,20,20,20	0
58	MG	2A	3755	1/1	0.98	0.11	50,50,50,50	0
58	MG	1A	3187	1/1	0.98	0.09	34,34,34,34	0
58	MG	1A	3518	1/1	0.98	0.20	31,31,31,31	0
58	MG	1A	3109	1/1	0.98	0.17	29,29,29,29	0
58	MG	1Q	204	1/1	0.98	0.05	45,45,45,45	0
58	MG	1A	3371	1/1	0.98	0.17	47,47,47,47	0
58	MG	2A	3761	1/1	0.98	0.07	47,47,47,47	0
58	MG	1A	3190	1/1	0.98	0.12	37,37,37,37	0
58	MG	1A	3443	1/1	0.98	0.19	27,27,27,27	0
58	MG	1A	3373	1/1	0.98	0.24	47,47,47,47	0
58	MG	1R	201	1/1	0.98	0.09	38,38,38,38	0
58	MG	2A	3516	1/1	0.98	0.06	41,41,41,41	0
58	MG	1A	3028	1/1	0.98	0.15	29,29,29,29	0
58	MG	2A	3768	1/1	0.98	0.08	53,53,53,53	0
58	MG	1a	1706	1/1	0.98	0.04	49,49,49,49	0
58	MG	1A	4030	1/1	0.98	0.04	43,43,43,43	0
58	MG	1A	3742	1/1	0.98	0.08	43,43,43,43	0
58	MG	1a	1709	1/1	0.98	0.17	42,42,42,42	0
58	MG	2A	3076	1/1	0.98	0.15	49,49,49,49	0
58	MG	2A	3523	1/1	0.98	0.12	38,38,38,38	0
58	MG	1A	3877	1/1	0.98	0.18	28,28,28,28	0
58	MG	1A	3042	1/1	0.98	0.08	30,30,30,30	0
58	MG	1A	3879	1/1	0.98	0.16	25,25,25,25	0
58	MG	2a	1693	1/1	0.98	0.14	62,62,62,62	0
58	MG	1A	3744	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	3012	1/1	0.98	0.04	34,34,34,34	0
58	MG	2A	3530	1/1	0.98	0.07	43,43,43,43	0
58	MG	1A	3044	1/1	0.98	0.09	38,38,38,38	0
58	MG	1A	3619	1/1	0.98	0.06	18,18,18,18	0
58	MG	2A	3084	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3748	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3620	1/1	0.98	0.06	34,34,34,34	0
58	MG	2A	3087	1/1	0.98	0.04	47,47,47,47	0
58	MG	2A	3538	1/1	0.98	0.06	31,31,31,31	0
58	MG	1a	1720	1/1	0.98	0.12	40,40,40,40	0
58	MG	2A	3540	1/1	0.98	0.16	44,44,44,44	0
58	MG	1A	3114	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3623	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3529	1/1	0.98	0.05	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	2A	3544	1/1	0.98	0.07	41,41,41,41	0
58	MG	1A	4045	1/1	0.98	0.05	30,30,30,30	0
58	MG	2a	1712	1/1	0.98	0.06	61,61,61,61	0
58	MG	1U	210	1/1	0.98	0.18	30,30,30,30	0
58	MG	2A	3311	1/1	0.98	0.08	52,52,52,52	0
58	MG	2A	3800	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3891	1/1	0.98	0.05	40,40,40,40	0
58	MG	1V	201	1/1	0.98	0.16	24,24,24,24	0
58	MG	1V	202	1/1	0.98	0.12	31,31,31,31	0
58	MG	1A	3115	1/1	0.98	0.07	25,25,25,25	0
58	MG	1a	1730	1/1	0.98	0.04	47,47,47,47	0
58	MG	2A	3099	1/1	0.98	0.17	45,45,45,45	0
58	MG	1A	3754	1/1	0.98	0.03	22,22,22,22	0
58	MG	1A	4049	1/1	0.98	0.05	42,42,42,42	0
58	MG	1A	3626	1/1	0.98	0.08	28,28,28,28	0
58	MG	2A	3103	1/1	0.98	0.18	53,53,53,53	0
58	MG	1A	3628	1/1	0.98	0.06	38,38,38,38	0
58	MG	1a	1735	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3531	1/1	0.98	0.21	26,26,26,26	0
58	MG	1A	4053	1/1	0.98	0.10	47,47,47,47	0
58	MG	2A	3562	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3632	1/1	0.98	0.04	50,50,50,50	0
58	MG	1W	204	1/1	0.98	0.07	29,29,29,29	0
58	MG	1A	3759	1/1	0.98	0.07	29,29,29,29	0
58	MG	1W	206	1/1	0.98	0.05	25,25,25,25	0
58	MG	1a	1742	1/1	0.98	0.05	41,41,41,41	0
58	MG	1A	3380	1/1	0.98	0.07	23,23,23,23	0
58	MG	1A	3030	1/1	0.98	0.13	35,35,35,35	0
58	MG	1A	3534	1/1	0.98	0.18	37,37,37,37	0
58	MG	1A	3065	1/1	0.98	0.11	33,33,33,33	0
58	MG	1A	4062	1/1	0.98	0.03	33,33,33,33	0
58	MG	1A	4063	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3154	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3638	1/1	0.98	0.07	46,46,46,46	0
58	MG	1A	3766	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3031	1/1	0.98	0.19	16,16,16,16	0
58	MG	2A	3580	1/1	0.98	0.08	45,45,45,45	0
58	MG	1A	3538	1/1	0.98	0.12	32,32,32,32	0
58	MG	2A	3582	1/1	0.98	0.05	38,38,38,38	0
58	MG	2A	3583	1/1	0.98	0.07	60,60,60,60	0
58	MG	1A	4071	1/1	0.98	0.06	56,56,56,56	0
58	MG	1a	1756	1/1	0.98	0.06	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3769	1/1	0.98	0.07	26,26,26,26	0
58	MG	1A	3770	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3641	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3119	1/1	0.98	0.11	23,23,23,23	0
58	MG	1A	3387	1/1	0.98	0.34	21,21,21,21	0
58	MG	2A	3847	1/1	0.98	0.12	44,44,44,44	0
58	MG	1A	4078	1/1	0.98	0.08	39,39,39,39	0
58	MG	1A	3541	1/1	0.98	0.09	19,19,19,19	0
58	MG	2A	3850	1/1	0.98	0.15	39,39,39,39	0
58	MG	1A	3458	1/1	0.98	0.07	30,30,30,30	0
58	MG	1A	3048	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3032	1/1	0.98	0.11	18,18,18,18	0
58	MG	1A	3050	1/1	0.98	0.10	30,30,30,30	0
58	MG	1a	1769	1/1	0.98	0.07	58,58,58,58	0
58	MG	1A	3779	1/1	0.98	0.04	14,14,14,14	0
58	MG	2A	3357	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3922	1/1	0.98	0.04	58,58,58,58	0
58	MG	12	102	1/1	0.98	0.08	40,40,40,40	0
58	MG	2a	1770	1/1	0.98	0.16	57,57,57,57	0
58	MG	1A	3160	1/1	0.98	0.12	24,24,24,24	0
58	MG	1A	3123	1/1	0.98	0.08	33,33,33,33	0
58	MG	2A	3362	1/1	0.98	0.10	37,37,37,37	0
58	MG	13	103	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3033	1/1	0.98	0.26	20,20,20,20	0
58	MG	1A	3784	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3465	1/1	0.98	0.12	24,24,24,24	0
58	MG	1A	3394	1/1	0.98	0.08	43,43,43,43	0
58	MG	2A	3610	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3098	1/1	0.98	0.06	27,27,27,27	0
58	MG	1a	1782	1/1	0.98	0.15	55,55,55,55	0
58	MG	1A	3099	1/1	0.98	0.11	18,18,18,18	0
58	MG	1A	3397	1/1	0.98	0.04	25,25,25,25	0
58	MG	15	106	1/1	0.98	0.17	42,42,42,42	0
58	MG	1A	4095	1/1	0.98	0.04	52,52,52,52	0
58	MG	15	108	1/1	0.98	0.07	35,35,35,35	0
58	MG	15	109	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	4096	1/1	0.98	0.06	35,35,35,35	0
58	MG	1A	3932	1/1	0.98	0.04	15,15,15,15	0
58	MG	2A	3621	1/1	0.98	0.06	38,38,38,38	0
58	MG	17	102	1/1	0.98	0.10	23,23,23,23	0
58	MG	1A	3554	1/1	0.98	0.09	27,27,27,27	0
58	MG	2A	3380	1/1	0.98	0.04	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	17	104	1/1	0.98	0.13	26,26,26,26	0
58	MG	1A	3934	1/1	0.98	0.07	54,54,54,54	0
58	MG	1A	3659	1/1	0.98	0.07	33,33,33,33	0
58	MG	18	102	1/1	0.98	0.19	40,40,40,40	0
58	MG	1A	3937	1/1	0.98	0.04	28,28,28,28	0
58	MG	1A	3076	1/1	0.98	0.05	28,28,28,28	0
58	MG	1A	3128	1/1	0.98	0.16	29,29,29,29	0
58	MG	1A	3023	1/1	0.98	0.04	14,14,14,14	0
58	MG	1A	3130	1/1	0.98	0.18	35,35,35,35	0
58	MG	1A	3797	1/1	0.98	0.07	50,50,50,50	0
58	MG	1A	3664	1/1	0.98	0.04	23,23,23,23	0
58	MG	1B	205	1/1	0.98	0.04	43,43,43,43	0
58	MG	1A	3945	1/1	0.98	0.06	56,56,56,56	0
58	MG	1A	3475	1/1	0.98	0.09	48,48,48,48	0
58	MG	2A	3175	1/1	0.98	0.12	34,34,34,34	0
58	MG	1A	3005	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3025	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3274	1/1	0.98	0.10	40,40,40,40	0
58	MG	1A	3133	1/1	0.98	0.04	35,35,35,35	0
58	MG	1A	3806	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3807	1/1	0.98	0.06	53,53,53,53	0
58	MG	2A	3182	1/1	0.98	0.09	34,34,34,34	0
58	MG	1A	3173	1/1	0.98	0.08	30,30,30,30	0
58	MG	1A	3809	1/1	0.98	0.08	21,21,21,21	0
58	MG	1A	3672	1/1	0.98	0.06	20,20,20,20	0
58	MG	2A	3186	1/1	0.98	0.06	47,47,47,47	0
58	MG	1B	217	1/1	0.98	0.03	31,31,31,31	0
58	MG	1B	218	1/1	0.98	0.08	30,30,30,30	0
58	MG	1A	3566	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3674	1/1	0.98	0.07	29,29,29,29	0
58	MG	1I	202	1/1	0.98	0.04	57,57,57,57	0
58	MG	1A	3567	1/1	0.98	0.24	32,32,32,32	0
58	MG	1A	3277	1/1	0.98	0.10	16,16,16,16	0
58	MG	1A	3221	1/1	0.98	0.03	49,49,49,49	0
58	MG	1A	3678	1/1	0.98	0.06	20,20,20,20	0
58	MG	1A	3222	1/1	0.98	0.08	26,26,26,26	0
58	MG	1A	3410	1/1	0.98	0.05	45,45,45,45	0
58	MG	1A	3174	1/1	0.98	0.18	24,24,24,24	0
58	MG	1A	3281	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3686	1/1	0.98	0.07	29,29,29,29	0
58	MG	1A	3175	1/1	0.98	0.10	24,24,24,24	0
58	MG	1A	3576	1/1	0.98	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	1A	3414	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3692	1/1	0.98	0.07	21,21,21,21	0
58	MG	1A	3826	1/1	0.98	0.05	27,27,27,27	0
58	MG	23	103	1/1	0.98	0.07	54,54,54,54	0
58	MG	23	104	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3693	1/1	0.98	0.04	23,23,23,23	0
58	MG	2A	3427	1/1	0.98	0.27	42,42,42,42	0
58	MG	2I	202	1/1	0.98	0.05	53,53,53,53	0
58	MG	1A	3828	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3694	1/1	0.98	0.07	31,31,31,31	0
58	MG	1a	1635	1/1	0.98	0.10	29,29,29,29	0
58	MG	1A	3283	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3225	1/1	0.98	0.08	40,40,40,40	0
58	MG	1A	3134	1/1	0.98	0.05	28,28,28,28	0
58	MG	1A	3833	1/1	0.98	0.12	35,35,35,35	0
58	MG	1D	309	1/1	0.98	0.11	26,26,26,26	0
58	MG	1D	310	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3348	1/1	0.98	0.16	28,28,28,28	0
58	MG	2A	3217	1/1	0.98	0.16	51,51,51,51	0
58	MG	1a	1643	1/1	0.98	0.11	48,48,48,48	0
58	MG	1A	3227	1/1	0.98	0.21	37,37,37,37	0
58	MG	1A	3038	1/1	0.98	0.09	24,24,24,24	0
58	MG	1A	3288	1/1	0.98	0.03	37,37,37,37	0
58	MG	1A	3585	1/1	0.98	0.07	40,40,40,40	0
58	MG	1A	3289	1/1	0.98	0.04	48,48,48,48	0
58	MG	2A	3445	1/1	0.98	0.13	28,28,28,28	0
58	MG	1E	303	1/1	0.98	0.07	21,21,21,21	0
58	MG	1A	3229	1/1	0.98	0.25	26,26,26,26	0
58	MG	2A	3226	1/1	0.98	0.08	34,34,34,34	0
58	MG	1A	3498	1/1	0.98	0.10	26,26,26,26	0
58	MG	1a	1652	1/1	0.98	0.05	48,48,48,48	0
58	MG	1a	1653	1/1	0.98	0.09	35,35,35,35	0
58	MG	1E	306	1/1	0.98	0.09	39,39,39,39	0
61	ZN	14	501	1/1	0.98	0.10	107,107,107,107	0
61	ZN	2Y	202	1/1	0.98	0.04	92,92,92,92	0
58	MG	1E	307	1/1	0.98	0.05	33,33,33,33	0
61	ZN	25	107	1/1	0.98	0.03	70,70,70,70	0
61	ZN	26	102	1/1	0.98	0.07	70,70,70,70	0
62	SF4	1d	302	8/8	0.98	0.06	58,63,68,71	0
62	SF4	2d	303	8/8	0.98	0.04	70,82,88,94	0
58	MG	17	101	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3631	1/1	0.99	0.03	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3700	1/1	0.99	0.03	32,32,32,32	0
58	MG	2A	3036	1/1	0.99	0.15	39,39,39,39	0
58	MG	1A	3250	1/1	0.99	0.07	32,32,32,32	0
58	MG	1A	3189	1/1	0.99	0.15	31,31,31,31	0
58	MG	1A	3045	1/1	0.99	0.03	34,34,34,34	0
58	MG	1A	4029	1/1	0.99	0.03	21,21,21,21	0
58	MG	1A	3191	1/1	0.99	0.22	32,32,32,32	0
58	MG	1A	3058	1/1	0.99	0.05	19,19,19,19	0
58	MG	1A	4032	1/1	0.99	0.03	43,43,43,43	0
58	MG	1A	3706	1/1	0.99	0.07	23,23,23,23	0
58	MG	1A	3193	1/1	0.99	0.17	23,23,23,23	0
58	MG	2A	3504	1/1	0.99	0.06	43,43,43,43	0
58	MG	1A	3234	1/1	0.99	0.13	36,36,36,36	0
58	MG	1A	3670	1/1	0.99	0.04	39,39,39,39	0
58	MG	1A	3079	1/1	0.99	0.07	36,36,36,36	0
58	MG	1A	3793	1/1	0.99	0.02	32,32,32,32	0
58	MG	1A	3010	1/1	0.99	0.09	29,29,29,29	0
58	MG	2a	1705	1/1	0.99	0.06	57,57,57,57	0
58	MG	1A	3883	1/1	0.99	0.06	49,49,49,49	0
58	MG	1A	3161	1/1	0.99	0.04	20,20,20,20	0
58	MG	1A	3305	1/1	0.99	0.03	31,31,31,31	0
58	MG	1F	302	1/1	0.99	0.16	26,26,26,26	0
58	MG	1A	3935	1/1	0.99	0.04	14,14,14,14	0
58	MG	1A	3146	1/1	0.99	0.14	27,27,27,27	0
58	MG	1A	3070	1/1	0.99	0.10	28,28,28,28	0
58	MG	1F	306	1/1	0.99	0.06	40,40,40,40	0
58	MG	1A	3094	1/1	0.99	0.08	21,21,21,21	0
58	MG	1A	3200	1/1	0.99	0.13	23,23,23,23	0
58	MG	1A	3890	1/1	0.99	0.06	46,46,46,46	0
58	MG	2A	3689	1/1	0.99	0.06	52,52,52,52	0
58	MG	2A	3137	1/1	0.99	0.10	44,44,44,44	0
58	MG	2A	3691	1/1	0.99	0.04	48,48,48,48	0
58	MG	1a	1758	1/1	0.99	0.06	33,33,33,33	0
58	MG	1A	3801	1/1	0.99	0.08	17,17,17,17	0
58	MG	1A	3993	1/1	0.99	0.08	43,43,43,43	0
58	MG	1X	105	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	3942	1/1	0.99	0.02	28,28,28,28	0
58	MG	2A	3527	1/1	0.99	0.05	47,47,47,47	0
58	MG	1A	3679	1/1	0.99	0.06	20,20,20,20	0
58	MG	1A	3082	1/1	0.99	0.16	24,24,24,24	0
58	MG	1A	3071	1/1	0.99	0.10	14,14,14,14	0
58	MG	1A	3805	1/1	0.99	0.05	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	3683	1/1	0.99	0.04	29,29,29,29	0
58	MG	1A	3948	1/1	0.99	0.03	49,49,49,49	0
58	MG	2A	3704	1/1	0.99	0.03	38,38,38,38	0
58	MG	2A	3792	1/1	0.99	0.07	38,38,38,38	0
58	MG	1A	4058	1/1	0.99	0.03	30,30,30,30	0
58	MG	2A	3794	1/1	0.99	0.06	49,49,49,49	0
58	MG	1A	4059	1/1	0.99	0.05	22,22,22,22	0
58	MG	1A	3072	1/1	0.99	0.08	22,22,22,22	0
58	MG	2A	3537	1/1	0.99	0.04	47,47,47,47	0
58	MG	1A	3650	1/1	0.99	0.05	27,27,27,27	0
58	MG	1a	1773	1/1	0.99	0.03	51,51,51,51	0
58	MG	1A	3073	1/1	0.99	0.13	26,26,26,26	0
58	MG	1A	3386	1/1	0.99	0.18	45,45,45,45	0
58	MG	1A	3688	1/1	0.99	0.05	17,17,17,17	0
58	MG	1A	4066	1/1	0.99	0.02	38,38,38,38	0
58	MG	11	102	1/1	0.99	0.04	40,40,40,40	0
58	MG	1A	3074	1/1	0.99	0.04	9,9,9,9	0
58	MG	2A	3807	1/1	0.99	0.07	32,32,32,32	0
58	MG	1A	3690	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3291	1/1	0.99	0.13	26,26,26,26	0
58	MG	1A	3905	1/1	0.99	0.11	29,29,29,29	0
58	MG	1A	3037	1/1	0.99	0.12	23,23,23,23	0
58	MG	2A	3812	1/1	0.99	0.09	54,54,54,54	0
58	MG	1A	4072	1/1	0.99	0.08	34,34,34,34	0
58	MG	1A	4011	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	4012	1/1	0.99	0.06	42,42,42,42	0
58	MG	1A	4013	1/1	0.99	0.07	24,24,24,24	0
58	MG	2A	3472	1/1	0.99	0.03	51,51,51,51	0
58	MG	1A	3570	1/1	0.99	0.26	33,33,33,33	0
58	MG	2A	3819	1/1	0.99	0.05	24,24,24,24	0
58	MG	1A	3003	1/1	0.99	0.05	16,16,16,16	0
58	MG	13	106	1/1	0.99	0.07	35,35,35,35	0
58	MG	1a	1791	1/1	0.99	0.10	43,43,43,43	0
58	MG	1a	1717	1/1	0.99	0.09	43,43,43,43	0
58	MG	1B	236	1/1	0.99	0.02	28,28,28,28	0
58	MG	2A	3825	1/1	0.99	0.10	22,22,22,22	0
58	MG	1A	3734	1/1	0.99	0.03	37,37,37,37	0
58	MG	1D	302	1/1	0.99	0.04	31,31,31,31	0
58	MG	1A	3627	1/1	0.99	0.05	19,19,19,19	0
58	MG	1A	3466	1/1	0.99	0.08	30,30,30,30	0
58	MG	1A	3737	1/1	0.99	0.07	18,18,18,18	0
58	MG	1D	306	1/1	0.99	0.01	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3629	1/1	0.99	0.05	38,38,38,38	0
58	MG	1A	3141	1/1	0.99	0.06	11,11,11,11	0
61	ZN	1Y	204	1/1	0.99	0.02	55,55,55,55	0
58	MG	1A	3916	1/1	0.99	0.07	28,28,28,28	0
61	ZN	16	102	1/1	0.99	0.05	43,43,43,43	0
61	ZN	1n	103	1/1	0.99	0.03	64,64,64,64	0
58	MG	2A	3488	1/1	0.99	0.03	57,57,57,57	0
58	MG	1A	3780	1/1	0.99	0.04	33,33,33,33	0
58	MG	2A	3572	1/1	0.99	0.03	40,40,40,40	0
58	MG	2A	3573	1/1	0.99	0.07	35,35,35,35	0
61	ZN	29	501	1/1	0.99	0.03	72,72,72,72	0
61	ZN	2n	501	1/1	0.99	0.03	88,88,88,88	0
58	MG	2A	3839	1/1	0.99	0.05	51,51,51,51	0
58	MG	2A	3490	1/1	0.99	0.05	54,54,54,54	0
61	ZN	19	102	1/1	1.00	0.05	44,44,44,44	0
58	MG	2A	3799	1/1	1.00	0.08	45,45,45,45	0
58	MG	1a	1743	1/1	1.00	0.07	31,31,31,31	0
58	MG	1A	4065	1/1	1.00	0.03	27,27,27,27	0
58	MG	1A	3622	1/1	1.00	0.05	29,29,29,29	0
58	MG	1a	1794	1/1	1.00	0.03	39,39,39,39	0
58	MG	1A	3910	1/1	1.00	0.06	32,32,32,32	0
58	MG	1A	3727	1/1	1.00	0.05	17,17,17,17	0
61	ZN	15	111	1/1	1.00	0.01	49,49,49,49	0
58	MG	1A	3681	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.