



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 09:33 AM EDT

PDB ID : 9O3K / pdb_00009o3k
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 fMAC-peptidyl-tRNA^{Met}, and deacylated E-site tRNA^{Lys} at 2.70Å 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 : 2.70 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

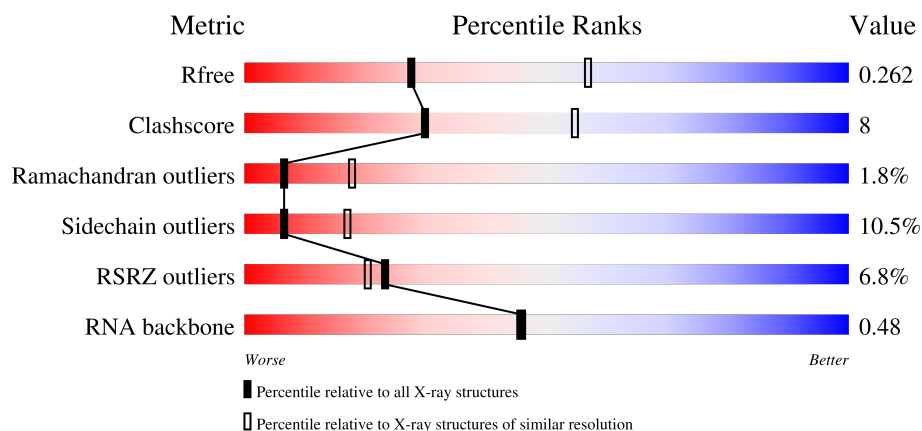
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

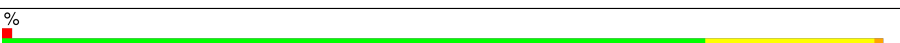
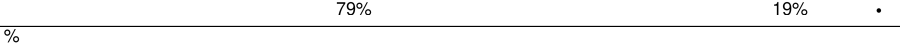
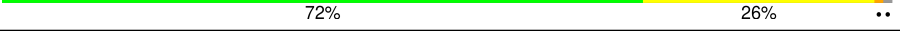
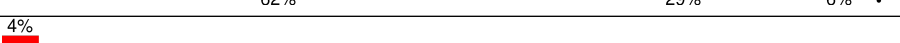
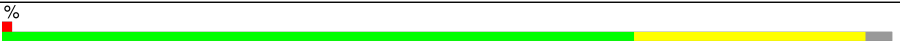
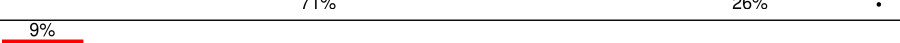
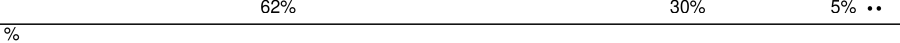
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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

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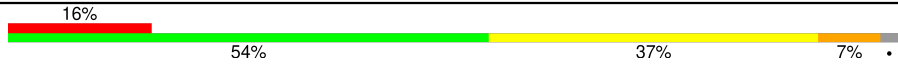
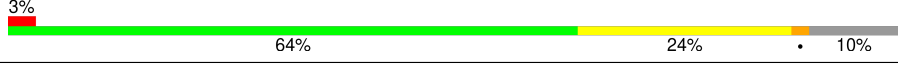
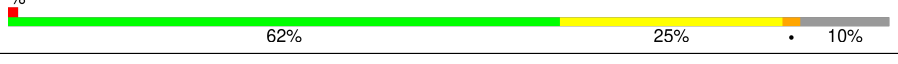
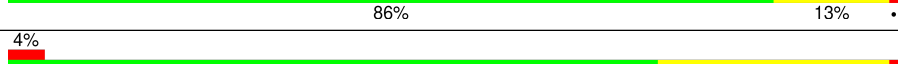
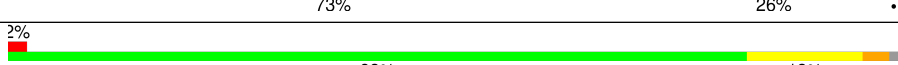
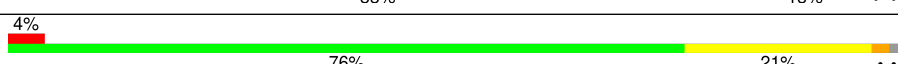
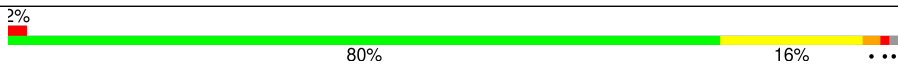
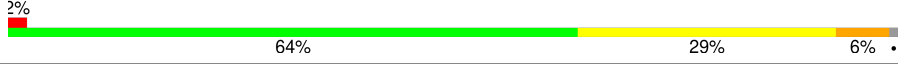
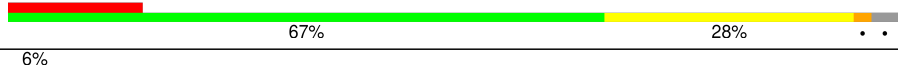
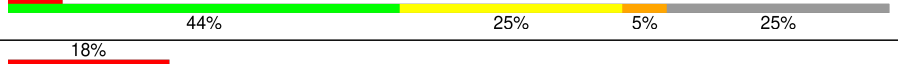
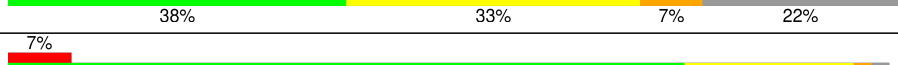
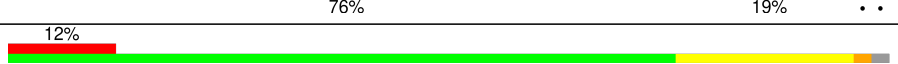
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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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
58	MG	1U	212	-	-	-	X
58	MG	2a	1613	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 298915 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	11	Total	C	N	O	P	0	0	0
			239	108	49	71	11			

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

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 fMAC-tRNA^{cys} 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 fMAC-tRNA^{cys} Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			

- Molecule 57 is a RNA chain called E-site Deacylated tRNA^{Lys}.

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	1096	Total	Mg	0	0
			1096	1096		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	35	Total 35	Mg 35	0	0
58	1D	11	Total 11	Mg 11	0	0
58	1E	13	Total 13	Mg 13	0	0
58	1F	12	Total 12	Mg 12	0	0
58	1G	4	Total 4	Mg 4	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	8	Total 8	Mg 8	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	6	Total 6	Mg 6	0	0
58	1S	2	Total 2	Mg 2	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	12	Total 12	Mg 12	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	4	Total 4	Mg 4	0	0
58	1Z	2	Total 2	Mg 2	0	0
58	10	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	4	Total 4	Mg 4	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	3	Total 3	Mg 3	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	4	Total 4	Mg 4	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	213	Total 213	Mg 213	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	2	Total 2	Mg 2	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1k	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1p	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1w	7	Total 7	Mg 7	0	0
58	1x	11	Total 11	Mg 11	0	0
58	2A	687	Total 687	Mg 687	0	0
58	2B	15	Total 15	Mg 15	0	0
58	2D	6	Total 6	Mg 6	0	0
58	2E	7	Total 7	Mg 7	0	0
58	2F	4	Total 4	Mg 4	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	1	Total 1	Mg 1	0	0
58	2P	1	Total 1	Mg 1	0	0
58	2Q	2	Total 2	Mg 2	0	0
58	2R	3	Total 3	Mg 3	0	0
58	2T	2	Total 2	Mg 2	0	0
58	2V	1	Total 1	Mg 1	0	0
58	2X	2	Total 2	Mg 2	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	3	Total 3	Mg 3	0	0
58	23	3	Total 3	Mg 3	0	0
58	25	4	Total 4	Mg 4	0	0
58	27	2	Total 2	Mg 2	0	0
58	28	1	Total 1	Mg 1	0	0

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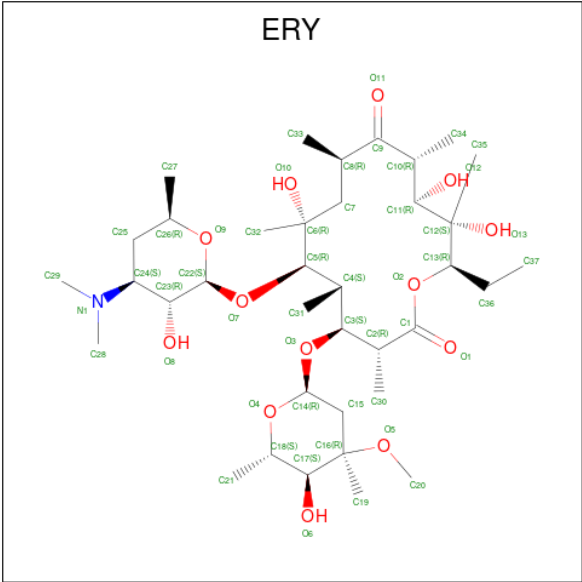
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2a	222	Total 222	Mg 222	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2l	6	Total 6	Mg 6	0	0
58	2q	2	Total 2	Mg 2	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	1	Total 1	Mg 1	0	0
58	2v	2	Total 2	Mg 2	0	0
58	2w	1	Total 1	Mg 1	0	0
58	2x	5	Total 5	Mg 5	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
59	2x	1	Total 1	K 1	0	0

- Molecule 60 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃) (labeled as "Ligand of Interest" by depositor).



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

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

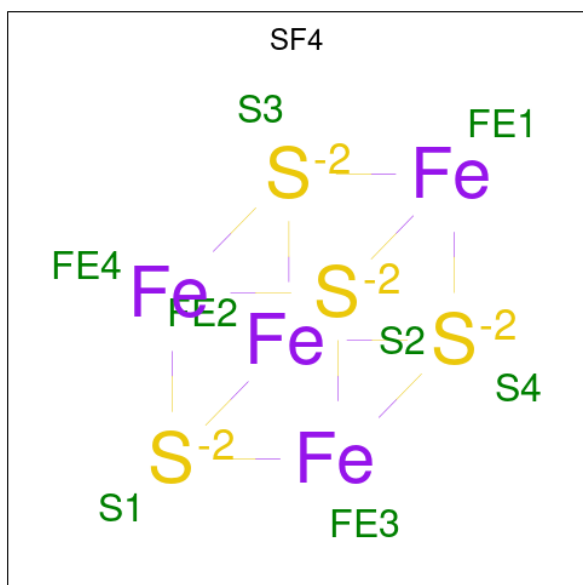
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Y	1	Total	Zn	0	0
			1	1		
61	14	1	Total	Zn	0	0
			1	1		
61	15	1	Total	Zn	0	0
			1	1		
61	16	1	Total	Zn	0	0
			1	1		
61	19	1	Total	Zn	0	0
			1	1		
61	1n	1	Total	Zn	0	0
			1	1		
61	2Y	1	Total	Zn	0	0
			1	1		
61	24	1	Total	Zn	0	0
			1	1		
61	25	1	Total	Zn	0	0
			1	1		
61	26	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	1715	Total	O	0	0
			1715	1715		
63	1B	53	Total	O	0	0
			53	53		
63	1D	28	Total	O	0	0
			28	28		
63	1E	25	Total	O	0	0
			25	25		
63	1F	13	Total	O	0	0
			13	13		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1G	3	Total 3	O 3	0	0
63	1H	2	Total 2	O 2	0	0
63	1N	3	Total 3	O 3	0	0
63	1O	4	Total 4	O 4	0	0
63	1P	17	Total 17	O 17	0	0
63	1Q	6	Total 6	O 6	0	0
63	1R	12	Total 12	O 12	0	0
63	1S	5	Total 5	O 5	0	0
63	1T	5	Total 5	O 5	0	0
63	1U	9	Total 9	O 9	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	8	Total 8	O 8	0	0
63	1X	7	Total 7	O 7	0	0
63	1Y	2	Total 2	O 2	0	0
63	1Z	1	Total 1	O 1	0	0
63	10	9	Total 9	O 9	0	0
63	11	8	Total 8	O 8	0	0
63	12	3	Total 3	O 3	0	0
63	13	4	Total 4	O 4	0	0
63	15	6	Total 6	O 6	0	0
63	16	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	17	9	Total 9	O 9	0	0
63	18	9	Total 9	O 9	0	0
63	1a	284	Total 284	O 284	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	5	Total 5	O 5	0	0
63	1m	2	Total 2	O 2	0	0
63	1o	1	Total 1	O 1	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	7	Total 7	O 7	0	0
63	1x	6	Total 6	O 6	0	0
63	1z	1	Total 1	O 1	0	0
63	1y	1	Total 1	O 1	0	0
63	2A	624	Total 624	O 624	0	0
63	2B	12	Total 12	O 12	0	0
63	2D	14	Total 14	O 14	0	0
63	2E	5	Total 5	O 5	0	0
63	2F	9	Total 9	O 9	0	0

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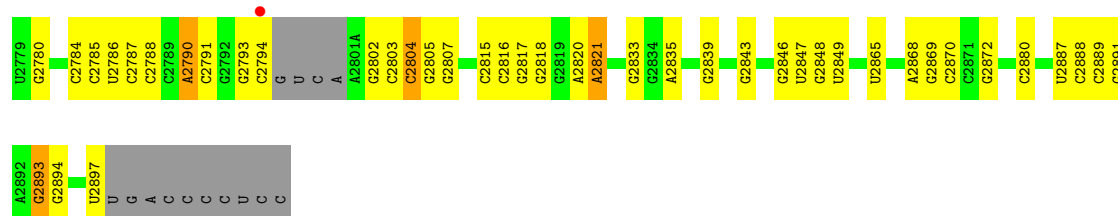
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2N	1	Total 1	O 1	0	0
63	2O	1	Total 1	O 1	0	0
63	2P	3	Total 3	O 3	0	0
63	2Q	1	Total 1	O 1	0	0
63	2R	1	Total 1	O 1	0	0
63	2T	4	Total 4	O 4	0	0
63	2U	1	Total 1	O 1	0	0
63	2W	3	Total 3	O 3	0	0
63	2Y	1	Total 1	O 1	0	0
63	20	1	Total 1	O 1	0	0
63	21	5	Total 5	O 5	0	0
63	26	1	Total 1	O 1	0	0
63	28	2	Total 2	O 2	0	0
63	2a	161	Total 161	O 161	0	0
63	2d	1	Total 1	O 1	0	0
63	2e	2	Total 2	O 2	0	0
63	2j	1	Total 1	O 1	0	0
63	2l	4	Total 4	O 4	0	0
63	2p	2	Total 2	O 2	0	0
63	2v	1	Total 1	O 1	0	0
63	2w	1	Total 1	O 1	0	0

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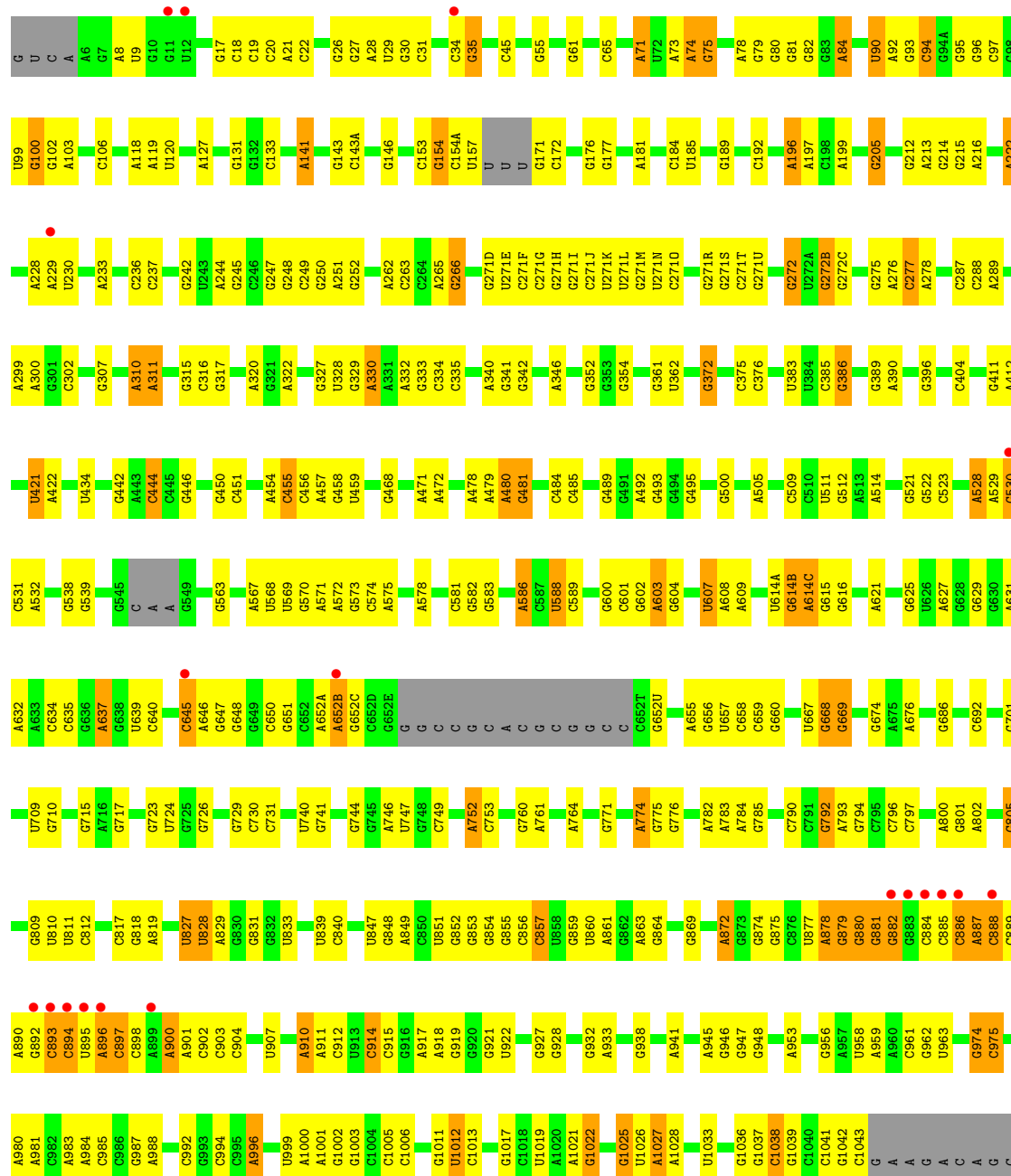
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2x	2	Total	O	0	0
			2	2		

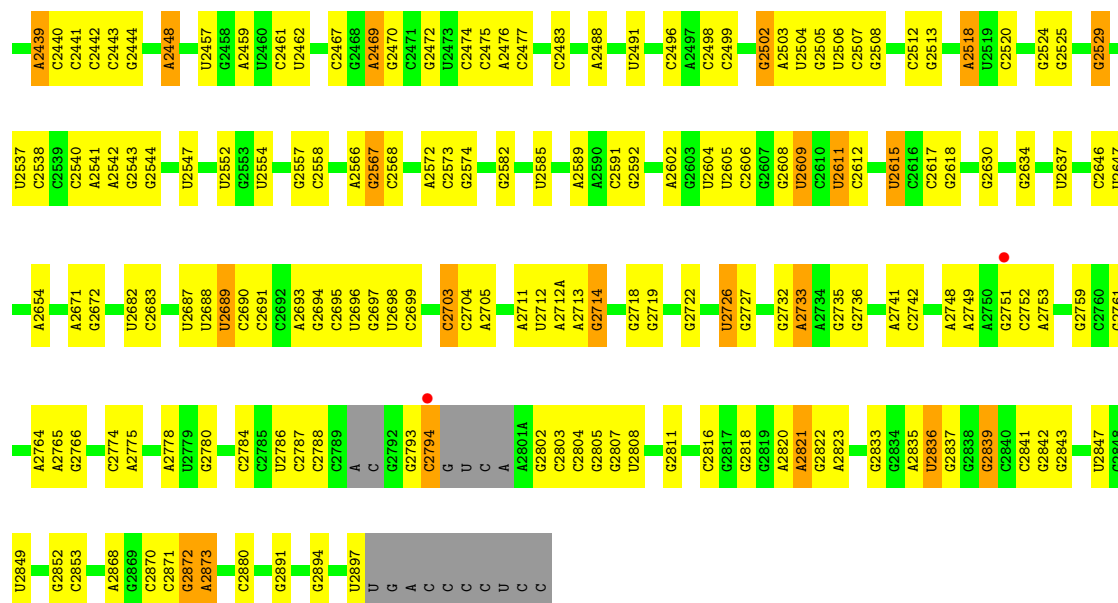
A2654	G2502	G2372	A2266	G2160	G2100	C1967	U1833	G1696	A1558	A1419	U1273	G1138	U1066
C2687	A2503	G2372	A2267	C2161	G2101	G1968	C1943	G1697	A1566	U1420	U1292	G1139	A1067
G2673	U2504	A2376	A2268	C2163	U2102	A1969	G1998	A1698	A1567	G1421	C1293	C1140	G1068
C2680	G2505	A2377	A2269	G2164	G2103	A1970	G1699	G1699	A1568	C1428	U1294	U1141	A1069
C2683	C2512	A2378	A2270	G2165	G2104	A1971	A1847	A1700	A1569	C1429	C1295	A1142A	G1070
U2684	G2513	G2379	A2271	U2167	G2106	A1972	G1858	G1702	U1578	C1430	G1296	A1143	C1072
U2685	A2518	G2383	A2272	G2168	C2107	U1991	U1858	G1703	U1579	U1431	U1300	G1144	A1073
U2686	G2519	G2384	A2273	A2169	U2108	G1992	U1864	G1704	A1580	U1301	G1149	G1074	G1076
U2687	G2520	G2385	A2274	G2170	U2109	U1993	G1865	A1720	G1581	A1301	G1149	G1075	G1077
U2688	G2521	G2386	A2275	A2171	G2110	U1997	G1866	G1721	U1578	A1308	A1156	G1078	U1078
U2689	G2522	G2387	A2276	U2172	G2111	G1997	A1876	A1722	G1584	A1309	G1156	G1079	U1079
C2690	G2523	G2388	A2277	G2173	G2112	G2002	G1877	U1739	A1586	G1448	G1164	G1080	U1081
A2693	G2524	G2389	A2278	A2174	U2113	G2006	G1878	G1740	A1587	C1315	U1165	U1082	U1083
G2694	G2525	G2390	A2279	C2175	A2114	C2006	G1882	A1741	C1588	G1450	G1167	G1168	A1084
G2697	G2526	G2391	A2280	G2176	G2115	G2006	G1883	G1746	C1589	U1453	G1169	A1085	A1086
C2701	G2527	G2392	A2281	U2177	G2116	G2012	G1889	G1756	G1593	G1461	A1342	G1170	A1086
U2702	G2528	G2393	A2282	C2178	A2117	A2013	A1890	A1762	U1602	G1467	G1343	G1173	G1087
C2703	G2529	G2394	A2283	C2179	U2118	A2014	A1891	G1764	A1608	C1467	G1344	A1174	A1088
G2706	G2530	G2395	A2284	U2180	U2119	G2028	G1903	A1773	A1609	G1482	U1352	U1175	G1089
A2711	G2531	G2396	A2285	G2181	G2120	G2029	G1906	U1778	A1610	U1493	A1353	G1176	G1090
U2712	G2532	G2397	A2286	G2182	A2121	A2030	G1907	G1779	A1614	C1494	A1354	A1177	G1091
A2712A	G2533	G2398	A2287	C2183	U2122	G2032	U1911	A1785	A1614	A1494	G1355	C1179	G1092
A2713	G2534	G2399	A2288	G2184	G2123	A2033	U1912	G1781	A1614	A1495	G1356	U1178	U1093
G2714	G2535	G2400	A2289	G2185	G2124	G2037	C1914	G1782	G1633	A1496	A1359	C1181	A1095
G2718	G2536	G2401	A2290	G2186	A2125	G2038	U1915	A1783	U1606	C1506	A1360	G1187	A1096
A2721	G2537	G2402	A2291	G2187	G2126	A2039	U1916	A1784	A1507	A1507	A1361	U1188	U1097
U2726	G2538	G2403	A2292	U2188	A2127	G2040	U1917	A1785	C1636	C1509	A1362	C1201	A1098
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A2733	G2540	G2405	A2294	G2190	G2129	G2042	A1919	A1786	A1641	U1512	U1372	A1220	U1101
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A2750	G2544	G2409	A2298	G2194	G2133	G2046	U1931	U1796	A1655	G1519	A1384	U1108	U1106
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C2763	G2550	G2415	A2304	G2200	C2139	G2053	C1942	A1803	U1671	U1538	U1406	C1258	G1113
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	G2615	G2480	A2369	G2265	G2204</								



• Molecule 1: 23S Ribosomal RNA

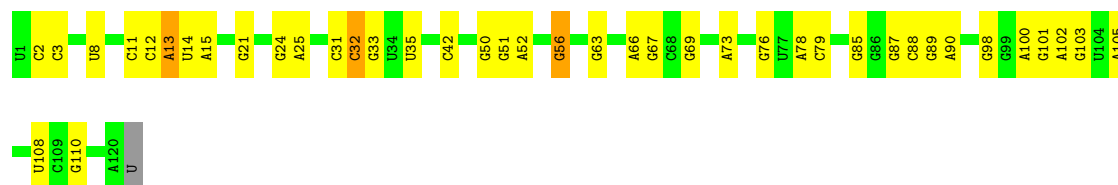






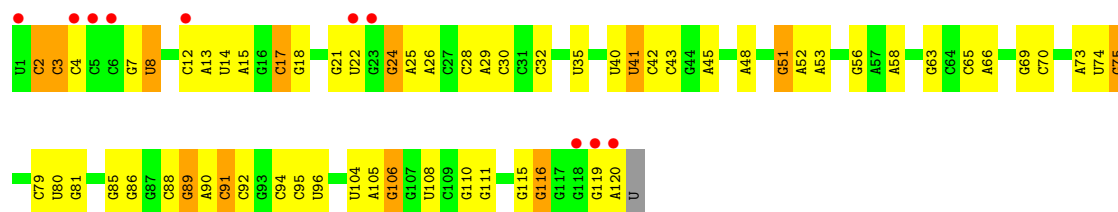
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 65% 31% ..



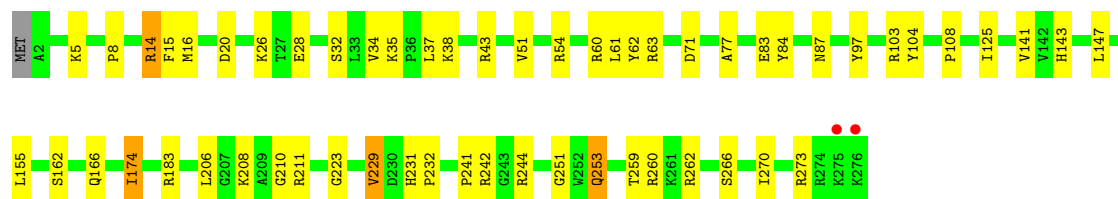
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 8% 47% 42% 10% .

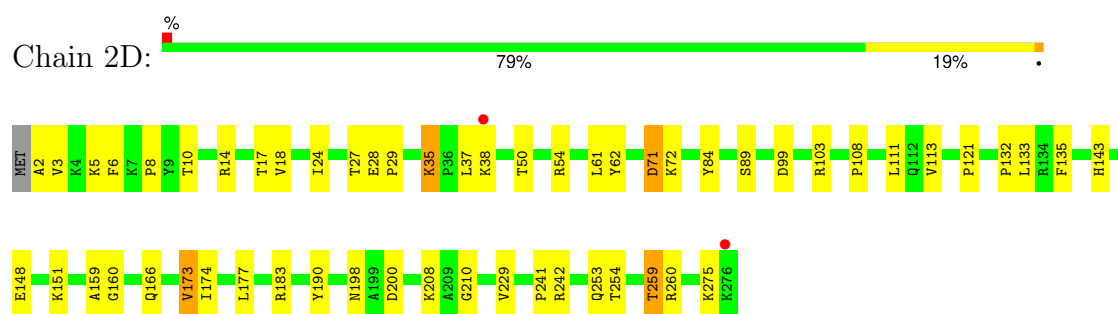


- Molecule 3: 50S ribosomal protein L2

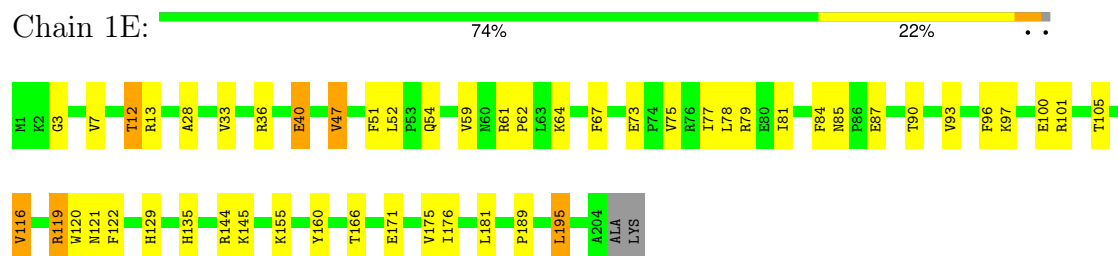
Chain 1D: 79% 19% .



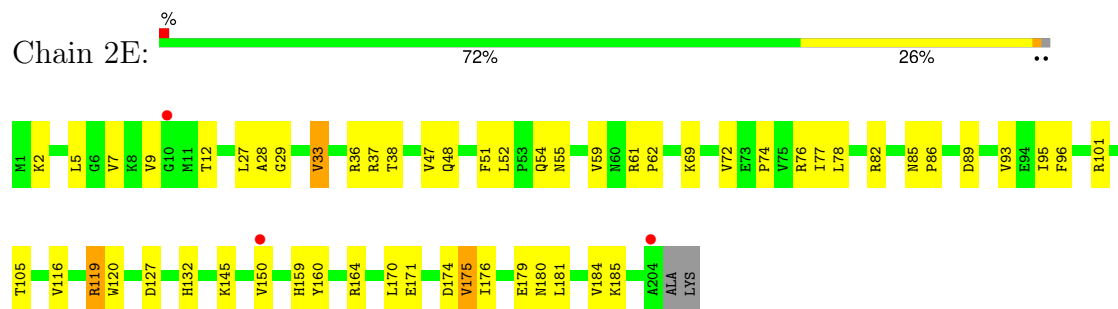
- Molecule 3: 50S ribosomal protein L2



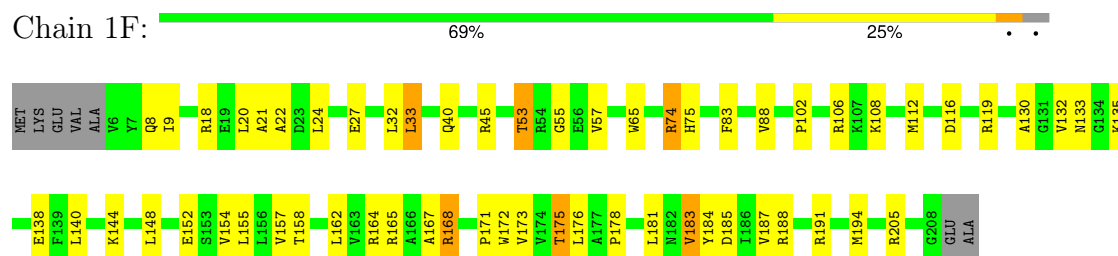
- Molecule 4: 50S ribosomal protein L3



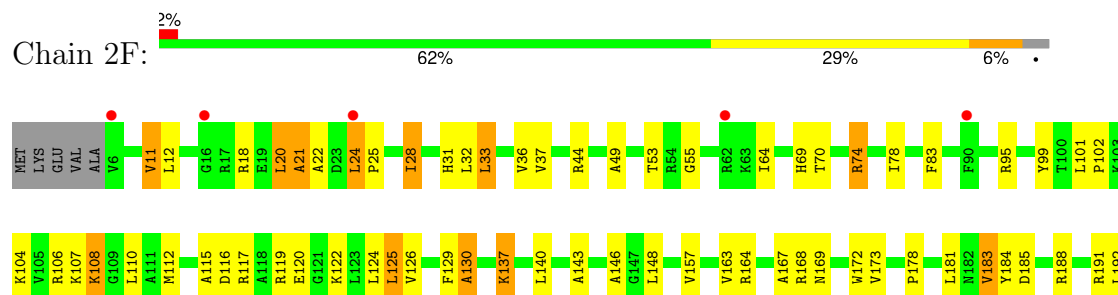
- Molecule 4: 50S ribosomal protein L3

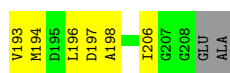


- Molecule 5: 50S ribosomal protein L4

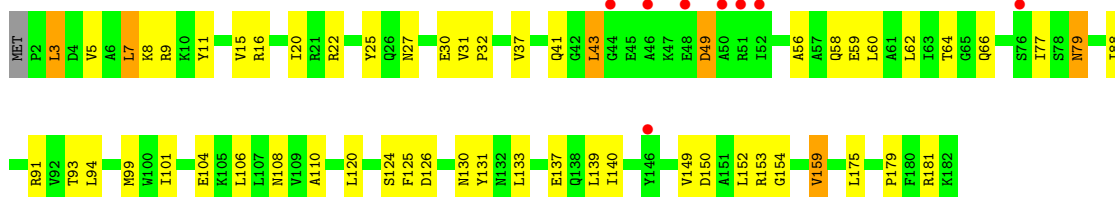


- Molecule 5: 50S ribosomal protein L4

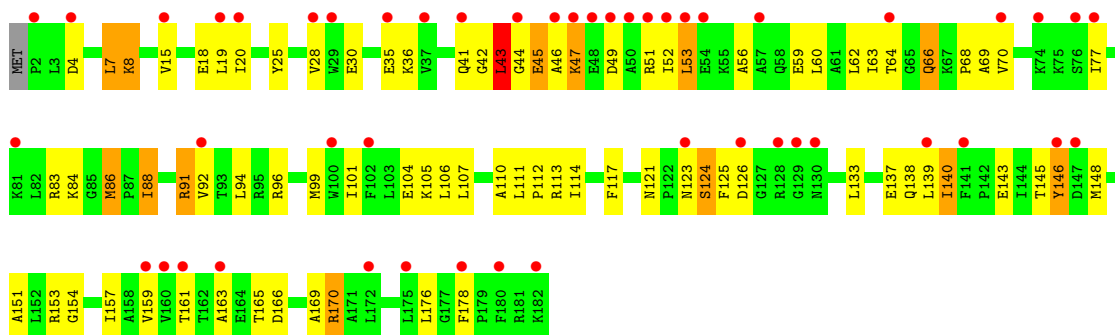




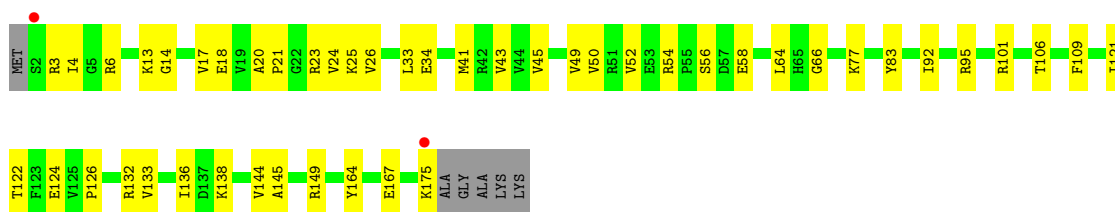
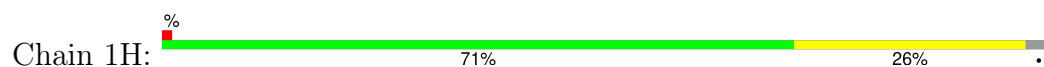
- Molecule 6: 50S ribosomal protein L5



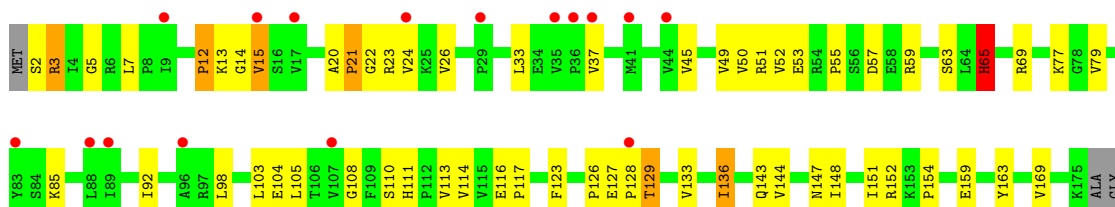
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



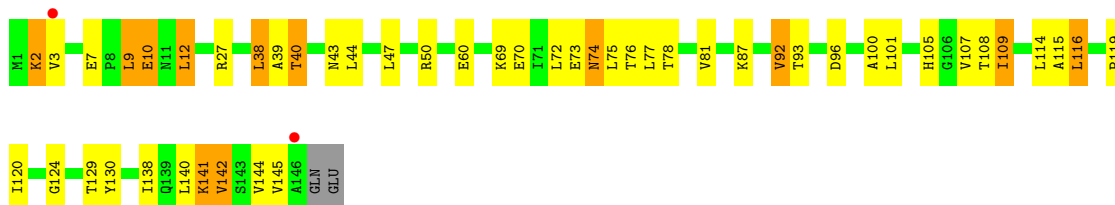
- Molecule 7: 50S ribosomal protein L6



ALA
LYS
LYS

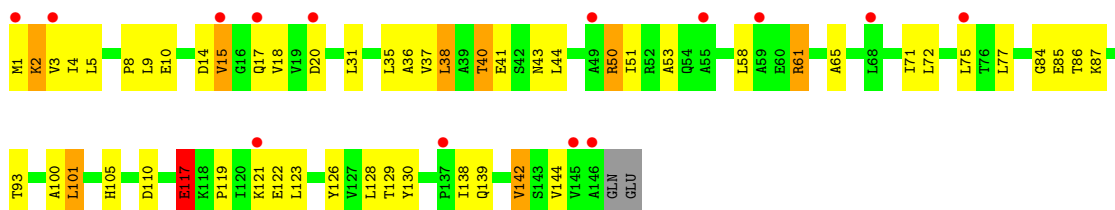
• Molecule 8: 50S ribosomal protein L9

Chain 1I:  66% 25% 8% .



• Molecule 8: 50S ribosomal protein L9

Chain 2I:  9% 62% 30% 5% ..



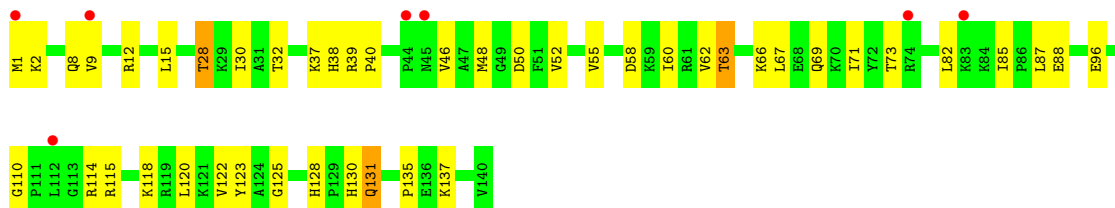
• Molecule 9: 50S ribosomal protein L13

Chain 1N:  79% 19% .



• Molecule 9: 50S ribosomal protein L13

Chain 2N:  5% 68% 30% .

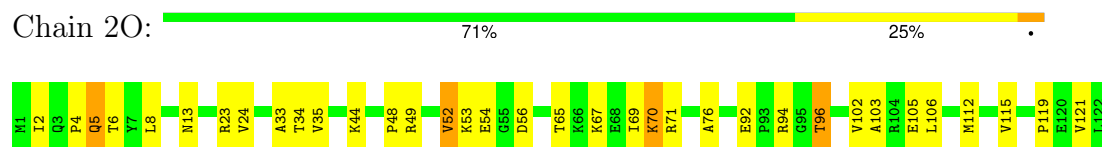


• Molecule 10: 50S ribosomal protein L14

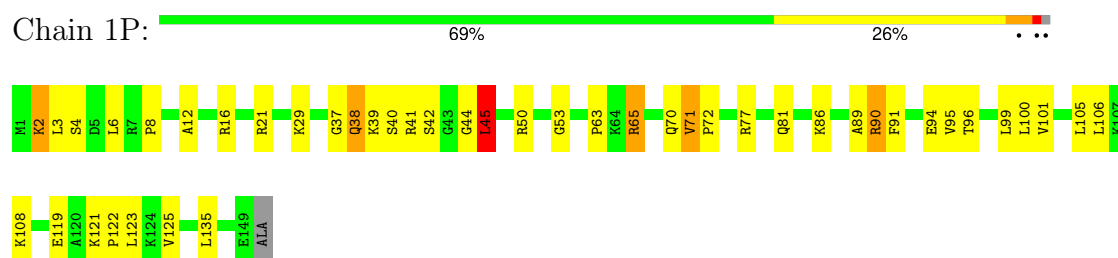
Chain 1O:  2% 80% 19% .



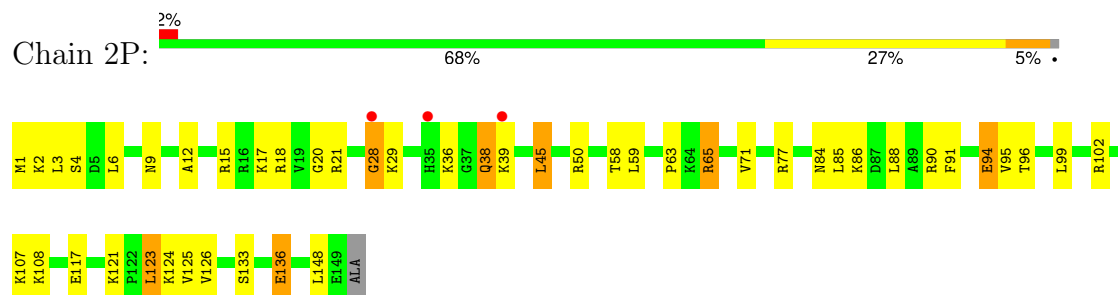
- Molecule 10: 50S ribosomal protein L14



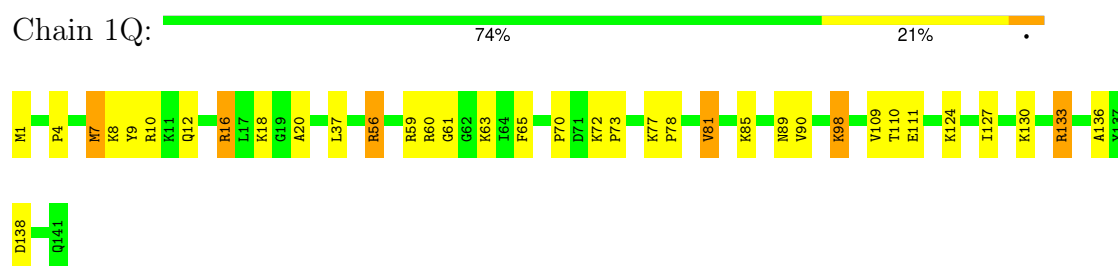
- Molecule 11: 50S ribosomal protein L15



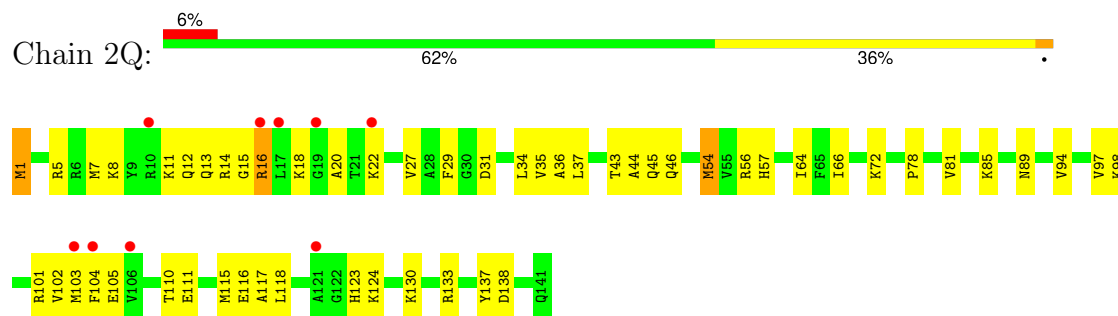
- Molecule 11: 50S ribosomal protein L15



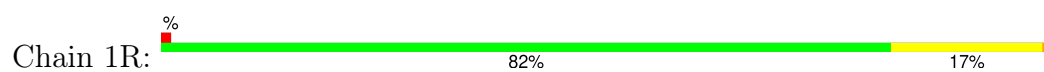
- Molecule 12: 50S ribosomal protein L16



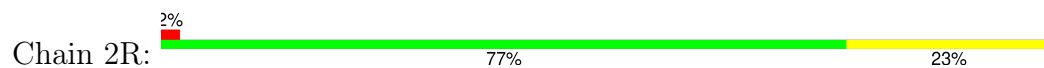
- Molecule 12: 50S ribosomal protein L16



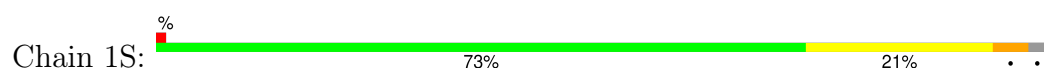
- Molecule 13: 50S ribosomal protein L17



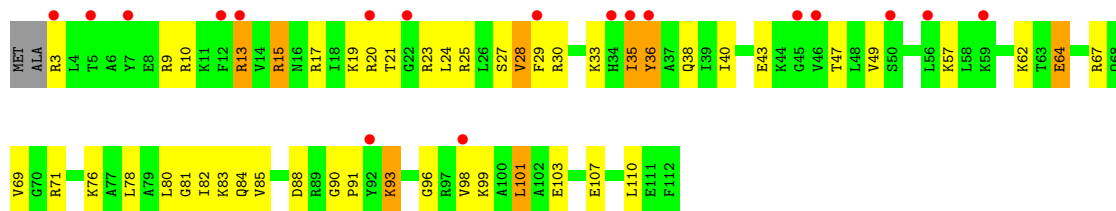
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

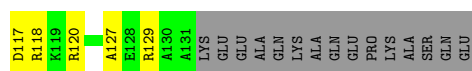


- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19





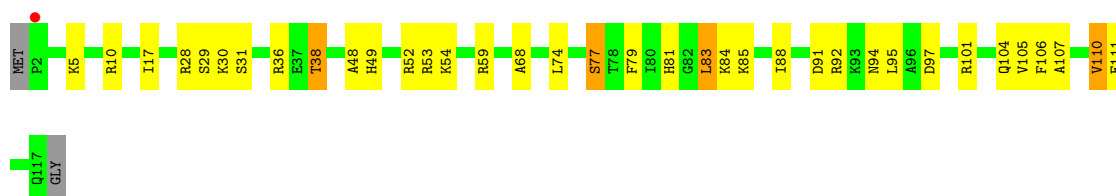
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 81% 16% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U: 68% 27% ..



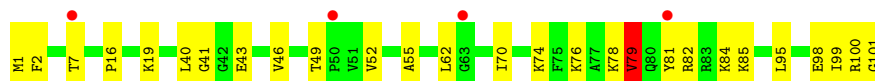
- Molecule 17: 50S ribosomal protein L21

Chain 1V: 86% 13% ..



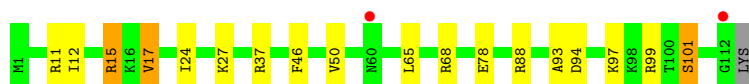
- Molecule 17: 50S ribosomal protein L21

Chain 2V: 73% 26% ..



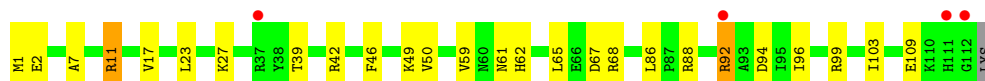
- Molecule 18: 50S ribosomal protein L22

Chain 1W: 83% 13% ..

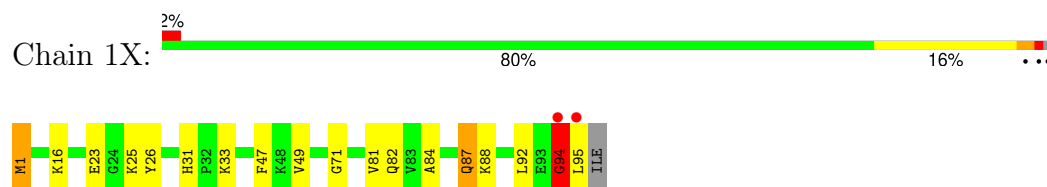


- Molecule 18: 50S ribosomal protein L22

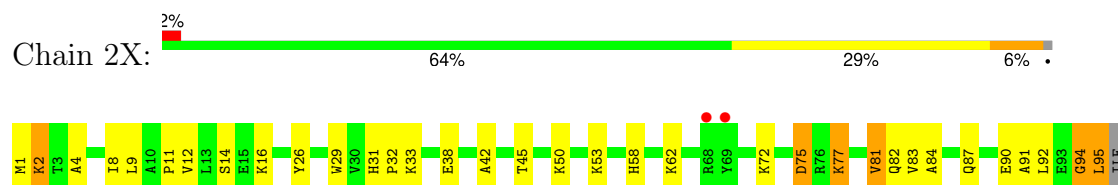
Chain 2W: 76% 21% ..



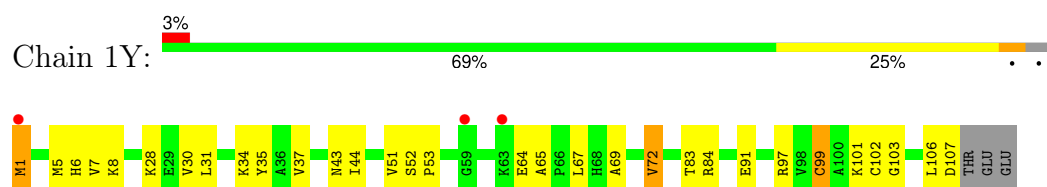
- Molecule 19: 50S ribosomal protein L23



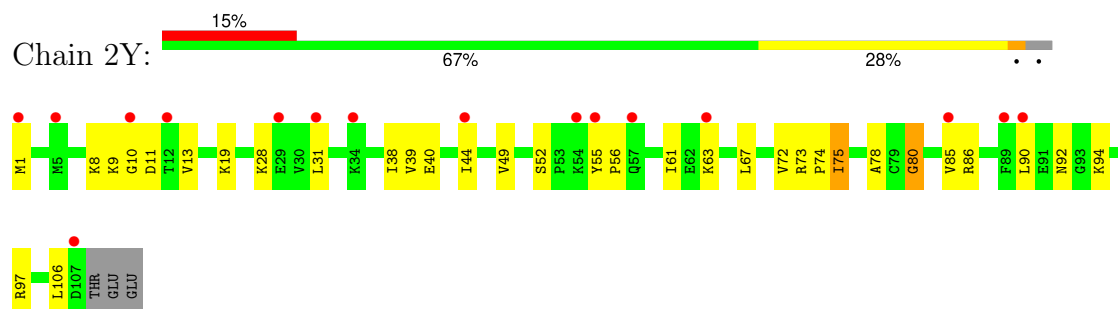
- Molecule 19: 50S ribosomal protein L23



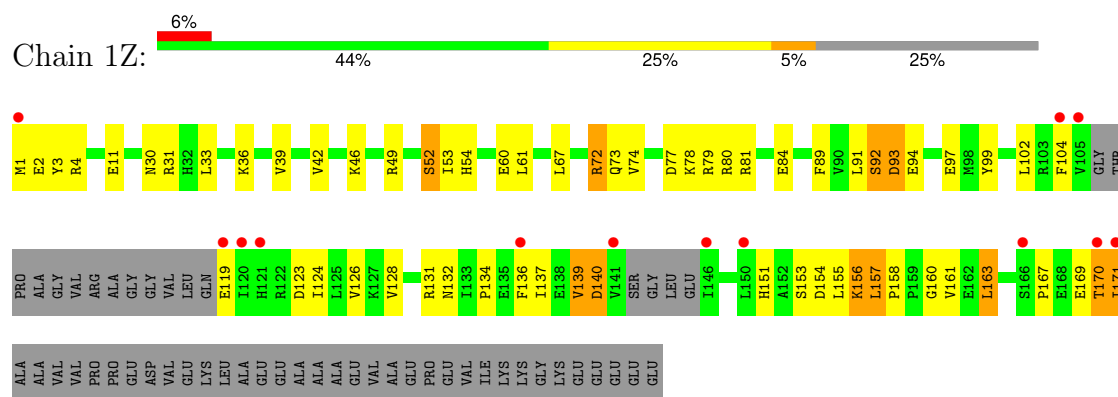
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

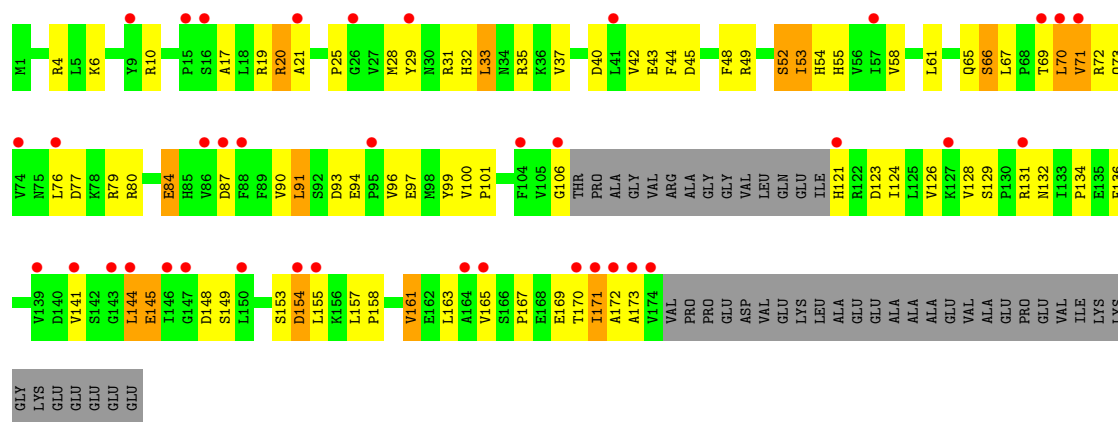


- Molecule 21: 50S ribosomal protein L25

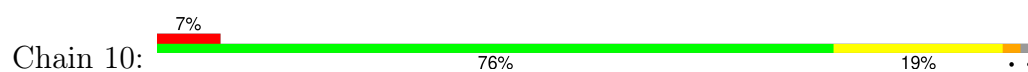


- Molecule 21: 50S ribosomal protein L25

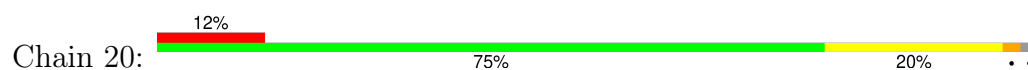




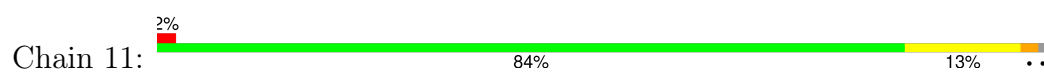
- Molecule 22: 50S ribosomal protein L27



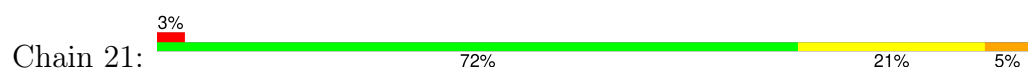
- Molecule 22: 50S ribosomal protein L27



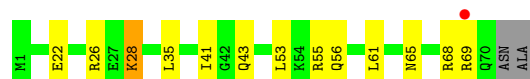
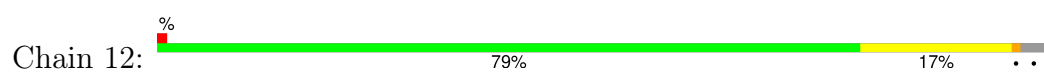
- Molecule 23: 50S ribosomal protein L28



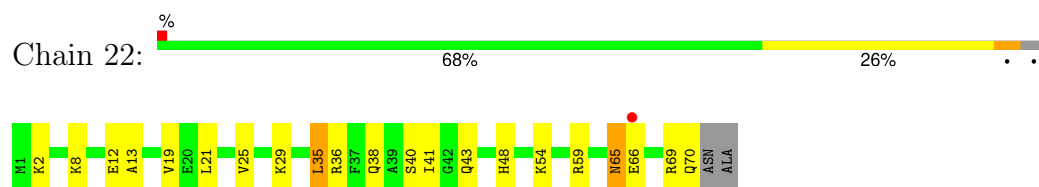
- Molecule 23: 50S ribosomal protein L28



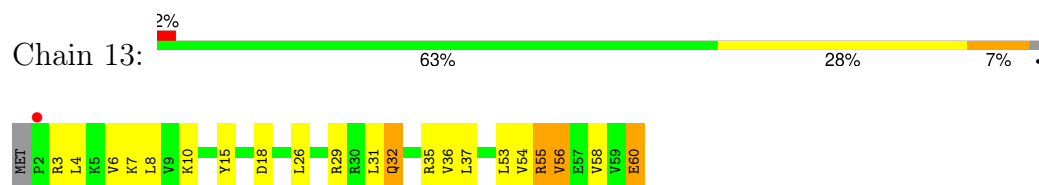
- Molecule 24: 50S ribosomal protein L29



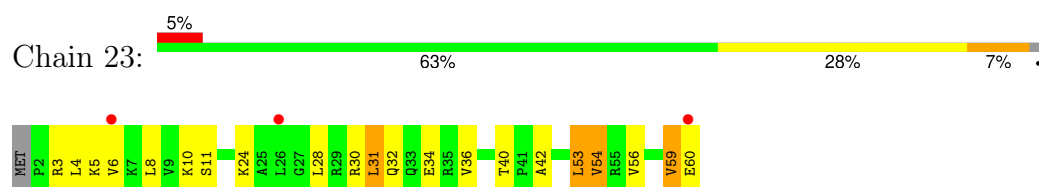
- Molecule 24: 50S ribosomal protein L29



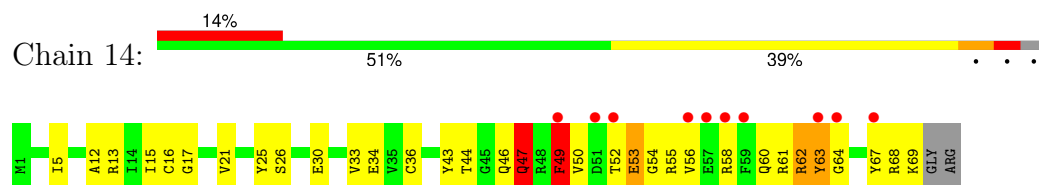
- Molecule 25: 50S ribosomal protein L30



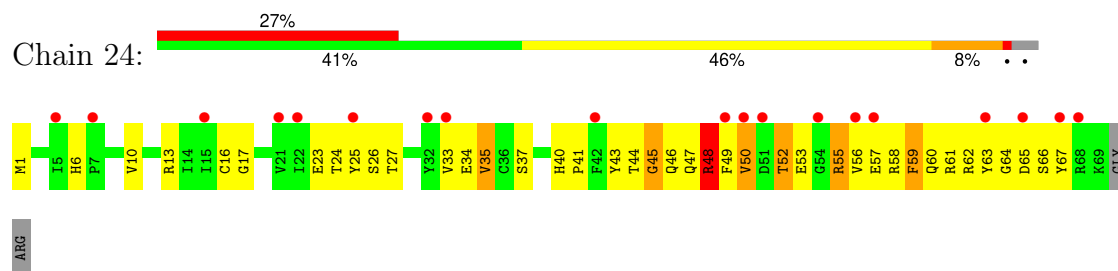
- Molecule 25: 50S ribosomal protein L30



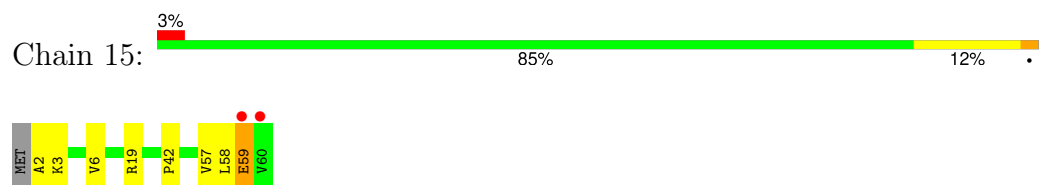
- Molecule 26: 50S ribosomal protein L31



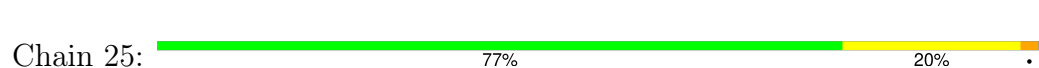
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

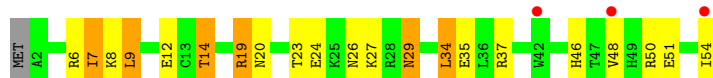




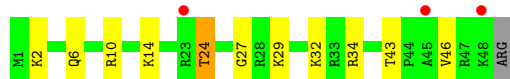
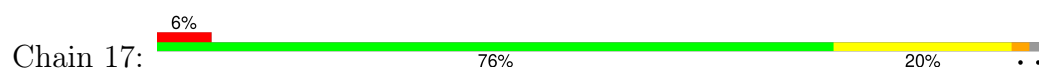
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



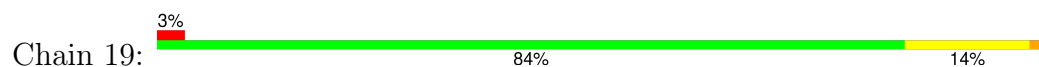
- Molecule 30: 50S ribosomal protein L35



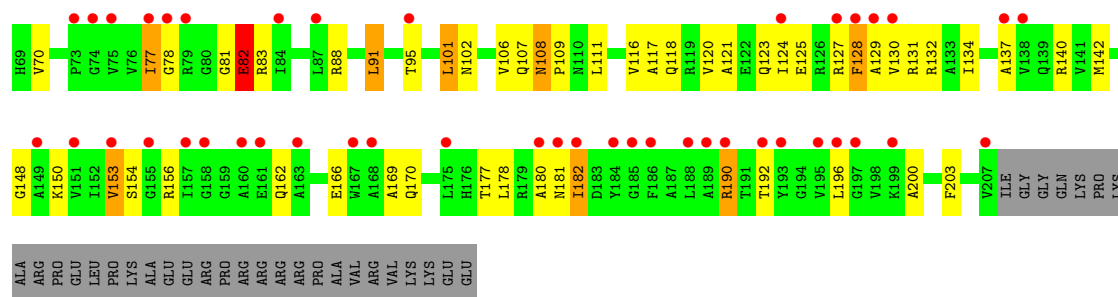
- Molecule 30: 50S ribosomal protein L35



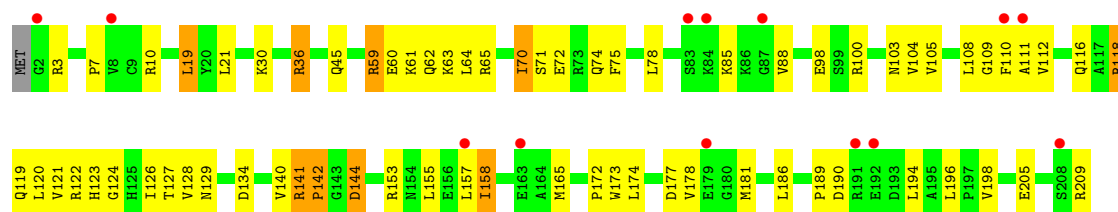
- Molecule 31: 50S ribosomal protein L36



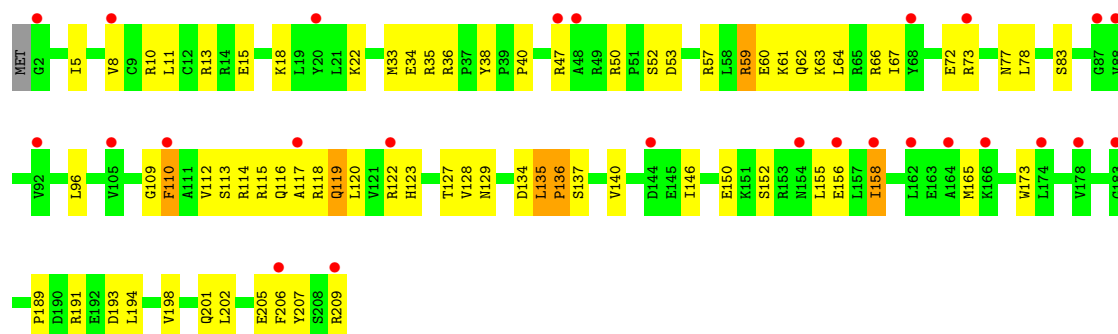




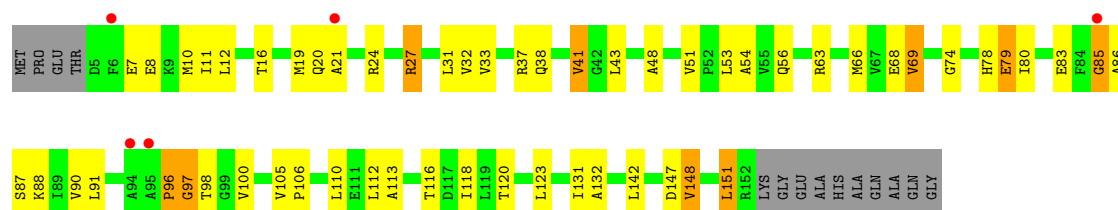
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

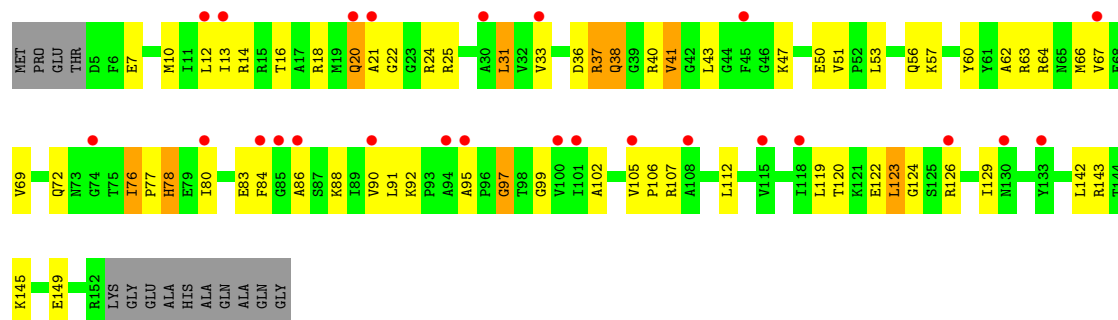


• Molecule 36: 30S ribosomal protein S5

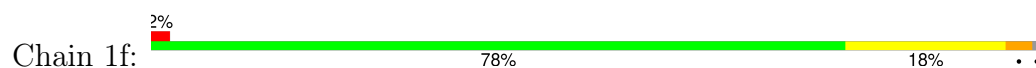


• Molecule 36: 30S ribosomal protein S5

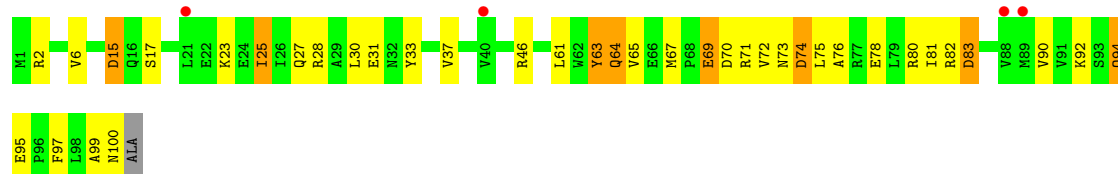




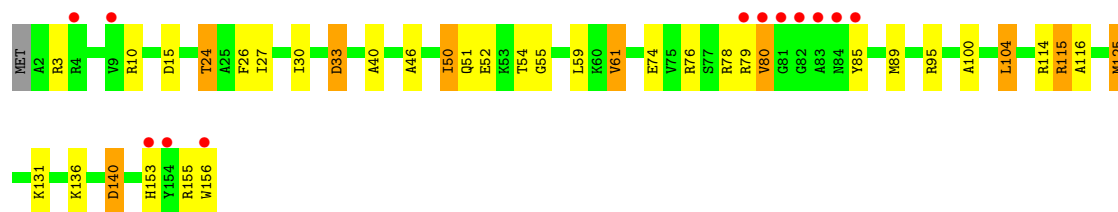
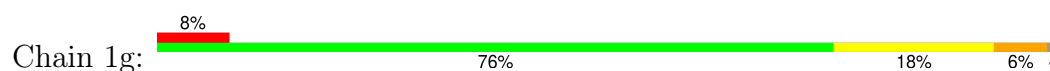
- Molecule 37: 30S ribosomal protein S6



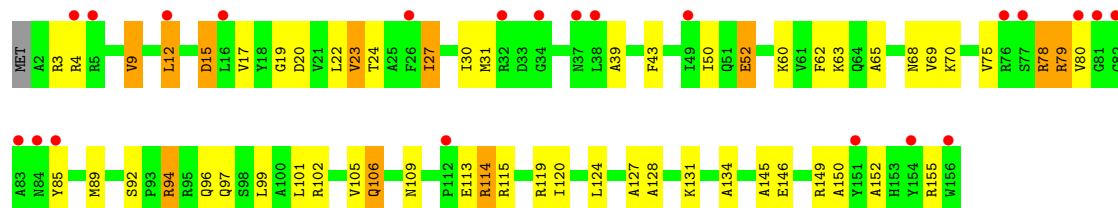
- Molecule 37: 30S ribosomal protein S6



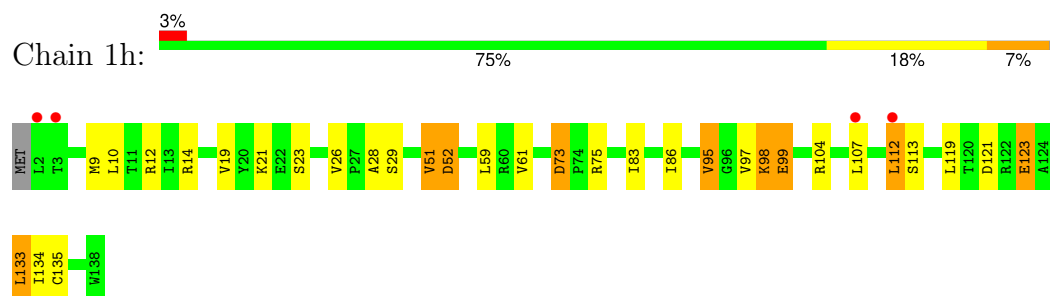
- Molecule 38: 30S ribosomal protein S7



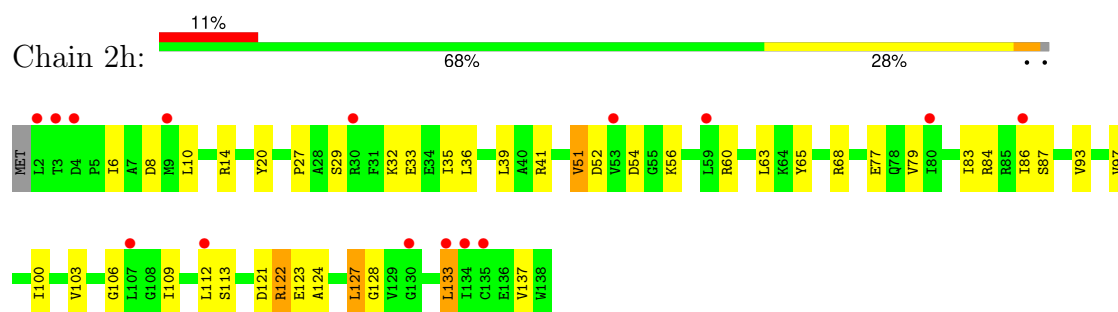
- Molecule 38: 30S ribosomal protein S7



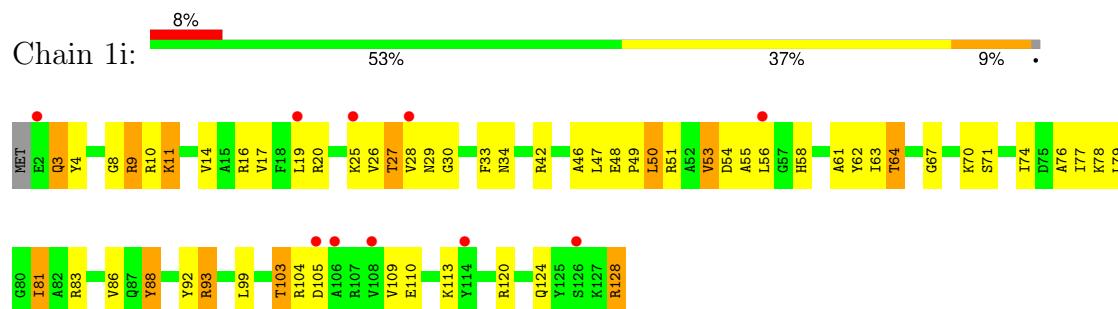
- Molecule 39: 30S ribosomal protein S8



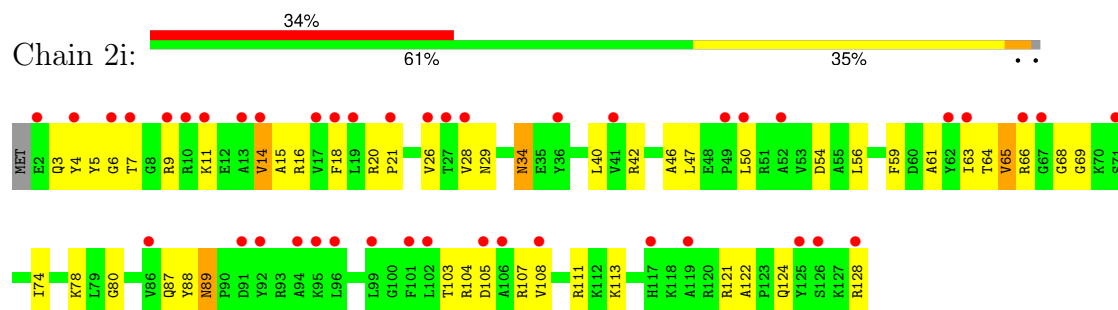
- Molecule 39: 30S ribosomal protein S8



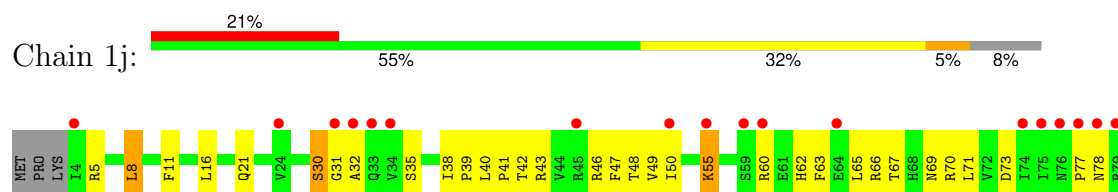
- Molecule 40: 30S ribosomal protein S9

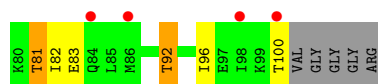


- Molecule 40: 30S ribosomal protein S9

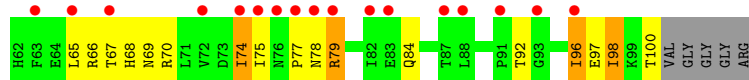
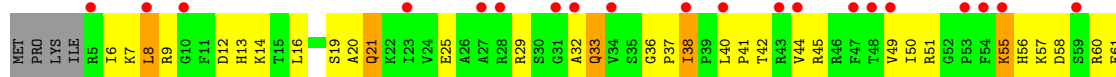
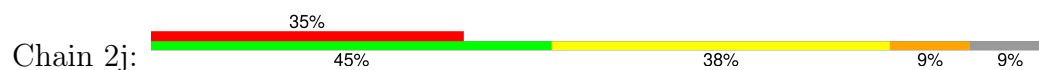


- Molecule 41: 30S ribosomal protein S10





• Molecule 41: 30S ribosomal protein S10



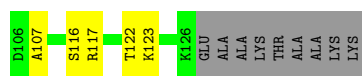
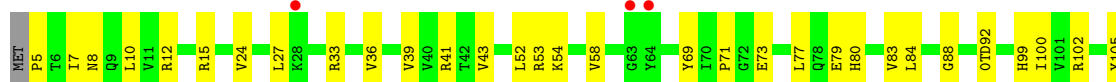
• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11

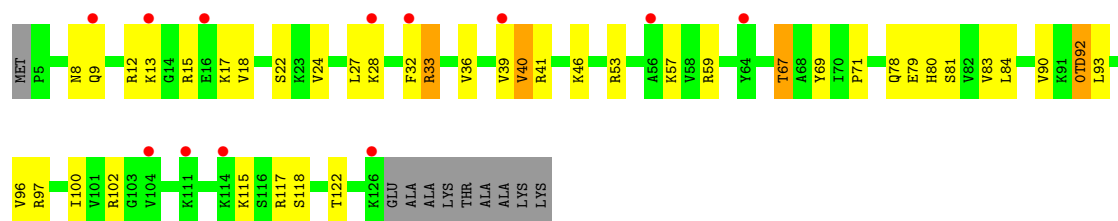


• Molecule 43: 30S ribosomal protein S12

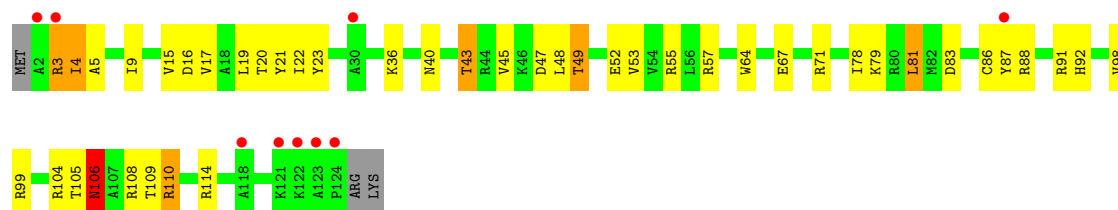


• Molecule 43: 30S ribosomal protein S12

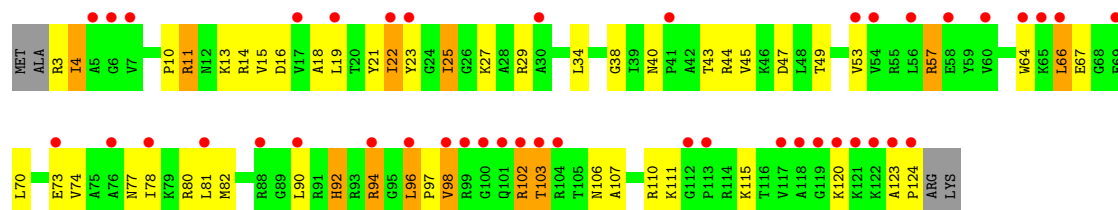




• Molecule 44: 30S ribosomal protein S13



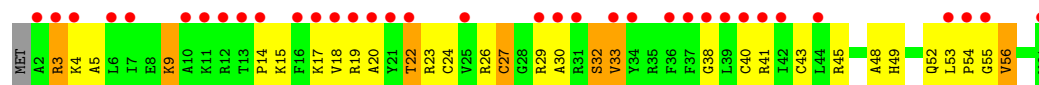
• Molecule 44: 30S ribosomal protein S13



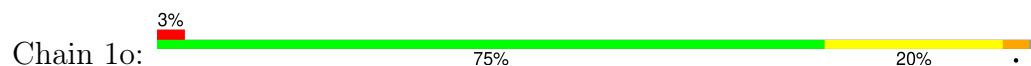
• Molecule 45: 30S ribosomal protein S14 type Z



• Molecule 45: 30S ribosomal protein S14 type Z

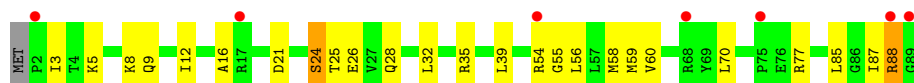


• Molecule 46: 30S ribosomal protein S15





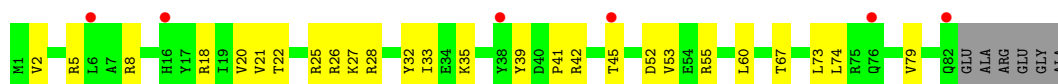
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



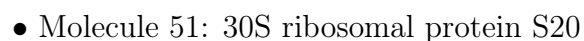
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18





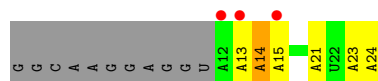
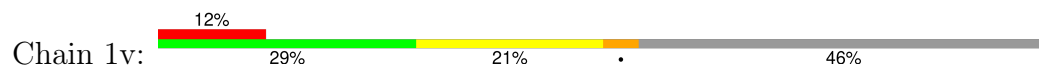
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



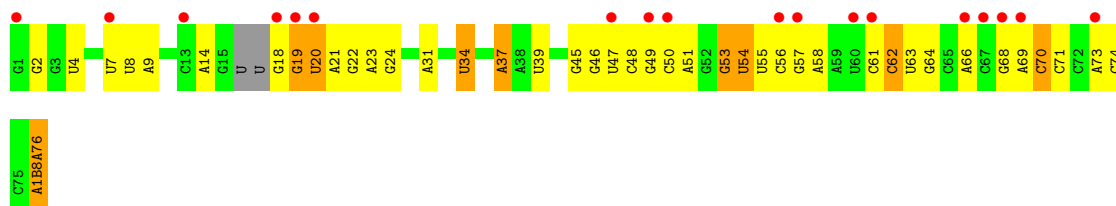
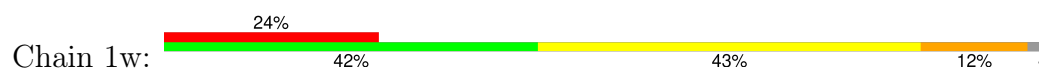
- Molecule 53: MET-LYS-mRNA



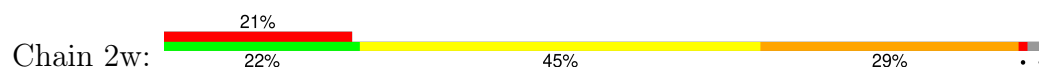
- Molecule 53: MET-LYS-mRNA

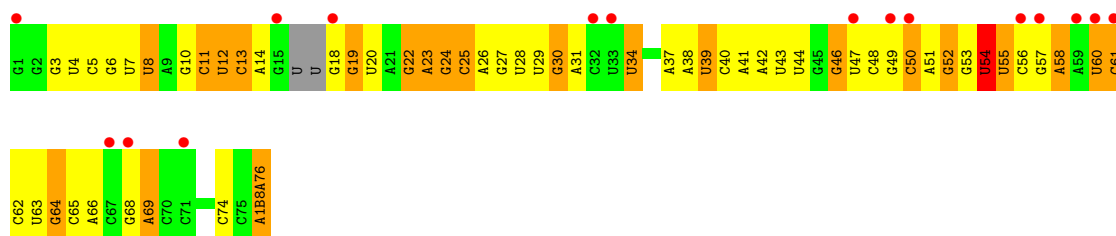


- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys

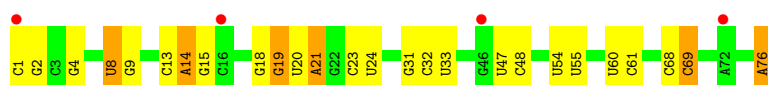


- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys





• Molecule 55: P-site Peptidyl-tRNA fMAC-tRNAcys RNA-part



• Molecule 55: P-site Peptidyl-tRNA fMAC-tRNAcys RNA-part



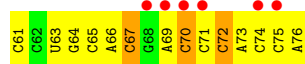
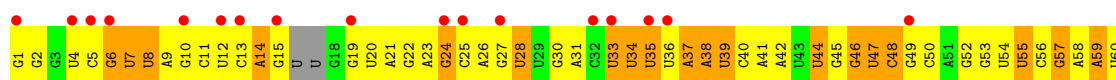
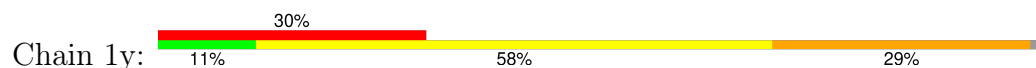
• Molecule 56: P-site Peptidyl-tRNA fMAC-tRNAcys Peptide-part



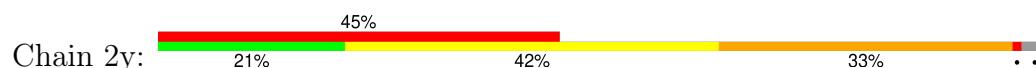
• Molecule 56: P-site Peptidyl-tRNA fMAC-tRNAcys Peptide-part

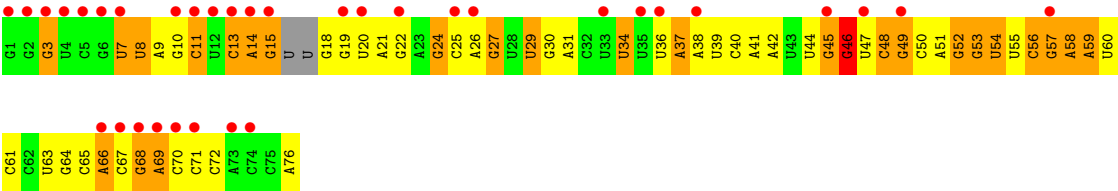


• Molecule 57: E-site Deacylated tRNAlys



• 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	209.69Å 447.93Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.21 – 2.70 152.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (152.21-2.70) 99.5 (152.21-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.217 , 0.262 0.219 , 0.262	Depositor DCC
R_{free} test set	79068 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	298915	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, A1B8A, 5MU, 4OC, MA6, 5MC, OMC, UR3, ERY, 0TD, U8U, ZN, 2MA, 8AN, 2MG, 4SU, G7M, FME, OMU, M2G, SF4, MG, T6A, K, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.27	1/69011 (0.0%)	0.44	2/107720 (0.0%)
1	2A	0.21	0/67295	0.39	1/105042 (0.0%)
2	1B	0.20	0/2882	0.38	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.47	0/2944
4	1E	0.25	0/1592	0.48	0/2149
4	2E	0.20	0/1592	0.44	0/2149
5	1F	0.24	0/1619	0.49	0/2193
5	2F	0.22	0/1615	0.47	2/2188 (0.1%)
6	1G	0.20	0/1448	0.44	0/1957
6	2G	0.20	0/1453	0.44	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.20	0/1356	0.40	0/1834
8	1I	0.19	0/1112	0.40	0/1514
8	2I	0.17	0/1079	0.39	0/1475
9	1N	0.23	0/1144	0.44	0/1543
9	2N	0.18	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.19	0/943	0.46	0/1269
11	1P	0.26	0/1152	0.52	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.26	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.48	0/1312
13	2R	0.19	0/982	0.44	0/1312
14	1S	0.22	0/883	0.46	0/1176
14	2S	0.22	0/880	0.52	0/1172
15	1T	0.23	0/1105	0.45	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.25	0/977	0.42	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.26	0/897	0.43	0/1205
18	2W	0.20	0/897	0.39	0/1205
19	1X	0.27	0/764	0.55	2/1025 (0.2%)
19	2X	0.22	0/764	0.57	2/1025 (0.2%)
20	1Y	0.22	0/819	0.45	0/1095
20	2Y	0.19	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.48	0/1717
21	2Z	0.22	0/1299	0.46	0/1763
22	10	0.24	0/662	0.45	0/881
22	20	0.20	0/662	0.44	0/881
23	11	0.26	0/762	0.45	0/1014
23	21	0.21	0/762	0.39	0/1014
24	12	0.26	0/590	0.47	0/781
24	22	0.18	0/590	0.36	0/781
25	13	0.24	0/474	0.44	0/635
25	23	0.17	0/469	0.39	0/630
26	14	0.26	0/565	0.65	0/761
26	24	0.23	0/545	0.53	0/737
27	15	0.25	0/469	0.44	0/635
27	25	0.21	0/469	0.44	0/635
28	16	0.26	0/460	0.43	0/613
28	26	0.22	0/456	0.46	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.27	0/525	0.50	0/691
30	28	0.20	0/525	0.42	0/691
31	19	0.24	0/310	0.57	0/407
31	29	0.19	0/310	0.41	0/407
32	1a	0.20	1/35795 (0.0%)	0.37	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.21	0/1881	0.46	0/2542
33	2b	0.24	0/1860	0.55	0/2518
34	1c	0.19	0/1572	0.40	0/2126
34	2c	0.23	0/1566	0.48	0/2119
35	1d	0.19	0/1685	0.42	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.24	0/1149	0.51	0/1548
37	1f	0.19	0/823	0.40	0/1115
37	2f	0.19	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.40	0/1679
38	2g	0.23	0/1254	0.44	0/1683
39	1h	0.18	0/1108	0.40	0/1494
39	2h	0.21	0/1108	0.50	1/1494 (0.1%)
40	1i	0.19	0/1002	0.50	1/1346 (0.1%)
40	2i	0.26	0/997	0.55	0/1343
41	1j	0.20	0/722	0.51	1/982 (0.1%)
41	2j	0.33	1/727 (0.1%)	0.47	0/988
42	1k	0.20	0/844	0.41	0/1145
42	2k	0.22	0/848	0.41	0/1149
43	1l	0.20	0/937	0.41	0/1260
43	2l	0.21	0/937	0.42	0/1260
44	1m	0.21	0/969	0.56	1/1302 (0.1%)
44	2m	0.22	0/961	0.48	1/1291 (0.1%)
45	1n	0.20	0/501	0.46	0/664
45	2n	0.20	0/501	0.47	0/664
46	1o	0.19	0/739	0.40	0/985
46	2o	0.16	0/739	0.39	0/985
47	1p	0.19	0/697	0.49	0/939
47	2p	0.18	0/693	0.47	0/935
48	1q	0.20	0/836	0.46	0/1117
48	2q	0.18	0/836	0.44	0/1117
49	1r	0.20	0/560	0.40	0/746
49	2r	0.17	0/560	0.41	0/746
50	1s	0.19	0/667	0.47	0/900
50	2s	0.26	0/661	0.62	0/893
51	1t	0.20	0/730	0.49	0/965
51	2t	0.21	0/729	0.46	0/965
52	1u	0.17	0/203	0.43	0/266
52	2u	0.22	0/203	0.49	0/266
53	1v	0.22	0/319	0.35	0/495
53	2v	0.20	0/269	0.35	0/417
54	1w	0.31	1/1593 (0.1%)	0.41	0/2474
54	2w	0.35	2/1593 (0.1%)	0.50	0/2474
55	1x	0.26	0/1723	0.40	0/2684
55	2x	0.24	0/1723	0.40	0/2684
56	1z	0.34	0/10	0.32	0/12
56	2z	0.13	0/10	0.27	0/12
57	1y	0.31	0/1618	0.44	0/2513
57	2y	0.32	2/1618 (0.1%)	0.45	0/2513
All	All	0.22	8/316745 (0.0%)	0.42	17/474198 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2j	79	ARG	CA-C	6.00	1.60	1.52
54	2w	46	G7M	O3'-P	5.49	1.61	1.56
57	2y	37	T6A	O3'-P	5.38	1.61	1.56
57	2y	46	G7M	O3'-P	5.19	1.61	1.56
54	1w	46	G7M	O3'-P	5.14	1.61	1.56

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2h	79	VAL	N-CA-C	-9.78	103.18	112.96
41	1j	82	ILE	N-CA-C	-7.58	103.51	112.98
19	2X	94	GLY	CA-C-N	7.38	134.99	121.70
19	2X	94	GLY	C-N-CA	7.38	134.99	121.70
1	1A	1992	G	C2'-C3'-O3'	6.88	119.81	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31197	555	0
1	2A	60322	0	30427	641	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	37	0
3	1D	2136	0	2218	44	0
3	2D	2136	0	2218	35	0
4	1E	1559	0	1618	36	0
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	56	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	48	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	33	0
8	1I	1097	0	1140	33	0
8	2I	1064	0	1082	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	24	0
10	1O	933	0	996	19	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	34	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	29	0
12	2Q	1122	0	1179	41	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	15	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	21	0
17	1V	771	0	830	8	0
17	2V	771	0	830	12	0
18	1W	886	0	940	10	0
18	2W	886	0	940	13	0
19	1X	750	0	814	12	0
19	2X	750	0	813	25	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	42	0
21	2Z	1271	0	1273	51	0
22	10	653	0	674	13	0
22	20	653	0	674	11	0
23	11	755	0	826	11	0
23	21	755	0	826	20	0
24	12	588	0	643	9	0
24	22	588	0	643	13	0
25	13	469	0	518	11	0
25	23	464	0	514	14	0
26	14	552	0	533	21	0
26	24	532	0	503	33	0
27	15	455	0	465	5	0
27	25	455	0	465	7	0
28	16	453	0	473	10	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	18	517	0	582	10	0
30	28	517	0	582	18	0
31	19	307	0	335	3	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	369	0
32	2a	32327	0	16338	487	0
33	1b	1846	0	1867	62	0
33	2b	1825	0	1828	82	0
34	1c	1548	0	1535	34	0
34	2c	1542	0	1517	65	0
35	1d	1655	0	1672	46	0
35	2d	1674	0	1714	51	0
36	1e	1129	0	1185	34	0
36	2e	1133	0	1191	39	0
37	1f	810	0	804	10	0
37	2f	816	0	808	26	0
38	1g	1231	0	1238	26	0
38	2g	1235	0	1249	41	0
39	1h	1088	0	1126	27	0
39	2h	1088	0	1126	25	0
40	1i	983	0	986	39	0
40	2i	978	0	966	34	0
41	1j	709	0	650	25	0
41	2j	714	0	672	29	0
42	1k	829	0	825	13	0
42	2k	833	0	835	21	0
43	1l	932	0	981	19	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	26	0
44	2m	950	0	988	43	0
45	1n	492	0	529	17	0
45	2n	492	0	529	38	0
46	1o	728	0	760	10	0
46	2o	728	0	760	17	0
47	1p	681	0	697	19	0
47	2p	677	0	686	15	0
48	1q	823	0	891	21	0
48	2q	823	0	891	20	0
49	1r	555	0	618	13	0
49	2r	555	0	618	19	0
50	1s	652	0	662	20	0
50	2s	646	0	644	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1t	728	0	798	21	0
51	2t	727	0	796	11	0
52	1u	199	0	208	8	0
52	2u	199	0	208	6	0
53	1v	283	0	142	4	0
53	2v	239	0	119	7	0
54	1w	1599	0	801	17	0
54	2w	1599	0	800	51	0
55	1x	1646	0	839	11	0
55	2x	1646	0	838	25	0
56	1z	21	0	20	0	0
56	2z	21	0	20	0	0
57	1y	1577	0	799	42	0
57	2y	1577	0	798	31	0
58	10	9	0	0	0	0
58	11	4	0	0	0	0
58	12	2	0	0	0	0
58	13	3	0	0	0	0
58	14	1	0	0	0	0
58	15	4	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	1096	0	0	0	0
58	1B	35	0	0	0	0
58	1D	11	0	0	0	0
58	1E	13	0	0	0	0
58	1F	12	0	0	0	0
58	1G	4	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	5	0	0	0	0
58	1P	8	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	6	0	0	0	0
58	1S	2	0	0	0	0
58	1T	2	0	0	0	0
58	1U	12	0	0	0	0
58	1V	7	0	0	0	0
58	1W	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1X	5	0	0	0	0
58	1Y	4	0	0	0	0
58	1Z	2	0	0	0	0
58	1a	213	0	0	0	0
58	1b	1	0	0	0	0
58	1d	2	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1k	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1p	1	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	7	0	0	0	0
58	1x	11	0	0	0	0
58	20	3	0	0	0	0
58	23	3	0	0	0	0
58	25	4	0	0	0	0
58	27	2	0	0	0	0
58	28	1	0	0	0	0
58	2A	687	0	0	0	0
58	2B	15	0	0	0	0
58	2D	6	0	0	0	0
58	2E	7	0	0	0	0
58	2F	4	0	0	0	0
58	2N	1	0	0	0	0
58	2O	1	0	0	0	0
58	2P	1	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	3	0	0	0	0
58	2T	2	0	0	0	0
58	2V	1	0	0	0	0
58	2X	2	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	222	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0	0	0	0
58	2w	1	0	0	0	0
58	2x	5	0	0	0	0
59	1A	1	0	0	0	0
59	2x	1	0	0	0	0
60	1A	51	0	67	1	0
60	2A	51	0	67	4	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	0	0
62	2d	8	0	0	1	0
63	10	9	0	0	0	0
63	11	8	0	0	0	0
63	12	3	0	0	1	0
63	13	4	0	0	0	0
63	15	6	0	0	0	0
63	16	1	0	0	0	0
63	17	9	0	0	0	0
63	18	9	0	0	1	0
63	1A	1715	0	0	85	0
63	1B	53	0	0	2	0
63	1D	28	0	0	0	0
63	1E	25	0	0	1	0
63	1F	13	0	0	0	0
63	1G	3	0	0	1	0
63	1H	2	0	0	0	0
63	1N	3	0	0	1	0
63	1O	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1P	17	0	0	1	0
63	1Q	6	0	0	0	0
63	1R	12	0	0	2	0
63	1S	5	0	0	0	0
63	1T	5	0	0	0	0
63	1U	9	0	0	1	0
63	1V	9	0	0	0	0
63	1W	8	0	0	0	0
63	1X	7	0	0	0	0
63	1Y	2	0	0	1	0
63	1Z	1	0	0	0	0
63	1a	284	0	0	23	0
63	1e	1	0	0	0	0
63	1f	1	0	0	0	0
63	1i	1	0	0	0	0
63	1l	5	0	0	0	0
63	1m	2	0	0	0	0
63	1o	1	0	0	0	0
63	1q	2	0	0	0	0
63	1u	1	0	0	1	0
63	1v	5	0	0	0	0
63	1w	7	0	0	0	0
63	1x	6	0	0	0	0
63	1y	1	0	0	0	0
63	1z	1	0	0	0	0
63	20	1	0	0	0	0
63	21	5	0	0	0	0
63	26	1	0	0	0	0
63	28	2	0	0	0	0
63	2A	624	0	0	49	0
63	2B	12	0	0	0	0
63	2D	14	0	0	2	0
63	2E	5	0	0	1	0
63	2F	9	0	0	0	0
63	2N	1	0	0	0	0
63	2O	1	0	0	0	0
63	2P	3	0	0	0	0
63	2Q	1	0	0	0	0
63	2R	1	0	0	0	0
63	2T	4	0	0	0	0
63	2U	1	0	0	1	0
63	2W	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	2Y	1	0	0	1	0
63	2a	161	0	0	13	0
63	2d	1	0	0	0	0
63	2e	2	0	0	0	0
63	2j	1	0	0	0	0
63	2l	4	0	0	0	0
63	2p	2	0	0	0	0
63	2v	1	0	0	0	0
63	2w	1	0	0	0	0
63	2x	2	0	0	0	0
All	All	298915	0	196861	4061	0

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

The worst 5 of 4061 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	1.43	1.14
54:2w:51:A:N6	54:2w:63:U:H3	1.45	1.13
54:2w:51:A:N6	54:2w:63:U:N3	2.04	0.99
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.48	0.95
12:1Q:12:GLN:HE21	12:1Q:73:PRO:HD2	1.32	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	255 (93%)	16 (6%)	2 (1%)	18	41
3	2D	273/276 (99%)	250 (92%)	20 (7%)	3 (1%)	11	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	48
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	48
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	48
5	2F	201/210 (96%)	182 (90%)	15 (8%)	4 (2%)	6	16
6	1G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11	29
6	2G	179/182 (98%)	149 (83%)	22 (12%)	8 (4%)	2	4
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	44
7	2H	172/180 (96%)	145 (84%)	20 (12%)	7 (4%)	2	5
8	1I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	18	41
8	2I	144/148 (97%)	123 (85%)	17 (12%)	4 (3%)	4	9
9	1N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	41
9	2N	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	5	14
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	107 (89%)	11 (9%)	2 (2%)	7	19
11	1P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	4	10
11	2P	147/150 (98%)	123 (84%)	17 (12%)	7 (5%)	2	3
12	1Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	41
12	2Q	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	5	14
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	94 (87%)	9 (8%)	5 (5%)	2	4
15	1T	129/146 (88%)	121 (94%)	4 (3%)	4 (3%)	3	8
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	16
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	16
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	2X	93/96 (97%)	84 (90%)	7 (8%)	2 (2%)	5	14
20	1Y	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12	32
20	2Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	12	32
21	1Z	148/206 (72%)	130 (88%)	12 (8%)	6 (4%)	2	5
21	2Z	156/206 (76%)	119 (76%)	32 (20%)	5 (3%)	3	7
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
22	20	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	29
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	29
24	12	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
24	22	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	2
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1	2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	34 (97%)	0	1 (3%)	3	9
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	1b	229/256 (90%)	187 (82%)	28 (12%)	14 (6%)	1	2
33	2b	229/256 (90%)	178 (78%)	39 (17%)	12 (5%)	1	3
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	12	32
34	2c	204/239 (85%)	157 (77%)	38 (19%)	9 (4%)	2	4
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24	48
35	2d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	24	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	1e	146/162 (90%)	131 (90%)	10 (7%)	5 (3%)	3	7
36	2e	146/162 (90%)	119 (82%)	21 (14%)	6 (4%)	2	5
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%)	134 (88%)	17 (11%)	2 (1%)	9	25
38	2g	153/156 (98%)	130 (85%)	19 (12%)	4 (3%)	4	11
39	1h	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18	41
39	2h	135/138 (98%)	119 (88%)	16 (12%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	15 (12%)	5 (4%)	2	5
40	2i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	7
41	2j	94/105 (90%)	77 (82%)	12 (13%)	5 (5%)	1	3
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	35
42	2k	112/129 (87%)	94 (84%)	16 (14%)	2 (2%)	6	18
43	1l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
43	2l	119/132 (90%)	100 (84%)	17 (14%)	2 (2%)	7	19
44	1m	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	4	11
44	2m	120/126 (95%)	100 (83%)	18 (15%)	2 (2%)	7	19
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	7
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	10	27
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	27
47	1p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9	25
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	32
48	2q	97/105 (92%)	84 (87%)	11 (11%)	2 (2%)	5	15
49	1r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	22
50	1s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	10	27
50	2s	81/93 (87%)	62 (76%)	16 (20%)	3 (4%)	2	6
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	2t	94/106 (89%)	83 (88%)	6 (6%)	5 (5%)	1	3
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	3
56	1z	1/3 (33%)	1 (100%)	0	0	100	100
56	2z	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11372/12134 (94%)	10199 (90%)	973 (9%)	200 (2%)	6	18

5 of 200 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
11	1P	38	GLN
21	1Z	93	ASP
26	14	47	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	206 (96%)	9 (4%)	26	55
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15	37
4	1E	164/166 (99%)	154 (94%)	10 (6%)	17	40
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	45
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	13
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	18
6	1G	143/156 (92%)	127 (89%)	16 (11%)	6	15
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	6
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19	44
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	20
8	1I	113/124 (91%)	92 (81%)	21 (19%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2	6
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	35
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	30
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	86
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	41
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	17
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	29
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	23
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	39
13	1R	101/101 (100%)	95 (94%)	6 (6%)	18	42
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	56
14	1S	86/88 (98%)	74 (86%)	12 (14%)	3	9
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	5
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	47
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	33
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	31
16	2U	93/94 (99%)	82 (88%)	11 (12%)	5	13
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	48
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	14
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	44
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	23
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	37
19	2X	77/78 (99%)	70 (91%)	7 (9%)	9	22
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	10
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	3	7
21	1Z	135/179 (75%)	115 (85%)	20 (15%)	3	8
21	2Z	137/179 (76%)	112 (82%)	25 (18%)	2	5
22	10	65/67 (97%)	60 (92%)	5 (8%)	12	30
22	20	65/67 (97%)	58 (89%)	7 (11%)	6	16
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	58
23	21	80/83 (96%)	71 (89%)	9 (11%)	5	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	12	65/67 (97%)	64 (98%)	1 (2%)	57	81
24	22	65/67 (97%)	57 (88%)	8 (12%)	4	12
25	13	51/52 (98%)	43 (84%)	8 (16%)	2	7
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	19
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	6
26	24	53/63 (84%)	44 (83%)	9 (17%)	2	6
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	41
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	28
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	19
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	6
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	12
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	12
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	21
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	59
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	67
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	23
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	6
33	2b	187/220 (85%)	141 (75%)	46 (25%)	1	2
34	1c	142/188 (76%)	128 (90%)	14 (10%)	7	19
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	16
35	1d	169/181 (93%)	148 (88%)	21 (12%)	4	11
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4	11
36	1e	113/123 (92%)	98 (87%)	15 (13%)	4	10
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	14
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	20
37	2f	85/90 (94%)	72 (85%)	13 (15%)	3	7
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	13
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	16
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	28
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	20
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	18
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	9
41	2j	69/92 (75%)	53 (77%)	16 (23%)	1	2
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	25
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	16
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	47
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5	14
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	13
44	2m	92/101 (91%)	76 (83%)	16 (17%)	2	5
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	12
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	8
46	1o	78/80 (98%)	69 (88%)	9 (12%)	5	14
46	2o	78/80 (98%)	76 (97%)	2 (3%)	40	70
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	18
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	18
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	25
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	32
49	1r	59/77 (77%)	49 (83%)	10 (17%)	2	6
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	13
50	1s	69/80 (86%)	66 (96%)	3 (4%)	26	54
50	2s	67/80 (84%)	55 (82%)	12 (18%)	2	5
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	10
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	10
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	44
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	15
56	1z	1/1 (100%)	1 (100%)	0	100	100
56	2z	1/1 (100%)	1 (100%)	0	100	100
All	All	9305/10066 (92%)	8326 (90%)	979 (10%)	6	17

5 of 979 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2E	33	VAL

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Mol	Chain	Res	Type
41	2j	96	ILE
13	2R	24	GLN
41	2j	29	ARG
48	2q	66	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	98	ASN
44	2m	77	ASN
35	2d	116	GLN
39	2h	78	GLN
50	2s	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	454 (15%)	22 (0%)
1	2A	2791/2915 (95%)	478 (17%)	29 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1497/1521 (98%)	259 (17%)	0
32	2a	1501/1521 (98%)	323 (21%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	10/24 (41%)	2 (20%)	0
54	1w	71/76 (93%)	26 (36%)	0
54	2w	71/76 (93%)	36 (50%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	12 (16%)	0
57	1y	72/76 (94%)	30 (41%)	0
57	2y	72/76 (94%)	35 (48%)	0
All	All	9348/9620 (97%)	1713 (18%)	51 (0%)

5 of 1713 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	72	U

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Mol	Chain	Res	Type
1	1A	74	A

5 of 51 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	310	A
1	2A	900	A
1	2A	2439	A
1	2A	528	A
1	2A	774	A

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	$\# Z > 2$
43	0TD	2l	92	43	8,9,10	4.44	2 (25%)	6,11,13	6.78	1 (16%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.47	0	33,38,41	2.11	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.27	5 (19%)
57	5MU	1y	54	57	19,22,23	1.41	5 (26%)	27,32,35	2.15	8 (29%)
54	U8U	1w	34	54,53	20,24,25	1.42	2 (10%)	22,34,37	1.17	4 (18%)
1	OMU	2A	2552	1,58	19,22,23	1.12	2 (10%)	25,31,34	1.88	5 (20%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.25	6 (22%)
55	8AN	1x	76	58,55,56	21,24,25	1.44	3 (14%)	26,35,38	2.32	10 (38%)
1	5MC	2A	1962	1,58	19,22,23	1.64	3 (15%)	26,32,35	1.15	2 (7%)
55	5MC	2x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.25	4 (15%)
57	T6A	1y	37	57	21,24,35	1.56	4 (19%)	30,35,52	2.01	7 (23%)
55	5MU	2x	54	55	19,22,23	1.38	6 (31%)	27,32,35	2.03	6 (22%)
1	2MA	2A	2503	1,58	22,25,26	1.51	4 (18%)	32,37,40	2.28	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1962	1,58	19,22,23	1.80	3 (15%)	26,32,35	1.20	3 (11%)
54	G7M	2w	46	54	23,26,27	1.49	4 (17%)	34,39,42	1.71	6 (17%)
57	PSU	1y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
54	G7M	1w	46	54	23,26,27	1.50	3 (13%)	34,39,42	1.68	5 (14%)
32	5MC	1a	1407	32	19,22,23	1.54	3 (15%)	26,32,35	1.14	3 (11%)
55	5MC	1x	32	55	19,22,23	1.58	3 (15%)	26,32,35	1.19	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.03	9 (27%)
55	5MU	1x	54	55	19,22,23	1.43	5 (26%)	27,32,35	1.94	5 (18%)
54	5MU	2w	54	54	19,22,23	1.54	6 (31%)	27,32,35	1.75	5 (18%)
57	G7M	2y	46	57	23,26,27	1.55	3 (13%)	34,39,42	1.69	4 (11%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.12	4 (19%)
56	FME	2z	1	56	8,9,10	1.00	0	8,9,11	1.57	2 (25%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.02	9 (27%)
54	A1B8A	1w	76	54	30,33,34	1.26	3 (10%)	36,46,49	1.88	9 (25%)
57	5MU	2y	54	57	19,22,23	1.49	5 (26%)	27,32,35	1.61	7 (25%)
54	U8U	2w	34	54,32,53	20,24,25	1.48	3 (15%)	22,34,37	1.73	2 (9%)
32	G7M	1a	527	32,58	23,26,27	1.51	3 (13%)	34,39,42	1.74	5 (14%)
1	OMU	1A	2552	1,58	19,22,23	1.22	3 (15%)	25,31,34	1.85	5 (20%)
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.19	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	1.96	3 (14%)
54	A1B8A	2w	76	54	30,33,34	1.24	3 (10%)	36,46,49	1.88	9 (25%)
55	4SU	2x	8	55	18,21,22	2.13	6 (33%)	25,30,33	1.32	4 (16%)
57	PSU	1y	39	57	18,21,22	1.39	2 (11%)	21,30,33	2.11	4 (19%)
54	PSU	2w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.09	3 (14%)
54	PSU	1w	55	54	18,21,22	1.37	1 (5%)	21,30,33	2.00	4 (19%)
32	5MC	1a	967	32	19,22,23	1.50	3 (15%)	26,32,35	1.07	2 (7%)
57	PSU	2y	39	57,42	18,21,22	1.42	2 (11%)	21,30,33	1.77	2 (9%)
32	UR3	2a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.65	3 (11%)
55	4SU	1x	8	55	18,21,22	2.29	5 (27%)	25,30,33	1.60	6 (24%)
43	0TD	1l	92	43	8,9,10	4.54	1 (12%)	6,11,13	2.98	2 (33%)
32	5MC	1a	1404	32	19,22,23	1.79	3 (15%)	26,32,35	1.25	4 (15%)
1	5MC	2A	1942	1	19,22,23	1.58	3 (15%)	26,32,35	1.11	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	21,30,33	2.01	4 (19%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.91	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	PSU	2y	55	57	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
1	OMG	2A	2251	55,1	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.25	7 (21%)
57	U8U	2y	34	57	17,21,25	1.56	3 (17%)	21,30,37	1.49	3 (14%)
32	2MG	1a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.28	9 (27%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.01	1 (4%)
54	5MU	1w	54	54	19,22,23	1.33	4 (21%)	27,32,35	2.68	6 (22%)
1	2MA	1A	2503	1,58	22,25,26	1.49	5 (22%)	32,37,40	2.29	9 (28%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
54	T6A	1w	37	54	31,34,35	1.41	5 (16%)	43,49,52	1.74	10 (23%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.14	3 (14%)
1	5MU	1A	1939	1,58	19,22,23	1.50	4 (21%)	27,32,35	2.08	6 (22%)
32	4OC	2a	1402	32,58	20,23,24	0.77	0	25,32,35	1.09	2 (8%)
57	T6A	2y	37	57	21,24,35	1.59	3 (14%)	30,35,52	2.03	8 (26%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.90	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.21	3 (11%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.19	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.04	9 (27%)
55	8AN	2x	76	58,55,59,56	21,24,25	1.41	3 (14%)	26,35,38	2.31	10 (38%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.91	1 (4%)
57	U8U	1y	34	57	17,21,25	1.56	4 (23%)	21,30,37	1.48	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.49	5 (26%)	27,32,35	2.04	5 (18%)
57	G7M	1y	46	57	23,26,27	1.56	4 (17%)	34,39,42	1.83	4 (11%)
1	5MC	1A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.19	3 (11%)
1	PSU	1A	2605	1,58	18,21,22	1.41	4 (22%)	21,30,33	2.20	4 (19%)
1	5MU	1A	1915	1	19,22,23	1.43	6 (31%)	27,32,35	2.12	7 (25%)
32	UR3	1a	1498	32	19,22,23	1.00	0	26,32,35	1.64	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.57	3 (15%)	26,32,35	1.18	3 (11%)
1	OMG	1A	2251	55,1,58	23,26,27	1.25	3 (13%)	32,38,41	2.04	6 (18%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	2.03	5 (23%)
32	G7M	2a	527	32,58	23,26,27	1.51	3 (13%)	34,39,42	1.70	5 (14%)
54	PSU	2w	55	54	18,21,22	1.33	2 (11%)	21,30,33	1.96	4 (19%)
32	PSU	1a	516	32	18,21,22	1.36	3 (16%)	21,30,33	1.89	4 (19%)
54	T6A	2w	37	54,53	31,34,35	1.39	4 (12%)	43,49,52	1.84	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.93	1 (4%)
56	FME	1z	1	56	8,9,10	0.95	1 (12%)	8,9,11	2.12	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	0TD	2l	92	43	-	4/7/12/14	-
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
54	U8U	1w	34	54,53	-	2/10/28/29	0/2/2/2
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	58,55,56	-	3/7/25/26	0/3/3/3
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
57	T6A	1y	37	57	-	1/7/25/42	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,58	-	0/7/25/26	0/3/3/3
1	5MC	1A	1962	1,58	-	2/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
57	PSU	1y	55	57	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	0/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	3/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	0/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	2/7/9/11	-
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	A1B8A	1w	76	54	-	6/20/38/39	0/3/3/3
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
54	U8U	2w	34	54,32,53	-	6/10/28/29	0/2/2/2

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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
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	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	PSU	1y	39	57	-	4/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57,42	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
57	PSU	2y	55	57	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
57	U8U	2y	34	57	-	0/7/25/29	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,58	-	0/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	T6A	1w	37	54	-	6/23/41/42	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,58	-	2/9/29/30	0/2/2/2
57	T6A	2y	37	57	-	1/7/25/42	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	8AN	2x	76	58,55,59,56	-	3/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
57	U8U	1y	34	57	-	0/7/25/29	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	0/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,58	-	0/9/27/28	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,58	-	3/7/25/26	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	T6A	2w	37	54,53	-	9/23/41/42	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-

The worst 5 of 241 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
43	2l	92	0TD	CB-SB	-12.04	1.70	1.82
1	1A	1962	5MC	C5-C4	6.74	1.49	1.44
32	2a	967	5MC	C5-C4	6.60	1.49	1.44
32	1a	1404	5MC	C5-C4	6.56	1.49	1.44

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	16.41	131.87	102.36
1	2A	2503	2MA	C5-C4-N3	-8.20	118.55	127.18
1	1A	2503	2MA	C5-C4-N3	-7.53	119.25	127.18
32	1a	1207	2MG	C2-N3-C4	7.19	120.99	112.00
32	2a	1207	2MG	C2-N3-C4	6.98	120.73	112.00

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	1y	39	PSU	C2'-C1'-C5-C4
32	2a	1400	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

45 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	1	0
32	1a	1519	MA6	1	0
32	2a	1400	5MC	1	0
54	1w	34	U8U	2	0
1	2A	1939	5MU	1	0
55	1x	76	8AN	1	0
1	2A	1962	5MC	1	0
57	1y	37	T6A	1	0
55	2x	54	5MU	1	0
57	1y	55	PSU	1	0
32	2a	1519	MA6	2	0
54	2w	54	5MU	4	0
57	2y	46	G7M	2	0
32	2a	1518	MA6	1	0
54	1w	76	A1B8A	1	0
57	2y	54	5MU	1	0
54	2w	34	U8U	1	0
1	1A	2552	OMU	1	0
32	2a	1404	5MC	1	0
54	2w	76	A1B8A	1	0
55	2x	8	4SU	2	0
57	1y	39	PSU	1	0
54	2w	39	PSU	4	0
55	1x	8	4SU	1	0
1	2A	2251	OMG	1	0
55	2x	55	PSU	1	0
32	2a	1207	2MG	3	0
57	2y	34	U8U	1	0
54	1w	54	5MU	1	0
1	2A	1911	PSU	1	0
54	1w	37	T6A	1	0
1	1A	1939	5MU	1	0
32	2a	1402	4OC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2y	37	T6A	1	0
32	1a	1400	5MC	1	0
32	2a	967	5MC	1	0
32	1a	1518	MA6	1	0
55	2x	76	8AN	2	0
1	2A	1920	OMC	1	0
57	1y	34	U8U	1	0
1	1A	2605	PSU	1	0
1	1A	1915	5MU	1	0
1	1A	2251	OMG	1	0
32	2a	516	PSU	2	0
54	2w	55	PSU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2540 ligands modelled in this entry, 2536 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	$\# Z > 2$
60	ERY	1A	4098	-	53,53,53	0.95	2 (3%)	82,82,82	1.49	12 (14%)
62	SF4	1d	303	35	0,12,12	-	-	-		
62	SF4	2d	303	35	0,12,12	-	-	-		
60	ERY	2A	3688	-	53,53,53	0.95	2 (3%)	82,82,82	1.36	9 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	ERY	1A	4098	-	-	1/72/107/107	0/3/3/3
62	SF4	1d	303	35	-	-	0/6/5/5
62	SF4	2d	303	35	-	-	0/6/5/5
60	ERY	2A	3688	-	-	5/72/107/107	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	2A	3688	ERY	O2-C1	4.85	1.45	1.34
60	1A	4098	ERY	O2-C1	4.77	1.45	1.34
60	1A	4098	ERY	O2-C13	-2.84	1.41	1.46
60	2A	3688	ERY	O2-C13	-2.41	1.42	1.46

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	2A	3688	ERY	C13-O2-C1	-5.08	109.32	118.20
60	1A	4098	ERY	O3-C3-C4	3.97	112.91	108.23
60	1A	4098	ERY	C6-C5-C4	-3.69	108.53	113.89
60	2A	3688	ERY	O5-C16-C15	-3.66	107.32	112.95
60	2A	3688	ERY	O5-C16-C17	3.58	109.05	103.86

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	2A	3688	ERY	C15-C16-O5-C20
60	2A	3688	ERY	C17-C16-O5-C20
60	2A	3688	ERY	C19-C16-O5-C20
60	1A	4098	ERY	C32-C6-C7-C8
60	2A	3688	ERY	C32-C6-C7-C8

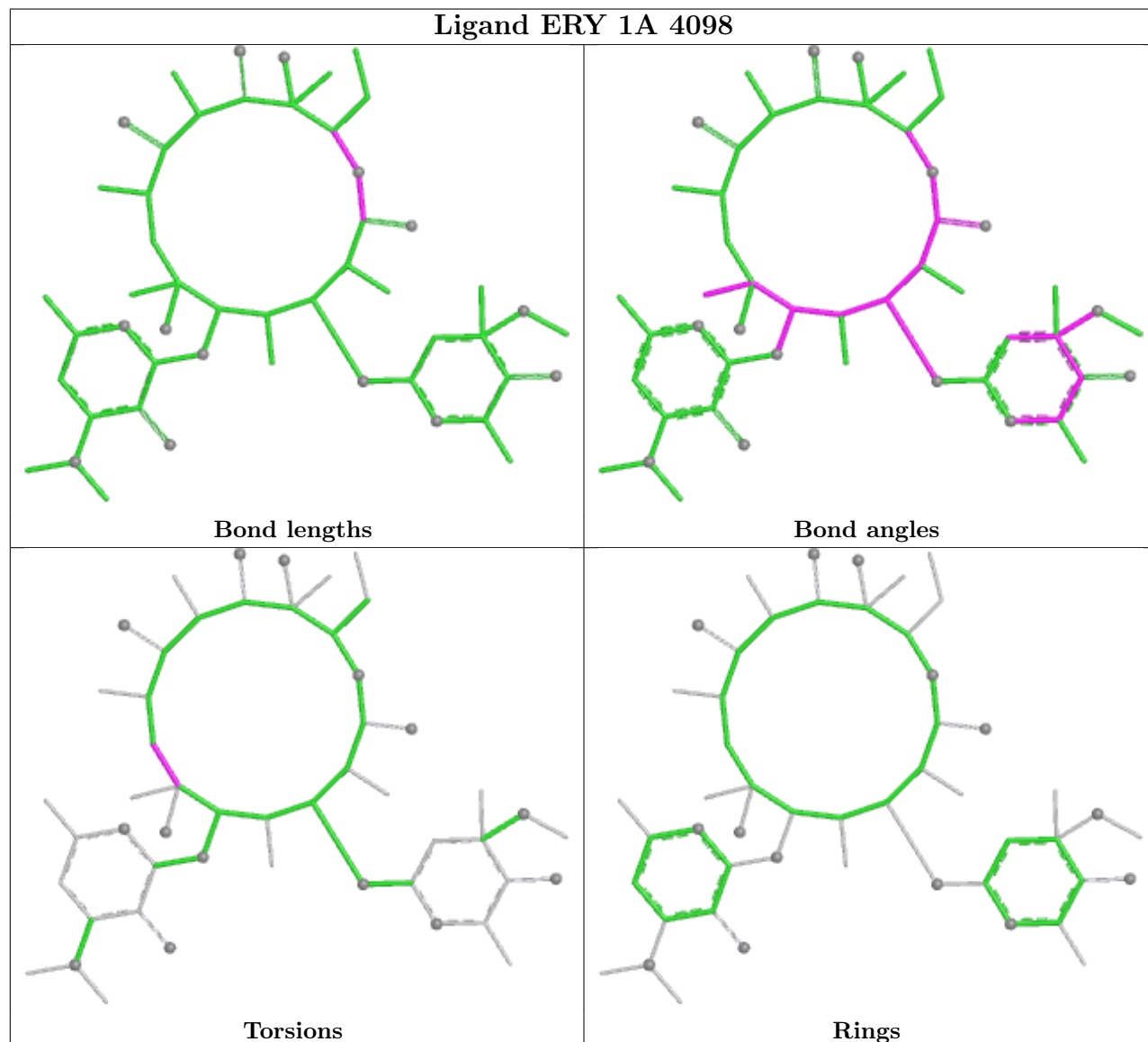
There are no ring outliers.

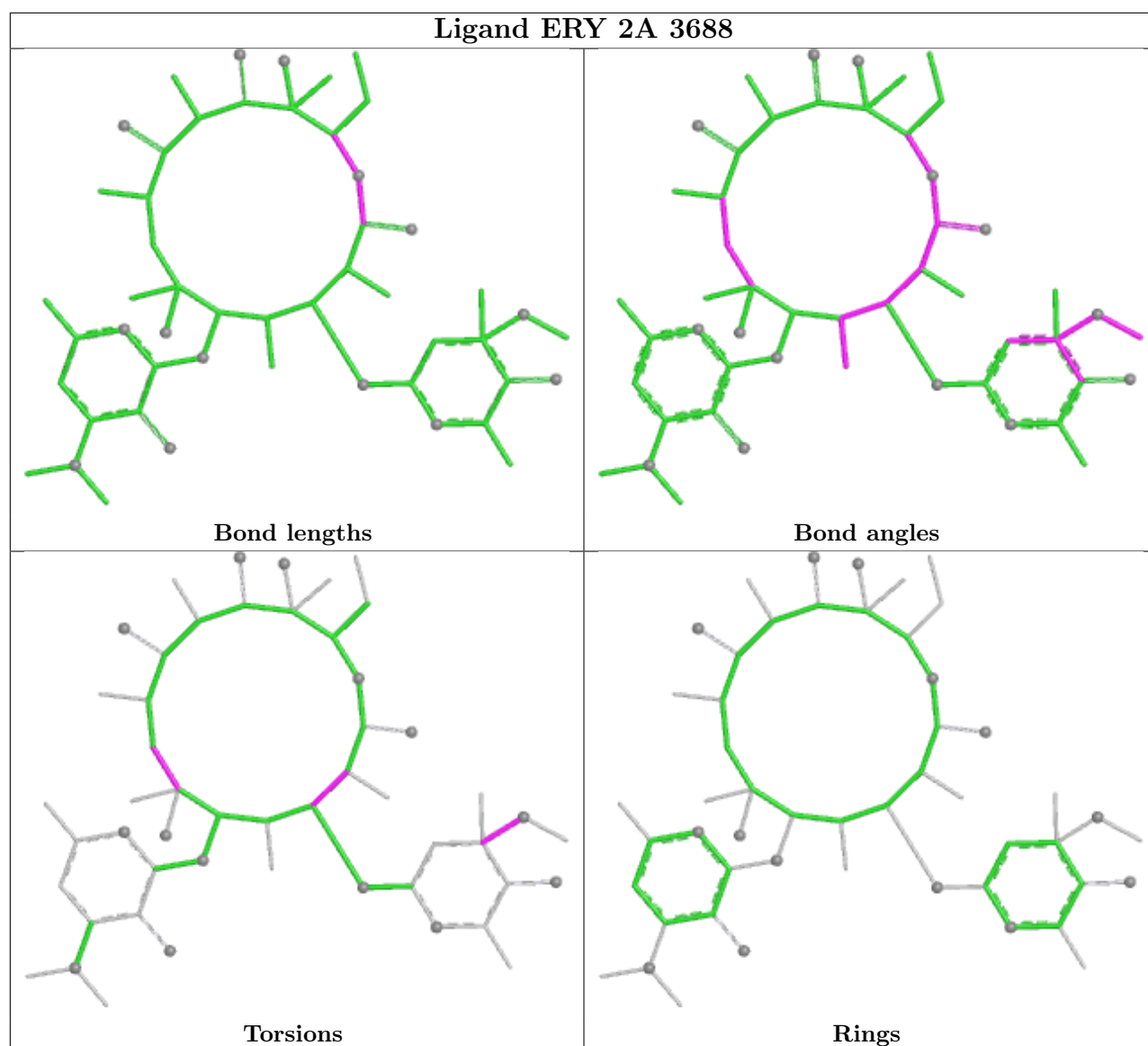
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1A	4098	ERY	1	0
62	2d	303	SF4	1	0
60	2A	3688	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.42	123 (4%)	40	36	19, 38, 99, 111	0
1	2A	2789/2915 (95%)	0.01	103 (3%)	45	41	33, 59, 95, 113	0
2	1B	120/121 (99%)	-0.34	0	100	100	31, 52, 66, 91	0
2	2B	120/121 (99%)	1.04	10 (8%)	17	14	64, 82, 90, 97	0
3	1D	275/276 (99%)	-0.12	2 (0%)	84	83	21, 38, 52, 80	0
3	2D	275/276 (99%)	0.27	2 (0%)	84	83	32, 51, 65, 79	0
4	1E	204/206 (99%)	-0.07	0	100	100	20, 44, 63, 72	0
4	2E	204/206 (99%)	0.29	3 (1%)	72	70	36, 60, 74, 84	0
5	1F	203/210 (96%)	-0.03	0	100	100	19, 44, 67, 85	0
5	2F	203/210 (96%)	0.46	5 (2%)	58	55	36, 71, 83, 88	0
6	1G	181/182 (99%)	0.54	8 (4%)	39	35	41, 61, 77, 86	0
6	2G	181/182 (99%)	1.55	48 (26%)	1	1	70, 82, 89, 96	0
7	1H	174/180 (96%)	0.32	2 (1%)	78	76	41, 56, 68, 71	0
7	2H	174/180 (96%)	1.11	16 (9%)	14	12	70, 83, 90, 93	0
8	1I	146/148 (98%)	0.62	2 (1%)	73	72	44, 75, 84, 88	0
8	2I	146/148 (98%)	0.90	14 (9%)	13	11	60, 75, 87, 90	0
9	1N	140/140 (100%)	0.08	1 (0%)	84	83	28, 44, 62, 81	0
9	2N	140/140 (100%)	0.81	7 (5%)	34	30	45, 66, 78, 88	0
10	1O	122/122 (100%)	0.09	2 (1%)	70	68	29, 42, 58, 69	0
10	2O	122/122 (100%)	0.34	0	100	100	46, 59, 71, 79	0
11	1P	149/150 (99%)	0.00	0	100	100	21, 45, 68, 77	0
11	2P	149/150 (99%)	0.60	3 (2%)	65	62	36, 69, 83, 89	0
12	1Q	141/141 (100%)	-0.05	0	100	100	27, 43, 59, 73	0
12	2Q	141/141 (100%)	0.89	9 (6%)	25	22	50, 69, 79, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.08	1 (0%) 82 81	28, 39, 53, 64	0
13	2R	118/118 (100%)	0.22	2 (1%) 69 67	40, 54, 65, 73	0
14	1S	110/112 (98%)	0.18	1 (0%) 81 80	38, 51, 63, 71	0
14	2S	110/112 (98%)	1.40	18 (16%) 4 4	65, 75, 84, 87	0
15	1T	131/146 (89%)	0.28	5 (3%) 44 40	34, 46, 71, 78	0
15	2T	131/146 (89%)	0.47	2 (1%) 72 70	50, 62, 76, 80	0
16	1U	116/118 (98%)	-0.15	0 100 100	26, 36, 55, 67	0
16	2U	116/118 (98%)	0.62	1 (0%) 81 80	46, 63, 78, 83	0
17	1V	101/101 (100%)	0.09	1 (0%) 79 78	25, 48, 64, 72	0
17	2V	101/101 (100%)	0.71	4 (3%) 42 38	45, 73, 81, 86	0
18	1W	112/113 (99%)	-0.04	2 (1%) 67 65	26, 37, 55, 82	0
18	2W	112/113 (99%)	0.54	4 (3%) 46 42	40, 52, 70, 96	0
19	1X	95/96 (98%)	0.01	2 (2%) 63 61	26, 40, 62, 77	0
19	2X	95/96 (98%)	0.63	2 (2%) 63 61	44, 62, 77, 82	0
20	1Y	107/110 (97%)	0.44	3 (2%) 55 51	35, 52, 71, 80	0
20	2Y	107/110 (97%)	1.24	16 (14%) 5 4	62, 74, 85, 89	0
21	1Z	154/206 (74%)	0.79	13 (8%) 17 14	46, 68, 90, 100	0
21	2Z	160/206 (77%)	1.52	38 (23%) 2 1	68, 83, 94, 99	0
22	10	83/85 (97%)	0.14	6 (7%) 21 18	29, 40, 60, 70	0
22	20	83/85 (97%)	1.26	10 (12%) 9 7	45, 67, 76, 81	0
23	11	97/98 (98%)	0.26	2 (2%) 63 61	27, 47, 71, 78	0
23	21	97/98 (98%)	0.51	3 (3%) 51 48	41, 58, 79, 80	0
24	12	70/72 (97%)	0.22	1 (1%) 73 72	35, 51, 63, 71	0
24	22	70/72 (97%)	0.84	1 (1%) 73 72	59, 73, 81, 85	0
25	13	59/60 (98%)	0.02	1 (1%) 69 67	29, 43, 65, 75	0
25	23	59/60 (98%)	0.81	3 (5%) 33 29	56, 68, 79, 92	0
26	14	69/71 (97%)	0.93	10 (14%) 6 5	55, 77, 89, 94	0
26	24	69/71 (97%)	1.54	19 (27%) 1 1	81, 89, 97, 100	0
27	15	59/60 (98%)	0.10	2 (3%) 48 44	24, 39, 69, 78	0
27	25	59/60 (98%)	0.26	0 100 100	39, 53, 71, 86	0
28	16	53/54 (98%)	-0.05	1 (1%) 66 63	31, 42, 57, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.85	3 (5%) 29 26	54, 64, 71, 75	0
29	17	48/49 (97%)	-0.18	3 (6%) 26 23	22, 28, 55, 63	0
29	27	48/49 (97%)	0.10	2 (4%) 40 37	32, 41, 64, 76	0
30	18	64/65 (98%)	-0.17	0 100 100	28, 35, 43, 55	0
30	28	64/65 (98%)	0.60	0 100 100	47, 58, 66, 74	0
31	19	37/37 (100%)	-0.15	1 (2%) 56 53	32, 43, 59, 67	0
31	29	37/37 (100%)	1.00	2 (5%) 31 27	64, 69, 80, 86	0
32	1a	1488/1521 (97%)	0.18	37 (2%) 58 55	36, 67, 94, 112	0
32	2a	1491/1521 (98%)	0.69	101 (6%) 23 20	52, 80, 98, 112	0
33	1b	231/256 (90%)	0.93	29 (12%) 8 7	66, 81, 89, 94	0
33	2b	231/256 (90%)	1.39	47 (20%) 3 2	75, 88, 93, 99	0
34	1c	206/239 (86%)	0.78	6 (2%) 53 50	61, 73, 82, 89	0
34	2c	206/239 (86%)	1.59	61 (29%) 1 1	75, 88, 93, 97	0
35	1d	208/209 (99%)	0.86	13 (6%) 26 23	58, 70, 81, 87	0
35	2d	208/209 (99%)	1.05	26 (12%) 8 7	62, 75, 85, 92	0
36	1e	148/162 (91%)	0.60	5 (3%) 48 44	51, 64, 75, 83	0
36	2e	148/162 (91%)	1.27	25 (16%) 4 3	69, 80, 87, 90	0
37	1f	100/101 (99%)	0.44	2 (2%) 65 62	58, 67, 77, 81	0
37	2f	100/101 (99%)	0.65	4 (4%) 42 38	64, 73, 80, 86	0
38	1g	155/156 (99%)	0.65	12 (7%) 19 17	61, 72, 89, 93	0
38	2g	155/156 (99%)	1.18	22 (14%) 6 5	74, 84, 91, 94	0
39	1h	137/138 (99%)	0.72	4 (2%) 53 50	58, 68, 76, 82	0
39	2h	137/138 (99%)	1.21	15 (10%) 10 9	71, 79, 85, 88	0
40	1i	127/128 (99%)	1.05	10 (7%) 18 16	56, 77, 85, 88	0
40	2i	127/128 (99%)	1.73	43 (33%) 1 1	76, 87, 93, 95	0
41	1j	97/105 (92%)	1.32	22 (22%) 2 2	59, 79, 87, 93	0
41	2j	96/105 (91%)	1.95	37 (38%) 1 0	75, 88, 94, 95	0
42	1k	114/129 (88%)	0.66	7 (6%) 27 24	45, 70, 81, 86	0
42	2k	114/129 (88%)	0.98	10 (8%) 15 13	60, 76, 85, 88	0
43	1l	121/132 (91%)	0.47	3 (2%) 58 55	41, 57, 68, 78	0
43	2l	121/132 (91%)	1.08	12 (9%) 13 10	57, 71, 80, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.95	9 (7%) 21 18	57, 72, 82, 97	0
44	2m	122/126 (96%)	1.95	43 (35%) 1 1	73, 86, 92, 95	0
45	1n	60/61 (98%)	0.72	3 (5%) 34 30	60, 68, 76, 77	0
45	2n	60/61 (98%)	2.37	35 (58%) 0 0	78, 88, 92, 95	0
46	1o	88/89 (98%)	0.67	3 (3%) 48 44	52, 65, 75, 81	0
46	2o	88/89 (98%)	0.89	7 (7%) 18 15	63, 76, 84, 91	0
47	1p	82/88 (93%)	1.34	19 (23%) 2 2	59, 71, 79, 89	0
47	2p	82/88 (93%)	0.91	6 (7%) 21 18	59, 71, 82, 86	0
48	1q	99/105 (94%)	0.71	3 (3%) 52 49	57, 68, 78, 82	0
48	2q	99/105 (94%)	1.08	12 (12%) 8 7	65, 74, 83, 87	0
49	1r	68/88 (77%)	0.43	1 (1%) 72 70	56, 67, 78, 81	0
49	2r	68/88 (77%)	0.66	1 (1%) 72 70	66, 75, 84, 87	0
50	1s	83/93 (89%)	0.65	3 (3%) 46 42	65, 74, 83, 86	0
50	2s	83/93 (89%)	1.89	35 (42%) 0 0	81, 89, 94, 98	0
51	1t	96/106 (90%)	0.88	12 (12%) 8 7	60, 72, 82, 86	0
51	2t	96/106 (90%)	0.74	4 (4%) 40 37	60, 72, 81, 87	0
52	1u	23/27 (85%)	0.80	2 (8%) 16 13	60, 67, 73, 79	0
52	2u	23/27 (85%)	2.04	14 (60%) 0 0	78, 83, 87, 88	0
53	1v	13/24 (54%)	1.06	3 (23%) 2 2	46, 72, 98, 103	0
53	2v	11/24 (45%)	1.38	3 (27%) 1 1	69, 83, 94, 96	0
54	1w	67/76 (88%)	1.33	18 (26%) 1 1	49, 93, 103, 108	0
54	2w	67/76 (88%)	1.49	16 (23%) 2 1	66, 100, 108, 110	0
55	1x	72/77 (93%)	0.59	4 (5%) 30 26	31, 67, 84, 89	0
55	2x	72/77 (93%)	0.81	3 (4%) 40 37	47, 84, 93, 96	0
56	1z	2/3 (66%)	0.54	0 100 100	37, 37, 37, 38	0
56	2z	2/3 (66%)	1.10	0 100 100	52, 52, 52, 56	0
57	1y	68/76 (89%)	1.84	23 (33%) 1 1	59, 104, 108, 109	0
57	2y	68/76 (89%)	2.01	34 (50%) 0 0	69, 106, 110, 111	0
All	All	20882/21754 (95%)	0.42	1414 (6%) 23 20	19, 66, 93, 113	0

The worst 5 of 1414 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	13.3
44	2m	123	ALA	10.1
44	1m	124	PRO	9.3
44	2m	102	ARG	9.2
44	1m	122	LYS	8.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	G7M	1y	46	24/25	0.35	0.17	95,104,109,118	0
57	G7M	2y	46	24/25	0.36	0.18	96,105,116,132	0
57	T6A	2y	37	22/33	0.41	0.18	89,102,113,126	0
57	U8U	1y	34	20/24	0.41	0.20	88,105,112,125	0
57	U8U	2y	34	20/24	0.42	0.23	97,108,116,129	0
57	T6A	1y	37	22/33	0.48	0.17	95,98,103,113	0
54	G7M	2w	46	24/25	0.52	0.14	91,102,116,128	0
54	PSU	2w	55	20/21	0.54	0.16	90,102,108,109	0
57	PSU	2y	55	20/21	0.55	0.15	97,107,113,117	0
54	G7M	1w	46	24/25	0.55	0.15	87,96,107,118	0
57	PSU	2y	39	20/21	0.57	0.16	93,101,106,120	0
54	PSU	1w	55	20/21	0.58	0.18	84,100,107,112	0
57	5MU	2y	54	21/22	0.58	0.14	97,105,113,122	0
57	PSU	1y	39	20/21	0.63	0.14	94,102,109,116	0
57	PSU	1y	55	20/21	0.65	0.11	99,102,112,123	0
54	5MU	2w	54	21/22	0.65	0.14	82,93,101,104	0
57	5MU	1y	54	21/22	0.66	0.12	95,101,104,119	0
54	5MU	1w	54	21/22	0.79	0.12	74,86,94,97	0
1	5MU	2A	1915	21/22	0.80	0.15	79,84,87,90	0
54	U8U	2w	34	23/24	0.80	0.20	78,89,97,100	0
32	2MG	2a	1207	24/25	0.81	0.15	81,90,101,106	0
54	PSU	2w	39	20/21	0.82	0.13	84,89,96,96	0
32	PSU	2a	516	20/21	0.83	0.14	73,85,91,92	0
54	T6A	2w	37	32/33	0.84	0.15	77,89,96,98	0
55	PSU	2x	55	20/21	0.84	0.13	79,84,89,90	0
55	4SU	2x	8	20/21	0.85	0.12	80,85,93,96	0
54	U8U	1w	34	23/24	0.86	0.14	69,76,84,87	0
55	5MU	2x	54	21/22	0.87	0.12	78,86,92,107	0
54	T6A	1w	37	32/33	0.88	0.14	60,72,81,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	FME	2z	1	10/11	0.88	0.24	51,59,66,70	0
55	PSU	1x	55	20/21	0.89	0.10	58,65,76,77	0
56	FME	1z	1	10/11	0.89	0.23	44,54,62,77	0
32	M2G	2a	966	25/26	0.89	0.16	62,72,88,91	0
32	5MC	2a	967	21/22	0.90	0.14	70,76,83,89	0
1	PSU	2A	1917	20/21	0.90	0.10	65,75,80,84	0
55	4SU	1x	8	20/21	0.91	0.12	59,65,71,77	0
55	5MU	1x	54	21/22	0.92	0.10	65,71,77,79	0
54	A1B8A	2w	76	31/32	0.92	0.12	41,56,64,65	0
43	0TD	2l	92	10/11	0.92	0.13	69,71,78,87	0
32	G7M	2a	527	24/25	0.92	0.11	59,68,74,83	0
32	5MC	2a	1404	21/22	0.93	0.11	55,62,71,74	0
1	PSU	2A	1911	20/21	0.93	0.10	57,70,78,80	0
1	5MU	1A	1915	21/22	0.93	0.10	52,59,63,68	0
54	PSU	1w	39	20/21	0.93	0.10	77,80,86,87	0
32	PSU	1a	516	20/21	0.93	0.09	62,67,70,70	0
43	0TD	1l	92	10/11	0.93	0.09	49,52,54,61	0
32	4OC	2a	1402	22/23	0.93	0.11	55,69,74,76	0
55	5MC	2x	32	21/22	0.94	0.12	71,75,82,85	0
32	5MC	2a	1407	21/22	0.94	0.11	54,60,67,69	0
54	A1B8A	1w	76	31/32	0.94	0.11	34,42,47,50	0
1	OMC	2A	1920	21/22	0.94	0.10	58,69,73,76	0
55	8AN	2x	76	22/23	0.94	0.11	42,50,56,58	0
32	5MC	2a	1400	21/22	0.94	0.14	72,77,81,84	0
1	5MC	2A	1962	21/22	0.95	0.09	39,51,58,70	0
32	MA6	1a	1519	24/25	0.95	0.10	35,45,48,51	0
32	G7M	1a	527	24/25	0.95	0.09	36,44,57,57	0
32	2MG	1a	1207	24/25	0.95	0.10	57,66,72,74	0
1	5MC	2A	1942	21/22	0.95	0.10	51,63,71,75	0
32	UR3	2a	1498	21/22	0.95	0.10	52,60,65,71	0
32	MA6	2a	1518	24/25	0.95	0.11	55,66,74,76	0
32	M2G	1a	966	25/26	0.96	0.09	51,54,62,63	0
1	OMG	2A	2251	24/25	0.96	0.09	37,43,45,48	0
1	PSU	2A	2605	20/21	0.96	0.07	31,41,44,45	0
55	5MC	1x	32	21/22	0.96	0.10	46,54,59,63	0
32	MA6	2a	1519	24/25	0.96	0.11	56,66,74,76	0
32	5MC	1a	967	21/22	0.96	0.10	50,57,64,67	0
1	5MC	1A	1942	21/22	0.96	0.10	38,42,48,59	0
55	8AN	1x	76	22/23	0.96	0.09	30,36,40,44	0
32	5MC	1a	1400	21/22	0.96	0.10	44,50,53,53	0
1	PSU	1A	1911	20/21	0.96	0.09	42,51,56,58	0
1	PSU	1A	1917	20/21	0.96	0.07	47,52,57,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	1A	1939	21/22	0.97	0.07	23,28,35,36	0
1	OMC	1A	1920	21/22	0.97	0.08	35,45,49,50	0
1	2MA	2A	2503	23/24	0.97	0.08	33,37,39,41	0
1	OMU	2A	2552	21/22	0.97	0.08	34,43,48,49	0
32	4OC	1a	1402	22/23	0.97	0.09	40,47,51,53	0
32	5MC	1a	1404	21/22	0.97	0.09	33,42,47,48	0
32	5MC	1a	1407	21/22	0.97	0.08	35,40,43,48	0
1	5MU	2A	1939	21/22	0.97	0.07	37,42,46,46	0
32	UR3	1a	1498	21/22	0.97	0.08	36,41,46,48	0
32	MA6	1a	1518	24/25	0.98	0.09	27,43,47,56	0
1	OMU	1A	2552	21/22	0.98	0.07	25,30,34,37	0
1	PSU	1A	2605	20/21	0.98	0.07	24,28,34,35	0
1	5MC	1A	1962	21/22	0.98	0.07	30,36,43,48	0
1	2MA	1A	2503	23/24	0.98	0.06	18,22,26,28	0
1	OMG	1A	2251	24/25	0.99	0.06	21,26,29,31	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	1753	1/1	0.40	0.16	93,93,93,93	0
58	MG	2a	1789	1/1	0.58	0.24	88,88,88,88	0
58	MG	2A	3538	1/1	0.59	0.31	77,77,77,77	0
58	MG	1A	3813	1/1	0.60	0.23	60,60,60,60	0
58	MG	2A	3668	1/1	0.60	0.15	73,73,73,73	0
58	MG	1A	3569	1/1	0.61	0.19	64,64,64,64	0
58	MG	2a	1606	1/1	0.62	0.31	81,81,81,81	0
58	MG	1a	1680	1/1	0.63	0.33	80,80,80,80	0
58	MG	2a	1741	1/1	0.63	0.29	84,84,84,84	0
58	MG	1v	101	1/1	0.64	0.27	88,88,88,88	0
58	MG	2A	3107	1/1	0.64	0.26	63,63,63,63	0
58	MG	2a	1802	1/1	0.64	0.14	82,82,82,82	0
58	MG	1A	3960	1/1	0.65	0.14	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	2a	1727	1/1	0.66	0.20	70,70,70,70	0
58	MG	2a	1762	1/1	0.66	0.15	81,81,81,81	0
58	MG	1a	1788	1/1	0.67	0.17	82,82,82,82	0
58	MG	1B	233	1/1	0.67	0.21	76,76,76,76	0
58	MG	1A	3998	1/1	0.68	0.30	83,83,83,83	0
58	MG	2A	3595	1/1	0.68	0.21	70,70,70,70	0
58	MG	1A	4094	1/1	0.68	0.21	79,79,79,79	0
58	MG	1a	1747	1/1	0.68	0.28	75,75,75,75	0
58	MG	2A	3535	1/1	0.68	0.20	79,79,79,79	0
58	MG	2A	3576	1/1	0.69	0.21	51,51,51,51	0
58	MG	2a	1708	1/1	0.69	0.15	88,88,88,88	0
58	MG	1A	4087	1/1	0.69	0.26	72,72,72,72	0
58	MG	2A	3243	1/1	0.69	0.28	83,83,83,83	0
58	MG	1a	1777	1/1	0.70	0.18	75,75,75,75	0
58	MG	1a	1812	1/1	0.70	0.20	79,79,79,79	0
58	MG	1U	212	1/1	0.71	0.44	60,60,60,60	0
58	MG	1a	1796	1/1	0.71	0.13	80,80,80,80	0
58	MG	2A	3610	1/1	0.71	0.21	89,89,89,89	0
58	MG	1A	3326	1/1	0.72	0.32	70,70,70,70	0
58	MG	2a	1644	1/1	0.72	0.12	79,79,79,79	0
58	MG	2a	1649	1/1	0.72	0.18	86,86,86,86	0
58	MG	2A	3341	1/1	0.72	0.22	73,73,73,73	0
58	MG	2A	3534	1/1	0.72	0.18	73,73,73,73	0
58	MG	1A	3512	1/1	0.73	0.17	75,75,75,75	0
58	MG	1A	3719	1/1	0.73	0.25	70,70,70,70	0
58	MG	2A	3025	1/1	0.74	0.25	61,61,61,61	0
58	MG	1B	229	1/1	0.74	0.21	71,71,71,71	0
58	MG	1a	1604	1/1	0.74	0.20	65,65,65,65	0
58	MG	2A	3553	1/1	0.74	0.18	50,50,50,50	0
58	MG	2a	1766	1/1	0.74	0.28	75,75,75,75	0
58	MG	1A	3796	1/1	0.74	0.18	80,80,80,80	0
58	MG	2A	3434	1/1	0.74	0.14	49,49,49,49	0
58	MG	2a	1808	1/1	0.74	0.28	63,63,63,63	0
58	MG	2v	101	1/1	0.74	0.18	69,69,69,69	0
58	MG	1A	3843	1/1	0.75	0.19	63,63,63,63	0
58	MG	1A	3883	1/1	0.75	0.36	76,76,76,76	0
58	MG	18	107	1/1	0.75	0.22	76,76,76,76	0
58	MG	1A	3926	1/1	0.75	0.13	44,44,44,44	0
58	MG	1a	1808	1/1	0.75	0.23	88,88,88,88	0
58	MG	1A	3266	1/1	0.75	0.20	68,68,68,68	0
58	MG	2l	201	1/1	0.75	0.18	69,69,69,69	0
58	MG	2l	206	1/1	0.75	0.14	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	2A	3526	1/1	0.75	0.15	82,82,82,82	0
58	MG	2B	212	1/1	0.76	0.17	73,73,73,73	0
58	MG	2A	3342	1/1	0.76	0.13	59,59,59,59	0
58	MG	2a	1625	1/1	0.76	0.37	76,76,76,76	0
58	MG	2a	1643	1/1	0.76	0.19	66,66,66,66	0
58	MG	2A	3356	1/1	0.76	0.11	51,51,51,51	0
58	MG	1A	4021	1/1	0.76	0.20	54,54,54,54	0
58	MG	1A	3369	1/1	0.76	0.24	65,65,65,65	0
58	MG	1a	1607	1/1	0.76	0.35	71,71,71,71	0
58	MG	1a	1665	1/1	0.76	0.29	68,68,68,68	0
58	MG	2a	1783	1/1	0.77	0.17	73,73,73,73	0
58	MG	1l	201	1/1	0.77	0.20	79,79,79,79	0
58	MG	2a	1613	1/1	0.77	0.41	77,77,77,77	0
58	MG	1A	3463	1/1	0.77	0.13	53,53,53,53	0
58	MG	2A	3371	1/1	0.77	0.29	65,65,65,65	0
58	MG	2A	3406	1/1	0.77	0.16	61,61,61,61	0
58	MG	1A	4078	1/1	0.77	0.15	67,67,67,67	0
58	MG	1A	3754	1/1	0.78	0.10	33,33,33,33	0
58	MG	2A	3318	1/1	0.78	0.25	71,71,71,71	0
58	MG	2a	1745	1/1	0.78	0.22	76,76,76,76	0
58	MG	1a	1809	1/1	0.78	0.21	73,73,73,73	0
58	MG	2a	1607	1/1	0.78	0.25	75,75,75,75	0
58	MG	1a	1741	1/1	0.78	0.24	68,68,68,68	0
58	MG	2A	3544	1/1	0.78	0.30	60,60,60,60	0
58	MG	2a	1785	1/1	0.78	0.17	83,83,83,83	0
58	MG	1A	3961	1/1	0.78	0.10	24,24,24,24	0
58	MG	1A	3523	1/1	0.78	0.23	71,71,71,71	0
58	MG	2a	1804	1/1	0.78	0.21	73,73,73,73	0
58	MG	1A	3942	1/1	0.78	0.11	22,22,22,22	0
58	MG	2a	1675	1/1	0.78	0.29	78,78,78,78	0
58	MG	2a	1691	1/1	0.78	0.35	85,85,85,85	0
58	MG	1A	4069	1/1	0.78	0.22	45,45,45,45	0
58	MG	1a	1707	1/1	0.79	0.25	68,68,68,68	0
58	MG	1a	1720	1/1	0.79	0.24	75,75,75,75	0
58	MG	2A	3614	1/1	0.79	0.14	50,50,50,50	0
58	MG	1a	1722	1/1	0.79	0.13	75,75,75,75	0
58	MG	2a	1748	1/1	0.79	0.14	79,79,79,79	0
58	MG	1A	3632	1/1	0.79	0.17	61,61,61,61	0
58	MG	1B	230	1/1	0.79	0.19	70,70,70,70	0
58	MG	2A	3057	1/1	0.79	0.11	56,56,56,56	0
58	MG	1A	3691	1/1	0.79	0.21	65,65,65,65	0
58	MG	1I	201	1/1	0.79	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	1788	1/1	0.79	0.18	70,70,70,70	0
58	MG	2a	1634	1/1	0.79	0.22	66,66,66,66	0
58	MG	2a	1799	1/1	0.79	0.25	79,79,79,79	0
58	MG	2a	1642	1/1	0.79	0.17	78,78,78,78	0
58	MG	2A	3260	1/1	0.79	0.29	59,59,59,59	0
58	MG	2a	1807	1/1	0.79	0.25	79,79,79,79	0
58	MG	2A	3306	1/1	0.79	0.15	50,50,50,50	0
58	MG	2d	301	1/1	0.79	0.17	75,75,75,75	0
58	MG	1a	1671	1/1	0.79	0.34	74,74,74,74	0
58	MG	2A	3572	1/1	0.79	0.16	72,72,72,72	0
58	MG	1A	3588	1/1	0.79	0.13	69,69,69,69	0
58	MG	2a	1703	1/1	0.80	0.20	70,70,70,70	0
58	MG	2A	3232	1/1	0.80	0.26	63,63,63,63	0
58	MG	2a	1723	1/1	0.80	0.23	81,81,81,81	0
58	MG	1A	3840	1/1	0.80	0.14	60,60,60,60	0
58	MG	1B	202	1/1	0.80	0.30	68,68,68,68	0
58	MG	1a	1781	1/1	0.80	0.15	64,64,64,64	0
58	MG	1a	1639	1/1	0.80	0.18	76,76,76,76	0
58	MG	1A	3656	1/1	0.80	0.20	55,55,55,55	0
58	MG	1A	4015	1/1	0.80	0.20	62,62,62,62	0
58	MG	1A	3264	1/1	0.80	0.27	72,72,72,72	0
58	MG	2a	1603	1/1	0.80	0.19	71,71,71,71	0
58	MG	2A	3361	1/1	0.80	0.25	80,80,80,80	0
58	MG	2A	3366	1/1	0.80	0.17	63,63,63,63	0
58	MG	1A	3381	1/1	0.80	0.28	66,66,66,66	0
58	MG	2a	1620	1/1	0.80	0.29	87,87,87,87	0
58	MG	2a	1800	1/1	0.80	0.30	65,65,65,65	0
58	MG	1O	202	1/1	0.80	0.25	69,69,69,69	0
58	MG	1A	3815	1/1	0.80	0.12	42,42,42,42	0
58	MG	2A	3444	1/1	0.80	0.21	39,39,39,39	0
58	MG	1a	1735	1/1	0.80	0.21	67,67,67,67	0
58	MG	1a	1737	1/1	0.80	0.15	80,80,80,80	0
58	MG	2A	3070	1/1	0.80	0.17	79,79,79,79	0
58	MG	1A	3824	1/1	0.80	0.14	60,60,60,60	0
58	MG	2A	3230	1/1	0.80	0.24	77,77,77,77	0
58	MG	2A	3247	1/1	0.81	0.15	73,73,73,73	0
58	MG	1A	3753	1/1	0.81	0.20	66,66,66,66	0
58	MG	2A	3541	1/1	0.81	0.17	60,60,60,60	0
58	MG	2a	1660	1/1	0.81	0.14	77,77,77,77	0
58	MG	1A	3972	1/1	0.81	0.12	66,66,66,66	0
58	MG	2A	3547	1/1	0.81	0.29	71,71,71,71	0
58	MG	1e	201	1/1	0.81	0.18	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	226	1/1	0.81	0.14	67,67,67,67	0
58	MG	2a	1709	1/1	0.81	0.26	65,65,65,65	0
58	MG	1A	3616	1/1	0.81	0.11	57,57,57,57	0
58	MG	1A	3462	1/1	0.81	0.15	75,75,75,75	0
58	MG	1A	3913	1/1	0.81	0.22	38,38,38,38	0
58	MG	2a	1743	1/1	0.81	0.40	86,86,86,86	0
58	MG	1a	1779	1/1	0.81	0.14	56,56,56,56	0
58	MG	2A	3666	1/1	0.81	0.22	73,73,73,73	0
58	MG	1A	3529	1/1	0.81	0.34	59,59,59,59	0
58	MG	2A	3682	1/1	0.81	0.18	56,56,56,56	0
58	MG	2B	201	1/1	0.81	0.29	76,76,76,76	0
58	MG	2B	208	1/1	0.81	0.27	79,79,79,79	0
58	MG	2A	3376	1/1	0.81	0.15	51,51,51,51	0
58	MG	2E	305	1/1	0.81	0.23	82,82,82,82	0
58	MG	2A	3404	1/1	0.81	0.26	71,71,71,71	0
58	MG	2A	3179	1/1	0.81	0.11	65,65,65,65	0
58	MG	2A	3198	1/1	0.81	0.30	71,71,71,71	0
58	MG	2a	1609	1/1	0.81	0.44	71,71,71,71	0
58	MG	2a	1612	1/1	0.81	0.50	80,80,80,80	0
58	MG	1a	1700	1/1	0.81	0.35	75,75,75,75	0
58	MG	2A	3466	1/1	0.81	0.10	52,52,52,52	0
58	MG	2a	1622	1/1	0.81	0.34	68,68,68,68	0
58	MG	2j	201	1/1	0.81	0.15	77,77,77,77	0
58	MG	2A	3495	1/1	0.81	0.20	67,67,67,67	0
58	MG	1A	3351	1/1	0.81	0.20	60,60,60,60	0
58	MG	1A	3401	1/1	0.81	0.24	63,63,63,63	0
58	MG	2A	3436	1/1	0.82	0.26	58,58,58,58	0
58	MG	2B	209	1/1	0.82	0.24	80,80,80,80	0
58	MG	2a	1722	1/1	0.82	0.24	81,81,81,81	0
58	MG	1A	3477	1/1	0.82	0.13	67,67,67,67	0
58	MG	2E	303	1/1	0.82	0.12	66,66,66,66	0
58	MG	2a	1737	1/1	0.82	0.46	78,78,78,78	0
58	MG	1b	301	1/1	0.82	0.14	79,79,79,79	0
58	MG	1A	3102	1/1	0.82	0.28	66,66,66,66	0
58	MG	2a	1604	1/1	0.82	0.25	80,80,80,80	0
58	MG	1A	3513	1/1	0.82	0.17	81,81,81,81	0
58	MG	1a	1669	1/1	0.82	0.34	77,77,77,77	0
58	MG	2A	3328	1/1	0.82	0.17	66,66,66,66	0
58	MG	2A	3335	1/1	0.82	0.25	68,68,68,68	0
58	MG	1a	1762	1/1	0.82	0.16	65,65,65,65	0
58	MG	2a	1618	1/1	0.82	0.20	76,76,76,76	0
58	MG	1A	3806	1/1	0.82	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3343	1/1	0.82	0.20	57,57,57,57	0
58	MG	2A	3353	1/1	0.82	0.18	67,67,67,67	0
58	MG	1A	3648	1/1	0.82	0.24	58,58,58,58	0
58	MG	2A	3360	1/1	0.82	0.19	55,55,55,55	0
58	MG	2A	3090	1/1	0.82	0.26	66,66,66,66	0
58	MG	1A	3412	1/1	0.82	0.27	74,74,74,74	0
58	MG	2A	3176	1/1	0.82	0.23	69,69,69,69	0
58	MG	2a	1812	1/1	0.82	0.32	73,73,73,73	0
58	MG	1A	4092	1/1	0.82	0.12	49,49,49,49	0
58	MG	1A	3185	1/1	0.82	0.15	68,68,68,68	0
58	MG	1A	3205	1/1	0.82	0.10	56,56,56,56	0
58	MG	2a	1701	1/1	0.82	0.29	71,71,71,71	0
58	MG	1a	1734	1/1	0.82	0.13	61,61,61,61	0
58	MG	2x	3303	1/1	0.82	0.24	79,79,79,79	0
58	MG	1a	1742	1/1	0.83	0.18	75,75,75,75	0
58	MG	1A	3362	1/1	0.83	0.36	51,51,51,51	0
58	MG	2A	3188	1/1	0.83	0.15	69,69,69,69	0
58	MG	2a	1652	1/1	0.83	0.28	71,71,71,71	0
58	MG	2a	1657	1/1	0.83	0.18	75,75,75,75	0
58	MG	1a	1758	1/1	0.83	0.18	64,64,64,64	0
58	MG	2A	3205	1/1	0.83	0.35	71,71,71,71	0
58	MG	2A	3222	1/1	0.83	0.30	80,80,80,80	0
58	MG	2A	3225	1/1	0.83	0.31	76,76,76,76	0
58	MG	1A	3767	1/1	0.83	0.11	18,18,18,18	0
58	MG	1a	1765	1/1	0.83	0.14	65,65,65,65	0
58	MG	1a	1772	1/1	0.83	0.19	78,78,78,78	0
58	MG	2a	1714	1/1	0.83	0.19	73,73,73,73	0
58	MG	1A	3422	1/1	0.83	0.23	71,71,71,71	0
58	MG	1a	1623	1/1	0.83	0.39	65,65,65,65	0
58	MG	2a	1726	1/1	0.83	0.21	73,73,73,73	0
58	MG	1A	3028	1/1	0.83	0.29	77,77,77,77	0
58	MG	1a	1652	1/1	0.83	0.20	68,68,68,68	0
58	MG	2a	1739	1/1	0.83	0.36	74,74,74,74	0
58	MG	2A	3319	1/1	0.83	0.12	68,68,68,68	0
58	MG	1A	3341	1/1	0.83	0.12	54,54,54,54	0
58	MG	1B	225	1/1	0.83	0.17	55,55,55,55	0
58	MG	2B	204	1/1	0.83	0.21	79,79,79,79	0
58	MG	1A	3473	1/1	0.83	0.10	62,62,62,62	0
58	MG	1A	3821	1/1	0.83	0.16	54,54,54,54	0
58	MG	2B	210	1/1	0.83	0.28	69,69,69,69	0
58	MG	1A	3705	1/1	0.83	0.10	55,55,55,55	0
58	MG	1A	3309	1/1	0.83	0.22	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	1709	1/1	0.83	0.30	62,62,62,62	0
58	MG	20	103	1/1	0.83	0.26	58,58,58,58	0
58	MG	1n	101	1/1	0.83	0.12	51,51,51,51	0
58	MG	1t	201	1/1	0.83	0.19	65,65,65,65	0
58	MG	1A	3597	1/1	0.83	0.35	42,42,42,42	0
58	MG	1w	101	1/1	0.83	0.09	66,66,66,66	0
58	MG	1N	201	1/1	0.83	0.20	52,52,52,52	0
58	MG	2A	3028	1/1	0.83	0.22	65,65,65,65	0
58	MG	1A	3871	1/1	0.83	0.17	39,39,39,39	0
58	MG	1T	202	1/1	0.83	0.21	52,52,52,52	0
58	MG	1A	4070	1/1	0.83	0.14	61,61,61,61	0
58	MG	2A	3102	1/1	0.83	0.32	79,79,79,79	0
58	MG	2A	3458	1/1	0.83	0.15	53,53,53,53	0
58	MG	2t	201	1/1	0.83	0.17	54,54,54,54	0
58	MG	1W	201	1/1	0.83	0.22	52,52,52,52	0
58	MG	2A	3119	1/1	0.83	0.18	72,72,72,72	0
58	MG	1A	3979	1/1	0.84	0.15	65,65,65,65	0
58	MG	2a	1640	1/1	0.84	0.16	59,59,59,59	0
58	MG	1a	1663	1/1	0.84	0.12	58,58,58,58	0
58	MG	2A	3531	1/1	0.84	0.16	76,76,76,76	0
58	MG	2A	3237	1/1	0.84	0.33	56,56,56,56	0
58	MG	1a	1759	1/1	0.84	0.13	60,60,60,60	0
58	MG	2A	3246	1/1	0.84	0.15	61,61,61,61	0
58	MG	2a	1654	1/1	0.84	0.13	79,79,79,79	0
58	MG	2A	3539	1/1	0.84	0.26	70,70,70,70	0
58	MG	1w	106	1/1	0.84	0.12	76,76,76,76	0
58	MG	1x	104	1/1	0.84	0.22	62,62,62,62	0
58	MG	2A	3267	1/1	0.84	0.35	66,66,66,66	0
58	MG	2A	3268	1/1	0.84	0.26	72,72,72,72	0
58	MG	2A	3557	1/1	0.84	0.20	66,66,66,66	0
58	MG	2A	3566	1/1	0.84	0.14	58,58,58,58	0
58	MG	2A	3273	1/1	0.84	0.24	62,62,62,62	0
58	MG	2A	3278	1/1	0.84	0.17	72,72,72,72	0
58	MG	2A	3582	1/1	0.84	0.18	63,63,63,63	0
58	MG	1x	109	1/1	0.84	0.32	67,67,67,67	0
58	MG	2A	3606	1/1	0.84	0.11	72,72,72,72	0
58	MG	2A	3307	1/1	0.84	0.28	70,70,70,70	0
58	MG	2A	3612	1/1	0.84	0.13	70,70,70,70	0
58	MG	1A	3270	1/1	0.84	0.14	54,54,54,54	0
58	MG	1P	202	1/1	0.84	0.20	46,46,46,46	0
58	MG	2A	3056	1/1	0.84	0.13	63,63,63,63	0
58	MG	2A	3330	1/1	0.84	0.35	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	2A	3333	1/1	0.84	0.23	62,62,62,62	0
58	MG	1A	3251	1/1	0.84	0.15	56,56,56,56	0
58	MG	2a	1756	1/1	0.84	0.30	66,66,66,66	0
58	MG	2B	205	1/1	0.84	0.24	73,73,73,73	0
58	MG	1A	3578	1/1	0.84	0.10	32,32,32,32	0
58	MG	2A	3089	1/1	0.84	0.24	69,69,69,69	0
58	MG	1a	1696	1/1	0.84	0.27	62,62,62,62	0
58	MG	1A	4042	1/1	0.84	0.17	57,57,57,57	0
58	MG	1Y	203	1/1	0.84	0.13	71,71,71,71	0
58	MG	2a	1795	1/1	0.84	0.22	64,64,64,64	0
58	MG	1A	3263	1/1	0.84	0.27	70,70,70,70	0
58	MG	2A	3127	1/1	0.84	0.10	71,71,71,71	0
58	MG	2A	3128	1/1	0.84	0.24	61,61,61,61	0
58	MG	1A	3870	1/1	0.84	0.20	46,46,46,46	0
58	MG	2a	1806	1/1	0.84	0.22	73,73,73,73	0
58	MG	1A	3593	1/1	0.84	0.29	60,60,60,60	0
58	MG	2A	3378	1/1	0.84	0.34	64,64,64,64	0
58	MG	2A	3180	1/1	0.84	0.22	59,59,59,59	0
58	MG	2a	1817	1/1	0.84	0.28	67,67,67,67	0
58	MG	2a	1820	1/1	0.84	0.33	75,75,75,75	0
58	MG	2a	1610	1/1	0.84	0.26	72,72,72,72	0
58	MG	1G	203	1/1	0.84	0.13	61,61,61,61	0
58	MG	1a	1630	1/1	0.84	0.34	59,59,59,59	0
58	MG	2l	204	1/1	0.84	0.28	73,73,73,73	0
58	MG	2A	3203	1/1	0.84	0.33	65,65,65,65	0
58	MG	1A	3878	1/1	0.84	0.27	63,63,63,63	0
58	MG	1a	1641	1/1	0.84	0.18	73,73,73,73	0
58	MG	1a	1647	1/1	0.84	0.25	70,70,70,70	0
58	MG	2A	3139	1/1	0.85	0.14	68,68,68,68	0
58	MG	1A	3603	1/1	0.85	0.30	71,71,71,71	0
58	MG	1A	3349	1/1	0.85	0.15	65,65,65,65	0
58	MG	1A	3896	1/1	0.85	0.28	81,81,81,81	0
58	MG	2A	3355	1/1	0.85	0.20	67,67,67,67	0
58	MG	1A	3033	1/1	0.85	0.18	38,38,38,38	0
58	MG	2A	3623	1/1	0.85	0.13	58,58,58,58	0
58	MG	2A	3628	1/1	0.85	0.11	35,35,35,35	0
58	MG	1d	301	1/1	0.85	0.39	61,61,61,61	0
58	MG	1a	1708	1/1	0.85	0.21	61,61,61,61	0
58	MG	2A	3671	1/1	0.85	0.17	67,67,67,67	0
58	MG	2A	3674	1/1	0.85	0.11	58,58,58,58	0
58	MG	2A	3678	1/1	0.85	0.13	60,60,60,60	0
58	MG	2A	3680	1/1	0.85	0.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1729	1/1	0.85	0.23	57,57,57,57	0
58	MG	1A	3920	1/1	0.85	0.14	47,47,47,47	0
58	MG	2A	3221	1/1	0.85	0.14	73,73,73,73	0
58	MG	2A	3373	1/1	0.85	0.19	64,64,64,64	0
58	MG	15	104	1/1	0.85	0.11	59,59,59,59	0
58	MG	1A	3441	1/1	0.85	0.12	52,52,52,52	0
58	MG	2A	3379	1/1	0.85	0.18	64,64,64,64	0
58	MG	2A	3400	1/1	0.85	0.22	64,64,64,64	0
58	MG	1A	3538	1/1	0.85	0.14	62,62,62,62	0
58	MG	1A	3954	1/1	0.85	0.16	65,65,65,65	0
58	MG	1w	104	1/1	0.85	0.09	83,83,83,83	0
58	MG	2V	201	1/1	0.85	0.16	62,62,62,62	0
58	MG	1a	1614	1/1	0.85	0.12	66,66,66,66	0
58	MG	28	101	1/1	0.85	0.19	64,64,64,64	0
58	MG	2A	3244	1/1	0.85	0.15	67,67,67,67	0
58	MG	1a	1619	1/1	0.85	0.18	61,61,61,61	0
58	MG	1A	3816	1/1	0.85	0.13	39,39,39,39	0
58	MG	2A	3005	1/1	0.85	0.20	66,66,66,66	0
58	MG	2A	3263	1/1	0.85	0.20	58,58,58,58	0
58	MG	2A	3528	1/1	0.85	0.15	62,62,62,62	0
58	MG	1A	3189	1/1	0.85	0.25	61,61,61,61	0
58	MG	1A	3193	1/1	0.85	0.14	54,54,54,54	0
58	MG	1A	3149	1/1	0.85	0.14	40,40,40,40	0
58	MG	1a	1644	1/1	0.85	0.18	65,65,65,65	0
58	MG	2a	1813	1/1	0.85	0.19	61,61,61,61	0
58	MG	1A	3346	1/1	0.85	0.12	52,52,52,52	0
58	MG	1a	1767	1/1	0.85	0.12	63,63,63,63	0
58	MG	1E	311	1/1	0.85	0.21	57,57,57,57	0
58	MG	2g	201	1/1	0.85	0.15	78,78,78,78	0
58	MG	1A	3404	1/1	0.85	0.10	55,55,55,55	0
58	MG	2A	3324	1/1	0.85	0.34	63,63,63,63	0
58	MG	1A	3758	1/1	0.85	0.17	56,56,56,56	0
58	MG	1A	4028	1/1	0.85	0.14	56,56,56,56	0
58	MG	2q	202	1/1	0.85	0.15	83,83,83,83	0
58	MG	2a	1645	1/1	0.85	0.19	77,77,77,77	0
58	MG	1A	4036	1/1	0.85	0.11	25,25,25,25	0
58	MG	1a	1678	1/1	0.85	0.19	68,68,68,68	0
58	MG	2A	3096	1/1	0.86	0.20	54,54,54,54	0
58	MG	1A	3514	1/1	0.86	0.16	75,75,75,75	0
58	MG	1A	3405	1/1	0.86	0.11	68,68,68,68	0
58	MG	2a	1674	1/1	0.86	0.28	69,69,69,69	0
58	MG	1A	4072	1/1	0.86	0.25	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	1689	1/1	0.86	0.22	71,71,71,71	0
58	MG	2A	3122	1/1	0.86	0.19	70,70,70,70	0
58	MG	2a	1700	1/1	0.86	0.16	72,72,72,72	0
58	MG	1A	3526	1/1	0.86	0.28	58,58,58,58	0
58	MG	2A	3638	1/1	0.86	0.11	45,45,45,45	0
58	MG	1A	3880	1/1	0.86	0.14	59,59,59,59	0
58	MG	1A	3350	1/1	0.86	0.13	53,53,53,53	0
58	MG	2A	3175	1/1	0.86	0.26	63,63,63,63	0
58	MG	1A	3166	1/1	0.86	0.37	63,63,63,63	0
58	MG	1A	3548	1/1	0.86	0.41	41,41,41,41	0
58	MG	1a	1648	1/1	0.86	0.26	60,60,60,60	0
58	MG	2A	3181	1/1	0.86	0.26	56,56,56,56	0
58	MG	1a	1802	1/1	0.86	0.10	60,60,60,60	0
58	MG	2a	1732	1/1	0.86	0.42	84,84,84,84	0
58	MG	1B	216	1/1	0.86	0.13	70,70,70,70	0
58	MG	1A	3756	1/1	0.86	0.11	64,64,64,64	0
58	MG	1A	3325	1/1	0.86	0.20	54,54,54,54	0
58	MG	1A	3937	1/1	0.86	0.12	61,61,61,61	0
58	MG	1A	3455	1/1	0.86	0.17	39,39,39,39	0
58	MG	1A	3584	1/1	0.86	0.19	71,71,71,71	0
58	MG	2a	1751	1/1	0.86	0.23	72,72,72,72	0
58	MG	1A	3025	1/1	0.86	0.18	52,52,52,52	0
58	MG	1A	3104	1/1	0.86	0.11	63,63,63,63	0
58	MG	1A	3967	1/1	0.86	0.15	53,53,53,53	0
58	MG	20	102	1/1	0.86	0.09	62,62,62,62	0
58	MG	1A	3814	1/1	0.86	0.15	38,38,38,38	0
58	MG	2A	3482	1/1	0.86	0.19	68,68,68,68	0
58	MG	2a	1787	1/1	0.86	0.24	68,68,68,68	0
58	MG	1A	3390	1/1	0.86	0.13	55,55,55,55	0
58	MG	1A	3994	1/1	0.86	0.11	34,34,34,34	0
58	MG	2a	1792	1/1	0.86	0.16	71,71,71,71	0
58	MG	1R	206	1/1	0.86	0.12	41,41,41,41	0
58	MG	1A	3997	1/1	0.86	0.20	83,83,83,83	0
58	MG	1A	3393	1/1	0.86	0.35	39,39,39,39	0
58	MG	2A	3264	1/1	0.86	0.19	54,54,54,54	0
58	MG	1x	111	1/1	0.86	0.33	69,69,69,69	0
58	MG	1A	3604	1/1	0.86	0.24	75,75,75,75	0
58	MG	2a	1617	1/1	0.86	0.17	70,70,70,70	0
58	MG	2A	3271	1/1	0.86	0.34	70,70,70,70	0
58	MG	2A	3023	1/1	0.86	0.21	54,54,54,54	0
58	MG	1A	3502	1/1	0.86	0.16	56,56,56,56	0
58	MG	10	104	1/1	0.86	0.24	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	1628	1/1	0.86	0.23	78,78,78,78	0
58	MG	1A	3107	1/1	0.86	0.15	52,52,52,52	0
58	MG	2a	1639	1/1	0.86	0.14	79,79,79,79	0
58	MG	2A	3560	1/1	0.86	0.18	47,47,47,47	0
58	MG	1a	1746	1/1	0.86	0.14	56,56,56,56	0
58	MG	2l	203	1/1	0.86	0.17	70,70,70,70	0
58	MG	1A	3090	1/1	0.86	0.12	53,53,53,53	0
58	MG	2A	3083	1/1	0.86	0.17	66,66,66,66	0
58	MG	1A	4040	1/1	0.86	0.16	56,56,56,56	0
58	MG	2r	101	1/1	0.86	0.24	74,74,74,74	0
58	MG	2A	3587	1/1	0.86	0.11	62,62,62,62	0
58	MG	1A	3856	1/1	0.86	0.14	48,48,48,48	0
58	MG	2a	1653	1/1	0.86	0.34	74,74,74,74	0
58	MG	2A	3655	1/1	0.87	0.12	60,60,60,60	0
58	MG	2a	1694	1/1	0.87	0.20	57,57,57,57	0
58	MG	2a	1699	1/1	0.87	0.13	78,78,78,78	0
58	MG	2A	3217	1/1	0.87	0.23	59,59,59,59	0
58	MG	1A	3912	1/1	0.87	0.21	44,44,44,44	0
58	MG	1a	1716	1/1	0.87	0.19	63,63,63,63	0
58	MG	1A	3027	1/1	0.87	0.19	69,69,69,69	0
58	MG	1A	3728	1/1	0.87	0.14	65,65,65,65	0
58	MG	1Z	301	1/1	0.87	0.07	55,55,55,55	0
58	MG	2a	1719	1/1	0.87	0.16	69,69,69,69	0
58	MG	1A	3924	1/1	0.87	0.14	64,64,64,64	0
58	MG	2A	3419	1/1	0.87	0.16	33,33,33,33	0
58	MG	2a	1725	1/1	0.87	0.38	52,52,52,52	0
58	MG	2A	3242	1/1	0.87	0.29	60,60,60,60	0
58	MG	1A	3491	1/1	0.87	0.20	72,72,72,72	0
58	MG	1A	4074	1/1	0.87	0.16	65,65,65,65	0
58	MG	2A	3006	1/1	0.87	0.26	56,56,56,56	0
58	MG	2a	1733	1/1	0.87	0.22	74,74,74,74	0
58	MG	1A	3831	1/1	0.87	0.12	56,56,56,56	0
58	MG	2A	3470	1/1	0.87	0.13	53,53,53,53	0
58	MG	2D	306	1/1	0.87	0.18	67,67,67,67	0
58	MG	1A	3605	1/1	0.87	0.14	49,49,49,49	0
58	MG	2A	3483	1/1	0.87	0.16	66,66,66,66	0
58	MG	2a	1747	1/1	0.87	0.34	79,79,79,79	0
58	MG	2A	3487	1/1	0.87	0.13	32,32,32,32	0
58	MG	1A	3943	1/1	0.87	0.14	38,38,38,38	0
58	MG	2A	3499	1/1	0.87	0.17	61,61,61,61	0
58	MG	2a	1754	1/1	0.87	0.22	70,70,70,70	0
58	MG	1A	3842	1/1	0.87	0.12	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	1A	3501	1/1	0.87	0.38	53,53,53,53	0
58	MG	1a	1627	1/1	0.87	0.12	49,49,49,49	0
58	MG	2a	1776	1/1	0.87	0.22	61,61,61,61	0
58	MG	1A	3854	1/1	0.87	0.13	47,47,47,47	0
58	MG	1A	3580	1/1	0.87	0.12	48,48,48,48	0
58	MG	2A	3277	1/1	0.87	0.21	55,55,55,55	0
58	MG	1A	3644	1/1	0.87	0.12	52,52,52,52	0
58	MG	1A	3343	1/1	0.87	0.20	55,55,55,55	0
58	MG	2A	3542	1/1	0.87	0.10	64,64,64,64	0
58	MG	1a	1778	1/1	0.87	0.14	36,36,36,36	0
58	MG	1A	3505	1/1	0.87	0.23	46,46,46,46	0
58	MG	1A	3530	1/1	0.87	0.27	71,71,71,71	0
58	MG	2a	1621	1/1	0.87	0.19	67,67,67,67	0
58	MG	1A	3881	1/1	0.87	0.10	29,29,29,29	0
58	MG	1A	4012	1/1	0.87	0.14	74,74,74,74	0
58	MG	2A	3562	1/1	0.87	0.12	51,51,51,51	0
58	MG	1a	1797	1/1	0.87	0.21	62,62,62,62	0
58	MG	1G	204	1/1	0.87	0.14	64,64,64,64	0
58	MG	2A	3573	1/1	0.87	0.14	53,53,53,53	0
58	MG	1A	3320	1/1	0.87	0.14	45,45,45,45	0
58	MG	1A	4017	1/1	0.87	0.21	63,63,63,63	0
58	MG	1N	204	1/1	0.87	0.13	57,57,57,57	0
58	MG	2d	302	1/1	0.87	0.24	53,53,53,53	0
58	MG	2f	202	1/1	0.87	0.15	72,72,72,72	0
58	MG	2A	3590	1/1	0.87	0.12	55,55,55,55	0
58	MG	2a	1647	1/1	0.87	0.23	63,63,63,63	0
58	MG	1A	3884	1/1	0.87	0.13	30,30,30,30	0
58	MG	2A	3602	1/1	0.87	0.25	75,75,75,75	0
58	MG	1A	3888	1/1	0.87	0.16	51,51,51,51	0
58	MG	2A	3186	1/1	0.87	0.15	63,63,63,63	0
58	MG	1A	4033	1/1	0.87	0.17	55,55,55,55	0
58	MG	1a	1705	1/1	0.87	0.26	73,73,73,73	0
58	MG	1A	3714	1/1	0.87	0.13	45,45,45,45	0
58	MG	1U	203	1/1	0.87	0.21	68,68,68,68	0
58	MG	2A	3215	1/1	0.87	0.12	66,66,66,66	0
58	MG	1A	3002	1/1	0.88	0.23	57,57,57,57	0
58	MG	2A	3386	1/1	0.88	0.23	65,65,65,65	0
58	MG	2A	3395	1/1	0.88	0.23	67,67,67,67	0
58	MG	1A	3704	1/1	0.88	0.11	32,32,32,32	0
58	MG	2A	3402	1/1	0.88	0.25	63,63,63,63	0
58	MG	1a	1712	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3154	1/1	0.88	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3370	1/1	0.88	0.20	45,45,45,45	0
58	MG	2a	1614	1/1	0.88	0.20	60,60,60,60	0
58	MG	1A	3718	1/1	0.88	0.10	52,52,52,52	0
58	MG	1E	308	1/1	0.88	0.12	30,30,30,30	0
58	MG	1A	3097	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3447	1/1	0.88	0.17	47,47,47,47	0
58	MG	2A	3151	1/1	0.88	0.27	71,71,71,71	0
58	MG	2A	3459	1/1	0.88	0.11	48,48,48,48	0
58	MG	1A	3271	1/1	0.88	0.10	45,45,45,45	0
58	MG	2a	1633	1/1	0.88	0.26	76,76,76,76	0
58	MG	1A	3730	1/1	0.88	0.20	55,55,55,55	0
58	MG	2a	1635	1/1	0.88	0.26	75,75,75,75	0
58	MG	2a	1637	1/1	0.88	0.14	55,55,55,55	0
58	MG	2A	3472	1/1	0.88	0.27	62,62,62,62	0
58	MG	2A	3474	1/1	0.88	0.20	46,46,46,46	0
58	MG	2A	3481	1/1	0.88	0.18	57,57,57,57	0
58	MG	1A	3731	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3739	1/1	0.88	0.15	51,51,51,51	0
58	MG	1A	3747	1/1	0.88	0.10	19,19,19,19	0
58	MG	2a	1646	1/1	0.88	0.09	65,65,65,65	0
58	MG	1A	3949	1/1	0.88	0.19	72,72,72,72	0
58	MG	1A	3041	1/1	0.88	0.14	52,52,52,52	0
58	MG	2A	3503	1/1	0.88	0.11	65,65,65,65	0
58	MG	2A	3509	1/1	0.88	0.29	43,43,43,43	0
58	MG	2A	3513	1/1	0.88	0.16	40,40,40,40	0
58	MG	2a	1655	1/1	0.88	0.30	81,81,81,81	0
58	MG	2A	3522	1/1	0.88	0.19	52,52,52,52	0
58	MG	1A	3054	1/1	0.88	0.11	52,52,52,52	0
58	MG	2A	3200	1/1	0.88	0.28	63,63,63,63	0
58	MG	1a	1764	1/1	0.88	0.11	70,70,70,70	0
58	MG	2a	1678	1/1	0.88	0.14	70,70,70,70	0
58	MG	1A	3190	1/1	0.88	0.20	42,42,42,42	0
58	MG	2a	1690	1/1	0.88	0.15	80,80,80,80	0
58	MG	1A	3063	1/1	0.88	0.17	61,61,61,61	0
58	MG	1A	3334	1/1	0.88	0.20	52,52,52,52	0
58	MG	1A	3773	1/1	0.88	0.14	44,44,44,44	0
58	MG	1A	3980	1/1	0.88	0.13	64,64,64,64	0
58	MG	1A	3336	1/1	0.88	0.09	50,50,50,50	0
58	MG	1A	3803	1/1	0.88	0.10	21,21,21,21	0
58	MG	2A	3546	1/1	0.88	0.15	49,49,49,49	0
58	MG	1A	3435	1/1	0.88	0.34	54,54,54,54	0
58	MG	2a	1710	1/1	0.88	0.28	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	3338	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3453	1/1	0.88	0.10	61,61,61,61	0
58	MG	1A	3340	1/1	0.88	0.17	39,39,39,39	0
58	MG	1A	3118	1/1	0.88	0.28	52,52,52,52	0
58	MG	1A	3594	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3567	1/1	0.88	0.13	64,64,64,64	0
58	MG	2A	3569	1/1	0.88	0.14	54,54,54,54	0
58	MG	1A	4032	1/1	0.88	0.12	55,55,55,55	0
58	MG	2A	3257	1/1	0.88	0.23	41,41,41,41	0
58	MG	2A	3574	1/1	0.88	0.11	78,78,78,78	0
58	MG	2a	1734	1/1	0.88	0.28	65,65,65,65	0
58	MG	2a	1735	1/1	0.88	0.20	65,65,65,65	0
58	MG	1A	3130	1/1	0.88	0.18	62,62,62,62	0
58	MG	2A	3577	1/1	0.88	0.15	61,61,61,61	0
58	MG	1A	3471	1/1	0.88	0.17	49,49,49,49	0
58	MG	1a	1631	1/1	0.88	0.16	61,61,61,61	0
58	MG	1A	3253	1/1	0.88	0.15	76,76,76,76	0
58	MG	1A	3258	1/1	0.88	0.15	64,64,64,64	0
58	MG	1p	101	1/1	0.88	0.23	64,64,64,64	0
58	MG	2A	3605	1/1	0.88	0.12	54,54,54,54	0
58	MG	1a	1643	1/1	0.88	0.20	59,59,59,59	0
58	MG	1A	4046	1/1	0.88	0.14	59,59,59,59	0
58	MG	2A	3611	1/1	0.88	0.10	62,62,62,62	0
58	MG	2a	1761	1/1	0.88	0.15	65,65,65,65	0
58	MG	1A	3486	1/1	0.88	0.12	61,61,61,61	0
58	MG	2A	3302	1/1	0.88	0.37	78,78,78,78	0
58	MG	2A	3615	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3617	1/1	0.88	0.10	26,26,26,26	0
58	MG	1w	105	1/1	0.88	0.23	79,79,79,79	0
58	MG	2A	3633	1/1	0.88	0.11	54,54,54,54	0
58	MG	2A	3315	1/1	0.88	0.16	63,63,63,63	0
58	MG	2A	3645	1/1	0.88	0.11	71,71,71,71	0
58	MG	1A	3260	1/1	0.88	0.12	51,51,51,51	0
58	MG	2A	3664	1/1	0.88	0.17	77,77,77,77	0
58	MG	2a	1798	1/1	0.88	0.22	67,67,67,67	0
58	MG	2A	3665	1/1	0.88	0.10	63,63,63,63	0
58	MG	1A	3493	1/1	0.88	0.12	51,51,51,51	0
58	MG	2a	1801	1/1	0.88	0.17	55,55,55,55	0
58	MG	1x	107	1/1	0.88	0.29	71,71,71,71	0
58	MG	1A	3139	1/1	0.88	0.36	36,36,36,36	0
58	MG	1x	110	1/1	0.88	0.30	65,65,65,65	0
58	MG	2A	3675	1/1	0.88	0.18	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3332	1/1	0.88	0.28	58,58,58,58	0
58	MG	1A	4081	1/1	0.88	0.12	47,47,47,47	0
58	MG	1A	4084	1/1	0.88	0.12	54,54,54,54	0
58	MG	1a	1672	1/1	0.88	0.15	62,62,62,62	0
58	MG	1A	3875	1/1	0.88	0.25	44,44,44,44	0
58	MG	1A	4088	1/1	0.88	0.22	63,63,63,63	0
58	MG	1a	1681	1/1	0.88	0.17	76,76,76,76	0
58	MG	2A	3041	1/1	0.88	0.14	68,68,68,68	0
58	MG	1a	1691	1/1	0.88	0.23	61,61,61,61	0
58	MG	1A	3361	1/1	0.88	0.18	43,43,43,43	0
58	MG	2A	3063	1/1	0.88	0.13	54,54,54,54	0
58	MG	1A	3663	1/1	0.88	0.16	52,52,52,52	0
58	MG	2A	3367	1/1	0.88	0.08	62,62,62,62	0
58	MG	2F	303	1/1	0.88	0.20	52,52,52,52	0
58	MG	2A	3075	1/1	0.88	0.10	70,70,70,70	0
58	MG	1a	1704	1/1	0.88	0.16	64,64,64,64	0
58	MG	1A	3685	1/1	0.88	0.13	46,46,46,46	0
58	MG	1A	3689	1/1	0.88	0.10	47,47,47,47	0
58	MG	2a	1602	1/1	0.88	0.14	74,74,74,74	0
58	MG	2x	3304	1/1	0.88	0.16	67,67,67,67	0
58	MG	1B	212	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1684	1/1	0.89	0.14	55,55,55,55	0
58	MG	1a	1689	1/1	0.89	0.32	64,64,64,64	0
58	MG	1A	3269	1/1	0.89	0.19	59,59,59,59	0
58	MG	2a	1608	1/1	0.89	0.53	72,72,72,72	0
58	MG	2A	3078	1/1	0.89	0.19	66,66,66,66	0
58	MG	1a	1692	1/1	0.89	0.31	55,55,55,55	0
58	MG	1A	3928	1/1	0.89	0.11	47,47,47,47	0
58	MG	2A	3407	1/1	0.89	0.17	43,43,43,43	0
58	MG	1A	3113	1/1	0.89	0.19	42,42,42,42	0
58	MG	2a	1616	1/1	0.89	0.10	72,72,72,72	0
58	MG	2A	3433	1/1	0.89	0.13	48,48,48,48	0
58	MG	1A	3776	1/1	0.89	0.12	27,27,27,27	0
58	MG	2A	3435	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3099	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3608	1/1	0.89	0.12	46,46,46,46	0
58	MG	2A	3106	1/1	0.89	0.10	52,52,52,52	0
58	MG	1B	231	1/1	0.89	0.13	54,54,54,54	0
58	MG	2A	3112	1/1	0.89	0.22	50,50,50,50	0
58	MG	1A	3945	1/1	0.89	0.15	65,65,65,65	0
58	MG	1A	3798	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3471	1/1	0.89	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3133	1/1	0.89	0.21	56,56,56,56	0
58	MG	1A	3291	1/1	0.89	0.15	59,59,59,59	0
58	MG	2A	3134	1/1	0.89	0.10	67,67,67,67	0
58	MG	1a	1718	1/1	0.89	0.27	69,69,69,69	0
58	MG	2A	3150	1/1	0.89	0.15	49,49,49,49	0
58	MG	1a	1719	1/1	0.89	0.27	59,59,59,59	0
58	MG	1A	3807	1/1	0.89	0.12	54,54,54,54	0
58	MG	1A	3304	1/1	0.89	0.36	62,62,62,62	0
58	MG	2A	3501	1/1	0.89	0.23	51,51,51,51	0
58	MG	2A	3177	1/1	0.89	0.43	71,71,71,71	0
58	MG	1a	1729	1/1	0.89	0.14	66,66,66,66	0
58	MG	1A	3348	1/1	0.89	0.44	44,44,44,44	0
58	MG	2A	3520	1/1	0.89	0.22	57,57,57,57	0
58	MG	1A	3974	1/1	0.89	0.16	70,70,70,70	0
58	MG	1O	201	1/1	0.89	0.09	65,65,65,65	0
58	MG	2a	1664	1/1	0.89	0.14	65,65,65,65	0
58	MG	2a	1668	1/1	0.89	0.30	59,59,59,59	0
58	MG	2a	1669	1/1	0.89	0.24	70,70,70,70	0
58	MG	1A	3416	1/1	0.89	0.08	58,58,58,58	0
58	MG	1O	205	1/1	0.89	0.18	56,56,56,56	0
58	MG	2a	1676	1/1	0.89	0.24	69,69,69,69	0
58	MG	1A	3420	1/1	0.89	0.14	52,52,52,52	0
58	MG	2a	1686	1/1	0.89	0.21	71,71,71,71	0
58	MG	2A	3201	1/1	0.89	0.20	63,63,63,63	0
58	MG	1P	206	1/1	0.89	0.24	57,57,57,57	0
58	MG	2A	3204	1/1	0.89	0.21	55,55,55,55	0
58	MG	1R	201	1/1	0.89	0.18	58,58,58,58	0
58	MG	2a	1696	1/1	0.89	0.13	76,76,76,76	0
58	MG	1A	3515	1/1	0.89	0.07	67,67,67,67	0
58	MG	1A	3995	1/1	0.89	0.12	24,24,24,24	0
58	MG	1A	3666	1/1	0.89	0.09	33,33,33,33	0
58	MG	1U	207	1/1	0.89	0.25	48,48,48,48	0
58	MG	1A	3164	1/1	0.89	0.43	35,35,35,35	0
58	MG	1a	1769	1/1	0.89	0.10	62,62,62,62	0
58	MG	1A	3053	1/1	0.89	0.24	46,46,46,46	0
58	MG	1A	4014	1/1	0.89	0.11	63,63,63,63	0
58	MG	2A	3239	1/1	0.89	0.12	61,61,61,61	0
58	MG	1A	3324	1/1	0.89	0.10	45,45,45,45	0
58	MG	1A	3695	1/1	0.89	0.12	25,25,25,25	0
58	MG	14	101	1/1	0.89	0.23	78,78,78,78	0
58	MG	1A	4018	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3851	1/1	0.89	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	2a	1728	1/1	0.89	0.33	80,80,80,80	0
58	MG	1a	1602	1/1	0.89	0.45	74,74,74,74	0
58	MG	1A	3442	1/1	0.89	0.09	43,43,43,43	0
58	MG	2A	3578	1/1	0.89	0.19	55,55,55,55	0
58	MG	1A	3452	1/1	0.89	0.15	64,64,64,64	0
58	MG	1a	1611	1/1	0.89	0.12	71,71,71,71	0
58	MG	1a	1811	1/1	0.89	0.10	65,65,65,65	0
58	MG	2A	3593	1/1	0.89	0.14	68,68,68,68	0
58	MG	1A	3167	1/1	0.89	0.09	33,33,33,33	0
58	MG	2A	3269	1/1	0.89	0.30	56,56,56,56	0
58	MG	2A	3270	1/1	0.89	0.27	61,61,61,61	0
58	MG	1A	3566	1/1	0.89	0.14	45,45,45,45	0
58	MG	1A	3874	1/1	0.89	0.18	33,33,33,33	0
58	MG	1a	1626	1/1	0.89	0.40	64,64,64,64	0
58	MG	1A	3221	1/1	0.89	0.23	44,44,44,44	0
58	MG	2A	3281	1/1	0.89	0.30	53,53,53,53	0
58	MG	2A	3285	1/1	0.89	0.23	63,63,63,63	0
58	MG	2A	3619	1/1	0.89	0.13	53,53,53,53	0
58	MG	1A	3329	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3304	1/1	0.89	0.30	60,60,60,60	0
58	MG	1A	4064	1/1	0.89	0.11	53,53,53,53	0
58	MG	2a	1778	1/1	0.89	0.18	55,55,55,55	0
58	MG	1a	1638	1/1	0.89	0.16	59,59,59,59	0
58	MG	1A	3265	1/1	0.89	0.12	61,61,61,61	0
58	MG	2A	3648	1/1	0.89	0.10	60,60,60,60	0
58	MG	2A	3654	1/1	0.89	0.11	36,36,36,36	0
58	MG	1A	3468	1/1	0.89	0.13	50,50,50,50	0
58	MG	1w	102	1/1	0.89	0.24	73,73,73,73	0
58	MG	2A	3321	1/1	0.89	0.18	63,63,63,63	0
58	MG	2A	3323	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1642	1/1	0.89	0.25	78,78,78,78	0
58	MG	1A	3587	1/1	0.89	0.16	64,64,64,64	0
58	MG	1A	3740	1/1	0.89	0.17	62,62,62,62	0
58	MG	1A	4077	1/1	0.89	0.14	54,54,54,54	0
58	MG	1x	106	1/1	0.89	0.20	73,73,73,73	0
58	MG	1A	3371	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3378	1/1	0.89	0.10	68,68,68,68	0
58	MG	1a	1659	1/1	0.89	0.24	72,72,72,72	0
58	MG	1A	3897	1/1	0.89	0.08	46,46,46,46	0
58	MG	2A	3345	1/1	0.89	0.14	46,46,46,46	0
58	MG	2a	1816	1/1	0.89	0.17	64,64,64,64	0
58	MG	2A	3348	1/1	0.89	0.17	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	1a	1664	1/1	0.89	0.15	64,64,64,64	0
58	MG	1A	3908	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3019	1/1	0.89	0.27	65,65,65,65	0
58	MG	2f	201	1/1	0.89	0.18	61,61,61,61	0
58	MG	2B	215	1/1	0.89	0.22	75,75,75,75	0
58	MG	1A	3379	1/1	0.89	0.12	63,63,63,63	0
58	MG	1A	4090	1/1	0.89	0.17	60,60,60,60	0
58	MG	2E	304	1/1	0.89	0.09	34,34,34,34	0
58	MG	2A	3363	1/1	0.89	0.23	54,54,54,54	0
58	MG	1A	3233	1/1	0.89	0.10	48,48,48,48	0
58	MG	2P	201	1/1	0.89	0.13	50,50,50,50	0
58	MG	2A	3031	1/1	0.89	0.24	63,63,63,63	0
58	MG	2Z	301	1/1	0.89	0.23	71,71,71,71	0
58	MG	2A	3033	1/1	0.89	0.22	56,56,56,56	0
58	MG	1A	3489	1/1	0.89	0.12	61,61,61,61	0
58	MG	2w	101	1/1	0.89	0.27	68,68,68,68	0
58	MG	2A	3043	1/1	0.89	0.12	69,69,69,69	0
58	MG	1A	3764	1/1	0.89	0.13	16,16,16,16	0
58	MG	2x	3305	1/1	0.89	0.28	66,66,66,66	0
58	MG	2A	3013	1/1	0.90	0.27	49,49,49,49	0
58	MG	2B	202	1/1	0.90	0.33	71,71,71,71	0
58	MG	2A	3018	1/1	0.90	0.31	43,43,43,43	0
58	MG	1A	3018	1/1	0.90	0.19	32,32,32,32	0
58	MG	1A	3804	1/1	0.90	0.10	40,40,40,40	0
58	MG	1a	1673	1/1	0.90	0.12	58,58,58,58	0
58	MG	1a	1674	1/1	0.90	0.28	68,68,68,68	0
58	MG	2A	3339	1/1	0.90	0.28	49,49,49,49	0
58	MG	1A	3311	1/1	0.90	0.26	57,57,57,57	0
58	MG	1A	3408	1/1	0.90	0.20	61,61,61,61	0
58	MG	2E	301	1/1	0.90	0.16	70,70,70,70	0
58	MG	2A	3034	1/1	0.90	0.09	62,62,62,62	0
58	MG	2A	3036	1/1	0.90	0.13	56,56,56,56	0
58	MG	2A	3040	1/1	0.90	0.20	67,67,67,67	0
58	MG	2A	3352	1/1	0.90	0.13	45,45,45,45	0
58	MG	1A	3618	1/1	0.90	0.15	52,52,52,52	0
58	MG	1A	3411	1/1	0.90	0.09	55,55,55,55	0
58	MG	2X	101	1/1	0.90	0.09	71,71,71,71	0
58	MG	2A	3045	1/1	0.90	0.23	71,71,71,71	0
58	MG	2A	3048	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	3503	1/1	0.90	0.16	70,70,70,70	0
58	MG	2A	3362	1/1	0.90	0.20	62,62,62,62	0
58	MG	2a	1601	1/1	0.90	0.16	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	3315	1/1	0.90	0.08	34,34,34,34	0
58	MG	2A	3364	1/1	0.90	0.26	63,63,63,63	0
58	MG	1A	3817	1/1	0.90	0.11	52,52,52,52	0
58	MG	2a	1605	1/1	0.90	0.32	71,71,71,71	0
58	MG	2A	3064	1/1	0.90	0.35	65,65,65,65	0
58	MG	1a	1695	1/1	0.90	0.28	72,72,72,72	0
58	MG	1A	3983	1/1	0.90	0.10	34,34,34,34	0
58	MG	1A	3655	1/1	0.90	0.11	58,58,58,58	0
58	MG	1a	1701	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3088	1/1	0.90	0.13	59,59,59,59	0
58	MG	2A	3383	1/1	0.90	0.17	50,50,50,50	0
58	MG	1A	3211	1/1	0.90	0.14	68,68,68,68	0
58	MG	2A	3390	1/1	0.90	0.31	73,73,73,73	0
58	MG	1A	3220	1/1	0.90	0.13	54,54,54,54	0
58	MG	2A	3399	1/1	0.90	0.36	66,66,66,66	0
58	MG	2a	1619	1/1	0.90	0.10	74,74,74,74	0
58	MG	2A	3092	1/1	0.90	0.14	50,50,50,50	0
58	MG	1A	3837	1/1	0.90	0.13	63,63,63,63	0
58	MG	1A	4004	1/1	0.90	0.10	37,37,37,37	0
58	MG	1A	4007	1/1	0.90	0.07	43,43,43,43	0
58	MG	1A	3354	1/1	0.90	0.13	62,62,62,62	0
58	MG	2A	3416	1/1	0.90	0.12	47,47,47,47	0
58	MG	1a	1715	1/1	0.90	0.23	55,55,55,55	0
58	MG	2A	3426	1/1	0.90	0.17	54,54,54,54	0
58	MG	2A	3429	1/1	0.90	0.13	56,56,56,56	0
58	MG	2a	1638	1/1	0.90	0.22	64,64,64,64	0
58	MG	1A	3683	1/1	0.90	0.09	26,26,26,26	0
58	MG	1A	3424	1/1	0.90	0.12	55,55,55,55	0
58	MG	2A	3121	1/1	0.90	0.28	63,63,63,63	0
58	MG	1T	201	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3442	1/1	0.90	0.20	41,41,41,41	0
58	MG	1A	4016	1/1	0.90	0.11	62,62,62,62	0
58	MG	1a	1721	1/1	0.90	0.29	71,71,71,71	0
58	MG	2A	3131	1/1	0.90	0.36	63,63,63,63	0
58	MG	2a	1648	1/1	0.90	0.11	81,81,81,81	0
58	MG	1A	3844	1/1	0.90	0.12	51,51,51,51	0
58	MG	2A	3135	1/1	0.90	0.20	73,73,73,73	0
58	MG	2A	3469	1/1	0.90	0.23	39,39,39,39	0
58	MG	2A	3136	1/1	0.90	0.10	50,50,50,50	0
58	MG	2A	3138	1/1	0.90	0.12	51,51,51,51	0
58	MG	2a	1656	1/1	0.90	0.14	59,59,59,59	0
58	MG	1U	205	1/1	0.90	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1658	1/1	0.90	0.30	76,76,76,76	0
58	MG	2A	3147	1/1	0.90	0.24	64,64,64,64	0
58	MG	2A	3477	1/1	0.90	0.27	64,64,64,64	0
58	MG	2a	1666	1/1	0.90	0.29	61,61,61,61	0
58	MG	2A	3479	1/1	0.90	0.17	45,45,45,45	0
58	MG	1A	3432	1/1	0.90	0.08	61,61,61,61	0
58	MG	1A	3852	1/1	0.90	0.23	44,44,44,44	0
58	MG	2A	3158	1/1	0.90	0.16	58,58,58,58	0
58	MG	2A	3486	1/1	0.90	0.14	35,35,35,35	0
58	MG	2A	3159	1/1	0.90	0.16	61,61,61,61	0
58	MG	2a	1680	1/1	0.90	0.22	64,64,64,64	0
58	MG	2a	1682	1/1	0.90	0.19	77,77,77,77	0
58	MG	2a	1684	1/1	0.90	0.28	68,68,68,68	0
58	MG	1A	4027	1/1	0.90	0.12	46,46,46,46	0
58	MG	1A	3433	1/1	0.90	0.13	49,49,49,49	0
58	MG	1A	3355	1/1	0.90	0.10	45,45,45,45	0
58	MG	10	101	1/1	0.90	0.10	42,42,42,42	0
58	MG	2A	3508	1/1	0.90	0.16	40,40,40,40	0
58	MG	1A	3075	1/1	0.90	0.20	57,57,57,57	0
58	MG	2a	1697	1/1	0.90	0.23	63,63,63,63	0
58	MG	1a	1757	1/1	0.90	0.20	68,68,68,68	0
58	MG	2A	3517	1/1	0.90	0.17	53,53,53,53	0
58	MG	10	107	1/1	0.90	0.15	61,61,61,61	0
58	MG	13	103	1/1	0.90	0.10	50,50,50,50	0
58	MG	2a	1706	1/1	0.90	0.18	75,75,75,75	0
58	MG	2A	3524	1/1	0.90	0.19	66,66,66,66	0
58	MG	2A	3525	1/1	0.90	0.26	63,63,63,63	0
58	MG	2A	3195	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3527	1/1	0.90	0.19	64,64,64,64	0
58	MG	2a	1718	1/1	0.90	0.19	70,70,70,70	0
58	MG	1A	3534	1/1	0.90	0.30	61,61,61,61	0
58	MG	15	102	1/1	0.90	0.37	34,34,34,34	0
58	MG	2A	3533	1/1	0.90	0.09	69,69,69,69	0
58	MG	2a	1724	1/1	0.90	0.17	64,64,64,64	0
58	MG	1A	3713	1/1	0.90	0.15	42,42,42,42	0
58	MG	2A	3202	1/1	0.90	0.28	61,61,61,61	0
58	MG	1A	3056	1/1	0.90	0.13	60,60,60,60	0
58	MG	1A	4043	1/1	0.90	0.11	56,56,56,56	0
58	MG	1a	1770	1/1	0.90	0.11	57,57,57,57	0
58	MG	2A	3208	1/1	0.90	0.34	47,47,47,47	0
58	MG	2A	3543	1/1	0.90	0.17	72,72,72,72	0
58	MG	2A	3211	1/1	0.90	0.13	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	3234	1/1	0.90	0.09	55,55,55,55	0
58	MG	1a	1605	1/1	0.90	0.13	51,51,51,51	0
58	MG	2A	3548	1/1	0.90	0.13	64,64,64,64	0
58	MG	2A	3551	1/1	0.90	0.28	61,61,61,61	0
58	MG	1A	3551	1/1	0.90	0.19	36,36,36,36	0
58	MG	1A	3564	1/1	0.90	0.42	39,39,39,39	0
58	MG	1A	3245	1/1	0.90	0.11	60,60,60,60	0
58	MG	2A	3229	1/1	0.90	0.21	46,46,46,46	0
58	MG	1a	1617	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1752	1/1	0.90	0.17	76,76,76,76	0
58	MG	1A	3335	1/1	0.90	0.19	53,53,53,53	0
58	MG	1a	1622	1/1	0.90	0.16	59,59,59,59	0
58	MG	2A	3238	1/1	0.90	0.36	78,78,78,78	0
58	MG	1A	3373	1/1	0.90	0.09	47,47,47,47	0
58	MG	1a	1806	1/1	0.90	0.38	73,73,73,73	0
58	MG	2a	1763	1/1	0.90	0.12	66,66,66,66	0
58	MG	2a	1764	1/1	0.90	0.20	70,70,70,70	0
58	MG	2a	1765	1/1	0.90	0.19	50,50,50,50	0
58	MG	1a	1624	1/1	0.90	0.18	60,60,60,60	0
58	MG	2a	1768	1/1	0.90	0.18	77,77,77,77	0
58	MG	2a	1771	1/1	0.90	0.18	73,73,73,73	0
58	MG	1A	4076	1/1	0.90	0.14	65,65,65,65	0
58	MG	1A	3249	1/1	0.90	0.34	67,67,67,67	0
58	MG	2a	1779	1/1	0.90	0.24	76,76,76,76	0
58	MG	2A	3579	1/1	0.90	0.15	40,40,40,40	0
58	MG	1A	3583	1/1	0.90	0.33	40,40,40,40	0
58	MG	1A	3465	1/1	0.90	0.30	54,54,54,54	0
58	MG	2A	3258	1/1	0.90	0.20	54,54,54,54	0
58	MG	2A	3591	1/1	0.90	0.16	52,52,52,52	0
58	MG	2a	1790	1/1	0.90	0.14	72,72,72,72	0
58	MG	1A	3586	1/1	0.90	0.14	44,44,44,44	0
58	MG	1A	4086	1/1	0.90	0.13	50,50,50,50	0
58	MG	2A	3597	1/1	0.90	0.12	61,61,61,61	0
58	MG	2A	3600	1/1	0.90	0.23	81,81,81,81	0
58	MG	1A	3122	1/1	0.90	0.17	40,40,40,40	0
58	MG	1A	3339	1/1	0.90	0.09	65,65,65,65	0
58	MG	1A	3760	1/1	0.90	0.08	32,32,32,32	0
58	MG	1A	3472	1/1	0.90	0.10	42,42,42,42	0
58	MG	1a	1645	1/1	0.90	0.18	49,49,49,49	0
58	MG	1A	3194	1/1	0.90	0.35	45,45,45,45	0
58	MG	1A	4095	1/1	0.90	0.13	55,55,55,55	0
58	MG	2a	1811	1/1	0.90	0.23	65,65,65,65	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	0.90	0.14	59,59,59,59	0
58	MG	1B	210	1/1	0.90	0.15	53,53,53,53	0
58	MG	2A	3620	1/1	0.90	0.12	76,76,76,76	0
58	MG	1a	1660	1/1	0.90	0.13	65,65,65,65	0
58	MG	2a	1818	1/1	0.90	0.14	74,74,74,74	0
58	MG	2a	1819	1/1	0.90	0.20	60,60,60,60	0
58	MG	1w	107	1/1	0.90	0.15	71,71,71,71	0
58	MG	2a	1821	1/1	0.90	0.27	70,70,70,70	0
58	MG	2A	3287	1/1	0.90	0.15	58,58,58,58	0
58	MG	2A	3296	1/1	0.90	0.20	54,54,54,54	0
58	MG	2A	3299	1/1	0.90	0.13	59,59,59,59	0
58	MG	1a	1661	1/1	0.90	0.20	66,66,66,66	0
58	MG	2A	3652	1/1	0.90	0.16	50,50,50,50	0
58	MG	1x	105	1/1	0.90	0.28	67,67,67,67	0
58	MG	2A	3305	1/1	0.90	0.11	55,55,55,55	0
58	MG	1a	1662	1/1	0.90	0.12	64,64,64,64	0
58	MG	1A	3479	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3309	1/1	0.90	0.17	69,69,69,69	0
58	MG	2A	3311	1/1	0.90	0.07	52,52,52,52	0
58	MG	2A	3313	1/1	0.90	0.37	55,55,55,55	0
58	MG	1B	215	1/1	0.90	0.17	60,60,60,60	0
58	MG	1A	3394	1/1	0.90	0.16	46,46,46,46	0
58	MG	1a	1666	1/1	0.90	0.26	64,64,64,64	0
58	MG	2x	3302	1/1	0.90	0.20	66,66,66,66	0
58	MG	1a	1667	1/1	0.90	0.22	63,63,63,63	0
58	MG	1A	3255	1/1	0.90	0.21	61,61,61,61	0
58	MG	2A	3685	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	3459	1/1	0.91	0.09	54,54,54,54	0
58	MG	2A	3493	1/1	0.91	0.14	77,77,77,77	0
58	MG	1x	102	1/1	0.91	0.16	68,68,68,68	0
58	MG	2A	3234	1/1	0.91	0.16	58,58,58,58	0
58	MG	2a	1624	1/1	0.91	0.12	66,66,66,66	0
58	MG	1A	3552	1/1	0.91	0.07	49,49,49,49	0
58	MG	2a	1626	1/1	0.91	0.25	63,63,63,63	0
58	MG	1A	3999	1/1	0.91	0.18	60,60,60,60	0
58	MG	1A	3183	1/1	0.91	0.21	49,49,49,49	0
58	MG	1A	4006	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3845	1/1	0.91	0.23	65,65,65,65	0
58	MG	2A	3514	1/1	0.91	0.23	52,52,52,52	0
58	MG	1A	4008	1/1	0.91	0.08	42,42,42,42	0
58	MG	2A	3518	1/1	0.91	0.25	66,66,66,66	0
58	MG	1O	204	1/1	0.91	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1641	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3847	1/1	0.91	0.08	65,65,65,65	0
58	MG	2A	3523	1/1	0.91	0.15	66,66,66,66	0
58	MG	2A	3248	1/1	0.91	0.16	67,67,67,67	0
58	MG	1a	1682	1/1	0.91	0.21	64,64,64,64	0
58	MG	1A	3386	1/1	0.91	0.27	43,43,43,43	0
58	MG	2A	3259	1/1	0.91	0.29	53,53,53,53	0
58	MG	1a	1688	1/1	0.91	0.31	46,46,46,46	0
58	MG	1A	3388	1/1	0.91	0.14	52,52,52,52	0
58	MG	2A	3022	1/1	0.91	0.18	51,51,51,51	0
58	MG	1A	3274	1/1	0.91	0.11	51,51,51,51	0
58	MG	1A	3579	1/1	0.91	0.15	37,37,37,37	0
58	MG	1S	202	1/1	0.91	0.10	73,73,73,73	0
58	MG	1A	3862	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3540	1/1	0.91	0.19	66,66,66,66	0
58	MG	2A	3032	1/1	0.91	0.13	57,57,57,57	0
58	MG	1a	1698	1/1	0.91	0.12	60,60,60,60	0
58	MG	1A	3280	1/1	0.91	0.31	48,48,48,48	0
58	MG	1A	3083	1/1	0.91	0.13	40,40,40,40	0
58	MG	1A	3293	1/1	0.91	0.07	38,38,38,38	0
58	MG	2A	3284	1/1	0.91	0.23	55,55,55,55	0
58	MG	1A	3402	1/1	0.91	0.15	49,49,49,49	0
58	MG	2A	3549	1/1	0.91	0.16	64,64,64,64	0
58	MG	1A	3067	1/1	0.91	0.22	66,66,66,66	0
58	MG	2a	1677	1/1	0.91	0.21	64,64,64,64	0
58	MG	2A	3552	1/1	0.91	0.11	54,54,54,54	0
58	MG	2a	1679	1/1	0.91	0.25	62,62,62,62	0
58	MG	2A	3294	1/1	0.91	0.15	62,62,62,62	0
58	MG	1A	4035	1/1	0.91	0.16	29,29,29,29	0
58	MG	2A	3559	1/1	0.91	0.11	61,61,61,61	0
58	MG	1W	202	1/1	0.91	0.14	49,49,49,49	0
58	MG	2A	3054	1/1	0.91	0.08	43,43,43,43	0
58	MG	1A	3745	1/1	0.91	0.10	59,59,59,59	0
58	MG	1A	3480	1/1	0.91	0.18	52,52,52,52	0
58	MG	2a	1692	1/1	0.91	0.19	57,57,57,57	0
58	MG	1A	3297	1/1	0.91	0.12	49,49,49,49	0
58	MG	1A	3300	1/1	0.91	0.18	44,44,44,44	0
58	MG	10	105	1/1	0.91	0.27	73,73,73,73	0
58	MG	2a	1698	1/1	0.91	0.12	78,78,78,78	0
58	MG	2A	3073	1/1	0.91	0.28	50,50,50,50	0
58	MG	1A	3093	1/1	0.91	0.28	53,53,53,53	0
58	MG	10	108	1/1	0.91	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3079	1/1	0.91	0.22	64,64,64,64	0
58	MG	2A	3081	1/1	0.91	0.19	56,56,56,56	0
58	MG	11	101	1/1	0.91	0.42	44,44,44,44	0
58	MG	2A	3086	1/1	0.91	0.24	53,53,53,53	0
58	MG	11	103	1/1	0.91	0.10	71,71,71,71	0
58	MG	13	102	1/1	0.91	0.15	59,59,59,59	0
58	MG	2a	1716	1/1	0.91	0.40	75,75,75,75	0
58	MG	1A	4047	1/1	0.91	0.19	46,46,46,46	0
58	MG	2A	3091	1/1	0.91	0.14	48,48,48,48	0
58	MG	1A	4050	1/1	0.91	0.10	47,47,47,47	0
58	MG	1A	3146	1/1	0.91	0.12	56,56,56,56	0
58	MG	2A	3601	1/1	0.91	0.15	59,59,59,59	0
58	MG	1A	3494	1/1	0.91	0.13	57,57,57,57	0
58	MG	2A	3340	1/1	0.91	0.16	58,58,58,58	0
58	MG	1A	3415	1/1	0.91	0.13	49,49,49,49	0
58	MG	2A	3105	1/1	0.91	0.13	50,50,50,50	0
58	MG	1a	1601	1/1	0.91	0.19	59,59,59,59	0
58	MG	1a	1751	1/1	0.91	0.12	53,53,53,53	0
58	MG	2A	3613	1/1	0.91	0.12	78,78,78,78	0
58	MG	1A	3116	1/1	0.91	0.07	50,50,50,50	0
58	MG	2A	3115	1/1	0.91	0.26	66,66,66,66	0
58	MG	1A	3198	1/1	0.91	0.31	52,52,52,52	0
58	MG	1A	3152	1/1	0.91	0.27	44,44,44,44	0
58	MG	1A	3921	1/1	0.91	0.09	60,60,60,60	0
58	MG	2A	3627	1/1	0.91	0.12	34,34,34,34	0
58	MG	2A	3358	1/1	0.91	0.12	70,70,70,70	0
58	MG	2a	1746	1/1	0.91	0.12	58,58,58,58	0
58	MG	1A	3507	1/1	0.91	0.14	56,56,56,56	0
58	MG	1A	4079	1/1	0.91	0.10	55,55,55,55	0
58	MG	1a	1615	1/1	0.91	0.14	55,55,55,55	0
58	MG	1A	3925	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3423	1/1	0.91	0.23	75,75,75,75	0
58	MG	1A	3322	1/1	0.91	0.11	51,51,51,51	0
58	MG	1a	1773	1/1	0.91	0.23	62,62,62,62	0
58	MG	2A	3657	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3661	1/1	0.91	0.09	55,55,55,55	0
58	MG	2A	3370	1/1	0.91	0.16	58,58,58,58	0
58	MG	1A	3117	1/1	0.91	0.18	38,38,38,38	0
58	MG	1A	3805	1/1	0.91	0.10	47,47,47,47	0
58	MG	1A	4089	1/1	0.91	0.12	54,54,54,54	0
58	MG	1a	1780	1/1	0.91	0.17	62,62,62,62	0
58	MG	2a	1770	1/1	0.91	0.16	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3152	1/1	0.91	0.14	58,58,58,58	0
58	MG	2a	1775	1/1	0.91	0.16	60,60,60,60	0
58	MG	2A	3381	1/1	0.91	0.25	48,48,48,48	0
58	MG	2a	1777	1/1	0.91	0.15	51,51,51,51	0
58	MG	2A	3153	1/1	0.91	0.22	63,63,63,63	0
58	MG	2A	3157	1/1	0.91	0.13	62,62,62,62	0
58	MG	2a	1780	1/1	0.91	0.11	62,62,62,62	0
58	MG	2A	3387	1/1	0.91	0.26	66,66,66,66	0
58	MG	2A	3389	1/1	0.91	0.29	63,63,63,63	0
58	MG	1A	3649	1/1	0.91	0.13	60,60,60,60	0
58	MG	1A	3650	1/1	0.91	0.18	34,34,34,34	0
58	MG	2A	3161	1/1	0.91	0.19	55,55,55,55	0
58	MG	2A	3168	1/1	0.91	0.15	45,45,45,45	0
58	MG	2B	206	1/1	0.91	0.15	57,57,57,57	0
58	MG	2B	207	1/1	0.91	0.15	72,72,72,72	0
58	MG	2a	1796	1/1	0.91	0.16	60,60,60,60	0
58	MG	1A	3948	1/1	0.91	0.26	66,66,66,66	0
58	MG	1a	1634	1/1	0.91	0.28	70,70,70,70	0
58	MG	1a	1636	1/1	0.91	0.15	61,61,61,61	0
58	MG	1a	1803	1/1	0.91	0.10	67,67,67,67	0
58	MG	1A	3812	1/1	0.91	0.45	36,36,36,36	0
58	MG	1A	3952	1/1	0.91	0.10	61,61,61,61	0
58	MG	2A	3185	1/1	0.91	0.18	68,68,68,68	0
58	MG	1A	3363	1/1	0.91	0.15	54,54,54,54	0
58	MG	1B	211	1/1	0.91	0.17	63,63,63,63	0
58	MG	2A	3191	1/1	0.91	0.20	68,68,68,68	0
58	MG	2F	301	1/1	0.91	0.09	54,54,54,54	0
58	MG	2F	302	1/1	0.91	0.11	63,63,63,63	0
58	MG	2a	1815	1/1	0.91	0.27	65,65,65,65	0
58	MG	1A	3006	1/1	0.91	0.15	64,64,64,64	0
58	MG	1a	1813	1/1	0.91	0.31	77,77,77,77	0
58	MG	2A	3199	1/1	0.91	0.17	63,63,63,63	0
58	MG	1B	213	1/1	0.91	0.12	44,44,44,44	0
58	MG	1A	3121	1/1	0.91	0.13	37,37,37,37	0
58	MG	2A	3449	1/1	0.91	0.29	58,58,58,58	0
58	MG	2A	3454	1/1	0.91	0.14	44,44,44,44	0
58	MG	23	101	1/1	0.91	0.31	70,70,70,70	0
58	MG	1A	3231	1/1	0.91	0.14	24,24,24,24	0
58	MG	1B	222	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3462	1/1	0.91	0.11	37,37,37,37	0
58	MG	2A	3464	1/1	0.91	0.21	57,57,57,57	0
58	MG	1A	3669	1/1	0.91	0.12	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	1A	3681	1/1	0.91	0.11	22,22,22,22	0
58	MG	1A	3977	1/1	0.91	0.11	65,65,65,65	0
58	MG	1A	3445	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3214	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3331	1/1	0.91	0.24	62,62,62,62	0
58	MG	1A	3832	1/1	0.91	0.14	47,47,47,47	0
58	MG	1w	103	1/1	0.91	0.10	65,65,65,65	0
58	MG	2v	102	1/1	0.91	0.17	74,74,74,74	0
58	MG	1A	3232	1/1	0.91	0.23	34,34,34,34	0
58	MG	1A	3081	1/1	0.91	0.12	65,65,65,65	0
58	MG	2A	3228	1/1	0.91	0.18	66,66,66,66	0
58	MG	2A	3484	1/1	0.91	0.17	54,54,54,54	0
58	MG	1F	310	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3155	1/1	0.92	0.06	51,51,51,51	0
58	MG	1A	3464	1/1	0.92	0.08	51,51,51,51	0
58	MG	1W	206	1/1	0.92	0.11	44,44,44,44	0
58	MG	1X	101	1/1	0.92	0.47	41,41,41,41	0
58	MG	2A	3160	1/1	0.92	0.15	48,48,48,48	0
58	MG	1A	3134	1/1	0.92	0.15	31,31,31,31	0
58	MG	1Y	204	1/1	0.92	0.20	51,51,51,51	0
58	MG	2A	3171	1/1	0.92	0.15	63,63,63,63	0
58	MG	2A	3172	1/1	0.92	0.14	40,40,40,40	0
58	MG	1A	3103	1/1	0.92	0.17	38,38,38,38	0
58	MG	2A	3453	1/1	0.92	0.17	34,34,34,34	0
58	MG	1A	3591	1/1	0.92	0.14	54,54,54,54	0
58	MG	2A	3455	1/1	0.92	0.16	45,45,45,45	0
58	MG	2A	3456	1/1	0.92	0.12	45,45,45,45	0
58	MG	1A	3169	1/1	0.92	0.08	31,31,31,31	0
58	MG	2A	3178	1/1	0.92	0.20	73,73,73,73	0
58	MG	1A	3170	1/1	0.92	0.14	40,40,40,40	0
58	MG	2A	3463	1/1	0.92	0.14	47,47,47,47	0
58	MG	1A	3144	1/1	0.92	0.15	53,53,53,53	0
58	MG	1a	1774	1/1	0.92	0.15	77,77,77,77	0
58	MG	1A	3406	1/1	0.92	0.12	56,56,56,56	0
58	MG	2a	1623	1/1	0.92	0.18	65,65,65,65	0
58	MG	1A	3819	1/1	0.92	0.15	70,70,70,70	0
58	MG	1A	3319	1/1	0.92	0.35	36,36,36,36	0
58	MG	2A	3189	1/1	0.92	0.17	66,66,66,66	0
58	MG	1A	3225	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3475	1/1	0.92	0.23	65,65,65,65	0
58	MG	1A	4025	1/1	0.92	0.10	54,54,54,54	0
58	MG	1a	1784	1/1	0.92	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3827	1/1	0.92	0.17	30,30,30,30	0
58	MG	1a	1790	1/1	0.92	0.09	73,73,73,73	0
58	MG	1A	3830	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3483	1/1	0.92	0.09	55,55,55,55	0
58	MG	1A	3609	1/1	0.92	0.08	41,41,41,41	0
58	MG	19	101	1/1	0.92	0.16	53,53,53,53	0
58	MG	1a	1804	1/1	0.92	0.15	60,60,60,60	0
58	MG	2A	3207	1/1	0.92	0.11	57,57,57,57	0
58	MG	2A	3496	1/1	0.92	0.15	41,41,41,41	0
58	MG	1A	3834	1/1	0.92	0.23	62,62,62,62	0
58	MG	2A	3209	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3227	1/1	0.92	0.14	58,58,58,58	0
58	MG	2A	3506	1/1	0.92	0.13	43,43,43,43	0
58	MG	1a	1603	1/1	0.92	0.20	71,71,71,71	0
58	MG	1A	3323	1/1	0.92	0.13	47,47,47,47	0
58	MG	1A	3490	1/1	0.92	0.17	45,45,45,45	0
58	MG	2A	3219	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3619	1/1	0.92	0.21	38,38,38,38	0
58	MG	1A	3626	1/1	0.92	0.12	35,35,35,35	0
58	MG	1a	1613	1/1	0.92	0.21	47,47,47,47	0
58	MG	2A	3521	1/1	0.92	0.22	70,70,70,70	0
58	MG	2a	1662	1/1	0.92	0.28	63,63,63,63	0
58	MG	1A	3357	1/1	0.92	0.16	57,57,57,57	0
58	MG	1f	202	1/1	0.92	0.20	66,66,66,66	0
58	MG	1A	4048	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3492	1/1	0.92	0.08	44,44,44,44	0
58	MG	2a	1671	1/1	0.92	0.23	59,59,59,59	0
58	MG	1A	4053	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3236	1/1	0.92	0.20	48,48,48,48	0
58	MG	1A	4061	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	4063	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3645	1/1	0.92	0.18	60,60,60,60	0
58	MG	1A	3417	1/1	0.92	0.26	47,47,47,47	0
58	MG	1A	3045	1/1	0.92	0.13	38,38,38,38	0
58	MG	1a	1629	1/1	0.92	0.28	61,61,61,61	0
58	MG	1A	3421	1/1	0.92	0.20	50,50,50,50	0
58	MG	1A	3858	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	4075	1/1	0.92	0.23	73,73,73,73	0
58	MG	1x	101	1/1	0.92	0.35	70,70,70,70	0
58	MG	1A	3096	1/1	0.92	0.21	53,53,53,53	0
58	MG	1A	3088	1/1	0.92	0.19	33,33,33,33	0
58	MG	2A	3545	1/1	0.92	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3659	1/1	0.92	0.11	40,40,40,40	0
58	MG	1A	3504	1/1	0.92	0.38	33,33,33,33	0
58	MG	1A	3327	1/1	0.92	0.23	59,59,59,59	0
58	MG	2A	3266	1/1	0.92	0.28	64,64,64,64	0
58	MG	1A	3426	1/1	0.92	0.13	58,58,58,58	0
58	MG	1A	3672	1/1	0.92	0.11	27,27,27,27	0
58	MG	1A	3510	1/1	0.92	0.11	47,47,47,47	0
58	MG	1A	3430	1/1	0.92	0.30	56,56,56,56	0
58	MG	1A	3431	1/1	0.92	0.11	53,53,53,53	0
58	MG	1A	3328	1/1	0.92	0.14	55,55,55,55	0
58	MG	1a	1656	1/1	0.92	0.15	63,63,63,63	0
58	MG	2a	1711	1/1	0.92	0.15	71,71,71,71	0
58	MG	2a	1713	1/1	0.92	0.22	63,63,63,63	0
58	MG	1a	1658	1/1	0.92	0.12	59,59,59,59	0
58	MG	1A	3191	1/1	0.92	0.18	34,34,34,34	0
58	MG	1A	4093	1/1	0.92	0.11	74,74,74,74	0
58	MG	2A	3571	1/1	0.92	0.21	53,53,53,53	0
58	MG	1A	3517	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3905	1/1	0.92	0.14	46,46,46,46	0
58	MG	2A	3288	1/1	0.92	0.25	43,43,43,43	0
58	MG	2A	3289	1/1	0.92	0.23	53,53,53,53	0
58	MG	1B	201	1/1	0.92	0.19	62,62,62,62	0
58	MG	2A	3295	1/1	0.92	0.21	70,70,70,70	0
58	MG	1A	3907	1/1	0.92	0.11	64,64,64,64	0
58	MG	2A	3581	1/1	0.92	0.08	52,52,52,52	0
58	MG	1B	204	1/1	0.92	0.28	67,67,67,67	0
58	MG	1B	207	1/1	0.92	0.15	69,69,69,69	0
58	MG	1A	3519	1/1	0.92	0.35	56,56,56,56	0
58	MG	1A	3521	1/1	0.92	0.48	49,49,49,49	0
58	MG	2A	3592	1/1	0.92	0.14	61,61,61,61	0
58	MG	1A	3114	1/1	0.92	0.16	34,34,34,34	0
58	MG	1A	3917	1/1	0.92	0.09	42,42,42,42	0
58	MG	2A	3308	1/1	0.92	0.09	51,51,51,51	0
58	MG	1A	3437	1/1	0.92	0.28	38,38,38,38	0
58	MG	2A	3046	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3715	1/1	0.92	0.08	53,53,53,53	0
58	MG	2A	3050	1/1	0.92	0.17	52,52,52,52	0
58	MG	2A	3316	1/1	0.92	0.17	60,60,60,60	0
58	MG	1A	3527	1/1	0.92	0.18	41,41,41,41	0
58	MG	1B	223	1/1	0.92	0.20	63,63,63,63	0
58	MG	1A	3439	1/1	0.92	0.24	39,39,39,39	0
58	MG	2A	3062	1/1	0.92	0.15	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	1758	1/1	0.92	0.07	50,50,50,50	0
58	MG	1A	3374	1/1	0.92	0.14	56,56,56,56	0
58	MG	1A	3333	1/1	0.92	0.26	52,52,52,52	0
58	MG	2A	3065	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3067	1/1	0.92	0.12	52,52,52,52	0
58	MG	1a	1687	1/1	0.92	0.21	47,47,47,47	0
58	MG	1A	3929	1/1	0.92	0.09	47,47,47,47	0
58	MG	2A	3338	1/1	0.92	0.27	65,65,65,65	0
58	MG	2a	1769	1/1	0.92	0.10	76,76,76,76	0
58	MG	1A	3281	1/1	0.92	0.28	32,32,32,32	0
58	MG	1A	3738	1/1	0.92	0.14	65,65,65,65	0
58	MG	2A	3644	1/1	0.92	0.10	69,69,69,69	0
58	MG	1E	302	1/1	0.92	0.23	35,35,35,35	0
58	MG	1A	3543	1/1	0.92	0.23	38,38,38,38	0
58	MG	1A	3446	1/1	0.92	0.13	51,51,51,51	0
58	MG	1F	307	1/1	0.92	0.10	52,52,52,52	0
58	MG	2A	3347	1/1	0.92	0.11	53,53,53,53	0
58	MG	1a	1699	1/1	0.92	0.22	52,52,52,52	0
58	MG	2A	3659	1/1	0.92	0.10	56,56,56,56	0
58	MG	1A	3550	1/1	0.92	0.29	44,44,44,44	0
58	MG	1A	3285	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3750	1/1	0.92	0.08	22,22,22,22	0
58	MG	1A	3247	1/1	0.92	0.17	54,54,54,54	0
58	MG	1A	3555	1/1	0.92	0.10	46,46,46,46	0
58	MG	2a	1793	1/1	0.92	0.14	76,76,76,76	0
58	MG	2A	3670	1/1	0.92	0.14	54,54,54,54	0
58	MG	1A	3556	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3966	1/1	0.92	0.11	41,41,41,41	0
58	MG	1A	3454	1/1	0.92	0.21	59,59,59,59	0
58	MG	2A	3676	1/1	0.92	0.13	66,66,66,66	0
58	MG	1A	3971	1/1	0.92	0.08	65,65,65,65	0
58	MG	1A	3387	1/1	0.92	0.12	65,65,65,65	0
58	MG	1A	3761	1/1	0.92	0.10	53,53,53,53	0
58	MG	2a	1805	1/1	0.92	0.10	62,62,62,62	0
58	MG	2A	3114	1/1	0.92	0.15	49,49,49,49	0
58	MG	2A	3686	1/1	0.92	0.20	58,58,58,58	0
58	MG	1A	3976	1/1	0.92	0.11	76,76,76,76	0
58	MG	2a	1810	1/1	0.92	0.18	57,57,57,57	0
58	MG	1A	3567	1/1	0.92	0.20	46,46,46,46	0
58	MG	2B	203	1/1	0.92	0.17	59,59,59,59	0
58	MG	2A	3120	1/1	0.92	0.15	46,46,46,46	0
58	MG	2a	1814	1/1	0.92	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	1R	205	1/1	0.92	0.11	32,32,32,32	0
58	MG	1A	3456	1/1	0.92	0.07	60,60,60,60	0
58	MG	1a	1724	1/1	0.92	0.18	59,59,59,59	0
58	MG	1A	3571	1/1	0.92	0.16	61,61,61,61	0
58	MG	2A	3129	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3384	1/1	0.92	0.14	68,68,68,68	0
58	MG	1a	1733	1/1	0.92	0.14	59,59,59,59	0
58	MG	2A	3132	1/1	0.92	0.20	53,53,53,53	0
58	MG	2D	305	1/1	0.92	0.16	45,45,45,45	0
58	MG	1A	3982	1/1	0.92	0.10	29,29,29,29	0
58	MG	1A	3572	1/1	0.92	0.14	51,51,51,51	0
58	MG	1U	201	1/1	0.92	0.29	40,40,40,40	0
58	MG	2A	3397	1/1	0.92	0.21	45,45,45,45	0
58	MG	1A	3057	1/1	0.92	0.09	35,35,35,35	0
58	MG	1A	3460	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3140	1/1	0.92	0.19	65,65,65,65	0
58	MG	2A	3403	1/1	0.92	0.16	60,60,60,60	0
58	MG	2O	201	1/1	0.92	0.12	61,61,61,61	0
58	MG	1a	1743	1/1	0.92	0.19	59,59,59,59	0
58	MG	1A	3461	1/1	0.92	0.25	54,54,54,54	0
58	MG	1A	3195	1/1	0.92	0.28	36,36,36,36	0
58	MG	2A	3408	1/1	0.92	0.10	52,52,52,52	0
58	MG	2A	3410	1/1	0.92	0.17	55,55,55,55	0
58	MG	1V	204	1/1	0.92	0.26	52,52,52,52	0
58	MG	1A	3197	1/1	0.92	0.36	34,34,34,34	0
58	MG	25	102	1/1	0.92	0.17	61,61,61,61	0
58	MG	27	102	1/1	0.92	0.08	49,49,49,49	0
58	MG	2A	3385	1/1	0.93	0.26	51,51,51,51	0
58	MG	1A	3962	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	3795	1/1	0.93	0.06	24,24,24,24	0
58	MG	1A	3089	1/1	0.93	0.26	41,41,41,41	0
58	MG	1A	3969	1/1	0.93	0.09	63,63,63,63	0
58	MG	1O	203	1/1	0.93	0.27	69,69,69,69	0
58	MG	2A	3396	1/1	0.93	0.19	55,55,55,55	0
58	MG	1A	3970	1/1	0.93	0.13	59,59,59,59	0
58	MG	2A	3398	1/1	0.93	0.26	63,63,63,63	0
58	MG	1A	3052	1/1	0.93	0.13	26,26,26,26	0
58	MG	2N	201	1/1	0.93	0.06	59,59,59,59	0
58	MG	1A	3802	1/1	0.93	0.11	24,24,24,24	0
58	MG	2A	3401	1/1	0.93	0.17	49,49,49,49	0
58	MG	1a	1725	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	3625	1/1	0.93	0.20	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	2X	102	1/1	0.93	0.21	54,54,54,54	0
58	MG	2A	3146	1/1	0.93	0.10	59,59,59,59	0
58	MG	1A	3236	1/1	0.93	0.20	44,44,44,44	0
58	MG	1A	3389	1/1	0.93	0.39	71,71,71,71	0
58	MG	1A	3640	1/1	0.93	0.10	57,57,57,57	0
58	MG	1S	201	1/1	0.93	0.10	56,56,56,56	0
58	MG	25	104	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3643	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3418	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3287	1/1	0.93	0.07	51,51,51,51	0
58	MG	2A	3423	1/1	0.93	0.21	58,58,58,58	0
58	MG	1A	3055	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3990	1/1	0.93	0.10	59,59,59,59	0
58	MG	1A	3992	1/1	0.93	0.07	46,46,46,46	0
58	MG	1a	1749	1/1	0.93	0.19	44,44,44,44	0
58	MG	1a	1750	1/1	0.93	0.17	55,55,55,55	0
58	MG	1A	3246	1/1	0.93	0.10	48,48,48,48	0
58	MG	1a	1756	1/1	0.93	0.15	54,54,54,54	0
58	MG	1U	206	1/1	0.93	0.28	42,42,42,42	0
58	MG	1A	3400	1/1	0.93	0.12	56,56,56,56	0
58	MG	2A	3448	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3125	1/1	0.93	0.16	47,47,47,47	0
58	MG	2a	1615	1/1	0.93	0.16	63,63,63,63	0
58	MG	2A	3450	1/1	0.93	0.10	47,47,47,47	0
58	MG	1a	1760	1/1	0.93	0.07	56,56,56,56	0
58	MG	1a	1761	1/1	0.93	0.13	66,66,66,66	0
58	MG	1A	3533	1/1	0.93	0.16	58,58,58,58	0
58	MG	1A	3818	1/1	0.93	0.10	50,50,50,50	0
58	MG	1A	4003	1/1	0.93	0.07	31,31,31,31	0
58	MG	2A	3183	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3461	1/1	0.93	0.23	40,40,40,40	0
58	MG	1W	205	1/1	0.93	0.17	31,31,31,31	0
58	MG	1A	3153	1/1	0.93	0.35	30,30,30,30	0
58	MG	1A	3403	1/1	0.93	0.16	56,56,56,56	0
58	MG	1Y	201	1/1	0.93	0.10	54,54,54,54	0
58	MG	2a	1629	1/1	0.93	0.28	69,69,69,69	0
58	MG	2A	3190	1/1	0.93	0.07	63,63,63,63	0
58	MG	1A	3540	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3192	1/1	0.93	0.14	59,59,59,59	0
58	MG	2a	1636	1/1	0.93	0.32	71,71,71,71	0
58	MG	2A	3193	1/1	0.93	0.13	62,62,62,62	0
58	MG	1A	3299	1/1	0.93	0.38	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	4011	1/1	0.93	0.12	57,57,57,57	0
58	MG	1A	3829	1/1	0.93	0.09	33,33,33,33	0
58	MG	1A	3196	1/1	0.93	0.17	32,32,32,32	0
58	MG	1A	3670	1/1	0.93	0.07	37,37,37,37	0
58	MG	10	106	1/1	0.93	0.10	48,48,48,48	0
58	MG	1A	3302	1/1	0.93	0.18	35,35,35,35	0
58	MG	1a	1787	1/1	0.93	0.11	58,58,58,58	0
58	MG	1A	3676	1/1	0.93	0.08	37,37,37,37	0
58	MG	1A	3467	1/1	0.93	0.23	56,56,56,56	0
58	MG	2A	3488	1/1	0.93	0.13	54,54,54,54	0
58	MG	2A	3489	1/1	0.93	0.15	54,54,54,54	0
58	MG	2a	1651	1/1	0.93	0.18	76,76,76,76	0
58	MG	2A	3490	1/1	0.93	0.20	44,44,44,44	0
58	MG	2A	3492	1/1	0.93	0.17	41,41,41,41	0
58	MG	11	102	1/1	0.93	0.20	51,51,51,51	0
58	MG	1A	3838	1/1	0.93	0.19	45,45,45,45	0
58	MG	1A	3303	1/1	0.93	0.17	40,40,40,40	0
58	MG	2A	3497	1/1	0.93	0.10	44,44,44,44	0
58	MG	1A	4026	1/1	0.93	0.07	43,43,43,43	0
58	MG	1A	3553	1/1	0.93	0.17	53,53,53,53	0
58	MG	1A	3470	1/1	0.93	0.18	41,41,41,41	0
58	MG	1A	4031	1/1	0.93	0.09	34,34,34,34	0
58	MG	2a	1665	1/1	0.93	0.13	62,62,62,62	0
58	MG	2A	3220	1/1	0.93	0.25	62,62,62,62	0
58	MG	1A	3410	1/1	0.93	0.13	51,51,51,51	0
58	MG	1A	3128	1/1	0.93	0.18	37,37,37,37	0
58	MG	2a	1670	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3696	1/1	0.93	0.13	21,21,21,21	0
58	MG	2a	1672	1/1	0.93	0.08	75,75,75,75	0
58	MG	2A	3515	1/1	0.93	0.11	56,56,56,56	0
58	MG	2A	3227	1/1	0.93	0.23	61,61,61,61	0
58	MG	1A	3849	1/1	0.93	0.16	45,45,45,45	0
58	MG	1A	4037	1/1	0.93	0.17	39,39,39,39	0
58	MG	1A	4039	1/1	0.93	0.12	43,43,43,43	0
58	MG	2A	3231	1/1	0.93	0.23	54,54,54,54	0
58	MG	1A	3699	1/1	0.93	0.10	26,26,26,26	0
58	MG	2a	1681	1/1	0.93	0.29	63,63,63,63	0
58	MG	1a	1606	1/1	0.93	0.06	69,69,69,69	0
58	MG	1A	3701	1/1	0.93	0.09	32,32,32,32	0
58	MG	1A	3307	1/1	0.93	0.22	56,56,56,56	0
58	MG	2a	1687	1/1	0.93	0.21	42,42,42,42	0
58	MG	1n	102	1/1	0.93	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3476	1/1	0.93	0.08	42,42,42,42	0
58	MG	2A	3240	1/1	0.93	0.14	60,60,60,60	0
58	MG	1A	3857	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	3712	1/1	0.93	0.10	49,49,49,49	0
58	MG	1a	1616	1/1	0.93	0.08	57,57,57,57	0
58	MG	1A	3859	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3051	1/1	0.93	0.09	42,42,42,42	0
58	MG	1a	1620	1/1	0.93	0.06	45,45,45,45	0
58	MG	2A	3252	1/1	0.93	0.23	41,41,41,41	0
58	MG	2A	3253	1/1	0.93	0.20	45,45,45,45	0
58	MG	2A	3254	1/1	0.93	0.24	52,52,52,52	0
58	MG	2a	1704	1/1	0.93	0.22	63,63,63,63	0
58	MG	2A	3255	1/1	0.93	0.21	52,52,52,52	0
58	MG	2a	1707	1/1	0.93	0.11	75,75,75,75	0
58	MG	1A	3863	1/1	0.93	0.08	48,48,48,48	0
58	MG	1A	4062	1/1	0.93	0.16	70,70,70,70	0
58	MG	1A	3867	1/1	0.93	0.08	25,25,25,25	0
58	MG	1A	3570	1/1	0.93	0.14	43,43,43,43	0
58	MG	1A	3131	1/1	0.93	0.15	39,39,39,39	0
58	MG	1A	3259	1/1	0.93	0.23	40,40,40,40	0
58	MG	2a	1715	1/1	0.93	0.18	62,62,62,62	0
58	MG	1A	3482	1/1	0.93	0.13	52,52,52,52	0
58	MG	2a	1717	1/1	0.93	0.42	60,60,60,60	0
58	MG	1A	3721	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3554	1/1	0.93	0.13	27,27,27,27	0
58	MG	2a	1720	1/1	0.93	0.24	51,51,51,51	0
58	MG	2a	1721	1/1	0.93	0.28	63,63,63,63	0
58	MG	2A	3556	1/1	0.93	0.12	38,38,38,38	0
58	MG	1A	3879	1/1	0.93	0.15	36,36,36,36	0
58	MG	1A	3132	1/1	0.93	0.09	64,64,64,64	0
58	MG	1A	3215	1/1	0.93	0.18	53,53,53,53	0
58	MG	1A	3218	1/1	0.93	0.24	49,49,49,49	0
58	MG	2A	3564	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3732	1/1	0.93	0.18	58,58,58,58	0
58	MG	2A	3275	1/1	0.93	0.22	59,59,59,59	0
58	MG	2A	3568	1/1	0.93	0.10	63,63,63,63	0
58	MG	2A	3276	1/1	0.93	0.28	50,50,50,50	0
58	MG	1A	3733	1/1	0.93	0.16	64,64,64,64	0
58	MG	2A	3007	1/1	0.93	0.17	53,53,53,53	0
58	MG	2A	3279	1/1	0.93	0.20	54,54,54,54	0
58	MG	1A	3894	1/1	0.93	0.07	33,33,33,33	0
58	MG	2A	3282	1/1	0.93	0.21	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	3283	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3014	1/1	0.93	0.15	48,48,48,48	0
58	MG	1A	3895	1/1	0.93	0.11	26,26,26,26	0
58	MG	1A	3364	1/1	0.93	0.24	47,47,47,47	0
58	MG	1A	3585	1/1	0.93	0.20	59,59,59,59	0
58	MG	2A	3585	1/1	0.93	0.17	41,41,41,41	0
58	MG	1A	3898	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3589	1/1	0.93	0.17	47,47,47,47	0
58	MG	1a	1650	1/1	0.93	0.19	46,46,46,46	0
58	MG	1A	3902	1/1	0.93	0.15	63,63,63,63	0
58	MG	1a	1653	1/1	0.93	0.11	51,51,51,51	0
58	MG	1a	1655	1/1	0.93	0.22	59,59,59,59	0
58	MG	1A	4091	1/1	0.93	0.24	57,57,57,57	0
58	MG	1a	1657	1/1	0.93	0.09	63,63,63,63	0
58	MG	2A	3599	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3903	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3365	1/1	0.93	0.14	49,49,49,49	0
58	MG	1A	3906	1/1	0.93	0.35	31,31,31,31	0
58	MG	1A	3741	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3742	1/1	0.93	0.08	43,43,43,43	0
58	MG	2A	3607	1/1	0.93	0.07	58,58,58,58	0
58	MG	2A	3609	1/1	0.93	0.12	79,79,79,79	0
58	MG	1A	3910	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3911	1/1	0.93	0.13	46,46,46,46	0
58	MG	2A	3314	1/1	0.93	0.27	58,58,58,58	0
58	MG	1A	3743	1/1	0.93	0.09	43,43,43,43	0
58	MG	1B	209	1/1	0.93	0.09	56,56,56,56	0
58	MG	2a	1782	1/1	0.93	0.14	67,67,67,67	0
58	MG	2A	3317	1/1	0.93	0.42	75,75,75,75	0
58	MG	2a	1784	1/1	0.93	0.14	73,73,73,73	0
58	MG	2A	3055	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3425	1/1	0.93	0.12	59,59,59,59	0
58	MG	2A	3621	1/1	0.93	0.12	52,52,52,52	0
58	MG	1a	1668	1/1	0.93	0.15	62,62,62,62	0
58	MG	2A	3058	1/1	0.93	0.16	61,61,61,61	0
58	MG	2A	3059	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	3746	1/1	0.93	0.10	52,52,52,52	0
58	MG	1a	1670	1/1	0.93	0.17	64,64,64,64	0
58	MG	2A	3640	1/1	0.93	0.13	46,46,46,46	0
58	MG	1A	3087	1/1	0.93	0.18	32,32,32,32	0
58	MG	1A	3429	1/1	0.93	0.29	55,55,55,55	0
58	MG	2A	3646	1/1	0.93	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3334	1/1	0.93	0.23	72,72,72,72	0
58	MG	2A	3650	1/1	0.93	0.07	74,74,74,74	0
58	MG	2A	3651	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3099	1/1	0.93	0.08	39,39,39,39	0
58	MG	1A	3181	1/1	0.93	0.19	35,35,35,35	0
58	MG	1a	1675	1/1	0.93	0.18	46,46,46,46	0
58	MG	1B	219	1/1	0.93	0.06	43,43,43,43	0
58	MG	2a	1809	1/1	0.93	0.28	64,64,64,64	0
58	MG	1B	220	1/1	0.93	0.09	37,37,37,37	0
58	MG	1A	3136	1/1	0.93	0.14	38,38,38,38	0
58	MG	2A	3080	1/1	0.93	0.10	34,34,34,34	0
58	MG	1A	3137	1/1	0.93	0.09	39,39,39,39	0
58	MG	1a	1683	1/1	0.93	0.23	68,68,68,68	0
58	MG	1A	3272	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3273	1/1	0.93	0.15	37,37,37,37	0
58	MG	1B	227	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3380	1/1	0.93	0.10	48,48,48,48	0
58	MG	1a	1690	1/1	0.93	0.33	50,50,50,50	0
58	MG	1A	3440	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3093	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3944	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3097	1/1	0.93	0.12	66,66,66,66	0
58	MG	2A	3683	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3772	1/1	0.93	0.11	26,26,26,26	0
58	MG	1D	306	1/1	0.93	0.15	43,43,43,43	0
58	MG	2A	3687	1/1	0.93	0.13	62,62,62,62	0
58	MG	1D	309	1/1	0.93	0.13	51,51,51,51	0
58	MG	2l	202	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3070	1/1	0.93	0.10	57,57,57,57	0
58	MG	1A	3385	1/1	0.93	0.11	63,63,63,63	0
58	MG	1A	3785	1/1	0.93	0.10	33,33,33,33	0
58	MG	2q	201	1/1	0.93	0.10	75,75,75,75	0
58	MG	1A	3791	1/1	0.93	0.06	30,30,30,30	0
58	MG	1A	3958	1/1	0.93	0.09	37,37,37,37	0
58	MG	1a	1706	1/1	0.93	0.15	45,45,45,45	0
58	MG	1F	312	1/1	0.93	0.07	49,49,49,49	0
58	MG	1A	3959	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3792	1/1	0.93	0.06	50,50,50,50	0
58	MG	2B	211	1/1	0.93	0.18	66,66,66,66	0
58	MG	1A	3794	1/1	0.93	0.07	45,45,45,45	0
58	MG	2B	213	1/1	0.93	0.21	59,59,59,59	0
58	MG	2B	214	1/1	0.93	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2x	3306	1/1	0.93	0.17	71,71,71,71	0
58	MG	1A	3040	1/1	0.94	0.19	31,31,31,31	0
58	MG	1A	4044	1/1	0.94	0.08	18,18,18,18	0
58	MG	1A	4045	1/1	0.94	0.15	50,50,50,50	0
58	MG	1A	3565	1/1	0.94	0.10	41,41,41,41	0
58	MG	23	102	1/1	0.94	0.08	63,63,63,63	0
58	MG	1a	1771	1/1	0.94	0.18	65,65,65,65	0
58	MG	2A	3445	1/1	0.94	0.19	43,43,43,43	0
58	MG	1A	3727	1/1	0.94	0.09	22,22,22,22	0
58	MG	1A	3174	1/1	0.94	0.16	43,43,43,43	0
58	MG	2A	3182	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3073	1/1	0.94	0.23	32,32,32,32	0
58	MG	17	104	1/1	0.94	0.15	31,31,31,31	0
58	MG	18	101	1/1	0.94	0.25	52,52,52,52	0
58	MG	2A	3187	1/1	0.94	0.09	50,50,50,50	0
58	MG	18	102	1/1	0.94	0.25	38,38,38,38	0
58	MG	18	105	1/1	0.94	0.14	45,45,45,45	0
58	MG	1A	4051	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3138	1/1	0.94	0.21	26,26,26,26	0
58	MG	1A	4057	1/1	0.94	0.06	25,25,25,25	0
58	MG	2a	1611	1/1	0.94	0.28	72,72,72,72	0
58	MG	1A	3885	1/1	0.94	0.07	28,28,28,28	0
58	MG	2A	3194	1/1	0.94	0.21	59,59,59,59	0
58	MG	1A	3886	1/1	0.94	0.09	35,35,35,35	0
58	MG	2A	3196	1/1	0.94	0.09	49,49,49,49	0
58	MG	1a	1795	1/1	0.94	0.07	77,77,77,77	0
58	MG	1A	3887	1/1	0.94	0.12	28,28,28,28	0
58	MG	1A	3474	1/1	0.94	0.22	55,55,55,55	0
58	MG	1A	4068	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3475	1/1	0.94	0.07	49,49,49,49	0
58	MG	1a	1609	1/1	0.94	0.13	59,59,59,59	0
58	MG	1A	3094	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	3574	1/1	0.94	0.07	53,53,53,53	0
58	MG	2A	3206	1/1	0.94	0.18	58,58,58,58	0
58	MG	1A	3576	1/1	0.94	0.08	41,41,41,41	0
58	MG	1A	3241	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3901	1/1	0.94	0.08	59,59,59,59	0
58	MG	2A	3210	1/1	0.94	0.09	71,71,71,71	0
58	MG	1A	3478	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3212	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3187	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3744	1/1	0.94	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4080	1/1	0.94	0.19	46,46,46,46	0
58	MG	2A	3218	1/1	0.94	0.22	52,52,52,52	0
58	MG	1e	202	1/1	0.94	0.19	60,60,60,60	0
58	MG	1f	201	1/1	0.94	0.13	51,51,51,51	0
58	MG	1A	3582	1/1	0.94	0.18	53,53,53,53	0
58	MG	2A	3500	1/1	0.94	0.09	36,36,36,36	0
58	MG	1k	201	1/1	0.94	0.19	58,58,58,58	0
58	MG	2A	3223	1/1	0.94	0.11	61,61,61,61	0
58	MG	2A	3224	1/1	0.94	0.17	58,58,58,58	0
58	MG	1A	3140	1/1	0.94	0.10	48,48,48,48	0
58	MG	2A	3226	1/1	0.94	0.09	44,44,44,44	0
58	MG	1a	1625	1/1	0.94	0.20	56,56,56,56	0
58	MG	1A	3481	1/1	0.94	0.15	47,47,47,47	0
58	MG	2a	1650	1/1	0.94	0.07	83,83,83,83	0
58	MG	1A	3748	1/1	0.94	0.12	31,31,31,31	0
58	MG	1A	3749	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3353	1/1	0.94	0.17	36,36,36,36	0
58	MG	1A	3141	1/1	0.94	0.18	37,37,37,37	0
58	MG	1a	1633	1/1	0.94	0.23	57,57,57,57	0
58	MG	1A	3916	1/1	0.94	0.09	26,26,26,26	0
58	MG	1A	3026	1/1	0.94	0.13	40,40,40,40	0
58	MG	1a	1637	1/1	0.94	0.21	51,51,51,51	0
58	MG	2a	1659	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3918	1/1	0.94	0.14	51,51,51,51	0
58	MG	2a	1661	1/1	0.94	0.09	62,62,62,62	0
58	MG	1A	3755	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3356	1/1	0.94	0.09	49,49,49,49	0
58	MG	1A	3590	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3145	1/1	0.94	0.14	62,62,62,62	0
58	MG	2A	3532	1/1	0.94	0.18	57,57,57,57	0
58	MG	2A	3245	1/1	0.94	0.15	64,64,64,64	0
58	MG	1A	3308	1/1	0.94	0.29	45,45,45,45	0
58	MG	1A	3252	1/1	0.94	0.25	36,36,36,36	0
58	MG	2A	3537	1/1	0.94	0.12	55,55,55,55	0
58	MG	2a	1673	1/1	0.94	0.13	67,67,67,67	0
58	MG	1A	3765	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3080	1/1	0.94	0.10	38,38,38,38	0
58	MG	1A	3313	1/1	0.94	0.14	52,52,52,52	0
58	MG	1A	3497	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3002	1/1	0.94	0.15	59,59,59,59	0
58	MG	2A	3003	1/1	0.94	0.23	53,53,53,53	0
58	MG	1A	3498	1/1	0.94	0.06	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	1B	214	1/1	0.94	0.15	57,57,57,57	0
58	MG	1A	3428	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3009	1/1	0.94	0.08	48,48,48,48	0
58	MG	2a	1685	1/1	0.94	0.24	74,74,74,74	0
58	MG	1A	3788	1/1	0.94	0.08	19,19,19,19	0
58	MG	1A	3314	1/1	0.94	0.16	47,47,47,47	0
58	MG	2a	1688	1/1	0.94	0.33	57,57,57,57	0
58	MG	1A	3613	1/1	0.94	0.10	24,24,24,24	0
58	MG	1A	3004	1/1	0.94	0.04	24,24,24,24	0
58	MG	1A	3957	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3318	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	3257	1/1	0.94	0.07	56,56,56,56	0
58	MG	2A	3272	1/1	0.94	0.35	55,55,55,55	0
58	MG	1A	3150	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3030	1/1	0.94	0.09	31,31,31,31	0
58	MG	1A	3624	1/1	0.94	0.13	15,15,15,15	0
58	MG	1A	3321	1/1	0.94	0.22	35,35,35,35	0
58	MG	1A	3963	1/1	0.94	0.08	62,62,62,62	0
58	MG	1B	232	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3280	1/1	0.94	0.15	50,50,50,50	0
58	MG	2a	1705	1/1	0.94	0.09	81,81,81,81	0
58	MG	1A	3964	1/1	0.94	0.12	47,47,47,47	0
58	MG	2A	3038	1/1	0.94	0.13	45,45,45,45	0
58	MG	2A	3039	1/1	0.94	0.25	70,70,70,70	0
58	MG	1D	301	1/1	0.94	0.31	34,34,34,34	0
58	MG	1A	3377	1/1	0.94	0.34	46,46,46,46	0
58	MG	1A	3630	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3044	1/1	0.94	0.13	53,53,53,53	0
58	MG	1D	310	1/1	0.94	0.07	40,40,40,40	0
58	MG	2A	3290	1/1	0.94	0.16	47,47,47,47	0
58	MG	2A	3580	1/1	0.94	0.12	59,59,59,59	0
58	MG	2A	3291	1/1	0.94	0.11	50,50,50,50	0
58	MG	1A	3631	1/1	0.94	0.11	49,49,49,49	0
58	MG	2A	3047	1/1	0.94	0.17	58,58,58,58	0
58	MG	1E	307	1/1	0.94	0.08	54,54,54,54	0
58	MG	1a	1676	1/1	0.94	0.20	65,65,65,65	0
58	MG	2A	3301	1/1	0.94	0.08	46,46,46,46	0
58	MG	1a	1677	1/1	0.94	0.19	54,54,54,54	0
58	MG	1A	3438	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3635	1/1	0.94	0.05	26,26,26,26	0
58	MG	1F	301	1/1	0.94	0.10	33,33,33,33	0
58	MG	1F	305	1/1	0.94	0.17	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	3598	1/1	0.94	0.14	73,73,73,73	0
58	MG	1A	3020	1/1	0.94	0.09	39,39,39,39	0
58	MG	2a	1730	1/1	0.94	0.30	68,68,68,68	0
58	MG	2a	1731	1/1	0.94	0.26	69,69,69,69	0
58	MG	1A	3642	1/1	0.94	0.06	26,26,26,26	0
58	MG	1a	1685	1/1	0.94	0.05	62,62,62,62	0
58	MG	1A	3084	1/1	0.94	0.27	38,38,38,38	0
58	MG	2A	3604	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3030	1/1	0.94	0.07	41,41,41,41	0
58	MG	1A	3518	1/1	0.94	0.11	43,43,43,43	0
58	MG	1A	3208	1/1	0.94	0.14	55,55,55,55	0
58	MG	2A	3608	1/1	0.94	0.12	59,59,59,59	0
58	MG	1A	3444	1/1	0.94	0.14	65,65,65,65	0
58	MG	1A	3382	1/1	0.94	0.21	56,56,56,56	0
58	MG	2A	3077	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3987	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3989	1/1	0.94	0.09	55,55,55,55	0
58	MG	1A	3524	1/1	0.94	0.23	40,40,40,40	0
58	MG	1A	3826	1/1	0.94	0.06	29,29,29,29	0
58	MG	2A	3617	1/1	0.94	0.06	48,48,48,48	0
58	MG	2a	1755	1/1	0.94	0.15	66,66,66,66	0
58	MG	2A	3082	1/1	0.94	0.14	64,64,64,64	0
58	MG	2a	1757	1/1	0.94	0.18	67,67,67,67	0
58	MG	1A	3158	1/1	0.94	0.23	45,45,45,45	0
58	MG	2A	3084	1/1	0.94	0.17	55,55,55,55	0
58	MG	1A	3213	1/1	0.94	0.15	45,45,45,45	0
58	MG	1A	3160	1/1	0.94	0.13	55,55,55,55	0
58	MG	1Q	202	1/1	0.94	0.19	38,38,38,38	0
58	MG	1Q	206	1/1	0.94	0.07	45,45,45,45	0
58	MG	2A	3635	1/1	0.94	0.10	52,52,52,52	0
58	MG	2A	3637	1/1	0.94	0.09	57,57,57,57	0
58	MG	1Q	207	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3105	1/1	0.94	0.17	38,38,38,38	0
58	MG	2A	3642	1/1	0.94	0.11	43,43,43,43	0
58	MG	2a	1773	1/1	0.94	0.12	60,60,60,60	0
58	MG	2a	1774	1/1	0.94	0.10	60,60,60,60	0
58	MG	1A	3668	1/1	0.94	0.07	28,28,28,28	0
58	MG	1a	1710	1/1	0.94	0.16	47,47,47,47	0
58	MG	1a	1711	1/1	0.94	0.37	66,66,66,66	0
58	MG	1A	3532	1/1	0.94	0.21	45,45,45,45	0
58	MG	2A	3100	1/1	0.94	0.09	69,69,69,69	0
58	MG	2A	3349	1/1	0.94	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3101	1/1	0.94	0.19	49,49,49,49	0
58	MG	1a	1713	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3354	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3103	1/1	0.94	0.11	61,61,61,61	0
58	MG	2a	1786	1/1	0.94	0.24	60,60,60,60	0
58	MG	1A	3165	1/1	0.94	0.19	49,49,49,49	0
58	MG	1A	4005	1/1	0.94	0.08	19,19,19,19	0
58	MG	2A	3662	1/1	0.94	0.12	57,57,57,57	0
58	MG	1A	3064	1/1	0.94	0.10	42,42,42,42	0
58	MG	2a	1791	1/1	0.94	0.15	60,60,60,60	0
58	MG	1A	3536	1/1	0.94	0.19	58,58,58,58	0
58	MG	1A	3457	1/1	0.94	0.20	47,47,47,47	0
58	MG	2a	1794	1/1	0.94	0.10	58,58,58,58	0
58	MG	1A	3391	1/1	0.94	0.19	43,43,43,43	0
58	MG	2A	3117	1/1	0.94	0.23	47,47,47,47	0
58	MG	1A	3541	1/1	0.94	0.26	54,54,54,54	0
58	MG	1A	3542	1/1	0.94	0.28	36,36,36,36	0
58	MG	1A	3223	1/1	0.94	0.13	51,51,51,51	0
58	MG	1a	1728	1/1	0.94	0.07	58,58,58,58	0
58	MG	2A	3677	1/1	0.94	0.13	69,69,69,69	0
58	MG	2A	3372	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3224	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3681	1/1	0.94	0.13	53,53,53,53	0
58	MG	1V	201	1/1	0.94	0.41	29,29,29,29	0
58	MG	1A	3549	1/1	0.94	0.16	35,35,35,35	0
58	MG	2A	3684	1/1	0.94	0.18	50,50,50,50	0
58	MG	1A	3397	1/1	0.94	0.09	53,53,53,53	0
58	MG	1a	1736	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3133	1/1	0.94	0.19	38,38,38,38	0
58	MG	1A	3398	1/1	0.94	0.06	48,48,48,48	0
58	MG	1a	1738	1/1	0.94	0.15	54,54,54,54	0
58	MG	1A	4024	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3703	1/1	0.94	0.14	35,35,35,35	0
58	MG	1W	207	1/1	0.94	0.12	55,55,55,55	0
58	MG	1a	1744	1/1	0.94	0.10	54,54,54,54	0
58	MG	2A	3142	1/1	0.94	0.16	55,55,55,55	0
58	MG	2A	3145	1/1	0.94	0.17	61,61,61,61	0
58	MG	1a	1745	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	3108	1/1	0.94	0.13	33,33,33,33	0
58	MG	1X	102	1/1	0.94	0.11	35,35,35,35	0
58	MG	2e	201	1/1	0.94	0.06	74,74,74,74	0
58	MG	1A	3337	1/1	0.94	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3709	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3711	1/1	0.94	0.13	40,40,40,40	0
58	MG	1a	1752	1/1	0.94	0.28	66,66,66,66	0
58	MG	1A	3001	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3229	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3868	1/1	0.94	0.20	54,54,54,54	0
58	MG	1A	3560	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3562	1/1	0.94	0.10	45,45,45,45	0
58	MG	2A	3411	1/1	0.94	0.13	24,24,24,24	0
58	MG	2A	3412	1/1	0.94	0.27	56,56,56,56	0
58	MG	2A	3163	1/1	0.94	0.20	42,42,42,42	0
58	MG	2A	3164	1/1	0.94	0.09	50,50,50,50	0
58	MG	1A	3872	1/1	0.94	0.18	37,37,37,37	0
58	MG	2A	3170	1/1	0.94	0.13	55,55,55,55	0
58	MG	1A	3717	1/1	0.94	0.12	51,51,51,51	0
58	MG	2Q	202	1/1	0.94	0.11	49,49,49,49	0
58	MG	2R	201	1/1	0.94	0.17	32,32,32,32	0
58	MG	1A	3563	1/1	0.94	0.21	43,43,43,43	0
58	MG	2A	3431	1/1	0.94	0.16	56,56,56,56	0
58	MG	2A	3173	1/1	0.94	0.10	60,60,60,60	0
59	K	2x	3301	1/1	0.94	0.08	59,59,59,59	0
61	ZN	14	102	1/1	0.94	0.11	121,121,121,121	0
61	ZN	24	501	1/1	0.94	0.12	136,136,136,136	0
58	MG	1a	1608	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3932	1/1	0.95	0.06	53,53,53,53	0
58	MG	2F	304	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3420	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3421	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3422	1/1	0.95	0.12	63,63,63,63	0
58	MG	2Q	201	1/1	0.95	0.10	64,64,64,64	0
58	MG	1a	1798	1/1	0.95	0.09	59,59,59,59	0
58	MG	2A	3425	1/1	0.95	0.11	46,46,46,46	0
58	MG	2T	201	1/1	0.95	0.11	60,60,60,60	0
58	MG	2T	202	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3936	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3161	1/1	0.95	0.09	32,32,32,32	0
58	MG	2A	3430	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3939	1/1	0.95	0.12	40,40,40,40	0
58	MG	1A	3162	1/1	0.95	0.23	38,38,38,38	0
58	MG	1a	1807	1/1	0.95	0.23	64,64,64,64	0
58	MG	1A	3100	1/1	0.95	0.12	25,25,25,25	0
58	MG	1A	3043	1/1	0.95	0.21	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	25	101	1/1	0.95	0.38	49,49,49,49	0
58	MG	2A	3437	1/1	0.95	0.13	38,38,38,38	0
58	MG	1a	1618	1/1	0.95	0.06	52,52,52,52	0
58	MG	27	101	1/1	0.95	0.16	49,49,49,49	0
58	MG	2A	3443	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3495	1/1	0.95	0.06	51,51,51,51	0
58	MG	1A	3496	1/1	0.95	0.19	47,47,47,47	0
58	MG	1A	3678	1/1	0.95	0.10	24,24,24,24	0
58	MG	1A	4096	1/1	0.95	0.14	46,46,46,46	0
58	MG	1d	302	1/1	0.95	0.18	50,50,50,50	0
58	MG	1A	3680	1/1	0.95	0.10	23,23,23,23	0
58	MG	2A	3451	1/1	0.95	0.25	58,58,58,58	0
58	MG	1A	3124	1/1	0.95	0.17	43,43,43,43	0
58	MG	1B	203	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3202	1/1	0.95	0.14	26,26,26,26	0
58	MG	1a	1628	1/1	0.95	0.20	56,56,56,56	0
58	MG	2A	3197	1/1	0.95	0.24	58,58,58,58	0
58	MG	1B	205	1/1	0.95	0.06	51,51,51,51	0
58	MG	1B	206	1/1	0.95	0.17	46,46,46,46	0
58	MG	1A	3500	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3687	1/1	0.95	0.05	32,32,32,32	0
58	MG	1A	3143	1/1	0.95	0.17	16,16,16,16	0
58	MG	1a	1635	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3690	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3575	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3694	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3206	1/1	0.95	0.13	27,27,27,27	0
58	MG	1A	3344	1/1	0.95	0.30	46,46,46,46	0
58	MG	1A	3447	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3345	1/1	0.95	0.20	40,40,40,40	0
58	MG	2A	3478	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3702	1/1	0.95	0.06	29,29,29,29	0
58	MG	2A	3480	1/1	0.95	0.12	50,50,50,50	0
58	MG	1B	221	1/1	0.95	0.07	39,39,39,39	0
58	MG	2a	1630	1/1	0.95	0.20	49,49,49,49	0
58	MG	2a	1631	1/1	0.95	0.30	54,54,54,54	0
58	MG	2a	1632	1/1	0.95	0.31	55,55,55,55	0
58	MG	2A	3213	1/1	0.95	0.08	41,41,41,41	0
58	MG	1x	103	1/1	0.95	0.23	63,63,63,63	0
58	MG	1a	1646	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3581	1/1	0.95	0.20	28,28,28,28	0
58	MG	1A	3015	1/1	0.95	0.09	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	1B	224	1/1	0.95	0.09	47,47,47,47	0
58	MG	1x	108	1/1	0.95	0.10	27,27,27,27	0
58	MG	1A	3209	1/1	0.95	0.14	43,43,43,43	0
58	MG	1A	3210	1/1	0.95	0.08	56,56,56,56	0
58	MG	1a	1654	1/1	0.95	0.17	47,47,47,47	0
58	MG	2A	3001	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3841	1/1	0.95	0.24	66,66,66,66	0
58	MG	1A	3254	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3498	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3004	1/1	0.95	0.29	57,57,57,57	0
58	MG	1A	3068	1/1	0.95	0.10	38,38,38,38	0
58	MG	1A	3981	1/1	0.95	0.05	54,54,54,54	0
58	MG	1A	3171	1/1	0.95	0.18	58,58,58,58	0
58	MG	1A	3516	1/1	0.95	0.09	74,74,74,74	0
58	MG	2A	3011	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3233	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3510	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3511	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3986	1/1	0.95	0.10	34,34,34,34	0
58	MG	1D	304	1/1	0.95	0.17	33,33,33,33	0
58	MG	1A	3173	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3988	1/1	0.95	0.08	47,47,47,47	0
58	MG	2A	3020	1/1	0.95	0.22	44,44,44,44	0
58	MG	2A	3519	1/1	0.95	0.26	62,62,62,62	0
58	MG	1A	3848	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3407	1/1	0.95	0.17	49,49,49,49	0
58	MG	2A	3024	1/1	0.95	0.08	51,51,51,51	0
58	MG	1A	3991	1/1	0.95	0.16	38,38,38,38	0
58	MG	1A	3850	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	3312	1/1	0.95	0.13	41,41,41,41	0
58	MG	1E	313	1/1	0.95	0.15	44,44,44,44	0
58	MG	1A	3409	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3251	1/1	0.95	0.19	68,68,68,68	0
58	MG	2A	3529	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3530	1/1	0.95	0.09	54,54,54,54	0
58	MG	1F	304	1/1	0.95	0.05	42,42,42,42	0
58	MG	1A	3853	1/1	0.95	0.09	52,52,52,52	0
58	MG	2A	3035	1/1	0.95	0.16	54,54,54,54	0
58	MG	1A	3216	1/1	0.95	0.06	47,47,47,47	0
58	MG	1F	309	1/1	0.95	0.09	47,47,47,47	0
58	MG	2A	3536	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3855	1/1	0.95	0.07	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1F	311	1/1	0.95	0.13	28,28,28,28	0
58	MG	2a	1683	1/1	0.95	0.17	60,60,60,60	0
58	MG	1A	4002	1/1	0.95	0.06	32,32,32,32	0
58	MG	2A	3262	1/1	0.95	0.09	40,40,40,40	0
58	MG	2A	3042	1/1	0.95	0.16	69,69,69,69	0
58	MG	1a	1679	1/1	0.95	0.18	69,69,69,69	0
58	MG	1G	201	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3722	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3598	1/1	0.95	0.12	39,39,39,39	0
58	MG	1A	3019	1/1	0.95	0.17	42,42,42,42	0
58	MG	1A	3525	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3049	1/1	0.95	0.06	44,44,44,44	0
58	MG	1A	3466	1/1	0.95	0.11	60,60,60,60	0
58	MG	2A	3051	1/1	0.95	0.18	55,55,55,55	0
58	MG	2A	3274	1/1	0.95	0.19	55,55,55,55	0
58	MG	2A	3052	1/1	0.95	0.16	50,50,50,50	0
58	MG	1A	3606	1/1	0.95	0.13	28,28,28,28	0
58	MG	1A	4010	1/1	0.95	0.12	40,40,40,40	0
58	MG	2a	1702	1/1	0.95	0.16	55,55,55,55	0
58	MG	1A	3607	1/1	0.95	0.17	48,48,48,48	0
58	MG	1A	3358	1/1	0.95	0.16	49,49,49,49	0
58	MG	1A	4013	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3561	1/1	0.95	0.13	61,61,61,61	0
58	MG	1P	201	1/1	0.95	0.21	31,31,31,31	0
58	MG	1A	3262	1/1	0.95	0.18	60,60,60,60	0
58	MG	1P	203	1/1	0.95	0.15	35,35,35,35	0
58	MG	1P	204	1/1	0.95	0.24	35,35,35,35	0
58	MG	1A	3612	1/1	0.95	0.08	48,48,48,48	0
58	MG	2a	1712	1/1	0.95	0.16	58,58,58,58	0
58	MG	2A	3286	1/1	0.95	0.17	48,48,48,48	0
58	MG	2A	3066	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3219	1/1	0.95	0.29	43,43,43,43	0
58	MG	1Q	205	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3072	1/1	0.95	0.07	43,43,43,43	0
58	MG	2A	3575	1/1	0.95	0.11	56,56,56,56	0
58	MG	1a	1702	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3873	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3076	1/1	0.95	0.12	50,50,50,50	0
58	MG	1A	3615	1/1	0.95	0.10	24,24,24,24	0
58	MG	2A	3297	1/1	0.95	0.13	51,51,51,51	0
58	MG	1A	4019	1/1	0.95	0.16	45,45,45,45	0
58	MG	1A	4020	1/1	0.95	0.08	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3583	1/1	0.95	0.19	51,51,51,51	0
58	MG	1A	3531	1/1	0.95	0.12	34,34,34,34	0
58	MG	1A	4023	1/1	0.95	0.16	24,24,24,24	0
58	MG	2A	3588	1/1	0.95	0.18	60,60,60,60	0
58	MG	1A	3017	1/1	0.95	0.12	65,65,65,65	0
58	MG	1A	3182	1/1	0.95	0.24	54,54,54,54	0
58	MG	1A	3222	1/1	0.95	0.09	47,47,47,47	0
58	MG	1A	3620	1/1	0.95	0.14	47,47,47,47	0
58	MG	2A	3087	1/1	0.95	0.15	49,49,49,49	0
58	MG	2A	3594	1/1	0.95	0.07	66,66,66,66	0
58	MG	2a	1736	1/1	0.95	0.24	54,54,54,54	0
58	MG	2A	3310	1/1	0.95	0.20	54,54,54,54	0
58	MG	2a	1738	1/1	0.95	0.16	60,60,60,60	0
58	MG	1A	3882	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3267	1/1	0.95	0.17	44,44,44,44	0
58	MG	1A	3268	1/1	0.95	0.15	45,45,45,45	0
58	MG	1A	3091	1/1	0.95	0.12	38,38,38,38	0
58	MG	1U	209	1/1	0.95	0.42	42,42,42,42	0
58	MG	1U	211	1/1	0.95	0.27	40,40,40,40	0
58	MG	2A	3094	1/1	0.95	0.11	43,43,43,43	0
58	MG	1A	3752	1/1	0.95	0.06	47,47,47,47	0
58	MG	1A	3060	1/1	0.95	0.11	41,41,41,41	0
58	MG	2A	3098	1/1	0.95	0.14	58,58,58,58	0
58	MG	1A	3078	1/1	0.95	0.23	45,45,45,45	0
58	MG	1V	206	1/1	0.95	0.14	63,63,63,63	0
58	MG	2A	3329	1/1	0.95	0.25	57,57,57,57	0
58	MG	1A	3891	1/1	0.95	0.11	25,25,25,25	0
58	MG	1A	3893	1/1	0.95	0.09	23,23,23,23	0
58	MG	1A	4041	1/1	0.95	0.09	25,25,25,25	0
58	MG	2A	3104	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3226	1/1	0.95	0.12	40,40,40,40	0
58	MG	2A	3616	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3544	1/1	0.95	0.28	50,50,50,50	0
58	MG	2A	3618	1/1	0.95	0.12	54,54,54,54	0
58	MG	1A	3636	1/1	0.95	0.11	29,29,29,29	0
58	MG	2A	3110	1/1	0.95	0.17	36,36,36,36	0
58	MG	1A	3759	1/1	0.95	0.15	30,30,30,30	0
58	MG	1X	105	1/1	0.95	0.09	47,47,47,47	0
58	MG	2a	1772	1/1	0.95	0.22	64,64,64,64	0
58	MG	2A	3625	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3061	1/1	0.95	0.15	51,51,51,51	0
58	MG	2A	3344	1/1	0.95	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3629	1/1	0.95	0.13	50,50,50,50	0
58	MG	2A	3631	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3062	1/1	0.95	0.06	42,42,42,42	0
58	MG	2A	3346	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3636	1/1	0.95	0.05	50,50,50,50	0
58	MG	2A	3118	1/1	0.95	0.06	36,36,36,36	0
58	MG	1A	3762	1/1	0.95	0.12	47,47,47,47	0
58	MG	1A	3279	1/1	0.95	0.28	37,37,37,37	0
58	MG	2A	3641	1/1	0.95	0.12	61,61,61,61	0
58	MG	1A	3332	1/1	0.95	0.15	51,51,51,51	0
58	MG	10	103	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3123	1/1	0.95	0.13	52,52,52,52	0
58	MG	2A	3124	1/1	0.95	0.06	57,57,57,57	0
58	MG	2A	3125	1/1	0.95	0.11	45,45,45,45	0
58	MG	1a	1748	1/1	0.95	0.20	48,48,48,48	0
58	MG	1A	3484	1/1	0.95	0.08	47,47,47,47	0
58	MG	1A	4054	1/1	0.95	0.13	14,14,14,14	0
58	MG	2A	3653	1/1	0.95	0.08	37,37,37,37	0
58	MG	2A	3130	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	4056	1/1	0.95	0.13	51,51,51,51	0
58	MG	2a	1797	1/1	0.95	0.24	56,56,56,56	0
58	MG	1A	3768	1/1	0.95	0.10	40,40,40,40	0
58	MG	2A	3365	1/1	0.95	0.14	63,63,63,63	0
58	MG	1A	3646	1/1	0.95	0.07	21,21,21,21	0
58	MG	1A	3647	1/1	0.95	0.08	19,19,19,19	0
58	MG	2A	3368	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3774	1/1	0.95	0.09	31,31,31,31	0
58	MG	1A	3485	1/1	0.95	0.26	68,68,68,68	0
58	MG	2A	3667	1/1	0.95	0.09	67,67,67,67	0
58	MG	12	101	1/1	0.95	0.14	48,48,48,48	0
58	MG	1A	4065	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3374	1/1	0.95	0.27	65,65,65,65	0
58	MG	2A	3672	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3375	1/1	0.95	0.17	46,46,46,46	0
58	MG	1A	4066	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3141	1/1	0.95	0.09	54,54,54,54	0
58	MG	1a	1763	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3380	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3143	1/1	0.95	0.10	54,54,54,54	0
58	MG	1A	3778	1/1	0.95	0.12	34,34,34,34	0
58	MG	15	101	1/1	0.95	0.20	42,42,42,42	0
58	MG	1a	1766	1/1	0.95	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	3782	1/1	0.95	0.09	39,39,39,39	0
58	MG	1A	3159	1/1	0.95	0.10	39,39,39,39	0
58	MG	2a	1822	1/1	0.95	0.09	56,56,56,56	0
58	MG	2A	3388	1/1	0.95	0.13	56,56,56,56	0
58	MG	1A	3487	1/1	0.95	0.31	42,42,42,42	0
58	MG	1A	3652	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3393	1/1	0.95	0.28	51,51,51,51	0
58	MG	2A	3394	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3654	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3156	1/1	0.95	0.10	49,49,49,49	0
58	MG	18	104	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3923	1/1	0.95	0.08	44,44,44,44	0
58	MG	18	106	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3558	1/1	0.95	0.15	33,33,33,33	0
58	MG	1A	3434	1/1	0.95	0.31	36,36,36,36	0
58	MG	2A	3162	1/1	0.95	0.23	59,59,59,59	0
58	MG	1A	3561	1/1	0.95	0.33	35,35,35,35	0
58	MG	1A	3927	1/1	0.95	0.09	34,34,34,34	0
58	MG	2A	3405	1/1	0.95	0.12	47,47,47,47	0
58	MG	2A	3166	1/1	0.95	0.12	43,43,43,43	0
58	MG	2D	302	1/1	0.95	0.17	43,43,43,43	0
58	MG	2D	304	1/1	0.95	0.22	41,41,41,41	0
58	MG	2A	3167	1/1	0.95	0.31	64,64,64,64	0
58	MG	1A	3661	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	4082	1/1	0.95	0.13	58,58,58,58	0
58	MG	1A	4083	1/1	0.95	0.12	61,61,61,61	0
58	MG	1A	3022	1/1	0.95	0.06	37,37,37,37	0
59	K	1A	3554	1/1	0.95	0.08	55,55,55,55	0
58	MG	2A	3415	1/1	0.95	0.14	51,51,51,51	0
58	MG	2E	306	1/1	0.95	0.13	52,52,52,52	0
58	MG	1A	4085	1/1	0.95	0.21	54,54,54,54	0
61	ZN	2n	501	1/1	0.95	0.07	103,103,103,103	0
58	MG	1V	207	1/1	0.96	0.09	66,66,66,66	0
58	MG	1A	3781	1/1	0.96	0.11	63,63,63,63	0
58	MG	1A	3660	1/1	0.96	0.07	34,34,34,34	0
58	MG	1a	1717	1/1	0.96	0.14	44,44,44,44	0
58	MG	2A	3069	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3512	1/1	0.96	0.07	54,54,54,54	0
58	MG	1A	3568	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3071	1/1	0.96	0.10	48,48,48,48	0
58	MG	1A	3787	1/1	0.96	0.14	55,55,55,55	0
58	MG	1A	3919	1/1	0.96	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3276	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3790	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3922	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3664	1/1	0.96	0.09	35,35,35,35	0
58	MG	1a	1726	1/1	0.96	0.14	57,57,57,57	0
58	MG	1Y	202	1/1	0.96	0.16	46,46,46,46	0
58	MG	2a	1627	1/1	0.96	0.06	71,71,71,71	0
58	MG	1A	3277	1/1	0.96	0.09	37,37,37,37	0
58	MG	1a	1730	1/1	0.96	0.07	40,40,40,40	0
58	MG	1a	1731	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3793	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3278	1/1	0.96	0.21	23,23,23,23	0
58	MG	1Z	302	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3032	1/1	0.96	0.29	28,28,28,28	0
58	MG	1A	3443	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3238	1/1	0.96	0.34	35,35,35,35	0
58	MG	1A	3799	1/1	0.96	0.15	53,53,53,53	0
58	MG	1A	3800	1/1	0.96	0.10	25,25,25,25	0
58	MG	1A	3673	1/1	0.96	0.05	23,23,23,23	0
58	MG	1A	3675	1/1	0.96	0.12	27,27,27,27	0
58	MG	2A	3095	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3298	1/1	0.96	0.27	44,44,44,44	0
58	MG	10	109	1/1	0.96	0.04	49,49,49,49	0
58	MG	2A	3300	1/1	0.96	0.12	46,46,46,46	0
58	MG	1A	3239	1/1	0.96	0.17	30,30,30,30	0
58	MG	1A	3577	1/1	0.96	0.12	46,46,46,46	0
58	MG	2A	3303	1/1	0.96	0.17	55,55,55,55	0
58	MG	1A	3098	1/1	0.96	0.19	37,37,37,37	0
58	MG	11	104	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3392	1/1	0.96	0.12	36,36,36,36	0
58	MG	13	101	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3946	1/1	0.96	0.10	57,57,57,57	0
58	MG	1a	1755	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	3509	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3684	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3950	1/1	0.96	0.11	61,61,61,61	0
58	MG	2A	3109	1/1	0.96	0.14	62,62,62,62	0
58	MG	2A	3555	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3448	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3111	1/1	0.96	0.12	54,54,54,54	0
58	MG	2A	3558	1/1	0.96	0.17	59,59,59,59	0
58	MG	1A	3953	1/1	0.96	0.12	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	1663	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3511	1/1	0.96	0.09	48,48,48,48	0
58	MG	17	105	1/1	0.96	0.06	44,44,44,44	0
58	MG	1A	3955	1/1	0.96	0.07	50,50,50,50	0
58	MG	2a	1667	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3688	1/1	0.96	0.12	25,25,25,25	0
58	MG	2A	3565	1/1	0.96	0.10	33,33,33,33	0
58	MG	18	103	1/1	0.96	0.19	46,46,46,46	0
58	MG	2A	3326	1/1	0.96	0.20	49,49,49,49	0
58	MG	2A	3327	1/1	0.96	0.30	63,63,63,63	0
58	MG	1A	3451	1/1	0.96	0.19	48,48,48,48	0
58	MG	1A	3244	1/1	0.96	0.15	41,41,41,41	0
58	MG	1a	1768	1/1	0.96	0.12	57,57,57,57	0
58	MG	1A	4097	1/1	0.96	0.16	45,45,45,45	0
58	MG	1A	3288	1/1	0.96	0.17	52,52,52,52	0
58	MG	1A	3692	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3396	1/1	0.96	0.05	47,47,47,47	0
58	MG	2A	3336	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3337	1/1	0.96	0.22	58,58,58,58	0
58	MG	1A	3289	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3290	1/1	0.96	0.11	47,47,47,47	0
58	MG	1a	1776	1/1	0.96	0.08	71,71,71,71	0
58	MG	1A	3697	1/1	0.96	0.06	28,28,28,28	0
58	MG	1A	3698	1/1	0.96	0.09	62,62,62,62	0
58	MG	1A	3968	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	3399	1/1	0.96	0.10	54,54,54,54	0
58	MG	1A	3342	1/1	0.96	0.05	55,55,55,55	0
58	MG	1a	1782	1/1	0.96	0.15	55,55,55,55	0
58	MG	1a	1783	1/1	0.96	0.08	56,56,56,56	0
58	MG	1A	3833	1/1	0.96	0.16	43,43,43,43	0
58	MG	1a	1610	1/1	0.96	0.12	27,27,27,27	0
58	MG	1A	3050	1/1	0.96	0.06	25,25,25,25	0
58	MG	1a	1789	1/1	0.96	0.10	55,55,55,55	0
58	MG	1a	1612	1/1	0.96	0.08	70,70,70,70	0
58	MG	2A	3144	1/1	0.96	0.10	43,43,43,43	0
58	MG	1a	1791	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3357	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3835	1/1	0.96	0.09	45,45,45,45	0
58	MG	2A	3359	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3204	1/1	0.96	0.14	37,37,37,37	0
58	MG	2A	3149	1/1	0.96	0.17	59,59,59,59	0
58	MG	1A	3142	1/1	0.96	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	218	1/1	0.96	0.09	46,46,46,46	0
58	MG	1a	1799	1/1	0.96	0.11	61,61,61,61	0
58	MG	1a	1801	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3839	1/1	0.96	0.07	36,36,36,36	0
58	MG	1A	3086	1/1	0.96	0.17	33,33,33,33	0
58	MG	1A	3706	1/1	0.96	0.09	28,28,28,28	0
58	MG	1A	3707	1/1	0.96	0.06	19,19,19,19	0
58	MG	1a	1621	1/1	0.96	0.18	51,51,51,51	0
58	MG	1A	3599	1/1	0.96	0.17	56,56,56,56	0
58	MG	1A	3985	1/1	0.96	0.08	23,23,23,23	0
58	MG	1a	1810	1/1	0.96	0.10	64,64,64,64	0
58	MG	1A	3600	1/1	0.96	0.11	43,43,43,43	0
58	MG	1A	3347	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3377	1/1	0.96	0.22	50,50,50,50	0
58	MG	2A	3165	1/1	0.96	0.07	62,62,62,62	0
58	MG	1A	3846	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3250	1/1	0.96	0.24	41,41,41,41	0
58	MG	1A	3528	1/1	0.96	0.19	39,39,39,39	0
58	MG	2A	3626	1/1	0.96	0.11	59,59,59,59	0
58	MG	2A	3382	1/1	0.96	0.14	45,45,45,45	0
58	MG	1A	3101	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3123	1/1	0.96	0.28	37,37,37,37	0
58	MG	2A	3630	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3172	1/1	0.96	0.09	34,34,34,34	0
58	MG	1B	234	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3174	1/1	0.96	0.14	46,46,46,46	0
58	MG	1A	3469	1/1	0.96	0.12	43,43,43,43	0
58	MG	1D	302	1/1	0.96	0.06	34,34,34,34	0
58	MG	1D	303	1/1	0.96	0.16	40,40,40,40	0
58	MG	2A	3391	1/1	0.96	0.32	52,52,52,52	0
58	MG	1l	202	1/1	0.96	0.13	61,61,61,61	0
58	MG	1A	3720	1/1	0.96	0.04	17,17,17,17	0
58	MG	2A	3643	1/1	0.96	0.10	32,32,32,32	0
58	MG	2a	1740	1/1	0.96	0.30	62,62,62,62	0
58	MG	1A	3610	1/1	0.96	0.06	22,22,22,22	0
58	MG	2a	1742	1/1	0.96	0.21	63,63,63,63	0
58	MG	1A	3611	1/1	0.96	0.08	42,42,42,42	0
58	MG	2a	1744	1/1	0.96	0.06	65,65,65,65	0
58	MG	1A	4000	1/1	0.96	0.19	44,44,44,44	0
58	MG	1A	4001	1/1	0.96	0.08	29,29,29,29	0
58	MG	2A	3649	1/1	0.96	0.08	26,26,26,26	0
58	MG	2A	3184	1/1	0.96	0.24	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	1749	1/1	0.96	0.09	64,64,64,64	0
58	MG	1E	304	1/1	0.96	0.16	34,34,34,34	0
58	MG	1E	305	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3723	1/1	0.96	0.07	59,59,59,59	0
58	MG	1A	3726	1/1	0.96	0.12	34,34,34,34	0
58	MG	1E	309	1/1	0.96	0.12	23,23,23,23	0
58	MG	2A	3656	1/1	0.96	0.07	48,48,48,48	0
58	MG	1A	3352	1/1	0.96	0.11	63,63,63,63	0
58	MG	1A	3014	1/1	0.96	0.10	28,28,28,28	0
58	MG	1a	1651	1/1	0.96	0.12	54,54,54,54	0
58	MG	1A	3861	1/1	0.96	0.11	51,51,51,51	0
58	MG	1A	3535	1/1	0.96	0.09	58,58,58,58	0
58	MG	1A	3016	1/1	0.96	0.27	56,56,56,56	0
58	MG	1A	4009	1/1	0.96	0.07	31,31,31,31	0
58	MG	2A	3414	1/1	0.96	0.13	74,74,74,74	0
58	MG	1F	308	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3669	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3413	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3417	1/1	0.96	0.11	32,32,32,32	0
58	MG	1A	3539	1/1	0.96	0.05	56,56,56,56	0
58	MG	1A	3735	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3414	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3256	1/1	0.96	0.07	57,57,57,57	0
58	MG	1A	3621	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3177	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3424	1/1	0.96	0.14	52,52,52,52	0
58	MG	1H	201	1/1	0.96	0.17	44,44,44,44	0
58	MG	1A	3180	1/1	0.96	0.05	33,33,33,33	0
58	MG	2a	1781	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3419	1/1	0.96	0.07	45,45,45,45	0
58	MG	1N	202	1/1	0.96	0.05	44,44,44,44	0
58	MG	1N	203	1/1	0.96	0.06	51,51,51,51	0
58	MG	2A	3008	1/1	0.96	0.05	45,45,45,45	0
58	MG	1A	3627	1/1	0.96	0.06	59,59,59,59	0
58	MG	2A	3010	1/1	0.96	0.12	48,48,48,48	0
58	MG	1A	3628	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3545	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3441	1/1	0.96	0.21	39,39,39,39	0
58	MG	1A	4022	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3015	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3546	1/1	0.96	0.18	37,37,37,37	0
58	MG	1A	3021	1/1	0.96	0.07	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3151	1/1	0.96	0.22	28,28,28,28	0
58	MG	1A	3077	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3751	1/1	0.96	0.25	61,61,61,61	0
58	MG	1A	3637	1/1	0.96	0.05	20,20,20,20	0
58	MG	1A	4029	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3452	1/1	0.96	0.09	35,35,35,35	0
58	MG	1P	208	1/1	0.96	0.09	64,64,64,64	0
58	MG	2D	301	1/1	0.96	0.07	41,41,41,41	0
58	MG	2a	1803	1/1	0.96	0.20	61,61,61,61	0
58	MG	1Q	201	1/1	0.96	0.13	42,42,42,42	0
58	MG	1A	3184	1/1	0.96	0.04	49,49,49,49	0
58	MG	1Q	204	1/1	0.96	0.11	60,60,60,60	0
58	MG	2A	3457	1/1	0.96	0.18	53,53,53,53	0
58	MG	1A	3890	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3641	1/1	0.96	0.10	28,28,28,28	0
58	MG	1A	3042	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3031	1/1	0.96	0.33	36,36,36,36	0
58	MG	2A	3037	1/1	0.96	0.14	39,39,39,39	0
58	MG	2E	307	1/1	0.96	0.10	49,49,49,49	0
58	MG	1R	204	1/1	0.96	0.29	43,43,43,43	0
58	MG	2A	3465	1/1	0.96	0.07	27,27,27,27	0
58	MG	2A	3235	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3188	1/1	0.96	0.15	37,37,37,37	0
58	MG	1A	3157	1/1	0.96	0.14	45,45,45,45	0
58	MG	1A	3557	1/1	0.96	0.20	33,33,33,33	0
58	MG	1a	1693	1/1	0.96	0.27	50,50,50,50	0
58	MG	2A	3473	1/1	0.96	0.11	40,40,40,40	0
58	MG	1a	1694	1/1	0.96	0.30	57,57,57,57	0
58	MG	2A	3241	1/1	0.96	0.14	56,56,56,56	0
58	MG	2R	202	1/1	0.96	0.20	60,60,60,60	0
58	MG	1A	3109	1/1	0.96	0.05	31,31,31,31	0
58	MG	1A	3900	1/1	0.96	0.13	42,42,42,42	0
58	MG	1a	1697	1/1	0.96	0.30	62,62,62,62	0
58	MG	1A	3112	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3192	1/1	0.96	0.29	32,32,32,32	0
58	MG	1A	3065	1/1	0.96	0.35	50,50,50,50	0
58	MG	1U	204	1/1	0.96	0.18	40,40,40,40	0
58	MG	1A	3904	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3651	1/1	0.96	0.07	29,29,29,29	0
58	MG	2A	3053	1/1	0.96	0.08	51,51,51,51	0
58	MG	23	103	1/1	0.96	0.25	54,54,54,54	0
58	MG	1A	3082	1/1	0.96	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4049	1/1	0.96	0.05	30,30,30,30	0
58	MG	2A	3256	1/1	0.96	0.22	50,50,50,50	0
58	MG	1U	210	1/1	0.96	0.17	39,39,39,39	0
58	MG	1A	3115	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3163	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3275	1/1	0.96	0.18	47,47,47,47	0
58	MG	2A	3261	1/1	0.96	0.33	58,58,58,58	0
58	MG	2A	3060	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3061	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3658	1/1	0.96	0.06	45,45,45,45	0
58	MG	2A	3265	1/1	0.96	0.32	54,54,54,54	0
58	MG	2A	3502	1/1	0.96	0.16	45,45,45,45	0
60	ERY	1A	4098	51/51	0.96	0.09	19,32,41,45	0
60	ERY	2A	3688	51/51	0.96	0.10	35,47,57,68	0
58	MG	1A	3330	1/1	0.96	0.18	49,49,49,49	0
61	ZN	2Y	501	1/1	0.96	0.06	104,104,104,104	0
58	MG	2A	3504	1/1	0.96	0.12	55,55,55,55	0
58	MG	2A	3505	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3126	1/1	0.97	0.17	53,53,53,53	0
58	MG	1A	3499	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3126	1/1	0.97	0.13	33,33,33,33	0
58	MG	1m	3001	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3186	1/1	0.97	0.04	36,36,36,36	0
58	MG	1U	208	1/1	0.97	0.15	28,28,28,28	0
58	MG	1A	3127	1/1	0.97	0.36	32,32,32,32	0
58	MG	1A	3036	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3066	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3384	1/1	0.97	0.28	32,32,32,32	0
58	MG	2A	3639	1/1	0.97	0.11	43,43,43,43	0
58	MG	1A	3573	1/1	0.97	0.05	52,52,52,52	0
58	MG	1V	202	1/1	0.97	0.16	35,35,35,35	0
58	MG	1A	3506	1/1	0.97	0.33	39,39,39,39	0
58	MG	2A	3292	1/1	0.97	0.06	50,50,50,50	0
58	MG	1V	205	1/1	0.97	0.08	43,43,43,43	0
58	MG	1A	3653	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3973	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3647	1/1	0.97	0.11	70,70,70,70	0
58	MG	1A	3039	1/1	0.97	0.15	33,33,33,33	0
58	MG	2A	3467	1/1	0.97	0.18	55,55,55,55	0
58	MG	2A	3468	1/1	0.97	0.09	44,44,44,44	0
58	MG	1a	1686	1/1	0.97	0.13	46,46,46,46	0
58	MG	1A	3975	1/1	0.97	0.12	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	1W	203	1/1	0.97	0.11	39,39,39,39	0
58	MG	2a	1693	1/1	0.97	0.20	64,64,64,64	0
58	MG	1W	204	1/1	0.97	0.15	43,43,43,43	0
58	MG	2a	1695	1/1	0.97	0.10	74,74,74,74	0
58	MG	2A	3148	1/1	0.97	0.18	54,54,54,54	0
58	MG	1A	3228	1/1	0.97	0.10	45,45,45,45	0
58	MG	1A	3005	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3658	1/1	0.97	0.18	55,55,55,55	0
58	MG	1A	3230	1/1	0.97	0.12	31,31,31,31	0
58	MG	2A	3660	1/1	0.97	0.10	60,60,60,60	0
58	MG	1A	3860	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3024	1/1	0.97	0.17	40,40,40,40	0
58	MG	2A	3663	1/1	0.97	0.07	46,46,46,46	0
58	MG	2A	3154	1/1	0.97	0.14	61,61,61,61	0
58	MG	1X	103	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	3072	1/1	0.97	0.09	19,19,19,19	0
58	MG	1A	3135	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3984	1/1	0.97	0.15	30,30,30,30	0
58	MG	2A	3485	1/1	0.97	0.11	56,56,56,56	0
58	MG	1A	3864	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3865	1/1	0.97	0.06	50,50,50,50	0
58	MG	1A	3662	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3111	1/1	0.97	0.23	37,37,37,37	0
58	MG	1A	3007	1/1	0.97	0.06	37,37,37,37	0
58	MG	2A	3491	1/1	0.97	0.10	35,35,35,35	0
58	MG	1A	3665	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3237	1/1	0.97	0.06	70,70,70,70	0
58	MG	2A	3494	1/1	0.97	0.07	40,40,40,40	0
58	MG	2A	3322	1/1	0.97	0.18	46,46,46,46	0
58	MG	1A	3667	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	3993	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3325	1/1	0.97	0.11	30,30,30,30	0
58	MG	1A	3092	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3282	1/1	0.97	0.27	35,35,35,35	0
58	MG	2A	3016	1/1	0.97	0.04	40,40,40,40	0
58	MG	1A	3996	1/1	0.97	0.09	44,44,44,44	0
58	MG	1A	3876	1/1	0.97	0.25	38,38,38,38	0
58	MG	2A	3331	1/1	0.97	0.22	66,66,66,66	0
58	MG	1A	3877	1/1	0.97	0.24	32,32,32,32	0
58	MG	1a	1714	1/1	0.97	0.14	37,37,37,37	0
58	MG	1A	3763	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3520	1/1	0.97	0.11	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	3458	1/1	0.97	0.13	32,32,32,32	0
58	MG	2A	3026	1/1	0.97	0.05	44,44,44,44	0
58	MG	12	102	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3589	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3674	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	3769	1/1	0.97	0.08	34,34,34,34	0
58	MG	2A	3516	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3771	1/1	0.97	0.05	26,26,26,26	0
58	MG	1B	228	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3522	1/1	0.97	0.24	44,44,44,44	0
58	MG	2D	303	1/1	0.97	0.04	30,30,30,30	0
58	MG	15	103	1/1	0.97	0.11	33,33,33,33	0
58	MG	1A	3074	1/1	0.97	0.04	13,13,13,13	0
58	MG	16	101	1/1	0.97	0.07	60,60,60,60	0
58	MG	17	103	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	3677	1/1	0.97	0.08	32,32,32,32	0
58	MG	2a	1750	1/1	0.97	0.11	71,71,71,71	0
58	MG	2A	3350	1/1	0.97	0.24	42,42,42,42	0
58	MG	1A	3592	1/1	0.97	0.09	34,34,34,34	0
58	MG	1A	3240	1/1	0.97	0.19	32,32,32,32	0
58	MG	1A	3200	1/1	0.97	0.19	37,37,37,37	0
58	MG	1A	3595	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3201	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3168	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3686	1/1	0.97	0.07	54,54,54,54	0
58	MG	2a	1760	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3009	1/1	0.97	0.04	34,34,34,34	0
58	MG	1D	308	1/1	0.97	0.15	41,41,41,41	0
58	MG	1A	3292	1/1	0.97	0.20	28,28,28,28	0
58	MG	1A	3095	1/1	0.97	0.07	19,19,19,19	0
58	MG	1D	311	1/1	0.97	0.14	36,36,36,36	0
58	MG	1A	3294	1/1	0.97	0.10	51,51,51,51	0
58	MG	2a	1767	1/1	0.97	0.04	82,82,82,82	0
58	MG	1A	3248	1/1	0.97	0.07	53,53,53,53	0
58	MG	2R	203	1/1	0.97	0.06	48,48,48,48	0
58	MG	1A	3296	1/1	0.97	0.07	48,48,48,48	0
58	MG	1E	306	1/1	0.97	0.07	52,52,52,52	0
58	MG	1A	3059	1/1	0.97	0.04	29,29,29,29	0
58	MG	2A	3369	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3797	1/1	0.97	0.09	54,54,54,54	0
58	MG	1a	1753	1/1	0.97	0.08	62,62,62,62	0
58	MG	1A	3207	1/1	0.97	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	1E	310	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3044	1/1	0.97	0.28	32,32,32,32	0
58	MG	1E	312	1/1	0.97	0.10	46,46,46,46	0
58	MG	2A	3550	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3301	1/1	0.97	0.10	29,29,29,29	0
58	MG	1A	3119	1/1	0.97	0.13	29,29,29,29	0
58	MG	25	103	1/1	0.97	0.07	52,52,52,52	0
58	MG	1F	302	1/1	0.97	0.21	28,28,28,28	0
58	MG	1F	303	1/1	0.97	0.11	44,44,44,44	0
58	MG	2A	3068	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3120	1/1	0.97	0.08	35,35,35,35	0
58	MG	1A	3700	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	4030	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3175	1/1	0.97	0.42	37,37,37,37	0
58	MG	1A	3614	1/1	0.97	0.13	48,48,48,48	0
58	MG	2A	3074	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3306	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3563	1/1	0.97	0.15	36,36,36,36	0
58	MG	1A	3212	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3418	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3079	1/1	0.97	0.14	38,38,38,38	0
58	MG	1G	202	1/1	0.97	0.19	51,51,51,51	0
58	MG	1A	4038	1/1	0.97	0.11	36,36,36,36	0
58	MG	1A	3359	1/1	0.97	0.13	45,45,45,45	0
58	MG	2A	3570	1/1	0.97	0.14	58,58,58,58	0
58	MG	1A	3214	1/1	0.97	0.31	37,37,37,37	0
58	MG	1A	3179	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3147	1/1	0.97	0.26	32,32,32,32	0
58	MG	2A	3085	1/1	0.97	0.18	50,50,50,50	0
58	MG	1A	3217	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3820	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3261	1/1	0.97	0.24	44,44,44,44	0
58	MG	1N	205	1/1	0.97	0.12	45,45,45,45	0
58	MG	1A	3822	1/1	0.97	0.27	25,25,25,25	0
58	MG	1A	3823	1/1	0.97	0.06	33,33,33,33	0
58	MG	1a	1785	1/1	0.97	0.12	62,62,62,62	0
58	MG	1A	3366	1/1	0.97	0.17	33,33,33,33	0
58	MG	1A	3933	1/1	0.97	0.06	50,50,50,50	0
58	MG	2A	3584	1/1	0.97	0.15	54,54,54,54	0
58	MG	1A	3825	1/1	0.97	0.07	23,23,23,23	0
58	MG	2A	3586	1/1	0.97	0.12	38,38,38,38	0
58	MG	2A	3409	1/1	0.97	0.13	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	3716	1/1	0.97	0.04	47,47,47,47	0
58	MG	2A	3249	1/1	0.97	0.10	55,55,55,55	0
58	MG	1A	3367	1/1	0.97	0.08	60,60,60,60	0
58	MG	1A	3940	1/1	0.97	0.08	55,55,55,55	0
58	MG	1A	3629	1/1	0.97	0.10	24,24,24,24	0
58	MG	1P	205	1/1	0.97	0.29	32,32,32,32	0
58	MG	1a	1649	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3368	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3010	1/1	0.97	0.08	40,40,40,40	0
58	MG	1A	3316	1/1	0.97	0.10	48,48,48,48	0
58	MG	1A	3633	1/1	0.97	0.06	20,20,20,20	0
58	MG	1A	3559	1/1	0.97	0.18	37,37,37,37	0
58	MG	1A	3724	1/1	0.97	0.15	40,40,40,40	0
58	MG	2A	3108	1/1	0.97	0.08	44,44,44,44	0
58	MG	1A	3836	1/1	0.97	0.17	61,61,61,61	0
58	MG	2l	205	1/1	0.97	0.06	67,67,67,67	0
58	MG	1A	3951	1/1	0.97	0.11	46,46,46,46	0
58	MG	2A	3427	1/1	0.97	0.09	60,60,60,60	0
58	MG	1A	3725	1/1	0.97	0.14	50,50,50,50	0
58	MG	1R	202	1/1	0.97	0.10	38,38,38,38	0
58	MG	2A	3113	1/1	0.97	0.11	41,41,41,41	0
58	MG	2A	3432	1/1	0.97	0.09	41,41,41,41	0
58	MG	1R	203	1/1	0.97	0.10	50,50,50,50	0
58	MG	1A	3317	1/1	0.97	0.11	50,50,50,50	0
58	MG	1A	4071	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3047	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3639	1/1	0.97	0.04	21,21,21,21	0
58	MG	2A	3438	1/1	0.97	0.09	44,44,44,44	0
58	MG	2A	3440	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3956	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3729	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3034	1/1	0.97	0.31	27,27,27,27	0
58	MG	1A	3375	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3622	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3436	1/1	0.97	0.16	36,36,36,36	0
58	MG	2A	3446	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3035	1/1	0.97	0.27	35,35,35,35	0
58	MG	2A	3507	1/1	0.98	0.12	51,51,51,51	0
58	MG	1A	3243	1/1	0.98	0.11	28,28,28,28	0
58	MG	1A	3203	1/1	0.98	0.06	33,33,33,33	0
58	MG	1a	1800	1/1	0.98	0.08	48,48,48,48	0
58	MG	1A	4034	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	2A	3634	1/1	0.98	0.08	45,45,45,45	0
58	MG	2A	3392	1/1	0.98	0.25	42,42,42,42	0
58	MG	1A	3376	1/1	0.98	0.06	26,26,26,26	0
58	MG	2A	3169	1/1	0.98	0.14	39,39,39,39	0
58	MG	1A	3708	1/1	0.98	0.11	20,20,20,20	0
58	MG	1A	3058	1/1	0.98	0.17	39,39,39,39	0
58	MG	1a	1805	1/1	0.98	0.04	57,57,57,57	0
58	MG	1A	3085	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3889	1/1	0.98	0.07	50,50,50,50	0
58	MG	1A	3965	1/1	0.98	0.10	20,20,20,20	0
58	MG	1A	3508	1/1	0.98	0.14	33,33,33,33	0
58	MG	1U	202	1/1	0.98	0.13	36,36,36,36	0
58	MG	1A	3828	1/1	0.98	0.03	34,34,34,34	0
58	MG	1A	3892	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3011	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3110	1/1	0.98	0.25	38,38,38,38	0
58	MG	1A	3622	1/1	0.98	0.10	19,19,19,19	0
58	MG	1A	3623	1/1	0.98	0.09	43,43,43,43	0
58	MG	1A	3076	1/1	0.98	0.05	32,32,32,32	0
58	MG	1B	235	1/1	0.98	0.07	30,30,30,30	0
58	MG	1A	3770	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3899	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3547	1/1	0.98	0.14	35,35,35,35	0
58	MG	2a	1759	1/1	0.98	0.21	50,50,50,50	0
58	MG	1A	4052	1/1	0.98	0.08	42,42,42,42	0
58	MG	1V	203	1/1	0.98	0.24	34,34,34,34	0
58	MG	1A	3012	1/1	0.98	0.04	26,26,26,26	0
58	MG	1D	307	1/1	0.98	0.07	35,35,35,35	0
58	MG	1a	1723	1/1	0.98	0.12	54,54,54,54	0
58	MG	1a	1632	1/1	0.98	0.10	28,28,28,28	0
58	MG	1A	3383	1/1	0.98	0.20	32,32,32,32	0
58	MG	1A	3155	1/1	0.98	0.10	30,30,30,30	0
58	MG	1a	1727	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	3775	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	3156	1/1	0.98	0.07	43,43,43,43	0
58	MG	1E	301	1/1	0.98	0.19	36,36,36,36	0
58	MG	2A	3312	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3777	1/1	0.98	0.05	63,63,63,63	0
58	MG	1A	3013	1/1	0.98	0.16	23,23,23,23	0
58	MG	1a	1640	1/1	0.98	0.23	53,53,53,53	0
58	MG	2A	3673	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3780	1/1	0.98	0.04	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	3909	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3449	1/1	0.98	0.10	44,44,44,44	0
58	MG	1A	3450	1/1	0.98	0.06	39,39,39,39	0
58	MG	2A	3320	1/1	0.98	0.14	46,46,46,46	0
58	MG	2A	3679	1/1	0.98	0.07	34,34,34,34	0
58	MG	1a	1739	1/1	0.98	0.05	39,39,39,39	0
58	MG	1a	1740	1/1	0.98	0.10	33,33,33,33	0
58	MG	2A	3439	1/1	0.98	0.11	38,38,38,38	0
58	MG	1A	3069	1/1	0.98	0.04	29,29,29,29	0
58	MG	1X	104	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3786	1/1	0.98	0.05	49,49,49,49	0
58	MG	1A	3679	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3048	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	4073	1/1	0.98	0.10	41,41,41,41	0
58	MG	2A	3216	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3789	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3129	1/1	0.98	0.23	39,39,39,39	0
58	MG	1A	3682	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3305	1/1	0.98	0.05	35,35,35,35	0
58	MG	10	102	1/1	0.98	0.09	42,42,42,42	0
58	MG	1A	3638	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3596	1/1	0.98	0.12	28,28,28,28	0
58	MG	1a	1754	1/1	0.98	0.07	54,54,54,54	0
58	MG	2A	3116	1/1	0.98	0.25	49,49,49,49	0
58	MG	1A	3734	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3235	1/1	0.98	0.06	47,47,47,47	0
58	MG	2A	3012	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3737	1/1	0.98	0.04	29,29,29,29	0
58	MG	2A	3460	1/1	0.98	0.12	42,42,42,42	0
58	MG	1A	3071	1/1	0.98	0.09	33,33,33,33	0
58	MG	1A	3037	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3199	1/1	0.98	0.05	43,43,43,43	0
58	MG	2A	3017	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3930	1/1	0.98	0.07	45,45,45,45	0
58	MG	1A	3931	1/1	0.98	0.03	20,20,20,20	0
58	MG	2E	302	1/1	0.98	0.06	45,45,45,45	0
58	MG	1A	3601	1/1	0.98	0.12	26,26,26,26	0
58	MG	2A	3021	1/1	0.98	0.04	45,45,45,45	0
58	MG	2A	3351	1/1	0.98	0.08	52,52,52,52	0
58	MG	1A	3602	1/1	0.98	0.03	22,22,22,22	0
58	MG	1A	3935	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3310	1/1	0.98	0.05	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3693	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3938	1/1	0.98	0.09	38,38,38,38	0
58	MG	1A	3866	1/1	0.98	0.06	49,49,49,49	0
58	MG	2A	3476	1/1	0.98	0.05	42,42,42,42	0
58	MG	2A	3029	1/1	0.98	0.14	44,44,44,44	0
58	MG	2A	3596	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3427	1/1	0.98	0.08	43,43,43,43	0
58	MG	2A	3137	1/1	0.98	0.14	37,37,37,37	0
58	MG	1A	3941	1/1	0.98	0.06	46,46,46,46	0
58	MG	1A	3283	1/1	0.98	0.27	28,28,28,28	0
58	MG	1A	3869	1/1	0.98	0.04	32,32,32,32	0
58	MG	2A	3250	1/1	0.98	0.13	35,35,35,35	0
58	MG	1A	3808	1/1	0.98	0.11	28,28,28,28	0
58	MG	1a	1775	1/1	0.98	0.05	40,40,40,40	0
58	MG	17	101	1/1	0.98	0.04	33,33,33,33	0
58	MG	17	102	1/1	0.98	0.17	33,33,33,33	0
58	MG	1A	3809	1/1	0.98	0.06	25,25,25,25	0
58	MG	20	101	1/1	0.98	0.09	53,53,53,53	0
58	MG	1A	3810	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3947	1/1	0.98	0.10	44,44,44,44	0
58	MG	1A	3811	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3284	1/1	0.98	0.12	43,43,43,43	0
58	MG	1B	208	1/1	0.98	0.07	52,52,52,52	0
58	MG	1A	3038	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3286	1/1	0.98	0.10	38,38,38,38	0
58	MG	1a	1786	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3106	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3148	1/1	0.98	0.19	31,31,31,31	0
58	MG	1Q	203	1/1	0.98	0.06	44,44,44,44	0
58	MG	1A	3372	1/1	0.98	0.07	42,42,42,42	0
58	MG	1A	3242	1/1	0.98	0.17	34,34,34,34	0
58	MG	1a	1792	1/1	0.98	0.04	46,46,46,46	0
58	MG	1a	1793	1/1	0.98	0.06	61,61,61,61	0
58	MG	1A	3537	1/1	0.98	0.08	58,58,58,58	0
58	MG	1A	3657	1/1	0.98	0.06	41,41,41,41	0
58	MG	1B	217	1/1	0.98	0.05	50,50,50,50	0
62	SF4	2d	303	8/8	0.98	0.05	71,78,88,104	0
58	MG	1A	3671	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3978	1/1	0.99	0.06	53,53,53,53	0
58	MG	1A	3008	1/1	0.99	0.06	27,27,27,27	0
58	MG	1D	305	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	3298	1/1	0.99	0.04	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	1A	3934	1/1	0.99	0.04	23,23,23,23	0
58	MG	1A	3757	1/1	0.99	0.04	41,41,41,41	0
58	MG	2A	3293	1/1	0.99	0.16	27,27,27,27	0
58	MG	1A	3029	1/1	0.99	0.15	30,30,30,30	0
58	MG	1A	3914	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	4058	1/1	0.99	0.04	44,44,44,44	0
58	MG	2A	3603	1/1	0.99	0.13	42,42,42,42	0
58	MG	1A	4059	1/1	0.99	0.07	52,52,52,52	0
58	MG	1A	4060	1/1	0.99	0.05	25,25,25,25	0
58	MG	1E	303	1/1	0.99	0.12	33,33,33,33	0
58	MG	1A	3915	1/1	0.99	0.02	22,22,22,22	0
58	MG	1A	3046	1/1	0.99	0.03	34,34,34,34	0
58	MG	2A	3413	1/1	0.99	0.08	36,36,36,36	0
58	MG	1A	3023	1/1	0.99	0.03	18,18,18,18	0
58	MG	1A	3003	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3395	1/1	0.99	0.21	39,39,39,39	0
58	MG	1A	3779	1/1	0.99	0.04	17,17,17,17	0
58	MG	1a	1794	1/1	0.99	0.04	57,57,57,57	0
58	MG	1A	4067	1/1	0.99	0.13	39,39,39,39	0
58	MG	1A	3049	1/1	0.99	0.17	32,32,32,32	0
58	MG	1A	3360	1/1	0.99	0.04	51,51,51,51	0
58	MG	1A	3801	1/1	0.99	0.07	24,24,24,24	0
58	MG	1A	3488	1/1	0.99	0.18	34,34,34,34	0
58	MG	1A	3783	1/1	0.99	0.04	20,20,20,20	0
58	MG	1a	1732	1/1	0.99	0.12	40,40,40,40	0
58	MG	1A	3784	1/1	0.99	0.03	24,24,24,24	0
58	MG	1P	207	1/1	0.99	0.04	32,32,32,32	0
58	MG	2A	3624	1/1	0.99	0.10	42,42,42,42	0
58	MG	2A	3428	1/1	0.99	0.05	40,40,40,40	0
58	MG	2A	3027	1/1	0.99	0.16	40,40,40,40	0
58	MG	1A	3766	1/1	0.99	0.09	40,40,40,40	0
61	ZN	1Y	205	1/1	0.99	0.02	66,66,66,66	0
58	MG	1A	3176	1/1	0.99	0.16	32,32,32,32	0
61	ZN	15	105	1/1	0.99	0.04	67,67,67,67	0
61	ZN	19	102	1/1	0.99	0.04	44,44,44,44	0
61	ZN	1n	103	1/1	0.99	0.03	67,67,67,67	0
58	MG	1a	1703	1/1	0.99	0.05	49,49,49,49	0
58	MG	1F	306	1/1	0.99	0.20	31,31,31,31	0
61	ZN	25	105	1/1	0.99	0.05	91,91,91,91	0
61	ZN	26	501	1/1	0.99	0.06	71,71,71,71	0
61	ZN	29	501	1/1	0.99	0.03	70,70,70,70	0
58	MG	1A	3634	1/1	0.99	0.04	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
62	SF4	1d	303	8/8	0.99	0.06	59,66,69,71	0
58	MG	1A	3710	1/1	0.99	0.05	31,31,31,31	0
58	MG	1A	4055	1/1	1.00	0.03	17,17,17,17	0
58	MG	1A	3178	1/1	1.00	0.06	19,19,19,19	0
58	MG	1A	3736	1/1	1.00	0.02	27,27,27,27	0
58	MG	2A	3632	1/1	1.00	0.06	28,28,28,28	0
61	ZN	16	102	1/1	1.00	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.