



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:19 AM UTC

PDB ID : 9O3J / pdb_00009o3j
Title : Crystal structure of the wild-type drug-free *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Lys-tRNA^{Lys}, P-site fM RC-peptidyl-tRNA^{Met}, and deacylated E-site tRNA^{Lys} at 2.60Å 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 : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

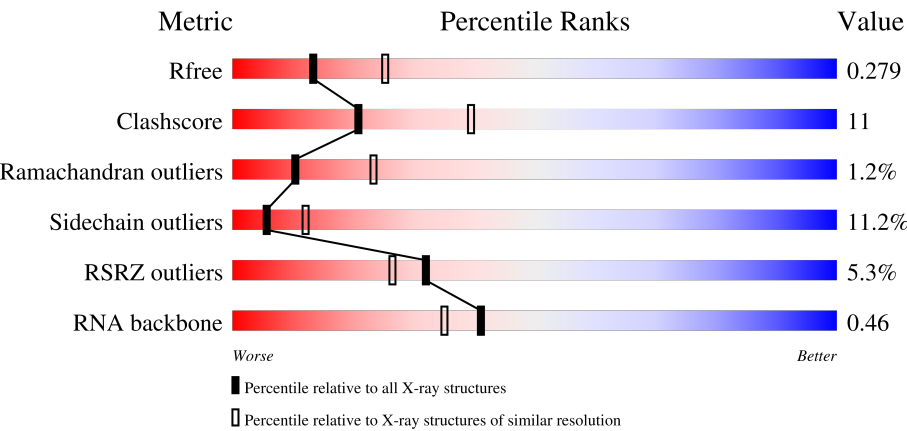
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

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

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Mol	Chain	Length	Quality of chain
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	
14	2S	112	

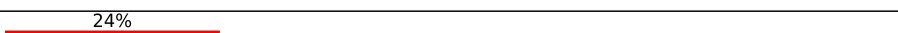
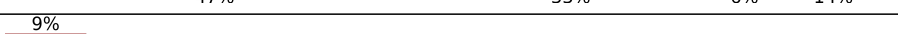
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Mol	Chain	Length	Quality of chain
15	1T	146	% 58% 29% 10%
15	2T	146	% 55% 34% 10%
16	1U	118	81% 16% ..
16	2U	118	63% 33% ..
17	1V	101	73% 25% .
17	2V	101	6% 54% 40% 5% .
18	1W	113	73% 24% ..
18	2W	113	2% 75% 23% ..
19	1X	96	% 72% 25% ..
19	2X	96	2% 73% 22% ..
20	1Y	110	2% 64% 27% 6% .
20	2Y	110	13% 60% 33% 5% .
21	1Z	206	7% 44% 24% 7% 25%
21	2Z	206	11% 41% 28% 9% 22%
22	10	85	5% 73% 21% ..
22	20	85	9% 68% 27% ..
23	11	98	% 64% 33% ..
23	21	98	3% 70% 23% 5% .
24	12	72	% 71% 22% . .
24	22	72	58% 36% . .
25	13	60	58% 37% ..
25	23	60	62% 33% ..
26	14	71	11% 51% 38% 6% . .
26	24	71	11% 41% 49% 7% .
27	15	60	2% 87% 12% .

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Mol	Chain	Length	Quality of chain
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	
39	2h	138	

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Mol	Chain	Length	Quality of chain
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	
52	1u	27	

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Mol	Chain	Length	Quality of chain
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	208	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299808 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1096	Total	Mg	0	0
			1096	1096		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	13	Total 13	Mg 13	0	0
58	1E	16	Total 16	Mg 16	0	0
58	1F	13	Total 13	Mg 13	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	4	Total 4	Mg 4	0	0
58	1P	6	Total 6	Mg 6	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	4	Total 4	Mg 4	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	9	Total 9	Mg 9	0	0
58	1V	9	Total 9	Mg 9	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	5	Total 5	Mg 5	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	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	5	Total 5	Mg 5	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	5	Total 5	Mg 5	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	6	Total 6	Mg 6	0	0
58	16	2	Total 2	Mg 2	0	0
58	17	6	Total 6	Mg 6	0	0
58	18	9	Total 9	Mg 9	0	0
58	1a	210	Total 210	Mg 210	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	1	Total 1	Mg 1	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
58	1w	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1x	11	Total 11 Mg 11	0	0
58	2A	863	Total 863 Mg 863	0	0
58	2B	20	Total 20 Mg 20	0	0
58	2D	7	Total 7 Mg 7	0	0
58	2E	7	Total 7 Mg 7	0	0
58	2F	7	Total 7 Mg 7	0	0
58	2G	1	Total 1 Mg 1	0	0
58	2O	2	Total 2 Mg 2	0	0
58	2P	3	Total 3 Mg 3	0	0
58	2Q	2	Total 2 Mg 2	0	0
58	2R	2	Total 2 Mg 2	0	0
58	2T	3	Total 3 Mg 3	0	0
58	2U	2	Total 2 Mg 2	0	0
58	2V	2	Total 2 Mg 2	0	0
58	2W	2	Total 2 Mg 2	0	0
58	2X	1	Total 1 Mg 1	0	0
58	2Y	1	Total 1 Mg 1	0	0
58	2Z	1	Total 1 Mg 1	0	0
58	20	4	Total 4 Mg 4	0	0
58	23	4	Total 4 Mg 4	0	0
58	25	5	Total 5 Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	27	3	Total 3	Mg 3	0	0
58	28	1	Total 1	Mg 1	0	0
58	2a	230	Total 230	Mg 230	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2i	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2k	1	Total 1	Mg 1	0	0
58	2l	4	Total 4	Mg 4	0	0
58	2n	1	Total 1	Mg 1	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	4	Total 4	Mg 4	0	0
58	2w	1	Total 1	Mg 1	0	0
58	2x	6	Total 6	Mg 6	0	0
58	2y	1	Total 1	Mg 1	0	0

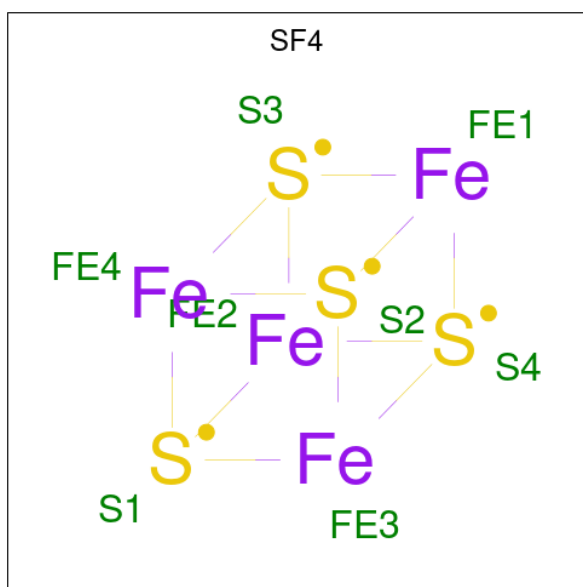
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1886	Total	O	0	0
			1886	1886		
62	1B	61	Total	O	0	0
			61	61		
62	1D	28	Total	O	0	0
			28	28		
62	1E	29	Total	O	0	0
			29	29		
62	1F	15	Total	O	0	0
			15	15		
62	1G	3	Total	O	0	0
			3	3		
62	1H	2	Total	O	0	0
			2	2		
62	1I	1	Total	O	0	0
			1	1		
62	1N	4	Total	O	0	0
			4	4		
62	1O	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	23	Total 23	O 23	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	16	Total 16	O 16	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	8	Total 8	O 8	0	0
62	1U	10	Total 10	O 10	0	0
62	1V	11	Total 11	O 11	0	0
62	1W	6	Total 6	O 6	0	0
62	1X	7	Total 7	O 7	0	0
62	1Y	1	Total 1	O 1	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	10	Total 10	O 10	0	0
62	11	12	Total 12	O 12	0	0
62	12	3	Total 3	O 3	0	0
62	13	4	Total 4	O 4	0	0
62	14	1	Total 1	O 1	0	0
62	15	7	Total 7	O 7	0	0
62	16	2	Total 2	O 2	0	0
62	17	11	Total 11	O 11	0	0
62	18	11	Total 11	O 11	0	0
62	1a	308	Total 308	O 308	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	7	Total 7	O 7	0	0
62	1m	2	Total 2	O 2	0	0
62	1o	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	8	Total 8	O 8	0	0
62	1x	6	Total 6	O 6	0	0
62	1z	1	Total 1	O 1	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	1000	Total 1000	O 1000	0	0
62	2B	22	Total 22	O 22	0	0
62	2D	24	Total 24	O 24	0	0
62	2E	9	Total 9	O 9	0	0
62	2F	15	Total 15	O 15	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2P	11	Total 11	O 11	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	5	Total 5	O 5	0	0
62	2U	3	Total 3	O 3	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	4	Total 4	O 4	0	0
62	2Y	1	Total 1	O 1	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	5	Total 5	O 5	0	0
62	21	13	Total 13	O 13	0	0
62	25	2	Total 2	O 2	0	0
62	27	1	Total 1	O 1	0	0
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	198	Total 198	O 198	0	0
62	2d	1	Total 1	O 1	0	0
62	2e	1	Total 1	O 1	0	0
62	2j	1	Total 1	O 1	0	0
62	2l	4	Total 4	O 4	0	0
62	2p	2	Total 2	O 2	0	0

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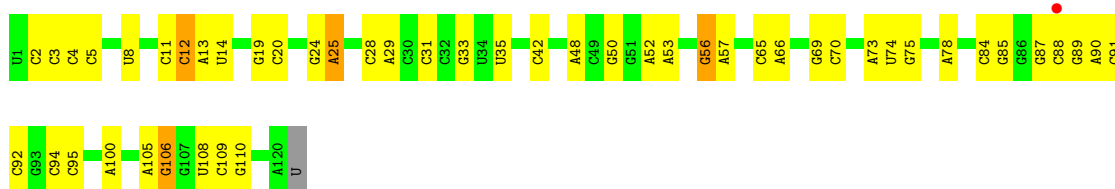
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2r	1	Total	O	0	0
			1	1		
62	2t	1	Total	O	0	0
			1	1		
62	2v	2	Total	O	0	0
			2	2		
62	2w	3	Total	O	0	0
			3	3		
62	2x	5	Total	O	0	0
			5	5		

C2292	C2195	G1950	G1826	G1718	C1588	A1494	G1371	A1247	G1149	A1077	A1010
G2302	A2198	U1951	C1827	G1719	C1589	U1497	U1372	G1252	C1150	U1078	G1011
G2305	A2199	A1952	G1828	U1720	G1594	U1497	A1373	A1253	C1151	C1079	U1012
A2306	C2200	A1953	A1829	U1721	G1595	C1504	A1379	G1256	C1152	C1080	U1013
G2307	C2203	U1955	A1847	A1722	U1602	C1506	G1380	A1256	G1153	U1081	U1014
G2308	C2205	C1962	U1851	G1739	U1607	A1507	A1384	G1264	A1155	U1083	G1015
U2312	G2206	U1963	C1852	G1740	C1607	A1508	G1385	A1265	A1156	A1084	G1016
G2315	G2207	G1964	A1808	A1741	A1608	C1509	U1394	G1266	G1164	A1085	G1022
G2316	U2218	C1965	A1610	G1753	A1609	A1509A	U1395	U1267	U1165	A1086	U1023
C2319	G2219	A1966	G1858	G1756	A1610	A1509B	U1396	A1268	C1166	A1088	G1024
A2320	G2222	U1968	U1864	U1757	A1614	U1512	C1399	G1271	U1167	U1089	G1025
A2328	A2225	A1969	G1865	G1759	C1615	C1513	C1399	U1272	G1171	U1090	U1026
G2325	G2226	A1970	C1866	A1762	G1633	U1514	U1405	A1273	G1173	C1091	A1027
A2327	A2227	A1971	A1876	G1763	G1634	G1515	U1406	A1274	U1094	U1093	U1033
G2329	G2228	A1972	G1878	G1764	G1636	U1518	C1407	A1275	A1174	A1095	G1034
G2330	G2229	U1984	C1882	G1770	A1641	G1520	G1416	A1278	U1175	A1096	U1035
G2331	G2233	U1993	G1883	A1773	G1642	A1528	C1417	G1281	A1177	U1097	U1036
G2334	G2234	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1178	A1098	G1037
A2335	G2235	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1179	A1099	G1038
A2336	G2236	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1180	U1101	G1039
G2337	G2237	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1181	C1102	G1041
G2345	G2238	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1182	C1103	G1042
A2346	G2239	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1183	A1103	C1043
A2347	G2240	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1184	C1104	G1044
G2348	G2241	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1185	C1105	A1045
G2349	G2242	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1186	C1106	G1106
G2350	G2243	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1187	C1107	G1047
G2351	G2244	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1188	C1108	A1048
G2352	G2245	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1189	C1109	G1049
G2353	G2246	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1190	C1110	A1050
G2354	G2247	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1191	C1111	G1051
G2355	G2248	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1192	C1112	G1052
G2356	G2249	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1193	C1113	G1053
G2357	G2250	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1194	C1114	G1054
A2377	G2251	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1195	C1115	G1055
A2378	G2252	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1196	C1116	G1056
G2381	G2253	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1197	C1117	G1057
G2382	G2254	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1198	C1118	G1058
G2383	G2255	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1199	C1119	G1059
G2384	G2256	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1200	C1120	U1060
G2385	G2257	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1201	C1121	U1061
G2386	G2258	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1202	C1122	G1062
G2387	G2259	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1203	C1123	G1063
A2377	G2260	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1204	C1124	G1064
A2378	G2261	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1205	C1125	U1065
G2381	G2262	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1206	C1126	U1066
G2382	G2263	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1207	C1127	U1067
G2383	G2264	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1208	C1128	G1068
G2384	G2265	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1209	C1129	A1069
G2385	G2266	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1210	C1130	A1070
G2386	G2267	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1211	C1131	G1071
G2387	G2268	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1212	C1132	C1072
U2390	G2269	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1213	C1133	A1073
G2394	G2270	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1214	C1134	G1074
G2395	G2271	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1215	C1135	G1075
G2396	G2272	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1216	C1136	G1076
G2397	G2273	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1217	C1137	G1077
G2398	G2274	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1218	C1138	G1078
G2399	G2275	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1219	C1139	G1079
G2400	G2276	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1220	C1140	G1080
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G2402	G2278	U1993	G1883	A1773	G1642	A1528	C1417	G1281	C1222	C1142	G1082
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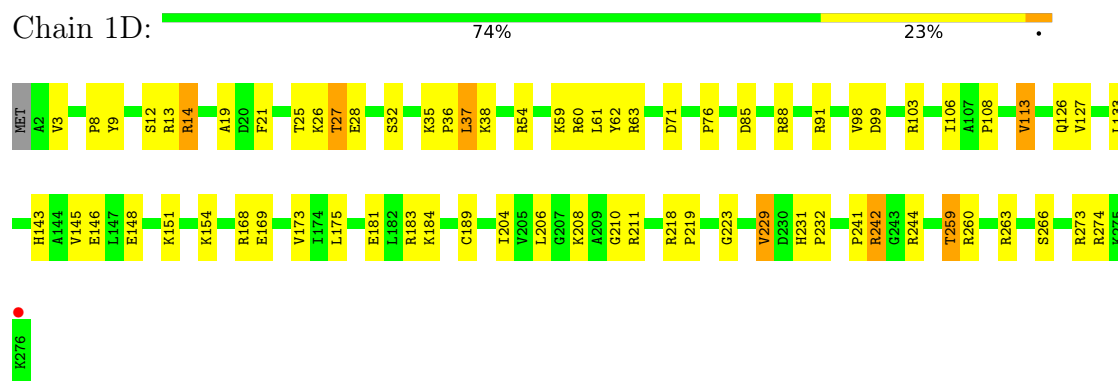
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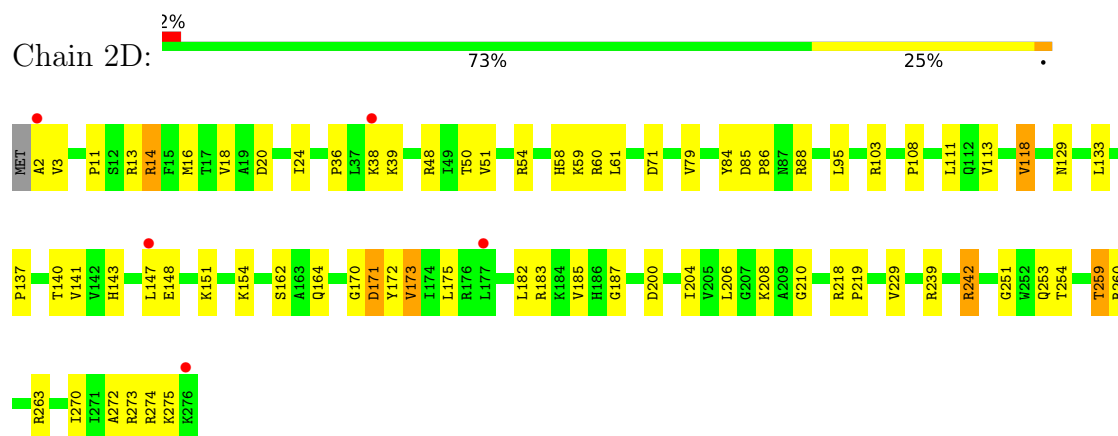
- Molecule 2: 5S Ribosomal RNA



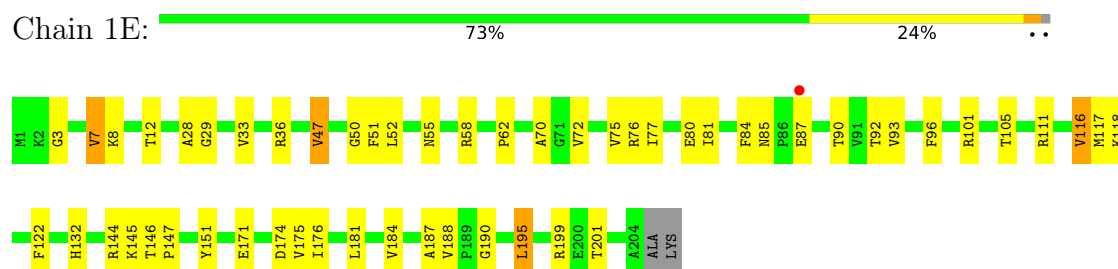
- Molecule 3: 50S ribosomal protein L2



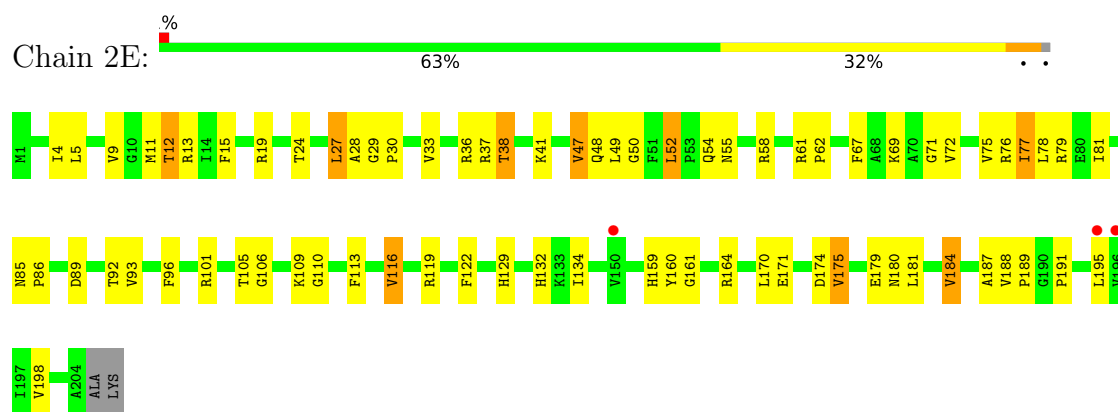
- Molecule 3: 50S ribosomal protein L2



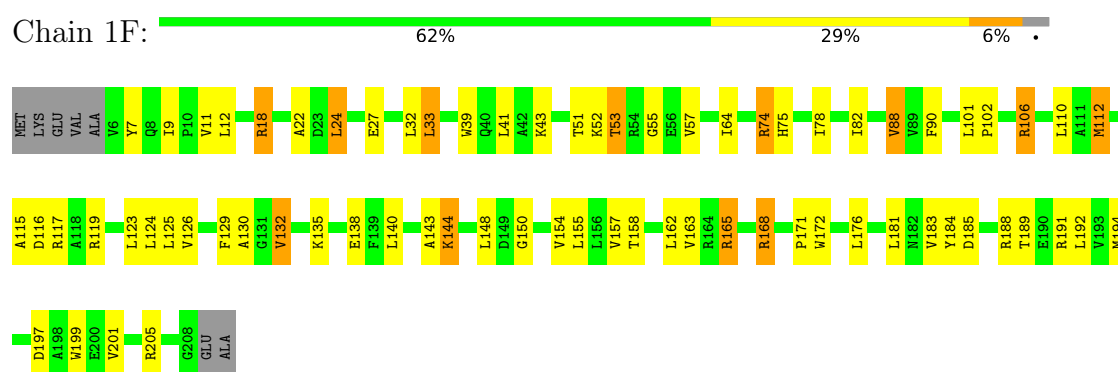
- Molecule 4: 50S ribosomal protein L3



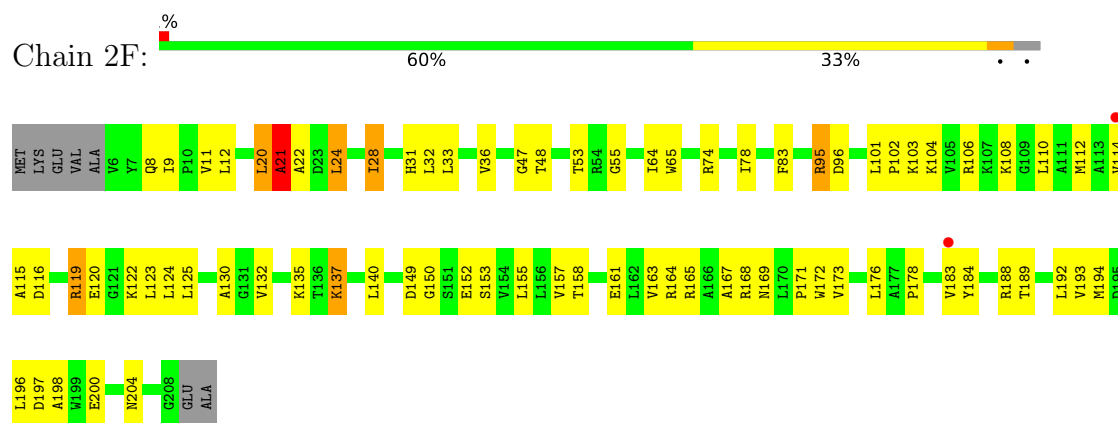
- Molecule 4: 50S ribosomal protein L3



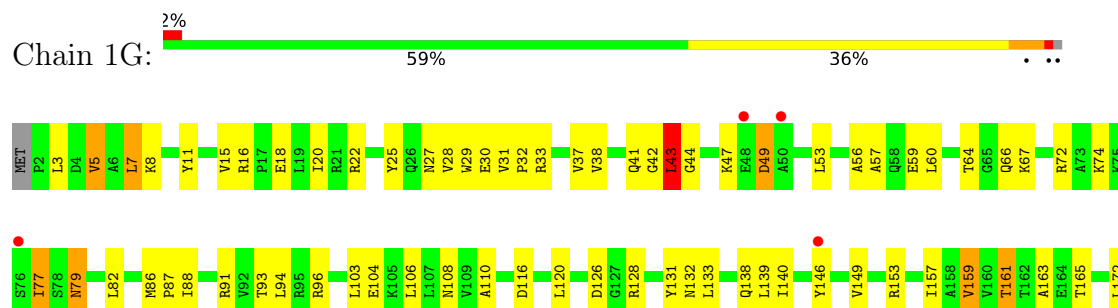
• Molecule 5: 50S ribosomal protein L4

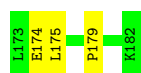


• Molecule 5: 50S ribosomal protein L4

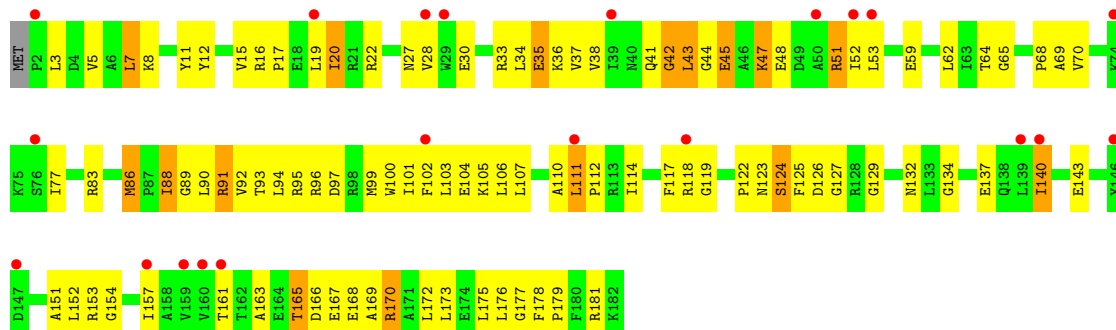
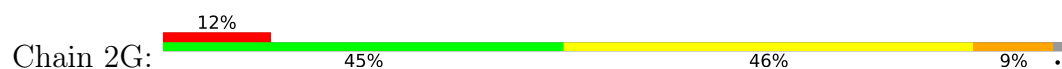


• Molecule 6: 50S ribosomal protein L5

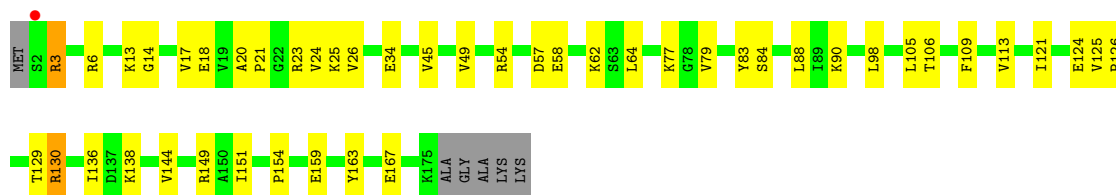
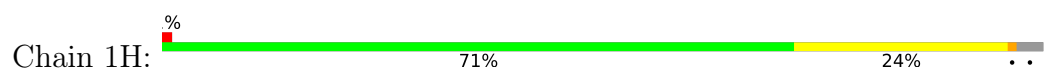




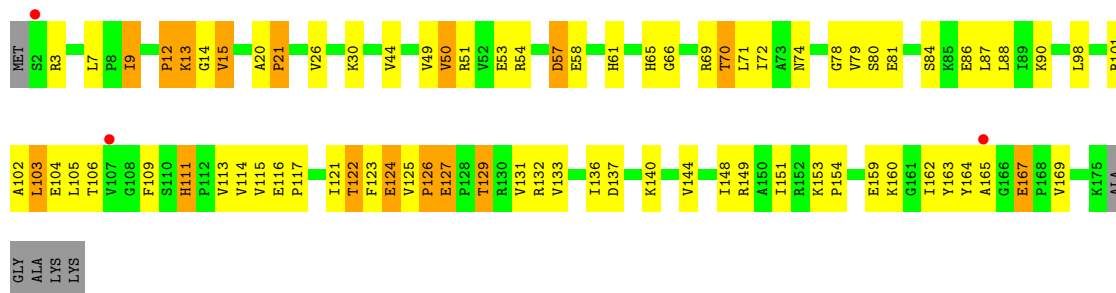
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

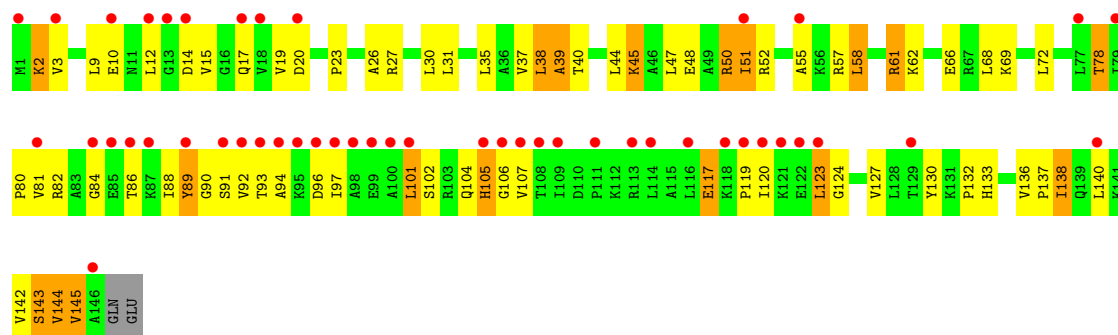


• Molecule 8: 50S ribosomal protein L9

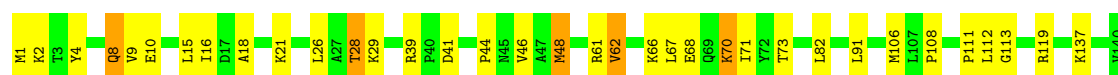
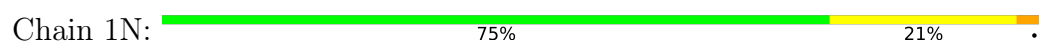




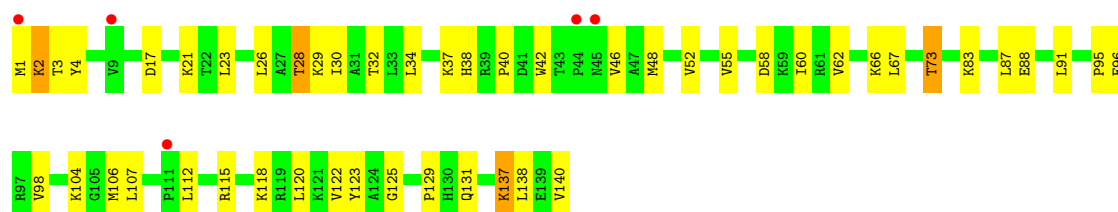
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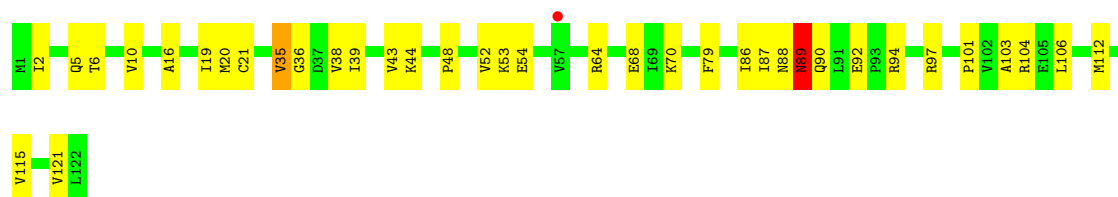
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

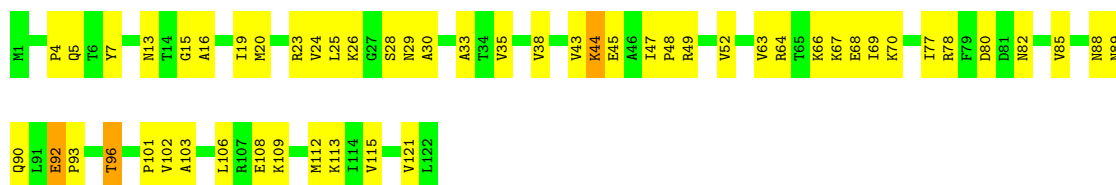


• Molecule 10: 50S ribosomal protein L14



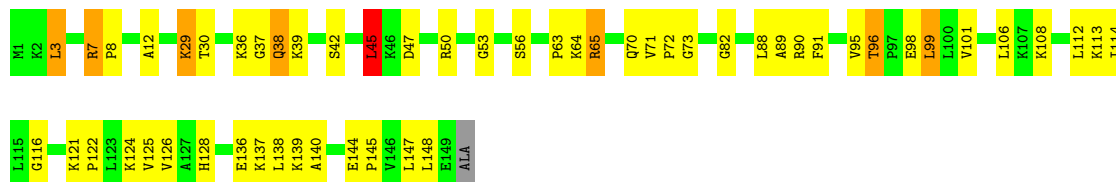
• Molecule 10: 50S ribosomal protein L14





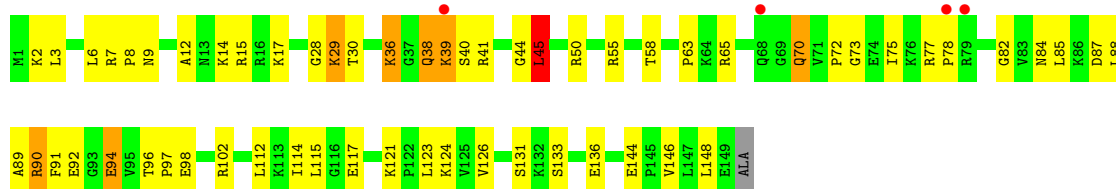
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 63% 31% 5% ..



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 3% 60% 34% 5% ..



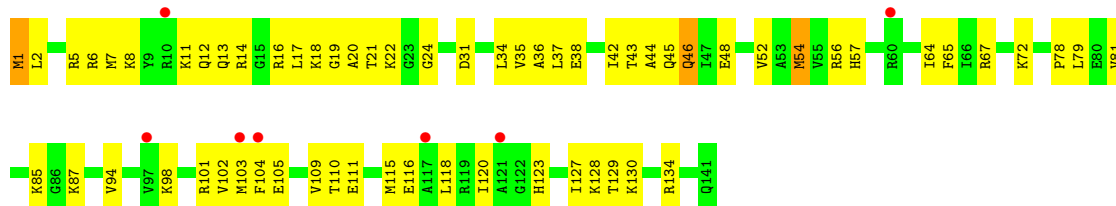
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 68% 28% .



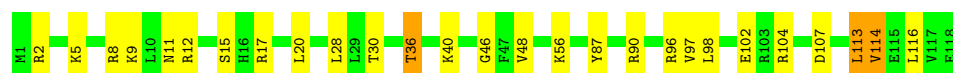
- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 5% 55% 43% .



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  77% 20% .



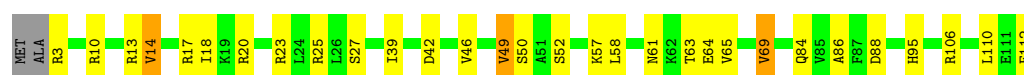
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  2% 74% 25% .



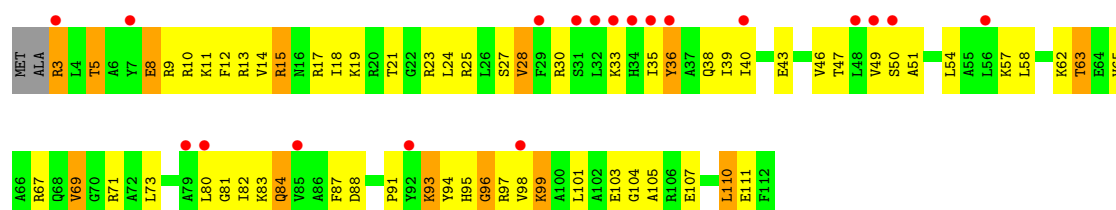
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  71% 24% . .



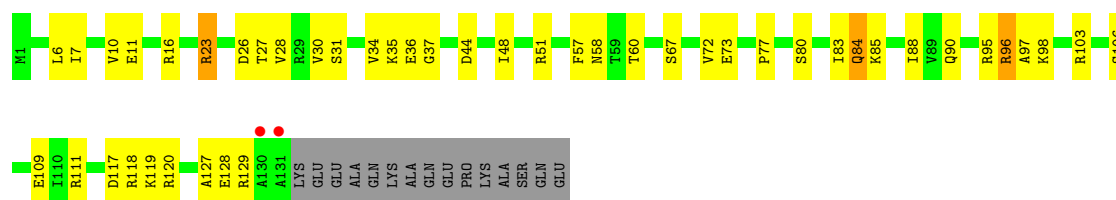
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  17% 41% 46% 12% .



- Molecule 15: 50S ribosomal protein L19

Chain 1T:  % 58% 29% 10% .



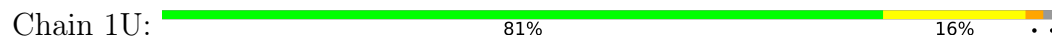
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  % 55% 34% 10% .

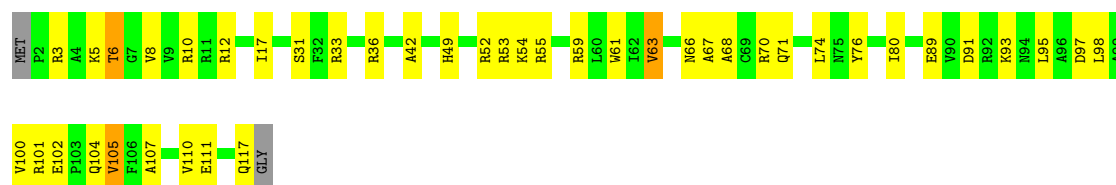




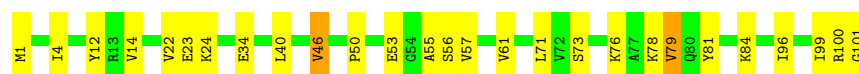
• Molecule 16: 50S ribosomal protein L20



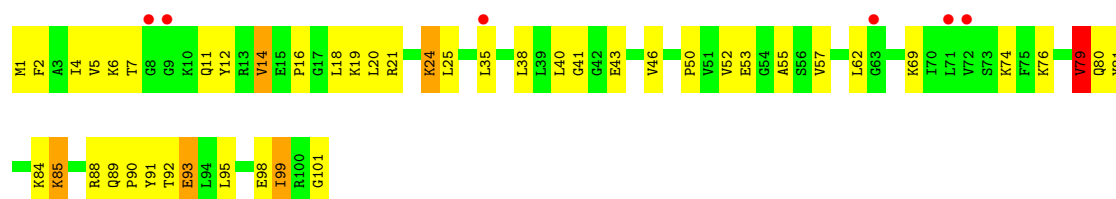
• Molecule 16: 50S ribosomal protein L20



• Molecule 17: 50S ribosomal protein L21



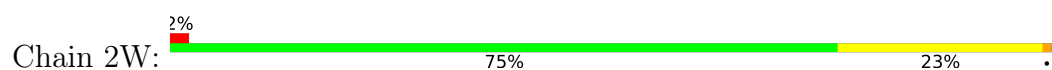
• Molecule 17: 50S ribosomal protein L21



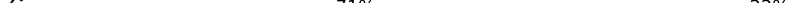
• Molecule 18: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L22





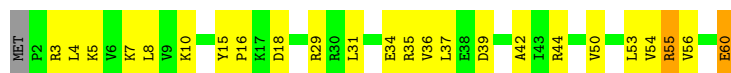
- Chain 12:  %



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



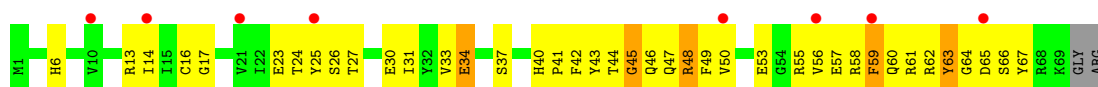
- Molecule 25: 50S ribosomal protein L30



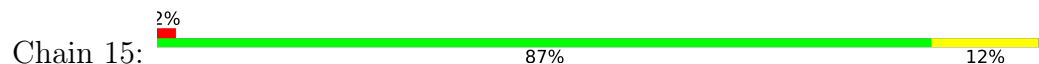
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31

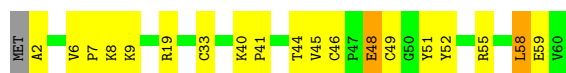


- Molecule 27: 50S ribosomal protein L32

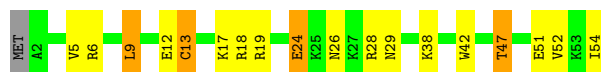


- Molecule 27: 50S ribosomal protein L32





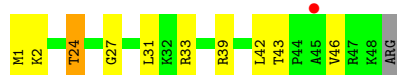
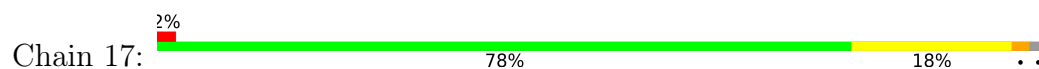
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



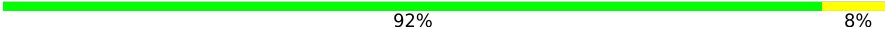
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



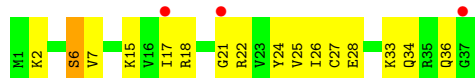
- Molecule 31: 50S ribosomal protein L36

Chain 19:  92% 8%



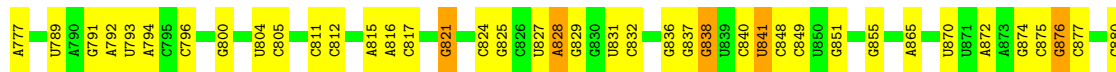
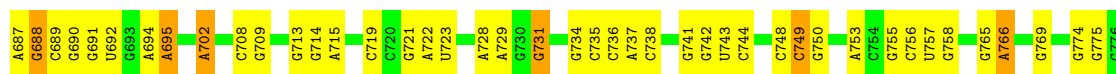
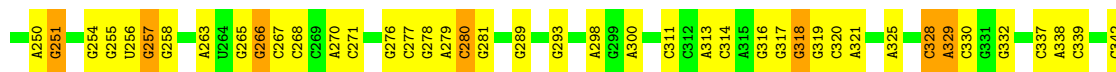
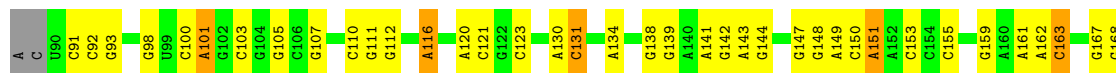
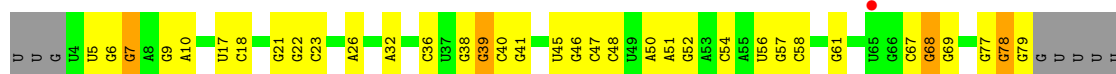
- Molecule 31: 50S ribosomal protein L36

Chain 29:  8% 57% 41%

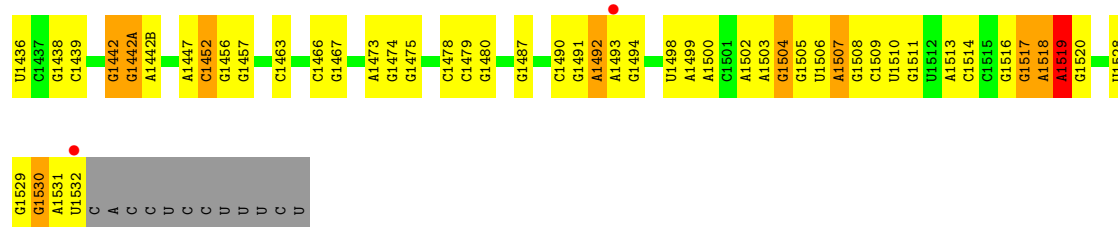


- Molecule 32: 16S Ribosomal RNA

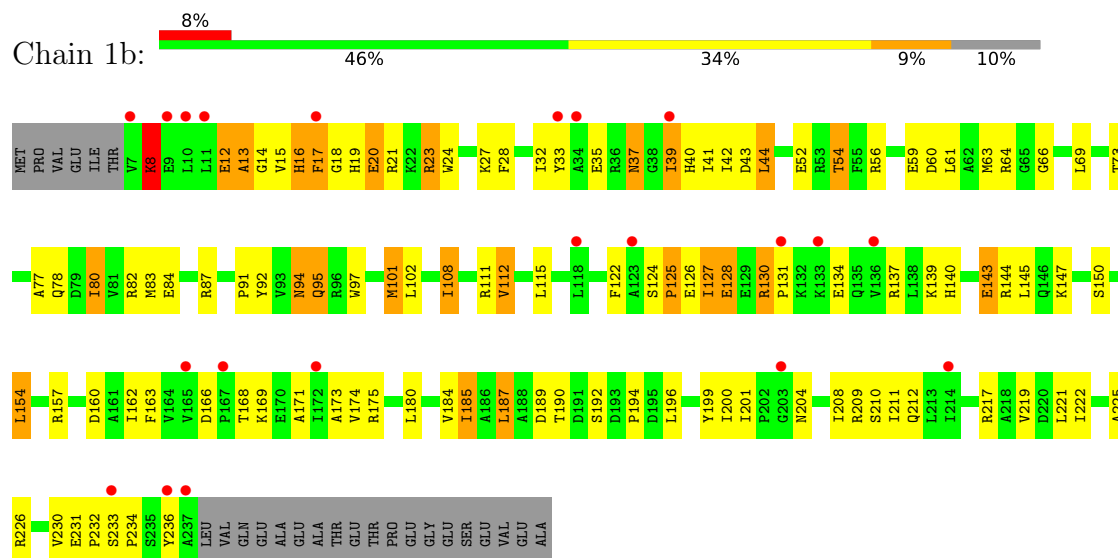
Chain 1a:  2% 49% 41% 8%



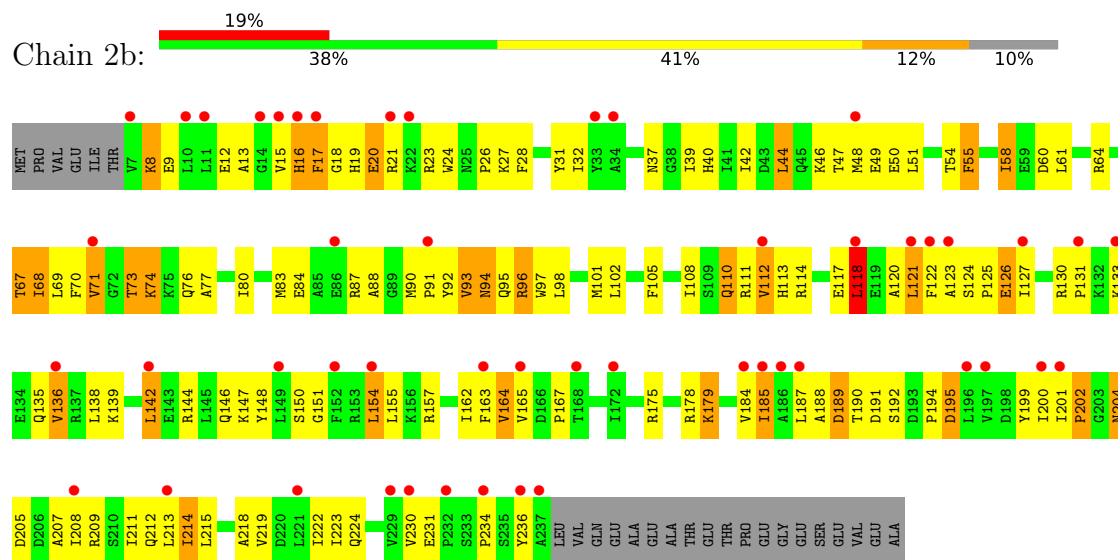
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G1294	G1295	C1228	G1160	C1098	A1030D	G973	A902	A778	G689	C600	C536	A453	C395
G1296	G1297	G1233	C1161	G1099	G1031	A974	G902	A779	G691	A601	G537	A454	G388
U1364	C1298	G1234	C1162	C1100	G1032	A975	G903	A780	G692	A602	G538	A455	A399
C1298	A1236	U1235	G1166	A1101	G1033	G976	U911	A781	G693	U603	A539	A456	C390
C1299	G1237	U1236	A1236	A1102	G1034	A977	C912	A782	G694	G460	G540	A457	G391
A1239	C1237	A1236	A1170	C1103	A1035	A978	G913	A783	A607	A461	G541	A458	G392
A1239	G1171	A1236	A1171	G1104	G1036	C979	A913	A784	A608	C470	G542	A459	A393
A1239	G1172	A1236	A1172	A1105	C1037	C980	A914	A785	A609	A471	G543	A460	A394
U1240	G1173	A1236	G1173	G1106	C1038	U981	A915	A786	G703	A472	G544	A461	U403
G1241	G1174	A1236	A1174	C1107	C1039	U982	G916	A787	G704	A473	G545	A462	U404
C1242	A1176	A1236	A1176	G1108	U1040	A983	G917	A788	C707	G474	G546	A463	U405
G1243	G1177	A1236	G1177	C1109	C1043	C984	A918	A789	C708	U480	A547	A464	G406
A1244	G1178	A1236	G1178	A1110	U1044	C985	A919	A790	G709	A481	U551	A465	G407
A1245	A1179	A1236	A1179	A1111	C1045	C986	A920	A791	G710	A482	U552	A466	C401
C1246	G1180	A1236	G1180	C1112	A1046	A987	U921	A792	G711	A483	A553	A467	C402
G1248	C1113	A1236	G1181	C1113	U1049	C988	G922	A793	G712	G484	C554	A468	U403
A1250	C1114	A1236	C1114	A923	G1050	C989	A924	A794	G713	G485	C555	A469	U404
A1251	C1115	A1236	C1115	G925	G1051	C990	G925	A795	G714	G486	C556	A470	U405
A1252	C1116	A1236	C1116	G926	G1052	U992	G926	A796	G715	A487	C557	A471	G406
G1253	C1117	A1236	G1182	C1117	G1053	G993	C931	A797	G716	A488	C558	A472	G407
G1254	C1118	A1236	A1183	C1118	G1054	U994	C932	A798	G717	A489	C559	A473	G408
G1255	C1119	A1236	G1184	C1119	A1055	A996	C933	A799	G718	A490	C560	A474	G409
A1256	C1120	A1236	G1185	C1120	G1056	U997	C934	A800	G719	A491	C561	A475	G410
A1257	C1121	A1236	G1186	C1121	G1057	U998	C935	A801	G720	A492	C562	A476	A411
A1258	C1122	A1236	G1187	C1122	G1058	U999	C936	A802	G721	A493	C563	A477	A412
A1259	C1123	A1236	G1188	C1123	G1059	U1000	C937	A803	G722	A494	C564	A478	A413
A1260	C1124	A1236	G1189	C1124	G1060	A1001	A938	A804	G723	A495	C565	A479	A414
A1261	C1125	A1236	G1190	C1125	G1061	G1001A	C939	A805	G724	A496	C566	A480	A415
C1262	C1126	A1236	A1191	C1126	G1062	G1002	A940	A806	G725	A497	C567	A481	G416
C1263	C1127	A1236	G1192	C1127	G1063	G1003	A941	A807	G726	A498	C568	A482	G417
C1264	C1128	A1236	G1193	C1128	G1064	G1004	C942	A808	G727	A499	C569	A483	G418
C1265	C1129	A1236	G1194	C1129	G1065	A1004	C943	A809	G728	A500	C570	A484	G419
C1266	C1130	A1236	G1195	C1130	G1066	A1005	C944	A810	G729	A501	C571	A485	U420
C1267	C1131	A1236	G1196	C1131	G1067	C1006	C945	A811	G730	A502	C572	A486	U421
G1270	C1132	A1236	U1199	C1132	G1068	C1007	C946	A812	G731	A503	C573	A487	G422
G1271	C1133	A1236	G1200	C1133	G1069	C1008	A947	A813	G732	A504	C574	A488	G423
G1272	C1134	A1236	G1201	C1134	G1070	G1009	C948	A814	G733	A505	C575	A489	G424
G1273	C1135	A1236	G1202	C1135	G1071	G1010	C949	A815	G734	A506	C576	A490	G425
G1274	C1136	A1236	G1203	C1136	G1072	G1011	C950	A816	G735	A507	C577	A491	G426
A1275	C1137	A1236	G1204	C1137	G1073	G1012	A951	A817	G736	A508	C578	A492	U427
G1276	C1138	A1236	G1205	C1138	G1074	G1013	C952	A818	G737	A509	C579	A493	U428
G1277	C1139	A1236	G1206	C1139	G1075	A1014	C953	A819	G738	A510	C580	A494	U429
A1278	G1405	A1236	G1207	G1405	G1076	G1015	G961	A820	G739	A511	C581	A495	A430
U1281	C1336	A1236	G1208	C1336	G1077	A1016	C962	A821	G740	A512	C582	A496	A431
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G1282	C1338	A1236	G1210	C1338	G1079	C1018	C964	A823	G742	A514	C584	A498	A433
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G1284	C1340	A1236	U1212	C1340	G1081	G1020	C966	A825	G744	A516	C586	A500	C435
A1285	C1341	A1236	G1213	C1341	G1082	U1021	C967	A826	G745	A517	C587	A501	G438
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A1287	C1343	A1236	G1214	C1343	G1084	G1023	C969	A828	G747	A519	C589	A503	A440
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G1289	C1345	A1236	G1216	C1345	U1086	G1025	C971	A830	G749	A521	C591	A505	A440
G1290	C1346	A1236	G1217	C1346	U1087	U1026	C972	A831	G750	A522	C592	A506	A441
G1291	C1347	A1236	G1218	C1347	G1088	G1027	C973	A832	G751	A523	C593	A507	C442
G1292	C1348	A1236	G1219	C1348	G1089	C1028	C974	A833	G752	A524	C594	A508	C443
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G1299	C1355	A1236	G1228	C1355	C1098	C1030B	C981	A840	G759	A531	C601	A515	A439
G1300	C1356	A1236	G1229	C1356	A1099	C1030B	C982	A841	G760	A532	C602	A516	A440
G1301	C1357	A1236	G1230	C1357	C1099	C1030B	C983	A842	G761	A533	C603	A517	A441
G1302	C1358	A1236	G1231	C1358	C1099	C1030B	C984	A843	G762	A534	C604	A518	A442
G1303	C1359	A1236	G1232	C1359	C1099	C1030B	C985	A844	G763	A535	C605	A519	C443
G1304	C1360	A1236	G1233	C1360	C1099	C1030B	C986	A845	G764	A536	C606	A520	C444
G1305	C1361	A1236	G1234	C1361	C1099	C1030B	C987	A846	G765	A537	C607	A521	G438
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G1307	C1363	A1236	G1236	C1363	C1099	C1030B	C989	A848	G767	A539	C609	A523	A440
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G1309	C1365	A1236	G1238	C1365	C1099	C1030B	C991	A850	G769	A541	C611	A525	A442
G1310	C1366	A1236	G1239	C1366	C1099	C1030B	C992	A851	G770	A542	C612	A526	C443
G1311	C1367	A1236	G1240	C1367	C1099	C1030B	C993	A852	G771	A543	C613	A527	C444
G1312	C1368	A1236	G1241	C1368	C1099	C1030B	C994	A853	G772	A544	C614	A528	G438
G1313	C1369	A1236	G1242	C1369	C1099	C1030B	C995	A854	G773	A545	C615	A529	A439
G1314	C1370	A1236	G1243	C1370	C1099	C1030B	C996	A855	G774	A546	C616	A530	A440
G1315	C1371	A1236	G1244	C1371	C1099	C1030B	C997	A856	G775	A547	C617	A531	C441
G1316	C1372	A1236	G1245	C1372	C1099	C1030B	C998	A857	G776	A548	C618	A532	A442
G1317	C1373	A1236	G1246	C1373	C1099	C1030B	C999	A858	G777	A549	C619	A533	C443
G1318	C1374	A1236	G1247	C1374	C1099	C1030B	C1000	A859	G778	A550	C620	A534	C444
G1319	C1375	A1236	G1248	C1375	C1099	C1030B	C1001	A860	G779	A551	C621	A535	G438
G1320	C1376	A1236	G1249	C1376	C1099	C1030B	C1002	A861	G780	A552	C622	A536	A439
G1321	C1377	A1236	G1250	C1377	C1099	C1030B	C1003	A862	G781	A553	C623	A537	A440
G1322	C1378	A1236	G1251	C1378	C1099	C1030B	C1004	A863	G782	A554	C624	A538	A441
G1323	C1379	A1236	G1252	C1379	C1099	C1030B	C1005	A864	G783	A555	C625	A539	C442
G1324	C1380	A1236	G1253	C1380	C1099	C1030B	C1006	A865	G784	A556	C626	A540	C443
G1325	C1381	A1236	G1254	C1381	C1099	C1030B	C1007	A866	G785	A557	C627	A541	C444
G1326	C1382	A1236	G1255	C1382	C1099	C1030B	C1008	A867	G786	A558	C628	A542	G438
G1327	C1383	A1236	G1256	C1383	C1099	C1030B	C1009	A868	G787	A559	C629	A543	A439
G1328	C1384	A1236	G1257	C1384	C1099	C1030B	C1010	A869	G788	A560	C630	A544	A440
G1329	C1385	A1236	G1258	C1385	C1099	C1030B	C1011	A870	G789	A561	C631	A545	C441
G1330	C1386	A1236	G1259	C1386	C1099	C1030B	C1012	A871	G790	A562	C632	A546	C442
G1331	C1387	A1236	G1260	C1387	C1099	C1030B	C1013	A872	G791	A563	C633	A547	A443
G1332	C1388	A1236	G1261	C1388	C1099	C1030B	C1014	A873	G792	A564	C634	A548	G438
G1333	C1389	A1236	G1262	C1389	C1099	C1030B	C1015	A874	G793	A565	C635	A549	A440
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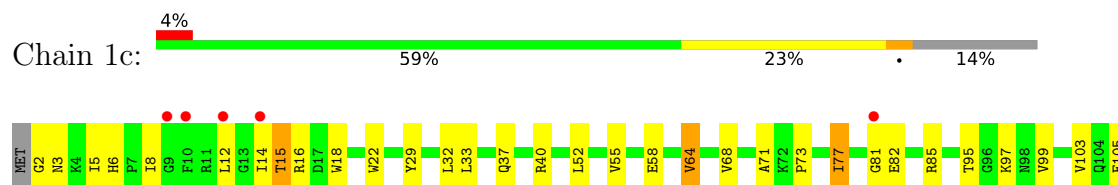
• Molecule 33: 30S ribosomal protein S2

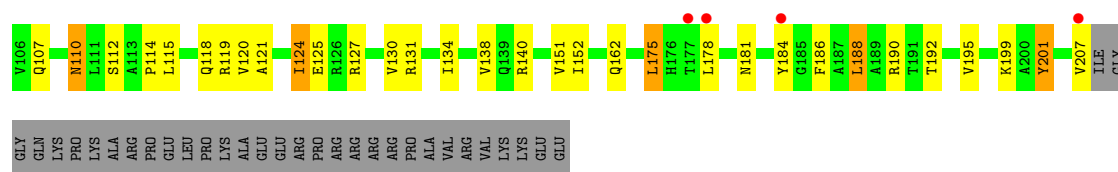


• Molecule 33: 30S ribosomal protein S2

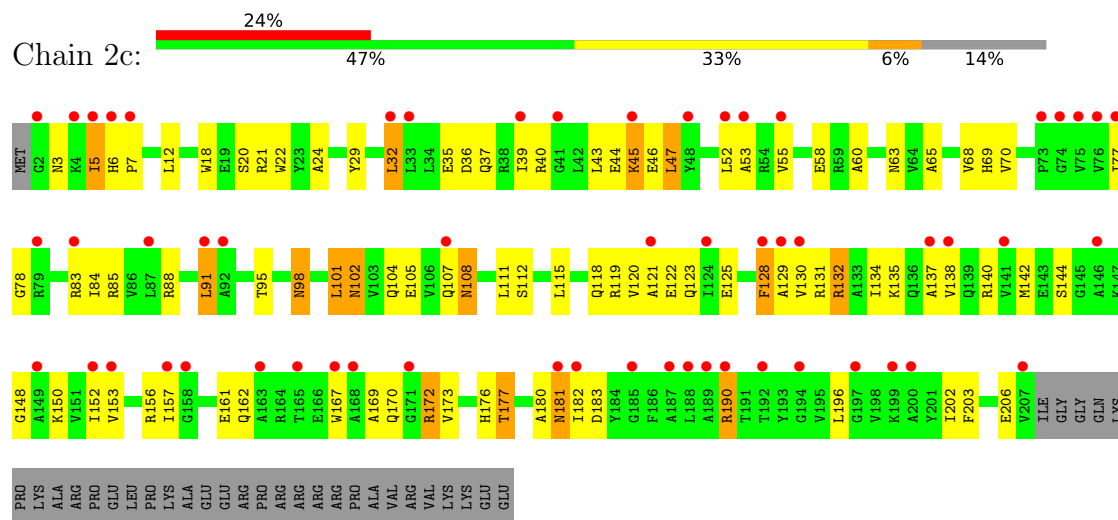


• Molecule 34: 30S ribosomal protein S3

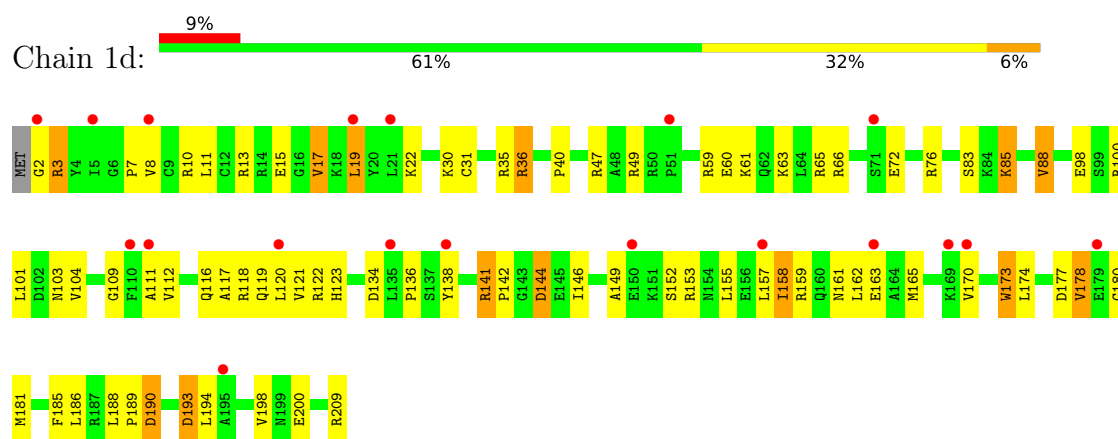




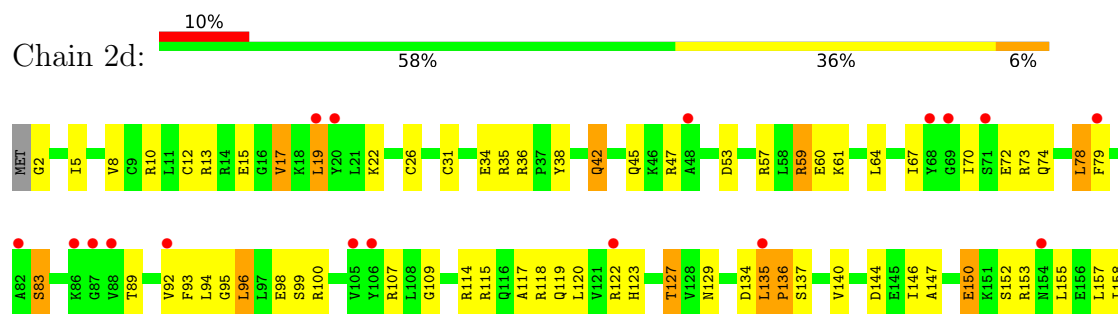
• Molecule 34: 30S ribosomal protein S3

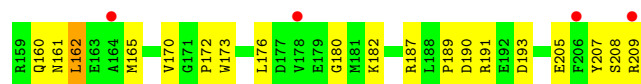


• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

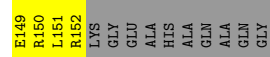
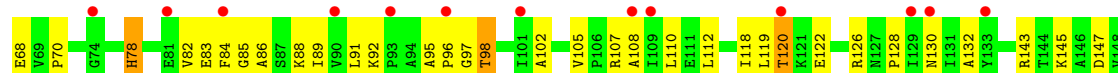




- Molecule 36: 30S ribosomal protein S5



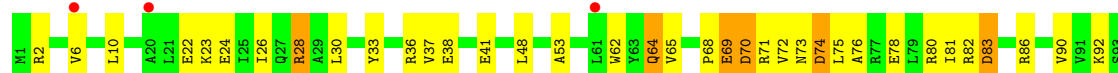
- Molecule 36: 30S ribosomal protein S5



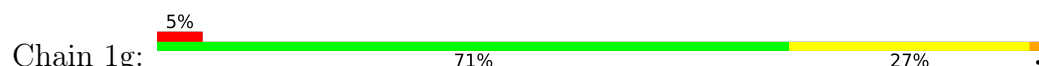
- Molecule 37: 30S ribosomal protein S6

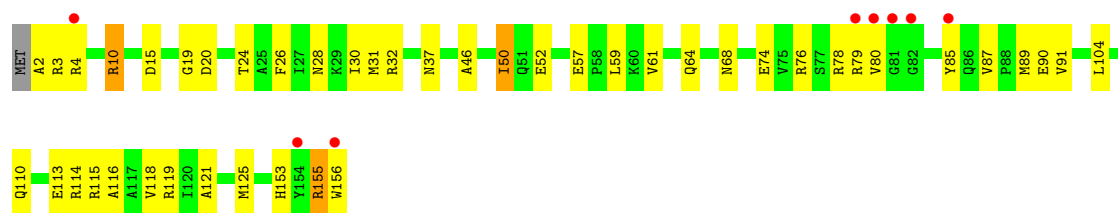


- Molecule 37: 30S ribosomal protein S6

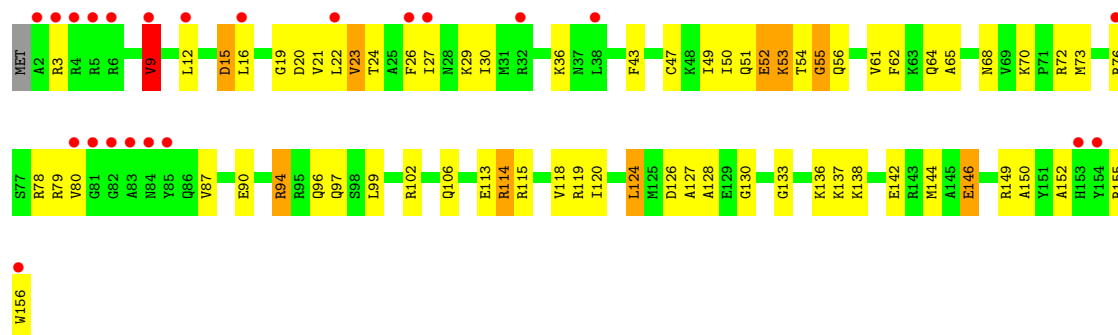


- Molecule 38: 30S ribosomal protein S7

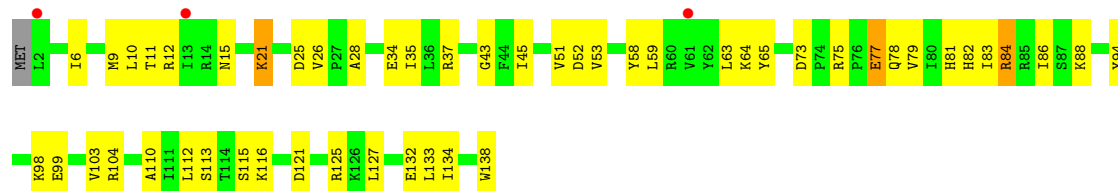




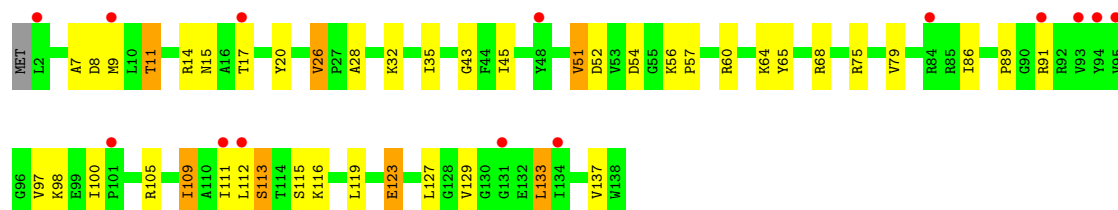
• Molecule 38: 30S ribosomal protein S7



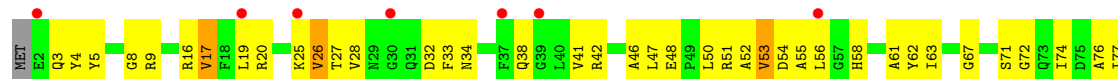
• Molecule 39: 30S ribosomal protein S8

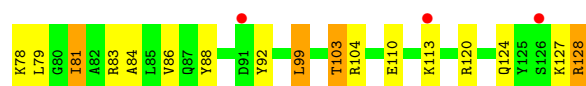


• Molecule 39: 30S ribosomal protein S8

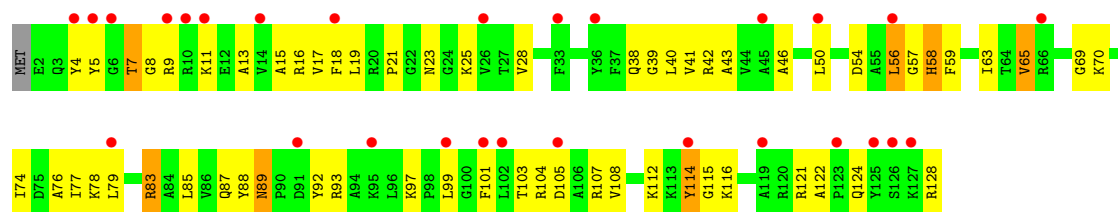


• Molecule 40: 30S ribosomal protein S9

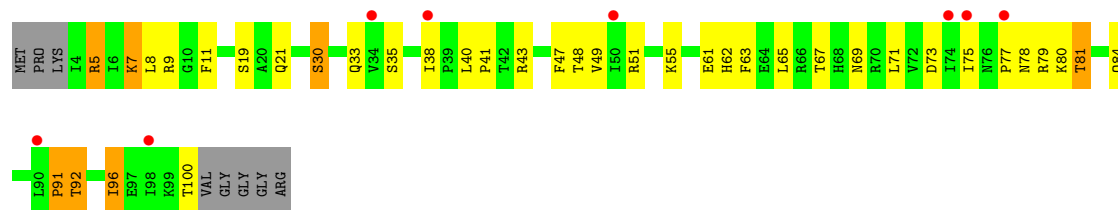




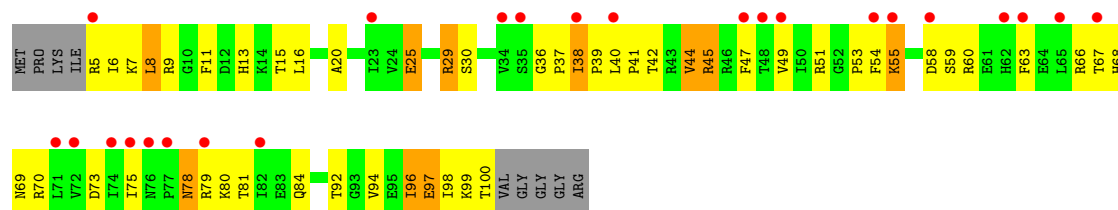
- Molecule 40: 30S ribosomal protein S9



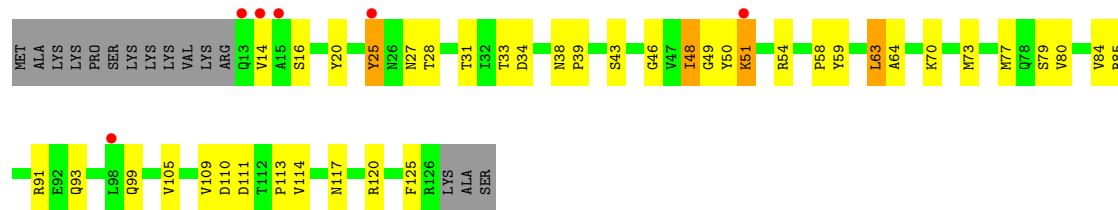
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11



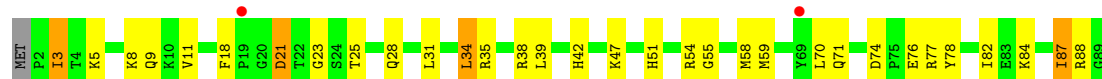
- Molecule 45: 30S ribosomal protein S14 type Z



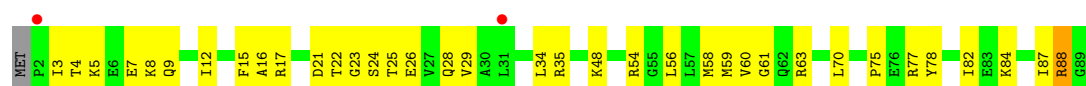
- Molecule 45: 30S ribosomal protein S14 type Z



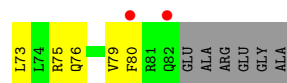
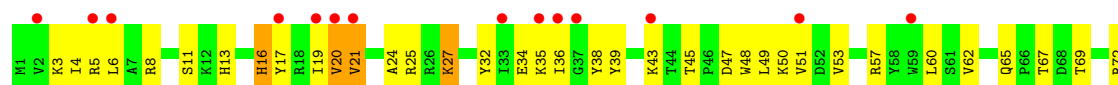
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

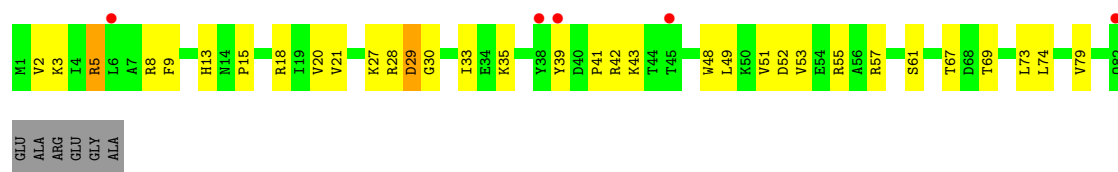


- Molecule 47: 30S ribosomal protein S16

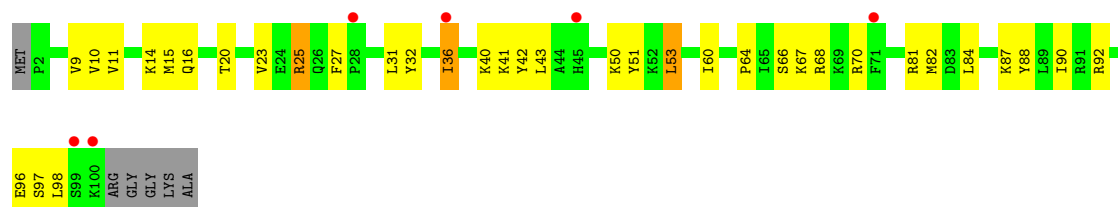


- Molecule 47: 30S ribosomal protein S16

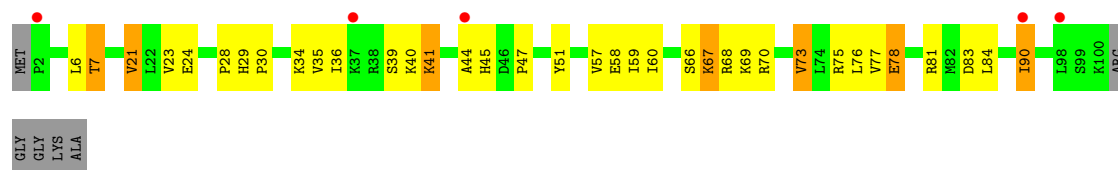




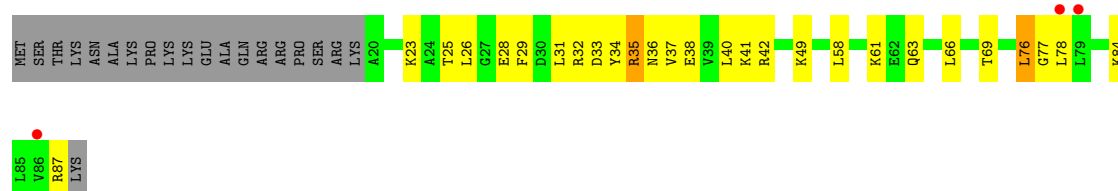
- Molecule 48: 30S ribosomal protein S17



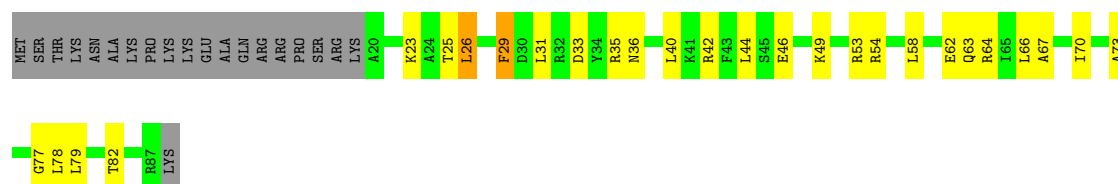
- Molecule 48: 30S ribosomal protein S17



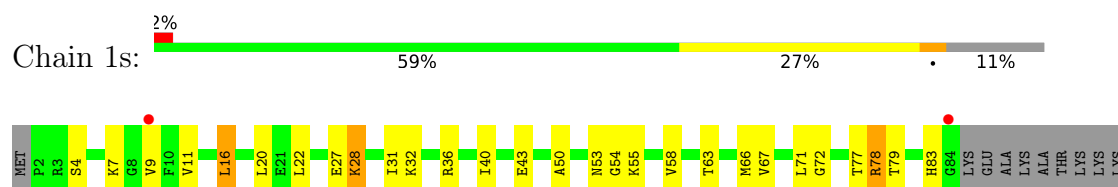
- Molecule 49: 30S ribosomal protein S18



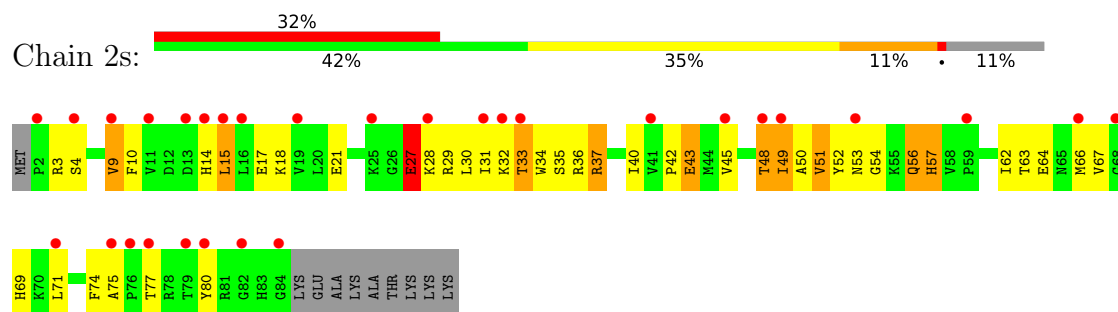
- Molecule 49: 30S ribosomal protein S18



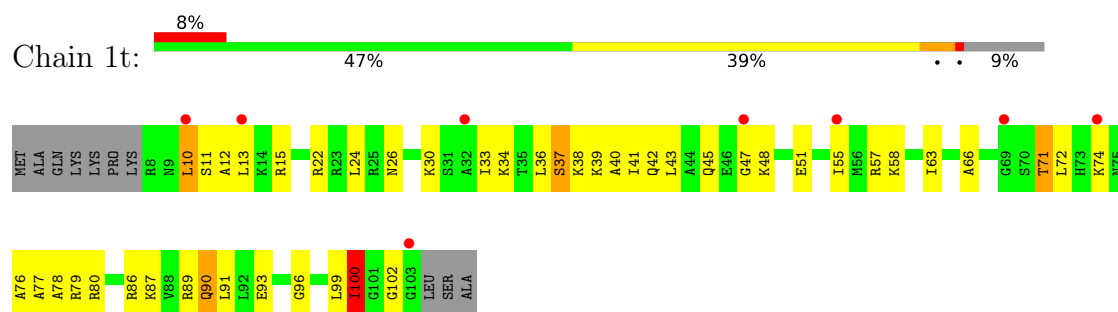
- Molecule 50: 30S ribosomal protein S19



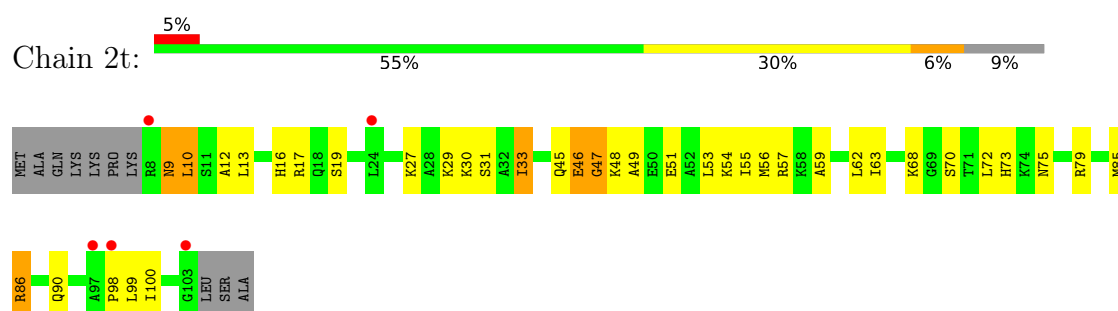
• Molecule 50: 30S ribosomal protein S19



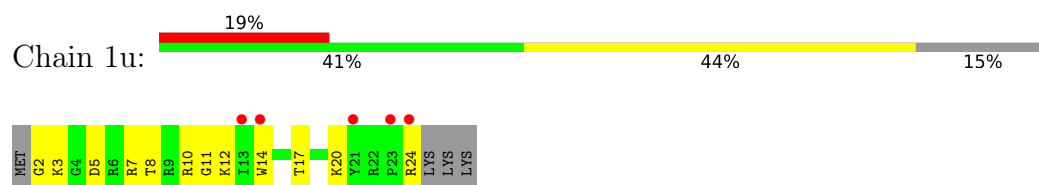
• Molecule 51: 30S ribosomal protein S20



• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx

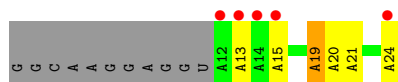
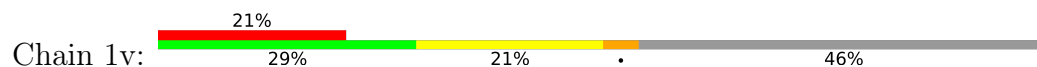


• Molecule 52: 30S ribosomal protein Thx

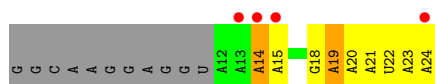




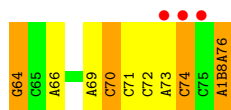
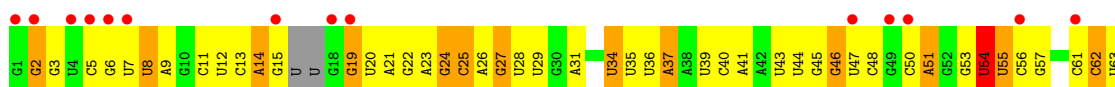
• Molecule 53: MET-LYS-mRNA



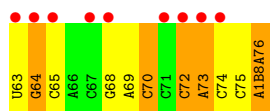
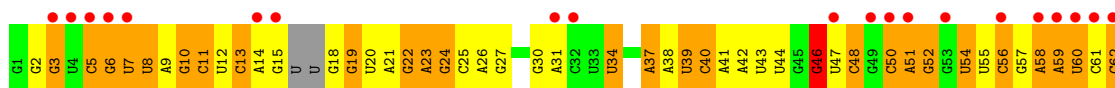
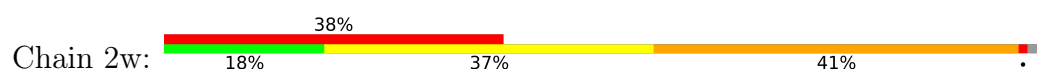
• Molecule 53: MET-LYS-mRNA



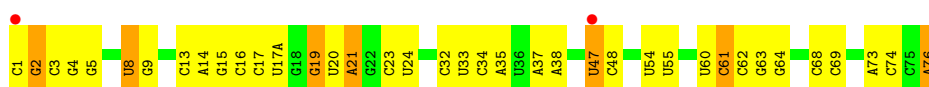
• Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys



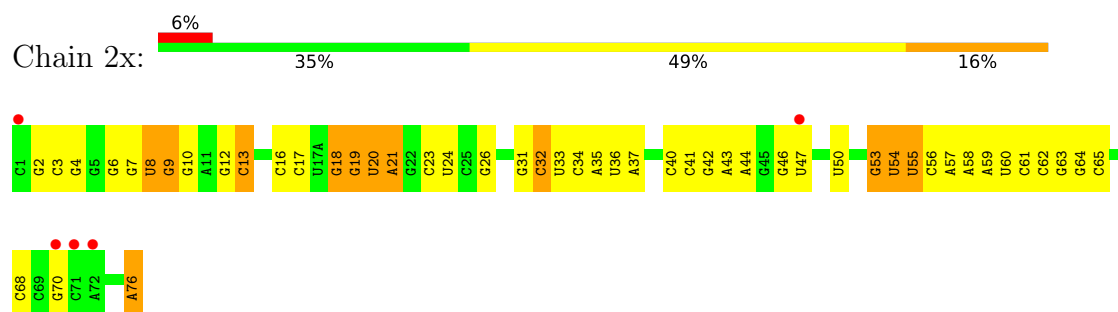
• Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys



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



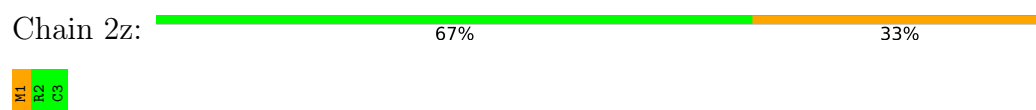
• Molecule 55: P-site Peptidyl-tRNA fMRC-tRNAcys RNA-part



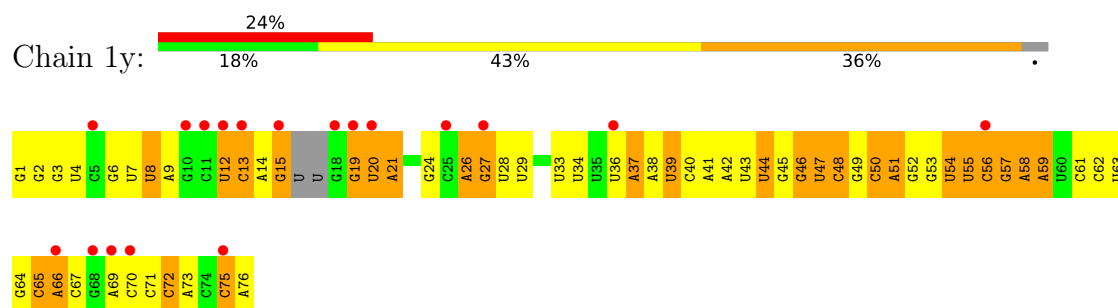
- Molecule 56: P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part



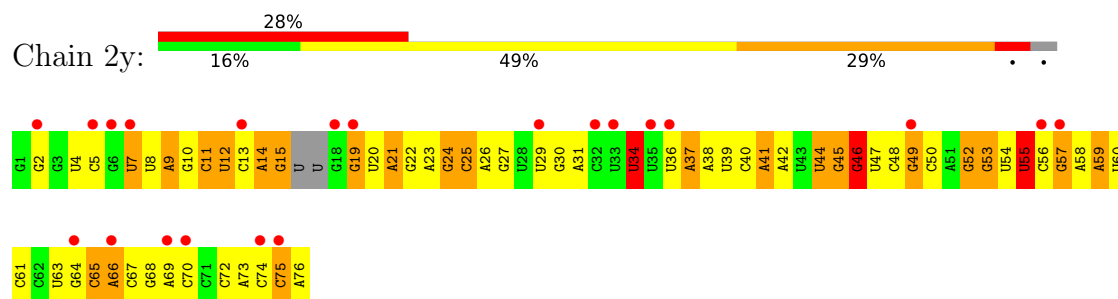
- Molecule 56: P-site Peptidyl-tRNA fMRC-tRNAcys Peptide-part



- Molecule 57: E-site Deacylated tRNAlys



- Molecule 57: E-site Deacylated tRNAlys



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.56Å 449.05Å 616.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.94 – 2.60 123.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (123.94-2.60) 99.9 (123.94-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.229 , 0.278 0.232 , 0.279	Depositor DCC
R_{free} test set	87740 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	299808	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: OMC, OMU, 2MA, G7M, 5MC, K, M2G, T6A, MG, ZN, SF4, 4OC, OMG, UR3, U8U, MA6, PSU, 2MG, 5MU, 8AN, A1B8A, 4SU, 0TD, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.29	1/69011 (0.0%)	0.47	1/107720 (0.0%)
1	2A	0.22	1/67295 (0.0%)	0.41	1/105042 (0.0%)
2	1B	0.24	0/2882	0.42	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.29	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.54	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.25	0/1619	0.48	0/2193
5	2F	0.22	0/1615	0.47	3/2188 (0.1%)
6	1G	0.22	0/1448	0.47	1/1957 (0.1%)
6	2G	0.23	0/1453	0.50	1/1963 (0.1%)
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.40	0/1834
8	1I	0.18	0/1112	0.42	0/1514
8	2I	0.22	0/1079	0.48	0/1475
9	1N	0.25	0/1144	0.49	0/1543
9	2N	0.20	0/1144	0.40	0/1543
10	1O	0.28	0/943	0.49	0/1269
10	2O	0.22	0/943	0.50	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.28	0/1143	0.49	0/1527
12	2Q	0.22	0/1143	0.47	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.22	0/982	0.46	0/1312
14	1S	0.21	0/883	0.48	0/1176
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.22	0/1097	0.48	0/1468
16	1U	0.28	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.41	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.18	0/782	0.39	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.44	0/1205
19	1X	0.26	0/764	0.55	2/1025 (0.2%)
19	2X	0.23	0/764	0.61	2/1025 (0.2%)
20	1Y	0.23	0/819	0.44	0/1095
20	2Y	0.20	0/819	0.47	1/1095 (0.1%)
21	1Z	0.23	0/1267	0.48	0/1717
21	2Z	0.22	0/1299	0.42	0/1763
22	10	0.27	0/662	0.52	0/881
22	20	0.23	0/662	0.53	0/881
23	11	0.27	0/762	0.46	0/1014
23	21	0.21	0/762	0.41	0/1014
24	12	0.23	0/590	0.43	0/781
24	22	0.22	0/590	0.42	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.18	0/469	0.39	0/630
26	14	0.25	0/565	0.58	1/761 (0.1%)
26	24	0.28	0/545	0.56	0/737
27	15	0.27	0/469	0.47	0/635
27	25	0.23	0/469	0.48	0/635
28	16	0.29	0/460	0.50	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.33	0/426	0.56	0/561
29	27	0.25	0/426	0.51	0/561
30	18	0.28	0/525	0.52	0/691
30	28	0.21	0/525	0.42	0/691
31	19	0.27	0/310	0.56	0/407
31	29	0.20	0/310	0.42	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.19	0/35886	0.38	1/56005 (0.0%)
33	1b	0.21	0/1881	0.47	0/2542
33	2b	0.26	0/1860	0.52	0/2518
34	1c	0.18	0/1572	0.39	0/2126
34	2c	0.23	0/1566	0.51	1/2119 (0.0%)
35	1d	0.20	0/1685	0.45	0/2262
35	2d	0.21	0/1704	0.46	0/2284
36	1e	0.22	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.48	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.20	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.20	0/1250	0.42	0/1679
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.19	0/1108	0.43	0/1494
40	1i	0.21	0/1002	0.49	0/1346
40	2i	0.23	0/997	0.55	0/1343
41	1j	0.22	0/722	0.47	0/982
41	2j	0.21	0/727	0.46	0/988
42	1k	0.23	0/844	0.43	0/1145
42	2k	0.20	0/848	0.41	0/1149
43	1l	0.20	0/937	0.42	0/1260
43	2l	0.20	0/937	0.45	0/1260
44	1m	0.21	0/969	0.51	0/1302
44	2m	0.21	0/961	0.45	0/1291
45	1n	0.19	0/501	0.41	0/664
45	2n	0.20	0/501	0.45	0/664
46	1o	0.19	0/739	0.43	0/985
46	2o	0.18	0/739	0.40	0/985
47	1p	0.20	0/697	0.45	0/939
47	2p	0.19	0/693	0.49	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.21	0/836	0.46	0/1117
49	1r	0.20	0/560	0.45	0/746
49	2r	0.19	0/560	0.47	0/746
50	1s	0.19	0/667	0.50	0/900
50	2s	0.24	0/661	0.58	2/893 (0.2%)
51	1t	0.21	0/730	0.48	0/965
51	2t	0.21	0/729	0.48	0/965
52	1u	0.19	0/203	0.43	0/266
52	2u	0.36	0/203	0.58	0/266
53	1v	0.23	0/319	0.40	0/495
53	2v	0.21	0/319	0.44	0/495
54	1w	0.32	2/1593 (0.1%)	0.39	0/2474
54	2w	0.36	2/1593 (0.1%)	0.52	0/2474
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.25	0/1723	0.40	0/2684
56	1z	0.54	0/16	0.89	0/19
56	2z	0.57	0/16	0.63	0/19
57	1y	0.31	1/1618 (0.1%)	0.45	0/2513
57	2y	0.35	2/1618 (0.1%)	0.53	0/2513
All	All	0.24	9/316807 (0.0%)	0.44	17/474290 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	1Q	0	1
26	24	0	1
33	1b	0	1
33	2b	0	1
51	1t	0	1
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	6.04	1.62	1.56
54	2w	46	G7M	O3'-P	5.90	1.62	1.56
57	2y	46	G7M	O3'-P	5.57	1.61	1.56
1	1A	2552	OMU	O3'-P	5.55	1.61	1.56
54	2w	37	T6A	O3'-P	5.41	1.61	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2X	94	GLY	CA-C-N	8.05	136.18	121.70
19	2X	94	GLY	C-N-CA	8.05	136.18	121.70
34	2c	84	ILE	N-CA-C	-6.13	105.04	113.00
6	1G	96	ARG	CB-CA-C	-5.96	109.69	116.54
1	1A	1992	G	C2'-C3'-O3'	5.83	118.25	109.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	15	GLY	Peptide
33	1b	130	ARG	Peptide
51	1t	99	LEU	Peptide
26	24	59	PHE	Peptide
33	2b	118	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31192	762	0
1	2A	60322	0	30422	849	0
2	1B	2577	0	1304	30	0
2	2B	2575	0	1303	61	0
3	1D	2136	0	2218	54	0
3	2D	2136	0	2218	55	0
4	1E	1559	0	1618	32	0
4	2E	1559	0	1618	49	0
5	1F	1584	0	1625	50	0
5	2F	1580	0	1619	55	0
6	1G	1423	0	1436	47	0
6	2G	1428	0	1438	73	0
7	1H	1330	0	1407	20	0
7	2H	1330	0	1407	48	0
8	1I	1097	0	1140	38	0
8	2I	1064	0	1082	55	0
9	1N	1117	0	1184	23	0
9	2N	1117	0	1184	33	0
10	1O	933	0	996	25	0
10	2O	933	0	996	33	0
11	1P	1135	0	1212	40	0
11	2P	1135	0	1212	44	0
12	1Q	1122	0	1179	30	0
12	2Q	1122	0	1179	47	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	19	0
14	2S	870	0	923	54	0
15	1T	1091	0	1151	30	0
15	2T	1083	0	1136	38	0
16	1U	959	0	1019	20	0
16	2U	959	0	1019	30	0
17	1V	771	0	830	16	0
17	2V	771	0	830	29	0
18	1W	886	0	940	18	0
18	2W	886	0	940	15	0
19	1X	750	0	814	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	813	23	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	23	0
21	1Z	1240	0	1240	38	0
21	2Z	1271	0	1273	56	0
22	10	653	0	674	21	0
22	20	653	0	674	18	0
23	11	755	0	826	24	0
23	21	755	0	825	20	0
24	12	588	0	643	9	0
24	22	588	0	643	22	0
25	13	469	0	518	18	0
25	23	464	0	514	13	0
26	14	552	0	533	21	0
26	24	532	0	503	32	0
27	15	455	0	465	4	0
27	25	455	0	465	11	0
28	16	453	0	473	10	0
28	26	449	0	469	16	0
29	17	418	0	467	6	0
29	27	418	0	467	11	0
30	18	517	0	582	14	0
30	28	517	0	582	14	0
31	19	307	0	335	2	0
31	29	307	0	335	13	0
32	1a	32246	0	16293	497	0
32	2a	32327	0	16338	653	0
33	1b	1846	0	1867	68	0
33	2b	1825	0	1828	93	0
34	1c	1548	0	1535	43	0
34	2c	1542	0	1517	69	0
35	1d	1655	0	1672	56	0
35	2d	1674	0	1714	63	0
36	1e	1129	0	1185	43	0
36	2e	1133	0	1191	48	0
37	1f	810	0	804	22	0
37	2f	816	0	808	27	0
38	1g	1231	0	1238	31	0
38	2g	1235	0	1249	47	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	28	0
40	1i	983	0	986	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	53	0
41	1j	709	0	650	31	0
41	2j	714	0	672	39	0
42	1k	829	0	825	23	0
42	2k	833	0	834	26	0
43	1l	932	0	981	21	0
43	2l	932	0	981	32	0
44	1m	958	0	1002	40	0
44	2m	950	0	988	46	0
45	1n	492	0	529	21	0
45	2n	492	0	529	25	0
46	1o	728	0	760	21	0
46	2o	728	0	760	22	0
47	1p	681	0	697	33	0
47	2p	677	0	686	22	0
48	1q	823	0	891	24	0
48	2q	823	0	891	26	0
49	1r	555	0	618	20	0
49	2r	555	0	618	19	0
50	1s	652	0	662	21	0
50	2s	646	0	644	38	0
51	1t	728	0	798	29	0
51	2t	727	0	796	26	0
52	1u	199	0	208	9	0
52	2u	199	0	208	11	0
53	1v	283	0	142	8	0
53	2v	283	0	141	7	0
54	1w	1599	0	801	35	0
54	2w	1599	0	801	65	0
55	1x	1646	0	839	22	0
55	2x	1646	0	839	33	0
56	1z	27	0	28	1	0
56	2z	27	0	28	1	0
57	1y	1577	0	799	42	0
57	2y	1577	0	798	47	0
58	10	9	0	0	0	0
58	11	5	0	0	0	0
58	12	2	0	0	0	0
58	13	5	0	0	0	0
58	14	1	0	0	0	0
58	15	6	0	0	0	0
58	16	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	17	6	0	0	0	0
58	18	9	0	0	0	0
58	1A	1096	0	0	0	0
58	1B	37	0	0	0	0
58	1D	13	0	0	0	0
58	1E	16	0	0	0	0
58	1F	13	0	0	0	0
58	1G	5	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	4	0	0	0	0
58	1P	6	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	4	0	0	0	0
58	1S	3	0	0	0	0
58	1T	2	0	0	0	0
58	1U	9	0	0	0	0
58	1V	9	0	0	0	0
58	1W	7	0	0	0	0
58	1X	5	0	0	0	0
58	1Y	3	0	0	0	0
58	1Z	2	0	0	0	0
58	1a	210	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	1	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	3	0	0	0	0
58	1x	11	0	0	0	0
58	20	4	0	0	0	0
58	23	4	0	0	0	0
58	25	5	0	0	0	0
58	27	3	0	0	0	0
58	28	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2A	863	0	0	0	0
58	2B	20	0	0	0	0
58	2D	7	0	0	0	0
58	2E	7	0	0	0	0
58	2F	7	0	0	0	0
58	2G	1	0	0	0	0
58	2O	2	0	0	0	0
58	2P	3	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	2	0	0	0	0
58	2T	3	0	0	0	0
58	2U	2	0	0	0	0
58	2V	2	0	0	0	0
58	2W	2	0	0	0	0
58	2X	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	230	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2i	1	0	0	0	0
58	2j	1	0	0	0	0
58	2k	1	0	0	0	0
58	2l	4	0	0	0	0
58	2n	1	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	4	0	0	0	0
58	2w	1	0	0	0	0
58	2x	6	0	0	0	0
58	2y	1	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	10	0	0	1	0
62	11	12	0	0	0	0
62	12	3	0	0	0	0
62	13	4	0	0	0	0
62	14	1	0	0	0	0
62	15	7	0	0	0	0
62	16	2	0	0	0	0
62	17	11	0	0	1	0
62	18	11	0	0	1	0
62	1A	1886	0	0	92	0
62	1B	61	0	0	1	0
62	1D	28	0	0	2	0
62	1E	29	0	0	2	0
62	1F	15	0	0	1	0
62	1G	3	0	0	0	0
62	1H	2	0	0	0	0
62	1I	1	0	0	0	0
62	1N	4	0	0	0	0
62	1O	4	0	0	0	0
62	1P	23	0	0	1	0
62	1Q	8	0	0	0	0
62	1R	16	0	0	2	0
62	1S	5	0	0	0	0
62	1T	8	0	0	0	0
62	1U	10	0	0	0	0
62	1V	11	0	0	1	0
62	1W	6	0	0	1	0
62	1X	7	0	0	0	0
62	1Y	1	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	308	0	0	25	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1i	1	0	0	0	0
62	1l	7	0	0	0	0
62	1m	2	0	0	0	0
62	1o	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	0	0
62	1v	5	0	0	0	0
62	1w	8	0	0	1	0
62	1x	6	0	0	0	0
62	1y	1	0	0	0	0
62	1z	1	0	0	1	0
62	20	5	0	0	0	0
62	21	13	0	0	1	0
62	25	2	0	0	1	0
62	27	1	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1000	0	0	92	0
62	2B	22	0	0	3	0
62	2D	24	0	0	1	0
62	2E	9	0	0	1	0
62	2F	15	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	11	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	3	0	0	0	0
62	2T	5	0	0	0	0
62	2U	3	0	0	2	0
62	2W	3	0	0	0	0
62	2X	4	0	0	0	0
62	2Y	1	0	0	0	0
62	2Z	1	0	0	0	0
62	2a	198	0	0	20	0
62	2d	1	0	0	0	0
62	2e	1	0	0	0	0
62	2j	1	0	0	0	0
62	2l	4	0	0	1	0
62	2p	2	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	0	0
62	2v	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2w	3	0	0	0	0
62	2x	5	0	0	0	0
All	All	299808	0	196752	5317	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5317 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	1.22	1.38
54:2w:51:A:N6	54:2w:63:U:H3	1.37	1.22
54:2w:51:A:N6	54:2w:63:U:N3	1.94	1.14
1:1A:1082:U:O4	1:1A:1086:A:N1	1.87	1.06
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.44	0.99

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%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	246 (90%)	26 (10%)	1 (0%)	30	51
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	46
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	46
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	46
5	2F	201/210 (96%)	187 (93%)	12 (6%)	2 (1%)	12	28
6	1G	179/182 (98%)	165 (92%)	11 (6%)	3 (2%)	7	15
6	2G	179/182 (98%)	146 (82%)	29 (16%)	4 (2%)	5	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	21	42
7	2H	172/180 (96%)	153 (89%)	16 (9%)	3 (2%)	7	15
8	1I	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
8	2I	144/148 (97%)	119 (83%)	20 (14%)	5 (4%)	3	4
9	1N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	38
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	38
10	1O	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	7	15
10	2O	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
11	1P	147/150 (98%)	131 (89%)	10 (7%)	6 (4%)	2	3
11	2P	147/150 (98%)	126 (86%)	17 (12%)	4 (3%)	4	7
12	1Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	38
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	3 (3%)	1 (1%)	14	30
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	96 (89%)	9 (8%)	3 (3%)	4	6
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	34
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	6	12
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	12
18	1W	110/113 (97%)	106 (96%)	4 (4%)	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	25
19	2X	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	11	25
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	126 (85%)	21 (14%)	1 (1%)	18	38
21	2Z	156/206 (76%)	125 (80%)	27 (17%)	4 (3%)	4	7
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2	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%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	43 (84%)	8 (16%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	23 (10%)	11 (5%)	2	2
33	2b	229/256 (90%)	182 (80%)	37 (16%)	10 (4%)	2	2
34	1c	204/239 (85%)	180 (88%)	21 (10%)	3 (2%)	8	18
34	2c	204/239 (85%)	160 (78%)	37 (18%)	7 (3%)	3	4
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	24	46
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	24	46
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	9	19
36	2e	146/162 (90%)	124 (85%)	19 (13%)	3 (2%)	5	11
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	28
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	18	38
38	2g	153/156 (98%)	135 (88%)	14 (9%)	4 (3%)	4	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	34
40	2i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	7	16
41	1j	95/105 (90%)	77 (81%)	13 (14%)	5 (5%)	1	1
41	2j	94/105 (90%)	76 (81%)	15 (16%)	3 (3%)	3	5
42	1k	112/129 (87%)	98 (88%)	12 (11%)	2 (2%)	6	14
42	2k	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	2	4
43	1l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
43	2l	119/132 (90%)	101 (85%)	16 (13%)	2 (2%)	7	15
44	1m	121/126 (96%)	106 (88%)	13 (11%)	2 (2%)	7	15
44	2m	120/126 (95%)	101 (84%)	18 (15%)	1 (1%)	16	34
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	15
46	1o	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	23
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9	21
48	1q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
48	2q	97/105 (92%)	84 (87%)	12 (12%)	1 (1%)	12	28
49	1r	66/88 (75%)	58 (88%)	7 (11%)	1 (2%)	8	18
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
50	2s	81/93 (87%)	67 (83%)	13 (16%)	1 (1%)	10	23
51	1t	94/106 (89%)	82 (87%)	9 (10%)	3 (3%)	3	5
51	2t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5	11
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	0	0
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	0	1 (100%)	0	100	100
All	All	11372/12134 (94%)	10242 (90%)	989 (9%)	141 (1%)	10	23

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	38	GLN
23	11	3	LYS
26	14	49	PHE
36	1e	96	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	17	37
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	31
4	1E	164/166 (99%)	152 (93%)	12 (7%)	13	29
4	2E	164/166 (99%)	151 (92%)	13 (8%)	11	26
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	12
5	2F	159/166 (96%)	145 (91%)	14 (9%)	9	21
6	1G	143/156 (92%)	123 (86%)	20 (14%)	3	6
6	2G	143/156 (92%)	121 (85%)	22 (15%)	2	5
7	1H	144/148 (97%)	130 (90%)	14 (10%)	8	17
7	2H	144/148 (97%)	123 (85%)	21 (15%)	3	6
8	1I	113/124 (91%)	90 (80%)	23 (20%)	1	2
8	2I	105/124 (85%)	83 (79%)	22 (21%)	1	2
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7	15
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	13
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	55
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9	20
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9	21
11	2P	115/116 (99%)	99 (86%)	16 (14%)	3	7
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	20
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	32
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	38
14	1S	86/88 (98%)	76 (88%)	10 (12%)	5	11
14	2S	85/88 (97%)	67 (79%)	18 (21%)	1	2
15	1T	115/127 (91%)	104 (90%)	11 (10%)	8	17
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	43
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	42
16	2U	93/94 (99%)	81 (87%)	12 (13%)	4	8
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	46
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	9
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	33
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	44
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	35
20	1Y	85/91 (93%)	72 (85%)	13 (15%)	3	5
20	2Y	85/91 (93%)	68 (80%)	17 (20%)	1	2
21	1Z	135/179 (75%)	110 (82%)	25 (18%)	1	3
21	2Z	137/179 (76%)	112 (82%)	25 (18%)	2	3
22	10	65/67 (97%)	62 (95%)	3 (5%)	24	49
22	20	65/67 (97%)	60 (92%)	5 (8%)	12	27
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	36
23	21	80/83 (96%)	71 (89%)	9 (11%)	5	12
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	13
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	13
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	26
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	25
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	4
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	5
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	25
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	10
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	6
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	17
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	40
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	21
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	4
33	2b	187/220 (85%)	146 (78%)	41 (22%)	1	2
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	9
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3	6
35	1d	169/181 (93%)	142 (84%)	27 (16%)	2	4
35	2d	173/181 (96%)	150 (87%)	23 (13%)	4	8
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	14
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4	9
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	14
37	2f	85/90 (94%)	74 (87%)	11 (13%)	4	8
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6	13
38	2g	120/127 (94%)	104 (87%)	16 (13%)	4	8
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	26
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	9
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	8
40	2i	89/99 (90%)	82 (92%)	7 (8%)	11	26
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	14
41	2j	69/92 (75%)	55 (80%)	14 (20%)	1	2
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	7
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17	37
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	52
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7	14
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	92/101 (91%)	78 (85%)	14 (15%)	3	5
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	24
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	6
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	20
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	35
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	6
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	21
48	1q	94/97 (97%)	84 (89%)	10 (11%)	6	14
48	2q	94/97 (97%)	85 (90%)	9 (10%)	8	17
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	15
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	7
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	21
50	2s	67/80 (84%)	53 (79%)	14 (21%)	1	2
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	8
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	8
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	12
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	40
56	1z	2/2 (100%)	2 (100%)	0	100	100
56	2z	2/2 (100%)	2 (100%)	0	100	100
All	All	9307/10068 (92%)	8260 (89%)	1047 (11%)	6	12

5 of 1047 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	2h	26	VAL
41	2j	58	ASP
39	2h	11	THR
51	2t	45	GLN
40	1i	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	42	GLN

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Mol	Chain	Res	Type
50	2s	83	HIS
35	2d	129	ASN
40	2i	87	GLN
35	1d	161	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	494 (17%)	22 (0%)
1	2A	2791/2915 (95%)	522 (18%)	27 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1497/1521 (98%)	273 (18%)	0
32	2a	1501/1521 (98%)	335 (22%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	32 (45%)	0
54	2w	71/76 (93%)	38 (53%)	0
55	1x	75/77 (97%)	14 (18%)	0
55	2x	75/77 (97%)	15 (20%)	0
57	1y	72/76 (94%)	35 (48%)	0
57	2y	72/76 (94%)	41 (56%)	0
All	All	9350/9620 (97%)	1850 (19%)	49 (0%)

5 of 1850 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	34	C
1	1A	45	C
1	1A	50	U
1	1A	55	G

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	277	C
1	2A	1026	U
1	2A	528	A
1	2A	827	U
1	2A	1275	A

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

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$
55	4SU	2x	8	55	18,21,22	2.25	5 (27%)	25,30,33	1.55	6 (24%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
55	4SU	1x	8	55	18,21,22	2.28	5 (27%)	25,30,33	1.53	6 (24%)
32	G7M	1a	527	58,32	23,26,27	1.52	3 (13%)	34,39,42	1.75	5 (14%)
32	G7M	2a	527	58,32	23,26,27	1.53	4 (17%)	34,39,42	1.72	5 (14%)
32	PSU	1a	516	58,32	18,21,22	1.44	3 (16%)	21,30,33	1.95	5 (23%)
54	A1B8A	2w	76	54	30,33,34	1.28	3 (10%)	36,46,49	1.87	8 (22%)
32	5MC	1a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.13	3 (11%)
56	FME	2z	1	56	8,9,10	0.99	0	8,9,11	1.04	1 (12%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.75	0
57	PSU	2y	55	57	18,21,22	1.42	2 (11%)	21,30,33	2.10	3 (14%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.83	6 (18%)
54	G7M	2w	46	54	23,26,27	1.45	3 (13%)	34,39,42	1.70	5 (14%)
32	M2G	2a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.87	6 (18%)
32	5MC	1a	967	32	19,22,23	1.51	3 (15%)	26,32,35	1.14	2 (7%)
57	U8U	1y	34	57	17,21,25	1.59	3 (17%)	21,30,37	1.46	3 (14%)
57	PSU	2y	39	57	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
1	OMG	2A	2251	1,55	23,26,27	1.25	4 (17%)	32,38,41	1.78	6 (18%)
57	5MU	2y	54	57	19,22,23	1.43	6 (31%)	27,32,35	2.11	6 (22%)
55	5MC	2x	32	55	19,22,23	1.70	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	2a	967	58,32	19,22,23	1.88	3 (15%)	26,32,35	1.17	3 (11%)
32	4OC	2a	1402	58,32	20,23,24	0.78	0	25,32,35	1.13	3 (12%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.01	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.10	10 (30%)
1	5MU	1A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.17	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)

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	4.46	1 (12%)	6,11,13	5.24	1 (16%)
54	A1B8A	1w	76	54	30,33,34	1.31	5 (16%)	36,46,49	1.81	8 (22%)
57	PSU	1y	55	57	18,21,22	1.40	2 (11%)	21,30,33	1.95	3 (14%)
1	5MC	1A	1942	1	19,22,23	1.67	3 (15%)	26,32,35	1.29	5 (19%)
32	2MG	1a	1207	58,32	23,26,27	1.24	2 (8%)	33,38,41	2.29	9 (27%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.95	1 (4%)
1	5MC	1A	1962	58,1	19,22,23	1.79	3 (15%)	26,32,35	1.18	3 (11%)
57	5MU	1y	54	57	19,22,23	1.36	5 (26%)	27,32,35	2.03	6 (22%)
1	PSU	1A	2605	58,1	18,21,22	1.40	4 (22%)	21,30,33	2.10	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.45	5 (26%)	27,32,35	2.07	6 (22%)
1	5MC	2A	1962	58,1	19,22,23	1.58	3 (15%)	26,32,35	1.15	3 (11%)
55	5MU	1x	54	55	19,22,23	1.45	5 (26%)	27,32,35	1.89	6 (22%)
54	T6A	1w	37	54	31,34,35	1.41	4 (12%)	43,49,52	1.87	10 (23%)
54	U8U	2w	34	54,53	20,24,25	1.30	2 (10%)	22,34,37	1.07	2 (9%)
57	T6A	1y	37	57	21,24,35	1.57	4 (19%)	30,35,52	2.06	9 (30%)
55	5MU	2x	54	55	19,22,23	1.36	4 (21%)	27,32,35	2.17	6 (22%)
54	5MU	2w	54	54	19,22,23	1.45	5 (26%)	27,32,35	1.67	5 (18%)
54	G7M	1w	46	54	23,26,27	1.50	3 (13%)	34,39,42	1.74	5 (14%)
54	5MU	1w	54	54	19,22,23	1.39	5 (26%)	27,32,35	2.11	6 (22%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.24	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
55	5MC	1x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.25	3 (11%)
57	G7M	1y	46	57	23,26,27	1.59	3 (13%)	34,39,42	1.72	3 (8%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.97	3 (14%)
54	U8U	1w	34	54,53	20,24,25	1.38	2 (10%)	22,34,37	1.34	4 (18%)
32	2MG	2a	1207	32	23,26,27	1.26	4 (17%)	33,38,41	2.17	7 (21%)
1	2MA	1A	2503	58,1	22,25,26	1.39	5 (22%)	32,37,40	2.38	10 (31%)
1	PSU	1A	1917	1	18,21,22	1.37	3 (16%)	21,30,33	1.96	4 (19%)
32	PSU	2a	516	58,32	18,21,22	1.41	3 (16%)	21,30,33	2.12	4 (19%)
55	8AN	2x	76	58,55	21,24,25	1.43	3 (14%)	26,35,38	2.58	9 (34%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.99	4 (19%)
57	U8U	2y	34	53,57	17,21,25	1.57	4 (23%)	21,30,37	1.54	3 (14%)
32	5MC	1a	1404	32	19,22,23	1.77	3 (15%)	26,32,35	1.13	2 (7%)
57	G7M	2y	46	57	23,26,27	1.59	3 (13%)	34,39,42	1.76	4 (11%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.73	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.10	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.12	2 (7%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.13	4 (19%)
1	2MA	2A	2503	58,1	22,25,26	1.42	4 (18%)	32,37,40	2.35	9 (28%)
57	PSU	1y	39	57	18,21,22	1.34	2 (11%)	21,30,33	2.04	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.27	3 (11%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	1.05	2 (8%)
32	5MC	2a	1400	32	19,22,23	1.83	3 (15%)	26,32,35	1.24	4 (15%)
54	T6A	2w	37	54,53	31,34,35	1.40	4 (12%)	43,49,52	1.86	9 (20%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	1.85	4 (19%)
54	PSU	2w	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.26	3 (14%)
1	OMU	2A	2552	58,1	19,22,23	1.20	2 (10%)	25,31,34	1.77	5 (20%)
57	T6A	2y	37	57,32	21,24,35	1.59	3 (14%)	30,35,52	2.02	8 (26%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.02	10 (30%)
1	OMU	1A	2552	58,1	19,22,23	1.18	3 (15%)	25,31,34	1.85	5 (20%)
1	5MU	1A	1915	1	19,22,23	1.37	5 (26%)	27,32,35	2.04	7 (25%)
55	8AN	1x	76	58,55	21,24,25	1.44	3 (14%)	26,35,38	2.31	10 (38%)
54	PSU	1w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	4 (19%)
1	5MU	2A	1939	1	19,22,23	1.40	5 (26%)	27,32,35	2.23	6 (22%)
32	UR3	1a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.78	4 (15%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	1.96	10 (30%)
43	0TD	1l	92	43	8,9,10	4.39	1 (12%)	6,11,13	4.50	2 (33%)
1	OMG	1A	2251	58,1,55	23,26,27	1.27	3 (13%)	32,38,41	2.00	6 (18%)
56	FME	1z	1	56	8,9,10	1.03	0	8,9,11	1.24	2 (25%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.02	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	58,32	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	2a	527	58,32	-	3/7/25/26	0/3/3/3
32	PSU	1a	516	58,32	-	0/7/25/26	0/2/2/2
54	A1B8A	2w	76	54	-	2/20/38/39	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
56	FME	2z	1	56	-	2/7/9/11	-
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
57	PSU	2y	55	57	-	2/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	1/11/29/30	0/3/3/3
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
57	U8U	1y	34	57	-	0/7/25/29	0/2/2/2
57	PSU	2y	39	57	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	1/9/27/28	0/3/3/3
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	58,32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	58,32	-	3/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
54	A1B8A	1w	76	54	-	2/20/38/39	0/3/3/3
57	PSU	1y	55	57	-	1/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	58,32	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MC	1A	1962	58,1	-	1/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	4/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	T6A	1w	37	54	-	6/23/41/42	0/3/3/3
54	U8U	2w	34	54,53	-	2/10/28/29	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
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	1w	46	54	-	2/7/25/26	0/3/3/3
54	5MU	1w	54	54	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	1/7/25/26	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	U8U	1w	34	54,53	-	2/10/28/29	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	2MA	1A	2503	58,1	-	1/7/25/26	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	58,32	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	58,55	-	0/7/25/26	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
57	U8U	2y	34	53,57	-	1/7/25/29	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	2/7/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	1/7/25/26	0/3/3/3
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
54	T6A	2w	37	54,53	-	4/23/41/42	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
57	T6A	2y	37	57,32	-	0/7/25/42	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	58,55	-	3/7/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1A	2251	58,1,55	-	0/9/27/28	0/3/3/3
56	FME	1z	1	56	-	4/7/9/11	-
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3

The worst 5 of 243 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.21	1.70	1.82
43	1l	92	0TD	CB-SB	-11.90	1.70	1.82
32	2a	967	5MC	C5-C4	7.05	1.49	1.44
32	2a	1400	5MC	C5-C4	6.88	1.49	1.44
1	1A	1962	5MC	C5-C4	6.79	1.49	1.44

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-12.58	79.76	102.36
43	1l	92	0TD	CSB-SB-CB	-10.57	83.37	102.36
1	2A	2503	2MA	C5-C4-N3	-8.14	118.61	127.18
1	1A	2503	2MA	C5-C4-N3	-7.55	119.22	127.18
32	1a	1207	2MG	C2-N3-C4	7.22	121.03	112.00

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

51 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	8	4SU	1	0
55	2x	55	PSU	2	0
55	1x	8	4SU	1	0
54	2w	76	A1B8A	1	0
56	2z	1	FME	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1920	OMC	1	0
57	2y	55	PSU	2	0
54	2w	46	G7M	1	0
1	2A	2251	OMG	1	0
55	2x	32	5MC	2	0
32	2a	967	5MC	1	0
32	2a	1402	4OC	3	0
32	2a	1519	MA6	2	0
1	1A	1939	5MU	2	0
43	2l	92	0TD	1	0
54	1w	76	A1B8A	3	0
57	1y	55	PSU	2	0
32	1a	1402	4OC	2	0
57	1y	54	5MU	2	0
54	1w	37	T6A	1	0
54	2w	34	U8U	1	0
57	1y	37	T6A	4	0
55	2x	54	5MU	1	0
54	2w	54	5MU	1	0
54	1w	54	5MU	1	0
1	1A	1911	PSU	1	0
54	1w	55	PSU	2	0
54	1w	34	U8U	4	0
32	2a	1207	2MG	2	0
1	1A	1917	PSU	1	0
32	2a	516	PSU	2	0
55	2x	76	8AN	2	0
57	2y	34	U8U	1	0
32	1a	1404	5MC	1	0
57	2y	46	G7M	1	0
1	2A	1942	5MC	1	0
32	2a	1404	5MC	1	0
1	2A	2503	2MA	3	0
57	1y	39	PSU	1	0
32	2a	1400	5MC	1	0
54	2w	37	T6A	1	0
54	2w	39	PSU	2	0
1	2A	2552	OMU	2	0
57	2y	37	T6A	1	0
32	1a	1519	MA6	2	0
1	1A	2552	OMU	1	0
55	1x	76	8AN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	2	0
32	1a	1518	MA6	2	0
1	1A	2251	OMG	1	0
32	2a	1518	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2750 ligands modelled in this entry, 2748 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	1A	2860/2915 (98%)	-0.57	83 (2%)	53	48	18, 36, 91, 104	0
1	2A	2789/2915 (95%)	-0.05	80 (2%)	53	48	32, 58, 88, 103	0
2	1B	120/121 (99%)	-0.49	1 (0%)	82	80	29, 49, 62, 81	0
2	2B	120/121 (99%)	0.75	8 (6%)	24	19	61, 78, 85, 93	0
3	1D	275/276 (99%)	-0.22	1 (0%)	88	86	19, 37, 50, 71	0
3	2D	275/276 (99%)	0.28	5 (1%)	67	63	30, 50, 63, 80	0
4	1E	204/206 (99%)	-0.14	1 (0%)	87	85	17, 42, 58, 69	0
4	2E	204/206 (99%)	0.29	3 (1%)	72	68	36, 57, 69, 78	0
5	1F	203/210 (96%)	-0.14	0	100	100	18, 43, 66, 78	0
5	2F	203/210 (96%)	0.47	2 (0%)	79	76	37, 66, 77, 82	0
6	1G	181/182 (99%)	0.38	4 (2%)	62	57	39, 57, 70, 80	0
6	2G	181/182 (99%)	1.17	21 (11%)	9	7	64, 77, 82, 92	0
7	1H	174/180 (96%)	0.22	1 (0%)	85	83	38, 51, 64, 68	0
7	2H	174/180 (96%)	0.86	3 (1%)	69	64	67, 77, 84, 87	0
8	1I	146/148 (98%)	0.61	4 (2%)	56	50	44, 70, 79, 82	0
8	2I	146/148 (98%)	1.64	48 (32%)	1	1	52, 79, 87, 92	0
9	1N	140/140 (100%)	-0.08	0	100	100	24, 40, 56, 73	0
9	2N	140/140 (100%)	0.59	5 (3%)	46	40	44, 63, 75, 79	0
10	1O	122/122 (100%)	-0.10	1 (0%)	82	80	26, 41, 57, 63	0
10	2O	122/122 (100%)	0.38	0	100	100	44, 56, 68, 73	0
11	1P	149/150 (99%)	-0.01	0	100	100	20, 45, 64, 73	0
11	2P	149/150 (99%)	0.54	4 (2%)	56	50	38, 66, 77, 85	0
12	1Q	141/141 (100%)	-0.05	2 (1%)	73	69	23, 40, 54, 67	0
12	2Q	141/141 (100%)	0.81	7 (4%)	34	28	49, 64, 73, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.24	0 100 100	26, 35, 46, 55	0
13	2R	118/118 (100%)	0.19	2 (1%) 69 64	38, 52, 60, 66	0
14	1S	110/112 (98%)	0.03	0 100 100	36, 48, 59, 64	0
14	2S	110/112 (98%)	1.22	19 (17%) 4 3	62, 72, 78, 82	0
15	1T	131/146 (89%)	0.14	2 (1%) 72 68	32, 46, 69, 74	0
15	2T	131/146 (89%)	0.43	1 (0%) 82 80	48, 59, 71, 75	0
16	1U	116/118 (98%)	-0.33	0 100 100	21, 32, 48, 55	0
16	2U	116/118 (98%)	0.33	0 100 100	45, 61, 73, 75	0
17	1V	101/101 (100%)	-0.21	0 100 100	21, 41, 57, 65	0
17	2V	101/101 (100%)	0.70	6 (5%) 28 23	45, 69, 75, 82	0
18	1W	112/113 (99%)	-0.33	0 100 100	24, 33, 51, 73	0
18	2W	112/113 (99%)	0.40	2 (1%) 67 63	35, 52, 64, 84	0
19	1X	95/96 (98%)	-0.15	1 (1%) 78 74	26, 38, 57, 64	0
19	2X	95/96 (98%)	0.50	2 (2%) 63 58	44, 58, 72, 78	0
20	1Y	107/110 (97%)	0.24	2 (1%) 66 61	35, 49, 65, 76	0
20	2Y	107/110 (97%)	1.05	14 (13%) 7 5	60, 69, 78, 82	0
21	1Z	154/206 (74%)	0.73	14 (9%) 15 11	40, 61, 82, 94	0
21	2Z	160/206 (77%)	1.23	22 (13%) 6 5	64, 77, 86, 94	0
22	10	83/85 (97%)	0.07	4 (4%) 35 30	27, 38, 62, 69	0
22	20	83/85 (97%)	1.05	8 (9%) 13 10	45, 64, 71, 84	0
23	11	97/98 (98%)	0.06	1 (1%) 79 76	26, 45, 67, 71	0
23	21	97/98 (98%)	0.34	3 (3%) 51 45	40, 56, 70, 75	0
24	12	70/72 (97%)	0.07	1 (1%) 73 69	35, 49, 57, 72	0
24	22	70/72 (97%)	0.76	0 100 100	59, 68, 75, 76	0
25	13	59/60 (98%)	-0.24	0 100 100	26, 37, 57, 64	0
25	23	59/60 (98%)	0.46	0 100 100	52, 63, 74, 77	0
26	14	69/71 (97%)	0.74	8 (11%) 9 7	55, 73, 85, 92	0
26	24	69/71 (97%)	1.27	8 (11%) 9 7	71, 82, 89, 94	0
27	15	59/60 (98%)	-0.34	1 (1%) 69 64	20, 33, 53, 66	0
27	25	59/60 (98%)	0.21	0 100 100	38, 51, 63, 77	0
28	16	53/54 (98%)	-0.21	0 100 100	32, 41, 53, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.68	1 (1%) 66 61	52, 62, 67, 73	0
29	17	48/49 (97%)	-0.30	1 (2%) 63 58	21, 26, 52, 59	0
29	27	48/49 (97%)	0.07	1 (2%) 63 58	35, 43, 60, 70	0
30	18	64/65 (98%)	-0.12	1 (1%) 70 66	28, 34, 42, 52	0
30	28	64/65 (98%)	0.68	2 (3%) 51 45	45, 56, 62, 69	0
31	19	37/37 (100%)	-0.21	0 100 100	29, 40, 60, 60	0
31	29	37/37 (100%)	1.13	3 (8%) 18 14	58, 65, 73, 75	0
32	1a	1488/1521 (97%)	0.19	26 (1%) 69 64	33, 66, 88, 100	0
32	2a	1491/1521 (98%)	0.50	53 (3%) 46 40	53, 77, 92, 102	0
33	1b	231/256 (90%)	0.82	21 (9%) 15 11	61, 75, 83, 86	0
33	2b	231/256 (90%)	1.30	49 (21%) 2 2	71, 81, 87, 90	0
34	1c	206/239 (86%)	0.70	9 (4%) 39 33	57, 69, 77, 84	0
34	2c	206/239 (86%)	1.53	57 (27%) 1 1	71, 82, 86, 90	0
35	1d	208/209 (99%)	0.87	19 (9%) 15 11	54, 67, 76, 80	0
35	2d	208/209 (99%)	1.02	21 (10%) 12 9	61, 71, 78, 85	0
36	1e	148/162 (91%)	0.41	1 (0%) 84 82	52, 62, 69, 79	0
36	2e	148/162 (91%)	1.12	19 (12%) 7 6	65, 75, 81, 88	0
37	1f	100/101 (99%)	0.50	2 (2%) 65 60	55, 65, 73, 76	0
37	2f	100/101 (99%)	0.55	3 (3%) 52 47	61, 71, 77, 79	0
38	1g	155/156 (99%)	0.63	8 (5%) 33 27	58, 69, 82, 87	0
38	2g	155/156 (99%)	1.19	23 (14%) 5 4	70, 78, 84, 87	0
39	1h	137/138 (99%)	0.60	3 (2%) 62 57	56, 65, 73, 76	0
39	2h	137/138 (99%)	1.13	14 (10%) 12 9	66, 74, 79, 83	0
40	1i	127/128 (99%)	1.03	10 (7%) 18 14	57, 73, 79, 82	0
40	2i	127/128 (99%)	1.45	28 (22%) 2 2	71, 80, 86, 88	0
41	1j	97/105 (92%)	1.04	8 (8%) 17 14	57, 74, 82, 85	0
41	2j	96/105 (91%)	1.50	24 (25%) 2 1	67, 81, 87, 89	0
42	1k	114/129 (88%)	0.79	6 (5%) 32 26	44, 66, 77, 82	0
42	2k	114/129 (88%)	0.89	8 (7%) 22 18	60, 73, 79, 82	0
43	1l	121/132 (91%)	0.49	5 (4%) 41 36	45, 58, 66, 72	0
43	2l	121/132 (91%)	0.71	9 (7%) 20 16	55, 69, 75, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.74	9 (7%) 21 17	56, 68, 77, 89	0
44	2m	122/126 (96%)	1.60	28 (22%) 2 1	70, 80, 86, 88	0
45	1n	60/61 (98%)	0.90	5 (8%) 17 13	58, 65, 71, 72	0
45	2n	60/61 (98%)	1.69	20 (33%) 1 1	70, 81, 85, 88	0
46	1o	88/89 (98%)	0.61	2 (2%) 61 55	49, 63, 73, 80	0
46	2o	88/89 (98%)	0.74	2 (2%) 61 55	62, 71, 79, 82	0
47	1p	82/88 (93%)	1.21	16 (19%) 3 2	58, 71, 76, 84	0
47	2p	82/88 (93%)	0.70	5 (6%) 27 22	53, 68, 74, 76	0
48	1q	99/105 (94%)	0.83	6 (6%) 27 22	56, 66, 74, 77	0
48	2q	99/105 (94%)	0.85	5 (5%) 33 28	60, 70, 77, 79	0
49	1r	68/88 (77%)	0.50	3 (4%) 39 33	53, 65, 74, 78	0
49	2r	68/88 (77%)	0.54	0 100 100	64, 71, 78, 81	0
50	1s	83/93 (89%)	0.70	2 (2%) 59 54	62, 71, 79, 83	0
50	2s	83/93 (89%)	1.73	30 (36%) 1 0	76, 83, 89, 91	0
51	1t	96/106 (90%)	0.98	8 (8%) 17 13	59, 68, 75, 79	0
51	2t	96/106 (90%)	0.59	5 (5%) 33 27	56, 68, 78, 82	0
52	1u	23/27 (85%)	1.16	5 (21%) 2 2	59, 67, 72, 75	0
52	2u	23/27 (85%)	2.11	12 (52%) 0 0	74, 77, 81, 81	0
53	1v	13/24 (54%)	1.48	5 (38%) 1 0	48, 77, 88, 91	0
53	2v	13/24 (54%)	1.99	4 (30%) 1 1	72, 87, 94, 96	0
54	1w	67/76 (88%)	1.52	17 (25%) 1 1	63, 95, 99, 102	0
54	2w	67/76 (88%)	1.93	29 (43%) 0 0	80, 96, 101, 104	0
55	1x	72/77 (93%)	0.48	2 (2%) 55 49	30, 63, 78, 84	0
55	2x	72/77 (93%)	0.89	5 (6%) 23 18	49, 79, 86, 93	0
56	1z	2/3 (66%)	0.65	0 100 100	39, 39, 39, 40	0
56	2z	2/3 (66%)	0.75	0 100 100	53, 53, 53, 58	0
57	1y	68/76 (89%)	1.59	18 (26%) 1 1	54, 95, 100, 102	0
57	2y	68/76 (89%)	1.69	21 (30%) 1 1	68, 96, 100, 102	0
All	All	20884/21754 (96%)	0.32	1104 (5%) 32 26	17, 63, 87, 104	0

The worst 5 of 1104 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	11.0
45	1n	2	ALA	7.1
44	2m	123	ALA	6.7
44	1m	123	ALA	6.2
21	2Z	174	VAL	5.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	2w	55	20/21	0.27	0.17	93,100,111,117	0
57	G7M	2y	46	24/25	0.42	0.15	89,98,109,123	0
54	G7M	2w	46	24/25	0.44	0.15	88,97,107,115	0
54	G7M	1w	46	24/25	0.45	0.15	80,94,105,110	0
54	5MU	2w	54	21/22	0.52	0.18	83,96,102,106	0
54	PSU	1w	55	20/21	0.57	0.17	82,96,103,105	0
57	U8U	2y	34	20/24	0.57	0.24	93,100,106,118	0
57	G7M	1y	46	24/25	0.60	0.15	86,93,98,107	0
57	PSU	2y	55	20/21	0.61	0.14	83,95,103,115	0
57	5MU	2y	54	21/22	0.63	0.14	88,95,104,117	0
57	PSU	2y	39	20/21	0.64	0.15	89,92,102,108	0
57	T6A	1y	37	22/33	0.66	0.16	81,91,100,107	0
57	PSU	1y	39	20/21	0.67	0.14	84,92,101,107	0
57	U8U	1y	34	20/24	0.69	0.17	82,92,98,102	0
57	PSU	1y	55	20/21	0.70	0.14	91,94,102,104	0
57	T6A	2y	37	22/33	0.72	0.17	85,93,99,105	0
54	U8U	1w	34	23/24	0.75	0.17	64,83,93,99	0
1	5MU	2A	1915	21/22	0.76	0.18	79,84,89,96	0
54	T6A	2w	37	32/33	0.76	0.17	71,91,100,108	0
54	5MU	1w	54	21/22	0.76	0.13	80,89,93,94	0
57	5MU	1y	54	21/22	0.78	0.12	83,91,96,103	0
54	U8U	2w	34	23/24	0.81	0.16	82,87,92,96	0
54	T6A	1w	37	32/33	0.82	0.14	70,79,82,83	0
32	2MG	2a	1207	24/25	0.83	0.13	78,83,89,94	0
54	PSU	2w	39	20/21	0.83	0.16	82,93,96,96	0
32	PSU	2a	516	20/21	0.84	0.12	75,82,90,90	0
54	A1B8A	2w	76	31/32	0.84	0.16	52,68,78,82	0
55	4SU	2x	8	20/21	0.85	0.12	74,78,83,87	0
32	M2G	2a	966	25/26	0.86	0.17	59,70,87,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	1w	39	20/21	0.86	0.12	76,82,88,94	0
55	5MU	2x	54	21/22	0.87	0.13	76,79,84,94	0
55	PSU	2x	55	20/21	0.87	0.11	69,76,80,89	0
54	A1B8A	1w	76	31/32	0.87	0.14	36,52,62,70	0
32	5MC	2a	967	21/22	0.87	0.15	66,71,81,83	0
43	0TD	1l	92	10/11	0.88	0.13	48,54,58,66	0
43	0TD	2l	92	10/11	0.90	0.12	68,70,73,87	0
1	PSU	2A	1911	20/21	0.90	0.12	64,70,78,82	0
1	5MU	1A	1915	21/22	0.90	0.10	53,61,69,79	0
32	PSU	1a	516	20/21	0.91	0.09	58,64,70,77	0
1	PSU	2A	1917	20/21	0.91	0.12	62,75,79,81	0
55	5MU	1x	54	21/22	0.92	0.11	60,66,70,74	0
32	2MG	1a	1207	24/25	0.92	0.11	59,68,74,81	0
32	5MC	2a	1400	21/22	0.92	0.15	65,72,76,78	0
56	FME	2z	1	10/11	0.92	0.16	49,55,58,65	0
32	G7M	2a	527	24/25	0.93	0.10	60,68,72,74	0
32	4OC	2a	1402	22/23	0.93	0.11	55,66,69,74	0
55	PSU	1x	55	20/21	0.93	0.09	49,58,67,71	0
1	OMC	2A	1920	21/22	0.94	0.11	57,65,72,74	0
55	5MC	1x	32	21/22	0.94	0.13	48,52,62,62	0
32	5MC	2a	1407	21/22	0.94	0.10	56,61,62,66	0
56	FME	1z	1	10/11	0.94	0.15	37,45,49,51	0
55	4SU	1x	8	20/21	0.94	0.11	59,64,69,73	0
32	UR3	2a	1498	21/22	0.95	0.11	55,60,66,73	0
32	MA6	2a	1518	24/25	0.95	0.11	52,66,70,72	0
1	5MC	2A	1942	21/22	0.95	0.10	46,60,65,69	0
1	5MC	2A	1962	21/22	0.95	0.11	42,52,56,76	0
55	5MC	2x	32	21/22	0.95	0.12	63,72,77,83	0
32	G7M	1a	527	24/25	0.95	0.09	41,47,54,58	0
32	5MC	1a	967	21/22	0.95	0.09	56,61,66,69	0
55	8AN	2x	76	22/23	0.95	0.10	43,52,58,59	0
32	5MC	2a	1404	21/22	0.95	0.10	53,62,64,67	0
1	PSU	1A	1917	20/21	0.95	0.07	46,55,62,62	0
32	M2G	1a	966	25/26	0.96	0.10	44,58,64,67	0
1	OMG	2A	2251	24/25	0.96	0.09	36,41,47,49	0
1	OMU	2A	2552	21/22	0.96	0.09	33,45,50,51	0
1	PSU	2A	2605	20/21	0.96	0.09	31,41,47,47	0
32	5MC	1a	1400	21/22	0.96	0.10	47,50,55,61	0
32	5MC	1a	1404	21/22	0.96	0.09	35,43,48,52	0
32	MA6	1a	1519	24/25	0.96	0.09	36,43,47,50	0
32	MA6	2a	1519	24/25	0.96	0.12	54,65,72,74	0
1	5MC	1A	1942	21/22	0.96	0.09	38,44,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	1a	1518	24/25	0.97	0.09	34,44,49,50	0
1	5MU	2A	1939	21/22	0.97	0.07	33,40,45,47	0
1	PSU	1A	1911	20/21	0.97	0.08	41,49,54,57	0
55	8AN	1x	76	22/23	0.97	0.08	24,34,42,44	0
32	4OC	1a	1402	22/23	0.97	0.09	43,48,53,57	0
1	2MA	2A	2503	23/24	0.97	0.08	26,37,41,47	0
1	OMC	1A	1920	21/22	0.97	0.07	34,45,50,52	0
32	5MC	1a	1407	21/22	0.97	0.07	33,42,47,48	0
1	PSU	1A	2605	20/21	0.98	0.07	21,28,34,34	0
1	5MU	1A	1939	21/22	0.98	0.05	22,29,31,35	0
1	5MC	1A	1962	21/22	0.98	0.06	22,31,36,45	0
1	OMG	1A	2251	24/25	0.98	0.05	21,26,29,31	0
32	UR3	1a	1498	21/22	0.98	0.07	33,42,44,45	0
1	2MA	1A	2503	23/24	0.98	0.06	16,23,27,27	0
1	OMU	1A	2552	21/22	0.98	0.06	23,28,32,35	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	1798	1/1	0.55	0.17	81,81,81,81	0
58	MG	2A	3385	1/1	0.58	0.16	84,84,84,84	0
58	MG	2a	1756	1/1	0.62	0.18	82,82,82,82	0
58	MG	1B	229	1/1	0.63	0.20	74,74,74,74	0
58	MG	2A	3451	1/1	0.63	0.28	83,83,83,83	0
58	MG	2A	3437	1/1	0.64	0.29	77,77,77,77	0
58	MG	1a	1804	1/1	0.65	0.18	72,72,72,72	0
58	MG	1A	3260	1/1	0.65	0.20	85,85,85,85	0
58	MG	1a	1738	1/1	0.65	0.21	77,77,77,77	0
58	MG	1B	230	1/1	0.66	0.23	78,78,78,78	0
58	MG	2A	3755	1/1	0.66	0.26	59,59,59,59	0
58	MG	1A	3683	1/1	0.67	0.20	63,63,63,63	0
58	MG	2A	3113	1/1	0.67	0.30	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	3171	1/1	0.68	0.20	80,80,80,80	0
58	MG	1A	3844	1/1	0.68	0.19	77,77,77,77	0
58	MG	2A	3669	1/1	0.68	0.18	77,77,77,77	0
58	MG	2A	3731	1/1	0.69	0.15	81,81,81,81	0
58	MG	2A	3608	1/1	0.69	0.20	63,63,63,63	0
58	MG	2A	3615	1/1	0.69	0.23	68,68,68,68	0
58	MG	2A	3175	1/1	0.69	0.23	68,68,68,68	0
58	MG	1A	3643	1/1	0.70	0.16	69,69,69,69	0
58	MG	2a	1789	1/1	0.70	0.20	70,70,70,70	0
58	MG	2a	1638	1/1	0.70	0.12	81,81,81,81	0
58	MG	1a	1809	1/1	0.71	0.18	72,72,72,72	0
58	MG	2G	201	1/1	0.71	0.23	75,75,75,75	0
58	MG	2A	3573	1/1	0.71	0.22	69,69,69,69	0
58	MG	1a	1733	1/1	0.72	0.17	85,85,85,85	0
58	MG	2A	3273	1/1	0.72	0.20	71,71,71,71	0
58	MG	2A	3332	1/1	0.73	0.25	72,72,72,72	0
58	MG	2A	3664	1/1	0.73	0.25	69,69,69,69	0
58	MG	1a	1802	1/1	0.73	0.24	81,81,81,81	0
58	MG	2a	1622	1/1	0.73	0.22	83,83,83,83	0
58	MG	2a	1607	1/1	0.74	0.36	67,67,67,67	0
58	MG	2A	3679	1/1	0.74	0.16	72,72,72,72	0
58	MG	2a	1805	1/1	0.74	0.20	68,68,68,68	0
58	MG	2A	3526	1/1	0.75	0.17	66,66,66,66	0
58	MG	2A	3704	1/1	0.75	0.20	69,69,69,69	0
58	MG	2a	1818	1/1	0.75	0.18	79,79,79,79	0
58	MG	2B	214	1/1	0.76	0.18	71,71,71,71	0
58	MG	1a	1731	1/1	0.76	0.18	66,66,66,66	0
58	MG	2a	1601	1/1	0.77	0.19	74,74,74,74	0
58	MG	1A	3772	1/1	0.77	0.14	20,20,20,20	0
58	MG	2A	3192	1/1	0.77	0.20	69,69,69,69	0
58	MG	1A	4083	1/1	0.77	0.16	58,58,58,58	0
58	MG	2a	1725	1/1	0.77	0.27	80,80,80,80	0
58	MG	1a	1760	1/1	0.77	0.12	67,67,67,67	0
58	MG	2A	3335	1/1	0.77	0.21	77,77,77,77	0
58	MG	2A	3833	1/1	0.77	0.20	65,65,65,65	0
58	MG	2A	3355	1/1	0.77	0.18	69,69,69,69	0
58	MG	2a	1812	1/1	0.77	0.18	83,83,83,83	0
58	MG	2a	1815	1/1	0.77	0.14	76,76,76,76	0
58	MG	1A	4089	1/1	0.77	0.17	45,45,45,45	0
58	MG	1A	3466	1/1	0.78	0.18	62,62,62,62	0
58	MG	1A	3882	1/1	0.78	0.13	23,23,23,23	0
58	MG	1x	109	1/1	0.78	0.34	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	2A	3327	1/1	0.78	0.16	71,71,71,71	0
58	MG	2A	3508	1/1	0.78	0.12	29,29,29,29	0
58	MG	2A	3690	1/1	0.78	0.12	70,70,70,70	0
58	MG	1A	4082	1/1	0.78	0.14	60,60,60,60	0
58	MG	1A	3267	1/1	0.78	0.20	62,62,62,62	0
58	MG	2a	1821	1/1	0.78	0.24	69,69,69,69	0
58	MG	2R	201	1/1	0.79	0.24	77,77,77,77	0
58	MG	1a	1755	1/1	0.79	0.12	60,60,60,60	0
58	MG	2A	3670	1/1	0.79	0.14	68,68,68,68	0
58	MG	1U	208	1/1	0.79	0.48	67,67,67,67	0
58	MG	1a	1622	1/1	0.79	0.20	66,66,66,66	0
58	MG	2a	1706	1/1	0.79	0.19	77,77,77,77	0
58	MG	1a	1697	1/1	0.79	0.17	66,66,66,66	0
58	MG	2A	3723	1/1	0.79	0.15	68,68,68,68	0
58	MG	1A	3752	1/1	0.79	0.13	65,65,65,65	0
58	MG	2A	3738	1/1	0.79	0.17	46,46,46,46	0
58	MG	1A	3468	1/1	0.79	0.13	56,56,56,56	0
58	MG	2A	3758	1/1	0.79	0.12	67,67,67,67	0
58	MG	1A	3687	1/1	0.79	0.13	64,64,64,64	0
58	MG	2A	3152	1/1	0.79	0.23	60,60,60,60	0
58	MG	2A	3380	1/1	0.79	0.29	76,76,76,76	0
58	MG	2j	201	1/1	0.79	0.20	71,71,71,71	0
58	MG	1A	3960	1/1	0.80	0.15	58,58,58,58	0
58	MG	2a	1655	1/1	0.80	0.17	80,80,80,80	0
58	MG	2A	3418	1/1	0.80	0.32	68,68,68,68	0
58	MG	2A	3653	1/1	0.80	0.14	65,65,65,65	0
58	MG	2A	3432	1/1	0.80	0.23	54,54,54,54	0
58	MG	1A	3957	1/1	0.80	0.10	46,46,46,46	0
58	MG	2A	3205	1/1	0.80	0.11	60,60,60,60	0
58	MG	2a	1800	1/1	0.80	0.17	86,86,86,86	0
58	MG	2A	3483	1/1	0.80	0.31	67,67,67,67	0
58	MG	2P	202	1/1	0.80	0.23	66,66,66,66	0
58	MG	2A	3097	1/1	0.80	0.15	72,72,72,72	0
58	MG	2A	3357	1/1	0.80	0.19	54,54,54,54	0
58	MG	2A	3705	1/1	0.80	0.18	59,59,59,59	0
58	MG	2A	3276	1/1	0.80	0.19	72,72,72,72	0
58	MG	2A	3024	1/1	0.81	0.15	61,61,61,61	0
58	MG	2A	3159	1/1	0.81	0.24	66,66,66,66	0
58	MG	2a	1733	1/1	0.81	0.22	70,70,70,70	0
58	MG	2a	1735	1/1	0.81	0.18	69,69,69,69	0
58	MG	1A	3326	1/1	0.81	0.11	65,65,65,65	0
58	MG	2A	3173	1/1	0.81	0.20	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3678	1/1	0.81	0.12	56,56,56,56	0
58	MG	2A	3106	1/1	0.81	0.30	72,72,72,72	0
58	MG	2A	3337	1/1	0.81	0.18	76,76,76,76	0
58	MG	1B	213	1/1	0.81	0.19	67,67,67,67	0
58	MG	2A	3115	1/1	0.81	0.22	62,62,62,62	0
58	MG	2A	3605	1/1	0.81	0.17	75,75,75,75	0
58	MG	2A	3256	1/1	0.81	0.14	58,58,58,58	0
58	MG	2A	3270	1/1	0.81	0.15	78,78,78,78	0
58	MG	2y	101	1/1	0.81	0.33	71,71,71,71	0
58	MG	2A	3773	1/1	0.82	0.10	46,46,46,46	0
58	MG	2A	3817	1/1	0.82	0.17	48,48,48,48	0
58	MG	1A	3878	1/1	0.82	0.12	61,61,61,61	0
58	MG	2B	208	1/1	0.82	0.10	62,62,62,62	0
58	MG	2A	3212	1/1	0.82	0.14	67,67,67,67	0
58	MG	2D	303	1/1	0.82	0.19	64,64,64,64	0
58	MG	2F	307	1/1	0.82	0.11	64,64,64,64	0
58	MG	2A	3502	1/1	0.82	0.16	55,55,55,55	0
58	MG	1B	234	1/1	0.82	0.16	66,66,66,66	0
58	MG	1A	3458	1/1	0.82	0.21	63,63,63,63	0
58	MG	20	104	1/1	0.82	0.11	55,55,55,55	0
58	MG	1A	3893	1/1	0.82	0.17	73,73,73,73	0
58	MG	2A	3600	1/1	0.82	0.17	55,55,55,55	0
58	MG	2A	3051	1/1	0.82	0.27	69,69,69,69	0
58	MG	2A	3291	1/1	0.82	0.14	59,59,59,59	0
58	MG	2A	3325	1/1	0.82	0.23	68,68,68,68	0
58	MG	2a	1704	1/1	0.82	0.14	55,55,55,55	0
58	MG	1a	1636	1/1	0.82	0.28	73,73,73,73	0
58	MG	1a	1683	1/1	0.82	0.28	68,68,68,68	0
58	MG	1A	3294	1/1	0.82	0.20	55,55,55,55	0
58	MG	1A	3707	1/1	0.82	0.11	29,29,29,29	0
58	MG	2A	3350	1/1	0.82	0.14	63,63,63,63	0
58	MG	2a	1757	1/1	0.82	0.09	89,89,89,89	0
58	MG	1A	3749	1/1	0.82	0.14	51,51,51,51	0
58	MG	1a	1737	1/1	0.82	0.24	62,62,62,62	0
58	MG	1A	3251	1/1	0.82	0.14	50,50,50,50	0
58	MG	1A	3536	1/1	0.82	0.12	59,59,59,59	0
58	MG	2A	3390	1/1	0.82	0.19	68,68,68,68	0
58	MG	2a	1814	1/1	0.82	0.20	63,63,63,63	0
58	MG	2A	3728	1/1	0.82	0.19	56,56,56,56	0
58	MG	1A	3809	1/1	0.82	0.14	51,51,51,51	0
58	MG	2A	3191	1/1	0.82	0.32	69,69,69,69	0
58	MG	1A	3383	1/1	0.82	0.14	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	2x	103	1/1	0.82	0.19	69,69,69,69	0
58	MG	2A	3444	1/1	0.82	0.12	67,67,67,67	0
58	MG	2A	3300	1/1	0.83	0.22	59,59,59,59	0
58	MG	2A	3472	1/1	0.83	0.10	72,72,72,72	0
58	MG	1A	4019	1/1	0.83	0.15	75,75,75,75	0
58	MG	2a	1641	1/1	0.83	0.28	67,67,67,67	0
58	MG	1A	3801	1/1	0.83	0.14	53,53,53,53	0
58	MG	2a	1681	1/1	0.83	0.24	71,71,71,71	0
58	MG	2a	1700	1/1	0.83	0.13	75,75,75,75	0
58	MG	1w	101	1/1	0.83	0.15	77,77,77,77	0
58	MG	1w	103	1/1	0.83	0.17	87,87,87,87	0
58	MG	2a	1714	1/1	0.83	0.28	67,67,67,67	0
58	MG	2a	1715	1/1	0.83	0.12	63,63,63,63	0
58	MG	1E	314	1/1	0.83	0.30	50,50,50,50	0
58	MG	2A	3023	1/1	0.83	0.20	71,71,71,71	0
58	MG	1A	3329	1/1	0.83	0.13	52,52,52,52	0
58	MG	2A	3782	1/1	0.83	0.14	79,79,79,79	0
58	MG	2A	3044	1/1	0.83	0.20	66,66,66,66	0
58	MG	1A	3923	1/1	0.83	0.13	30,30,30,30	0
58	MG	2A	3646	1/1	0.83	0.13	77,77,77,77	0
58	MG	2A	3384	1/1	0.83	0.15	66,66,66,66	0
58	MG	2B	216	1/1	0.83	0.16	72,72,72,72	0
58	MG	2A	3052	1/1	0.83	0.22	67,67,67,67	0
58	MG	2A	3065	1/1	0.83	0.17	77,77,77,77	0
58	MG	2A	3075	1/1	0.83	0.17	72,72,72,72	0
58	MG	2A	3672	1/1	0.83	0.17	68,68,68,68	0
58	MG	1A	3626	1/1	0.83	0.16	48,48,48,48	0
58	MG	1a	1680	1/1	0.83	0.19	67,67,67,67	0
58	MG	2l	202	1/1	0.83	0.23	68,68,68,68	0
58	MG	2x	102	1/1	0.83	0.18	65,65,65,65	0
58	MG	28	101	1/1	0.83	0.26	64,64,64,64	0
58	MG	1A	3470	1/1	0.83	0.15	60,60,60,60	0
58	MG	20	103	1/1	0.84	0.16	59,59,59,59	0
58	MG	2A	3364	1/1	0.84	0.14	71,71,71,71	0
58	MG	2a	1742	1/1	0.84	0.26	77,77,77,77	0
58	MG	2a	1752	1/1	0.84	0.10	71,71,71,71	0
58	MG	2A	3089	1/1	0.84	0.14	58,58,58,58	0
58	MG	2A	3457	1/1	0.84	0.17	72,72,72,72	0
58	MG	1x	105	1/1	0.84	0.32	69,69,69,69	0
58	MG	2A	3634	1/1	0.84	0.15	41,41,41,41	0
58	MG	2A	3849	1/1	0.84	0.17	61,61,61,61	0
58	MG	1A	3992	1/1	0.84	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3313	1/1	0.84	0.13	59,59,59,59	0
58	MG	2A	3654	1/1	0.84	0.21	73,73,73,73	0
58	MG	2B	220	1/1	0.84	0.18	76,76,76,76	0
58	MG	2A	3729	1/1	0.84	0.16	66,66,66,66	0
58	MG	1a	1670	1/1	0.84	0.18	55,55,55,55	0
58	MG	2d	302	1/1	0.84	0.14	70,70,70,70	0
58	MG	2A	3197	1/1	0.84	0.16	66,66,66,66	0
58	MG	2k	201	1/1	0.84	0.12	64,64,64,64	0
58	MG	2A	3743	1/1	0.84	0.21	48,48,48,48	0
58	MG	2a	1717	1/1	0.84	0.20	76,76,76,76	0
58	MG	2a	1720	1/1	0.84	0.16	68,68,68,68	0
58	MG	2A	3359	1/1	0.84	0.12	75,75,75,75	0
58	MG	2A	3193	1/1	0.85	0.23	62,62,62,62	0
58	MG	2A	3530	1/1	0.85	0.22	63,63,63,63	0
58	MG	2A	3554	1/1	0.85	0.15	55,55,55,55	0
58	MG	2a	1674	1/1	0.85	0.22	67,67,67,67	0
58	MG	2A	3195	1/1	0.85	0.15	69,69,69,69	0
58	MG	2a	1684	1/1	0.85	0.22	62,62,62,62	0
58	MG	2A	3746	1/1	0.85	0.15	61,61,61,61	0
58	MG	2A	3582	1/1	0.85	0.19	81,81,81,81	0
58	MG	1a	1743	1/1	0.85	0.18	64,64,64,64	0
58	MG	1A	3810	1/1	0.85	0.14	46,46,46,46	0
58	MG	2A	3366	1/1	0.85	0.16	57,57,57,57	0
58	MG	2A	3792	1/1	0.85	0.10	73,73,73,73	0
58	MG	1a	1628	1/1	0.85	0.11	56,56,56,56	0
58	MG	1a	1776	1/1	0.85	0.11	66,66,66,66	0
58	MG	2A	3635	1/1	0.85	0.12	46,46,46,46	0
58	MG	2A	3862	1/1	0.85	0.18	62,62,62,62	0
58	MG	2B	203	1/1	0.85	0.20	63,63,63,63	0
58	MG	2B	204	1/1	0.85	0.16	70,70,70,70	0
58	MG	2B	206	1/1	0.85	0.17	58,58,58,58	0
58	MG	2A	3091	1/1	0.85	0.12	70,70,70,70	0
58	MG	2a	1781	1/1	0.85	0.14	63,63,63,63	0
58	MG	2a	1787	1/1	0.85	0.13	72,72,72,72	0
58	MG	2a	1788	1/1	0.85	0.15	65,65,65,65	0
58	MG	1B	222	1/1	0.85	0.17	58,58,58,58	0
58	MG	2A	3391	1/1	0.85	0.12	66,66,66,66	0
58	MG	1A	3245	1/1	0.85	0.12	59,59,59,59	0
58	MG	2A	3667	1/1	0.85	0.18	56,56,56,56	0
58	MG	1A	3956	1/1	0.85	0.10	45,45,45,45	0
58	MG	1A	3236	1/1	0.85	0.21	42,42,42,42	0
58	MG	1a	1687	1/1	0.85	0.31	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	3388	1/1	0.85	0.17	61,61,61,61	0
58	MG	1G	203	1/1	0.85	0.10	68,68,68,68	0
58	MG	1P	206	1/1	0.85	0.24	55,55,55,55	0
58	MG	2A	3482	1/1	0.85	0.17	54,54,54,54	0
58	MG	1A	4094	1/1	0.85	0.17	53,53,53,53	0
58	MG	1W	207	1/1	0.85	0.19	32,32,32,32	0
58	MG	2t	201	1/1	0.85	0.19	48,48,48,48	0
58	MG	2w	101	1/1	0.85	0.27	84,84,84,84	0
58	MG	2a	1608	1/1	0.85	0.35	78,78,78,78	0
58	MG	1a	1739	1/1	0.85	0.15	62,62,62,62	0
58	MG	2a	1633	1/1	0.85	0.21	73,73,73,73	0
58	MG	1a	1768	1/1	0.86	0.14	64,64,64,64	0
58	MG	2A	3264	1/1	0.86	0.19	67,67,67,67	0
58	MG	2a	1630	1/1	0.86	0.17	62,62,62,62	0
58	MG	1A	3946	1/1	0.86	0.19	67,67,67,67	0
58	MG	2A	3434	1/1	0.86	0.20	59,59,59,59	0
58	MG	2A	3701	1/1	0.86	0.11	39,39,39,39	0
58	MG	2A	3703	1/1	0.86	0.17	63,63,63,63	0
58	MG	2A	3272	1/1	0.86	0.17	66,66,66,66	0
58	MG	1A	3191	1/1	0.86	0.18	53,53,53,53	0
58	MG	1A	3595	1/1	0.86	0.10	52,52,52,52	0
58	MG	1A	3833	1/1	0.86	0.13	46,46,46,46	0
58	MG	2a	1702	1/1	0.86	0.16	55,55,55,55	0
58	MG	2A	3292	1/1	0.86	0.30	73,73,73,73	0
58	MG	1b	301	1/1	0.86	0.20	81,81,81,81	0
58	MG	2A	3302	1/1	0.86	0.16	62,62,62,62	0
58	MG	2A	3739	1/1	0.86	0.14	72,72,72,72	0
58	MG	2A	3485	1/1	0.86	0.20	61,61,61,61	0
58	MG	2A	3495	1/1	0.86	0.15	64,64,64,64	0
58	MG	2A	3126	1/1	0.86	0.09	66,66,66,66	0
58	MG	1A	3599	1/1	0.86	0.22	73,73,73,73	0
58	MG	2a	1734	1/1	0.86	0.17	70,70,70,70	0
58	MG	2A	3763	1/1	0.86	0.20	74,74,74,74	0
58	MG	2A	3509	1/1	0.86	0.18	65,65,65,65	0
58	MG	2A	3153	1/1	0.86	0.14	62,62,62,62	0
58	MG	2a	1754	1/1	0.86	0.12	67,67,67,67	0
58	MG	1a	1714	1/1	0.86	0.24	58,58,58,58	0
58	MG	2A	3541	1/1	0.86	0.09	46,46,46,46	0
58	MG	2a	1766	1/1	0.86	0.17	79,79,79,79	0
58	MG	2A	3165	1/1	0.86	0.08	41,41,41,41	0
58	MG	2A	3561	1/1	0.86	0.09	35,35,35,35	0
58	MG	2A	3859	1/1	0.86	0.33	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1730	1/1	0.86	0.11	69,69,69,69	0
58	MG	2A	3348	1/1	0.86	0.17	59,59,59,59	0
58	MG	1A	3864	1/1	0.86	0.13	52,52,52,52	0
58	MG	1A	4061	1/1	0.86	0.14	45,45,45,45	0
58	MG	2a	1806	1/1	0.86	0.25	61,61,61,61	0
58	MG	1A	4078	1/1	0.86	0.12	49,49,49,49	0
58	MG	2A	3613	1/1	0.86	0.18	65,65,65,65	0
58	MG	2A	3358	1/1	0.86	0.11	70,70,70,70	0
58	MG	2A	3029	1/1	0.86	0.20	77,77,77,77	0
58	MG	2A	3362	1/1	0.86	0.17	65,65,65,65	0
58	MG	2a	1829	1/1	0.86	0.21	72,72,72,72	0
58	MG	1A	3610	1/1	0.86	0.12	35,35,35,35	0
58	MG	2A	3649	1/1	0.86	0.14	70,70,70,70	0
58	MG	1A	3621	1/1	0.86	0.12	33,33,33,33	0
58	MG	1A	3502	1/1	0.86	0.13	45,45,45,45	0
58	MG	2n	101	1/1	0.86	0.29	72,72,72,72	0
58	MG	2A	3657	1/1	0.86	0.13	64,64,64,64	0
58	MG	1A	3531	1/1	0.86	0.21	50,50,50,50	0
58	MG	2A	3206	1/1	0.86	0.17	66,66,66,66	0
58	MG	2A	3389	1/1	0.86	0.11	68,68,68,68	0
58	MG	1B	203	1/1	0.86	0.22	49,49,49,49	0
58	MG	1A	3889	1/1	0.87	0.12	34,34,34,34	0
58	MG	2A	3607	1/1	0.87	0.11	31,31,31,31	0
58	MG	2A	3103	1/1	0.87	0.20	58,58,58,58	0
58	MG	2A	3387	1/1	0.87	0.14	57,57,57,57	0
58	MG	1a	1631	1/1	0.87	0.32	59,59,59,59	0
58	MG	2a	1707	1/1	0.87	0.29	69,69,69,69	0
58	MG	2A	3804	1/1	0.87	0.13	55,55,55,55	0
58	MG	1A	3435	1/1	0.87	0.11	59,59,59,59	0
58	MG	1a	1664	1/1	0.87	0.17	59,59,59,59	0
58	MG	2A	3412	1/1	0.87	0.18	54,54,54,54	0
58	MG	1A	4093	1/1	0.87	0.11	69,69,69,69	0
58	MG	1A	3791	1/1	0.87	0.10	31,31,31,31	0
58	MG	2A	3864	1/1	0.87	0.16	64,64,64,64	0
58	MG	1A	3525	1/1	0.87	0.11	52,52,52,52	0
58	MG	1A	3951	1/1	0.87	0.18	65,65,65,65	0
58	MG	2a	1744	1/1	0.87	0.24	65,65,65,65	0
58	MG	2A	3317	1/1	0.87	0.18	52,52,52,52	0
58	MG	1x	101	1/1	0.87	0.32	62,62,62,62	0
58	MG	2B	210	1/1	0.87	0.14	71,71,71,71	0
58	MG	1a	1690	1/1	0.87	0.23	63,63,63,63	0
58	MG	1A	3244	1/1	0.87	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3334	1/1	0.87	0.25	70,70,70,70	0
58	MG	1A	3646	1/1	0.87	0.11	35,35,35,35	0
58	MG	2D	306	1/1	0.87	0.24	53,53,53,53	0
58	MG	1A	3824	1/1	0.87	0.08	35,35,35,35	0
58	MG	2A	3686	1/1	0.87	0.12	45,45,45,45	0
58	MG	2A	3338	1/1	0.87	0.11	73,73,73,73	0
58	MG	1A	3335	1/1	0.87	0.20	64,64,64,64	0
58	MG	1A	3543	1/1	0.87	0.09	62,62,62,62	0
58	MG	1A	4043	1/1	0.87	0.12	45,45,45,45	0
58	MG	1O	204	1/1	0.87	0.14	71,71,71,71	0
58	MG	2A	3721	1/1	0.87	0.12	69,69,69,69	0
58	MG	2a	1817	1/1	0.87	0.22	73,73,73,73	0
58	MG	1A	3187	1/1	0.87	0.10	52,52,52,52	0
58	MG	2A	3067	1/1	0.87	0.23	58,58,58,58	0
58	MG	1A	4076	1/1	0.87	0.21	47,47,47,47	0
58	MG	2a	1623	1/1	0.87	0.10	59,59,59,59	0
58	MG	2A	3232	1/1	0.87	0.43	54,54,54,54	0
58	MG	2A	3572	1/1	0.87	0.19	55,55,55,55	0
58	MG	2a	1637	1/1	0.87	0.36	67,67,67,67	0
58	MG	1A	3261	1/1	0.87	0.14	52,52,52,52	0
58	MG	2A	3740	1/1	0.87	0.20	60,60,60,60	0
58	MG	2a	1650	1/1	0.87	0.10	57,57,57,57	0
58	MG	2A	3576	1/1	0.87	0.10	55,55,55,55	0
58	MG	2A	3376	1/1	0.87	0.12	61,61,61,61	0
58	MG	2x	106	1/1	0.87	0.11	59,59,59,59	0
58	MG	1A	3472	1/1	0.87	0.31	64,64,64,64	0
58	MG	2B	218	1/1	0.88	0.16	76,76,76,76	0
58	MG	2A	3594	1/1	0.88	0.09	35,35,35,35	0
58	MG	1a	1774	1/1	0.88	0.11	54,54,54,54	0
58	MG	2A	3601	1/1	0.88	0.22	71,71,71,71	0
58	MG	1A	3913	1/1	0.88	0.08	30,30,30,30	0
58	MG	1A	3457	1/1	0.88	0.19	61,61,61,61	0
58	MG	1A	3584	1/1	0.88	0.10	34,34,34,34	0
58	MG	1A	3486	1/1	0.88	0.11	46,46,46,46	0
58	MG	1a	1642	1/1	0.88	0.19	65,65,65,65	0
58	MG	1B	211	1/1	0.88	0.09	44,44,44,44	0
58	MG	2A	3185	1/1	0.88	0.23	63,63,63,63	0
58	MG	1A	3208	1/1	0.88	0.17	63,63,63,63	0
58	MG	1A	3839	1/1	0.88	0.27	65,65,65,65	0
58	MG	1x	102	1/1	0.88	0.23	65,65,65,65	0
58	MG	1A	3507	1/1	0.88	0.11	59,59,59,59	0
58	MG	2A	3370	1/1	0.88	0.33	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	3372	1/1	0.88	0.12	67,67,67,67	0
58	MG	1a	1684	1/1	0.88	0.10	62,62,62,62	0
58	MG	2A	3668	1/1	0.88	0.10	57,57,57,57	0
58	MG	2A	3198	1/1	0.88	0.26	64,64,64,64	0
58	MG	1A	3848	1/1	0.88	0.12	61,61,61,61	0
58	MG	2a	1642	1/1	0.88	0.24	69,69,69,69	0
58	MG	1A	3386	1/1	0.88	0.24	27,27,27,27	0
58	MG	2A	3676	1/1	0.88	0.16	59,59,59,59	0
58	MG	2a	1657	1/1	0.88	0.10	61,61,61,61	0
58	MG	2a	1663	1/1	0.88	0.15	84,84,84,84	0
58	MG	1a	1694	1/1	0.88	0.19	49,49,49,49	0
58	MG	2a	1677	1/1	0.88	0.22	63,63,63,63	0
58	MG	2A	3213	1/1	0.88	0.12	53,53,53,53	0
58	MG	2a	1682	1/1	0.88	0.11	75,75,75,75	0
58	MG	1E	311	1/1	0.88	0.08	29,29,29,29	0
58	MG	2A	3687	1/1	0.88	0.14	58,58,58,58	0
58	MG	2a	1701	1/1	0.88	0.17	73,73,73,73	0
58	MG	2A	3237	1/1	0.88	0.19	57,57,57,57	0
58	MG	2A	3395	1/1	0.88	0.11	65,65,65,65	0
58	MG	2A	3404	1/1	0.88	0.20	52,52,52,52	0
58	MG	2A	3243	1/1	0.88	0.14	60,60,60,60	0
58	MG	2a	1708	1/1	0.88	0.14	66,66,66,66	0
58	MG	2A	3247	1/1	0.88	0.12	64,64,64,64	0
58	MG	2A	3422	1/1	0.88	0.32	68,68,68,68	0
58	MG	1E	313	1/1	0.88	0.14	61,61,61,61	0
58	MG	1A	3167	1/1	0.88	0.10	38,38,38,38	0
58	MG	1A	3881	1/1	0.88	0.13	49,49,49,49	0
58	MG	2a	1728	1/1	0.88	0.15	61,61,61,61	0
58	MG	1A	3781	1/1	0.88	0.10	36,36,36,36	0
58	MG	2A	3733	1/1	0.88	0.12	77,77,77,77	0
58	MG	2A	3737	1/1	0.88	0.19	69,69,69,69	0
58	MG	2a	1737	1/1	0.88	0.09	66,66,66,66	0
58	MG	1A	3639	1/1	0.88	0.09	41,41,41,41	0
58	MG	1A	3367	1/1	0.88	0.15	47,47,47,47	0
58	MG	2a	1750	1/1	0.88	0.14	74,74,74,74	0
58	MG	2A	3280	1/1	0.88	0.19	67,67,67,67	0
58	MG	2A	3288	1/1	0.88	0.28	65,65,65,65	0
58	MG	1A	3897	1/1	0.88	0.10	35,35,35,35	0
58	MG	1Z	301	1/1	0.88	0.09	70,70,70,70	0
58	MG	2a	1761	1/1	0.88	0.21	65,65,65,65	0
58	MG	2A	3757	1/1	0.88	0.14	76,76,76,76	0
58	MG	2A	3295	1/1	0.88	0.09	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	1784	1/1	0.88	0.16	86,86,86,86	0
58	MG	2A	3297	1/1	0.88	0.16	60,60,60,60	0
58	MG	2A	3098	1/1	0.88	0.14	77,77,77,77	0
58	MG	2A	3775	1/1	0.88	0.10	62,62,62,62	0
58	MG	2a	1794	1/1	0.88	0.20	66,66,66,66	0
58	MG	2A	3776	1/1	0.88	0.12	62,62,62,62	0
58	MG	1a	1747	1/1	0.88	0.07	49,49,49,49	0
58	MG	2a	1801	1/1	0.88	0.19	60,60,60,60	0
58	MG	2a	1802	1/1	0.88	0.26	68,68,68,68	0
58	MG	2A	3783	1/1	0.88	0.11	69,69,69,69	0
58	MG	2A	3510	1/1	0.88	0.10	44,44,44,44	0
58	MG	2A	3522	1/1	0.88	0.10	43,43,43,43	0
58	MG	2A	3809	1/1	0.88	0.09	37,37,37,37	0
58	MG	2A	3304	1/1	0.88	0.12	69,69,69,69	0
58	MG	1Z	302	1/1	0.88	0.13	55,55,55,55	0
58	MG	2A	3846	1/1	0.88	0.11	69,69,69,69	0
58	MG	2A	3540	1/1	0.88	0.12	50,50,50,50	0
58	MG	2a	1825	1/1	0.88	0.30	68,68,68,68	0
58	MG	2a	1826	1/1	0.88	0.14	58,58,58,58	0
58	MG	2A	3852	1/1	0.88	0.14	68,68,68,68	0
58	MG	2A	3110	1/1	0.88	0.08	72,72,72,72	0
58	MG	2A	3860	1/1	0.88	0.22	70,70,70,70	0
58	MG	2A	3324	1/1	0.88	0.12	51,51,51,51	0
58	MG	2l	201	1/1	0.88	0.09	66,66,66,66	0
58	MG	10	105	1/1	0.88	0.13	66,66,66,66	0
58	MG	2A	3564	1/1	0.88	0.16	55,55,55,55	0
58	MG	1a	1761	1/1	0.88	0.11	62,62,62,62	0
58	MG	2A	3329	1/1	0.88	0.25	72,72,72,72	0
58	MG	1a	1602	1/1	0.88	0.32	62,62,62,62	0
58	MG	2A	3578	1/1	0.88	0.19	60,60,60,60	0
58	MG	2x	105	1/1	0.88	0.26	68,68,68,68	0
58	MG	2A	3127	1/1	0.88	0.12	68,68,68,68	0
58	MG	2A	3585	1/1	0.88	0.09	60,60,60,60	0
58	MG	1A	3131	1/1	0.89	0.10	42,42,42,42	0
58	MG	1A	4047	1/1	0.89	0.07	17,17,17,17	0
58	MG	20	102	1/1	0.89	0.26	69,69,69,69	0
58	MG	1a	1677	1/1	0.89	0.21	52,52,52,52	0
58	MG	2A	3090	1/1	0.89	0.15	49,49,49,49	0
58	MG	1A	3590	1/1	0.89	0.24	59,59,59,59	0
58	MG	2A	3092	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	3265	1/1	0.89	0.21	66,66,66,66	0
58	MG	2A	3636	1/1	0.89	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1610	1/1	0.89	0.12	59,59,59,59	0
58	MG	2a	1612	1/1	0.89	0.12	64,64,64,64	0
58	MG	2a	1621	1/1	0.89	0.25	69,69,69,69	0
58	MG	2A	3642	1/1	0.89	0.10	51,51,51,51	0
58	MG	1A	3817	1/1	0.89	0.09	52,52,52,52	0
58	MG	2a	1624	1/1	0.89	0.20	56,56,56,56	0
58	MG	2a	1627	1/1	0.89	0.19	66,66,66,66	0
58	MG	1A	3350	1/1	0.89	0.22	59,59,59,59	0
58	MG	1A	3601	1/1	0.89	0.10	47,47,47,47	0
58	MG	1A	3253	1/1	0.89	0.09	44,44,44,44	0
58	MG	1a	1695	1/1	0.89	0.26	60,60,60,60	0
58	MG	2A	3662	1/1	0.89	0.14	64,64,64,64	0
58	MG	1A	3840	1/1	0.89	0.10	47,47,47,47	0
58	MG	2a	1644	1/1	0.89	0.14	56,56,56,56	0
58	MG	1a	1701	1/1	0.89	0.17	54,54,54,54	0
58	MG	2a	1653	1/1	0.89	0.16	63,63,63,63	0
58	MG	1A	3372	1/1	0.89	0.27	50,50,50,50	0
58	MG	2A	3136	1/1	0.89	0.13	52,52,52,52	0
58	MG	2A	3146	1/1	0.89	0.21	66,66,66,66	0
58	MG	2a	1665	1/1	0.89	0.13	63,63,63,63	0
58	MG	1A	3254	1/1	0.89	0.16	62,62,62,62	0
58	MG	1A	3480	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3374	1/1	0.89	0.11	59,59,59,59	0
58	MG	1A	3866	1/1	0.89	0.14	52,52,52,52	0
58	MG	1A	3870	1/1	0.89	0.08	38,38,38,38	0
58	MG	1A	3306	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3689	1/1	0.89	0.17	63,63,63,63	0
58	MG	1A	3496	1/1	0.89	0.12	53,53,53,53	0
58	MG	1A	3651	1/1	0.89	0.13	55,55,55,55	0
58	MG	1B	235	1/1	0.89	0.11	61,61,61,61	0
58	MG	1a	1754	1/1	0.89	0.12	76,76,76,76	0
58	MG	1E	302	1/1	0.89	0.14	36,36,36,36	0
58	MG	2A	3707	1/1	0.89	0.14	65,65,65,65	0
58	MG	2A	3716	1/1	0.89	0.12	60,60,60,60	0
58	MG	1A	3888	1/1	0.89	0.10	23,23,23,23	0
58	MG	1A	3321	1/1	0.89	0.13	47,47,47,47	0
58	MG	1A	3394	1/1	0.89	0.18	75,75,75,75	0
58	MG	1a	1773	1/1	0.89	0.10	37,37,37,37	0
58	MG	1A	3518	1/1	0.89	0.09	82,82,82,82	0
58	MG	2A	3423	1/1	0.89	0.23	52,52,52,52	0
58	MG	2A	3425	1/1	0.89	0.18	58,58,58,58	0
58	MG	1G	205	1/1	0.89	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3433	1/1	0.89	0.21	56,56,56,56	0
58	MG	1a	1793	1/1	0.89	0.10	60,60,60,60	0
58	MG	1a	1795	1/1	0.89	0.24	69,69,69,69	0
58	MG	2A	3441	1/1	0.89	0.22	51,51,51,51	0
58	MG	2A	3216	1/1	0.89	0.29	73,73,73,73	0
58	MG	2A	3224	1/1	0.89	0.18	57,57,57,57	0
58	MG	1A	3905	1/1	0.89	0.09	51,51,51,51	0
58	MG	2a	1760	1/1	0.89	0.19	73,73,73,73	0
58	MG	2A	3470	1/1	0.89	0.11	53,53,53,53	0
58	MG	2A	3236	1/1	0.89	0.18	67,67,67,67	0
58	MG	2a	1772	1/1	0.89	0.09	85,85,85,85	0
58	MG	2a	1776	1/1	0.89	0.12	70,70,70,70	0
58	MG	1A	3405	1/1	0.89	0.18	43,43,43,43	0
58	MG	1A	3414	1/1	0.89	0.10	57,57,57,57	0
58	MG	1A	3934	1/1	0.89	0.14	51,51,51,51	0
58	MG	1t	201	1/1	0.89	0.18	57,57,57,57	0
58	MG	2A	3501	1/1	0.89	0.11	46,46,46,46	0
58	MG	2A	3260	1/1	0.89	0.16	56,56,56,56	0
58	MG	1A	3429	1/1	0.89	0.12	46,46,46,46	0
58	MG	1A	3539	1/1	0.89	0.12	59,59,59,59	0
58	MG	2A	3827	1/1	0.89	0.12	68,68,68,68	0
58	MG	1A	3783	1/1	0.89	0.14	54,54,54,54	0
58	MG	2A	3837	1/1	0.89	0.09	51,51,51,51	0
58	MG	2A	3841	1/1	0.89	0.12	54,54,54,54	0
58	MG	1a	1601	1/1	0.89	0.13	61,61,61,61	0
58	MG	1A	3785	1/1	0.89	0.10	62,62,62,62	0
58	MG	1a	1618	1/1	0.89	0.23	55,55,55,55	0
58	MG	2A	3853	1/1	0.89	0.11	51,51,51,51	0
58	MG	2A	3856	1/1	0.89	0.14	73,73,73,73	0
58	MG	1A	3958	1/1	0.89	0.08	23,23,23,23	0
58	MG	2A	3290	1/1	0.89	0.14	55,55,55,55	0
58	MG	1A	3202	1/1	0.89	0.09	47,47,47,47	0
58	MG	1A	3985	1/1	0.89	0.07	24,24,24,24	0
58	MG	2A	3563	1/1	0.89	0.09	40,40,40,40	0
58	MG	1a	1635	1/1	0.89	0.10	50,50,50,50	0
58	MG	1A	3798	1/1	0.89	0.09	20,20,20,20	0
58	MG	1a	1637	1/1	0.89	0.23	55,55,55,55	0
58	MG	2A	3574	1/1	0.89	0.16	60,60,60,60	0
58	MG	2A	3055	1/1	0.89	0.09	63,63,63,63	0
58	MG	2A	3058	1/1	0.89	0.21	58,58,58,58	0
58	MG	2v	101	1/1	0.89	0.13	63,63,63,63	0
58	MG	2v	102	1/1	0.89	0.18	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	2v	103	1/1	0.89	0.48	72,72,72,72	0
58	MG	2v	104	1/1	0.89	0.17	67,67,67,67	0
58	MG	2A	3309	1/1	0.89	0.26	56,56,56,56	0
58	MG	2A	3063	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3799	1/1	0.89	0.10	39,39,39,39	0
58	MG	2A	3598	1/1	0.89	0.15	57,57,57,57	0
58	MG	2A	3321	1/1	0.89	0.21	61,61,61,61	0
58	MG	2A	3066	1/1	0.89	0.15	52,52,52,52	0
58	MG	1A	3592	1/1	0.90	0.20	63,63,63,63	0
58	MG	1A	3059	1/1	0.90	0.10	36,36,36,36	0
58	MG	1a	1608	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3369	1/1	0.90	0.24	53,53,53,53	0
58	MG	2A	3042	1/1	0.90	0.24	61,61,61,61	0
58	MG	2E	303	1/1	0.90	0.08	47,47,47,47	0
58	MG	1A	3971	1/1	0.90	0.11	58,58,58,58	0
58	MG	2A	3046	1/1	0.90	0.14	59,59,59,59	0
58	MG	2O	201	1/1	0.90	0.17	71,71,71,71	0
58	MG	2A	3580	1/1	0.90	0.12	49,49,49,49	0
58	MG	1A	3974	1/1	0.90	0.11	71,71,71,71	0
58	MG	2A	3301	1/1	0.90	0.14	60,60,60,60	0
58	MG	1A	3212	1/1	0.90	0.07	50,50,50,50	0
58	MG	2A	3303	1/1	0.90	0.08	63,63,63,63	0
58	MG	1A	3811	1/1	0.90	0.09	36,36,36,36	0
58	MG	1A	3995	1/1	0.90	0.09	25,25,25,25	0
58	MG	2A	3310	1/1	0.90	0.11	58,58,58,58	0
58	MG	1A	3815	1/1	0.90	0.18	58,58,58,58	0
58	MG	1a	1639	1/1	0.90	0.17	53,53,53,53	0
58	MG	2a	1611	1/1	0.90	0.18	66,66,66,66	0
58	MG	2A	3320	1/1	0.90	0.15	69,69,69,69	0
58	MG	2a	1616	1/1	0.90	0.12	65,65,65,65	0
58	MG	2a	1618	1/1	0.90	0.11	52,52,52,52	0
58	MG	1A	4020	1/1	0.90	0.11	53,53,53,53	0
58	MG	1a	1659	1/1	0.90	0.13	65,65,65,65	0
58	MG	1A	4027	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3083	1/1	0.90	0.15	65,65,65,65	0
58	MG	2a	1625	1/1	0.90	0.12	64,64,64,64	0
58	MG	2A	3641	1/1	0.90	0.09	42,42,42,42	0
58	MG	1A	4030	1/1	0.90	0.10	63,63,63,63	0
58	MG	2a	1631	1/1	0.90	0.25	64,64,64,64	0
58	MG	2a	1632	1/1	0.90	0.08	74,74,74,74	0
58	MG	1a	1672	1/1	0.90	0.16	59,59,59,59	0
58	MG	1A	4034	1/1	0.90	0.13	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	3375	1/1	0.90	0.11	39,39,39,39	0
58	MG	2a	1639	1/1	0.90	0.14	55,55,55,55	0
58	MG	1a	1681	1/1	0.90	0.12	48,48,48,48	0
58	MG	1A	3820	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3344	1/1	0.90	0.18	72,72,72,72	0
58	MG	2a	1649	1/1	0.90	0.09	73,73,73,73	0
58	MG	1A	3380	1/1	0.90	0.10	45,45,45,45	0
58	MG	2A	3666	1/1	0.90	0.12	51,51,51,51	0
58	MG	1A	4068	1/1	0.90	0.08	44,44,44,44	0
58	MG	1A	3259	1/1	0.90	0.21	72,72,72,72	0
58	MG	2a	1658	1/1	0.90	0.10	62,62,62,62	0
58	MG	1A	3638	1/1	0.90	0.09	45,45,45,45	0
58	MG	2A	3114	1/1	0.90	0.20	63,63,63,63	0
58	MG	2a	1666	1/1	0.90	0.16	69,69,69,69	0
58	MG	1A	3292	1/1	0.90	0.23	56,56,56,56	0
58	MG	2A	3675	1/1	0.90	0.19	67,67,67,67	0
58	MG	2a	1680	1/1	0.90	0.26	59,59,59,59	0
58	MG	1A	3481	1/1	0.90	0.11	42,42,42,42	0
58	MG	2A	3363	1/1	0.90	0.24	63,63,63,63	0
58	MG	1A	3332	1/1	0.90	0.31	68,68,68,68	0
58	MG	2a	1687	1/1	0.90	0.19	67,67,67,67	0
58	MG	2A	3680	1/1	0.90	0.12	51,51,51,51	0
58	MG	2A	3684	1/1	0.90	0.09	57,57,57,57	0
58	MG	2A	3128	1/1	0.90	0.16	51,51,51,51	0
58	MG	2A	3368	1/1	0.90	0.19	61,61,61,61	0
58	MG	1A	3391	1/1	0.90	0.10	64,64,64,64	0
58	MG	2A	3371	1/1	0.90	0.24	63,63,63,63	0
58	MG	2A	3696	1/1	0.90	0.14	48,48,48,48	0
58	MG	2a	1711	1/1	0.90	0.08	71,71,71,71	0
58	MG	2A	3140	1/1	0.90	0.28	65,65,65,65	0
58	MG	1a	1718	1/1	0.90	0.30	66,66,66,66	0
58	MG	2a	1716	1/1	0.90	0.13	64,64,64,64	0
58	MG	1A	3661	1/1	0.90	0.07	25,25,25,25	0
58	MG	1A	3868	1/1	0.90	0.14	42,42,42,42	0
58	MG	2a	1724	1/1	0.90	0.14	76,76,76,76	0
58	MG	1B	208	1/1	0.90	0.11	63,63,63,63	0
58	MG	2A	3710	1/1	0.90	0.13	61,61,61,61	0
58	MG	2a	1731	1/1	0.90	0.24	47,47,47,47	0
58	MG	1B	210	1/1	0.90	0.10	50,50,50,50	0
58	MG	2A	3719	1/1	0.90	0.16	67,67,67,67	0
58	MG	2A	3386	1/1	0.90	0.09	52,52,52,52	0
58	MG	2A	3168	1/1	0.90	0.13	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	1740	1/1	0.90	0.23	52,52,52,52	0
58	MG	2A	3726	1/1	0.90	0.10	49,49,49,49	0
58	MG	1A	3680	1/1	0.90	0.08	43,43,43,43	0
58	MG	2a	1749	1/1	0.90	0.13	71,71,71,71	0
58	MG	1A	3877	1/1	0.90	0.14	28,28,28,28	0
58	MG	1A	3023	1/1	0.90	0.26	51,51,51,51	0
58	MG	2A	3179	1/1	0.90	0.16	68,68,68,68	0
58	MG	2A	3401	1/1	0.90	0.29	58,58,58,58	0
58	MG	1B	225	1/1	0.90	0.09	57,57,57,57	0
58	MG	2A	3187	1/1	0.90	0.19	60,60,60,60	0
58	MG	2A	3190	1/1	0.90	0.33	69,69,69,69	0
58	MG	1A	3403	1/1	0.90	0.14	52,52,52,52	0
58	MG	2A	3745	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3692	1/1	0.90	0.08	13,13,13,13	0
58	MG	1A	3404	1/1	0.90	0.13	51,51,51,51	0
58	MG	1A	3715	1/1	0.90	0.16	64,64,64,64	0
58	MG	1D	312	1/1	0.90	0.16	40,40,40,40	0
58	MG	1A	3891	1/1	0.90	0.08	29,29,29,29	0
58	MG	1A	3338	1/1	0.90	0.11	42,42,42,42	0
58	MG	2a	1790	1/1	0.90	0.11	59,59,59,59	0
58	MG	2a	1792	1/1	0.90	0.13	62,62,62,62	0
58	MG	1A	3894	1/1	0.90	0.08	37,37,37,37	0
58	MG	2a	1795	1/1	0.90	0.22	63,63,63,63	0
58	MG	1a	1788	1/1	0.90	0.10	70,70,70,70	0
58	MG	2A	3779	1/1	0.90	0.15	64,64,64,64	0
58	MG	2A	3447	1/1	0.90	0.16	65,65,65,65	0
58	MG	1a	1791	1/1	0.90	0.09	75,75,75,75	0
58	MG	2A	3454	1/1	0.90	0.10	65,65,65,65	0
58	MG	2A	3801	1/1	0.90	0.09	80,80,80,80	0
58	MG	1A	3407	1/1	0.90	0.15	46,46,46,46	0
58	MG	2A	3469	1/1	0.90	0.24	65,65,65,65	0
58	MG	2A	3812	1/1	0.90	0.09	53,53,53,53	0
58	MG	2A	3218	1/1	0.90	0.24	59,59,59,59	0
58	MG	2A	3826	1/1	0.90	0.22	69,69,69,69	0
58	MG	1A	3757	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	3348	1/1	0.90	0.14	50,50,50,50	0
58	MG	1A	3418	1/1	0.90	0.14	65,65,65,65	0
58	MG	2A	3484	1/1	0.90	0.14	66,66,66,66	0
58	MG	2A	3845	1/1	0.90	0.10	67,67,67,67	0
58	MG	2e	201	1/1	0.90	0.09	73,73,73,73	0
58	MG	1A	3927	1/1	0.90	0.15	47,47,47,47	0
58	MG	2A	3848	1/1	0.90	0.15	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	3238	1/1	0.90	0.14	64,64,64,64	0
58	MG	2A	3241	1/1	0.90	0.10	48,48,48,48	0
58	MG	1A	3299	1/1	0.90	0.07	26,26,26,26	0
58	MG	1d	301	1/1	0.90	0.34	62,62,62,62	0
58	MG	2A	3253	1/1	0.90	0.21	73,73,73,73	0
58	MG	2A	3254	1/1	0.90	0.11	62,62,62,62	0
58	MG	1A	3939	1/1	0.90	0.10	26,26,26,26	0
58	MG	1Y	203	1/1	0.90	0.31	49,49,49,49	0
58	MG	1A	3544	1/1	0.90	0.08	62,62,62,62	0
58	MG	1A	3357	1/1	0.90	0.08	55,55,55,55	0
58	MG	1A	3448	1/1	0.90	0.13	61,61,61,61	0
58	MG	2A	3542	1/1	0.90	0.12	38,38,38,38	0
58	MG	1x	104	1/1	0.90	0.23	57,57,57,57	0
58	MG	14	101	1/1	0.90	0.17	69,69,69,69	0
58	MG	2B	209	1/1	0.91	0.10	67,67,67,67	0
58	MG	2A	3007	1/1	0.91	0.21	63,63,63,63	0
58	MG	1A	3393	1/1	0.91	0.25	69,69,69,69	0
58	MG	1A	3760	1/1	0.91	0.08	16,16,16,16	0
58	MG	1A	3887	1/1	0.91	0.07	39,39,39,39	0
58	MG	2B	219	1/1	0.91	0.19	77,77,77,77	0
58	MG	2A	3551	1/1	0.91	0.16	40,40,40,40	0
58	MG	2A	3035	1/1	0.91	0.06	31,31,31,31	0
58	MG	2A	3036	1/1	0.91	0.15	53,53,53,53	0
58	MG	2A	3287	1/1	0.91	0.09	56,56,56,56	0
58	MG	2E	307	1/1	0.91	0.18	63,63,63,63	0
58	MG	2F	303	1/1	0.91	0.07	40,40,40,40	0
58	MG	2F	304	1/1	0.91	0.13	66,66,66,66	0
58	MG	2A	3038	1/1	0.91	0.13	35,35,35,35	0
58	MG	2A	3568	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3571	1/1	0.91	0.09	45,45,45,45	0
58	MG	2A	3039	1/1	0.91	0.21	58,58,58,58	0
58	MG	1A	3768	1/1	0.91	0.09	27,27,27,27	0
58	MG	2R	202	1/1	0.91	0.14	62,62,62,62	0
58	MG	2T	3501	1/1	0.91	0.24	65,65,65,65	0
58	MG	2W	201	1/1	0.91	0.18	60,60,60,60	0
58	MG	1A	3051	1/1	0.91	0.11	34,34,34,34	0
58	MG	2A	3045	1/1	0.91	0.08	75,75,75,75	0
58	MG	1a	1646	1/1	0.91	0.15	68,68,68,68	0
58	MG	27	103	1/1	0.91	0.08	44,44,44,44	0
58	MG	2A	3047	1/1	0.91	0.17	72,72,72,72	0
58	MG	1a	1651	1/1	0.91	0.12	46,46,46,46	0
58	MG	2a	1602	1/1	0.91	0.23	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	2a	1606	1/1	0.91	0.22	67,67,67,67	0
58	MG	1a	1656	1/1	0.91	0.13	62,62,62,62	0
58	MG	1A	3401	1/1	0.91	0.12	47,47,47,47	0
58	MG	2A	3596	1/1	0.91	0.10	58,58,58,58	0
58	MG	1a	1661	1/1	0.91	0.17	56,56,56,56	0
58	MG	2A	3599	1/1	0.91	0.12	60,60,60,60	0
58	MG	2A	3307	1/1	0.91	0.16	65,65,65,65	0
58	MG	2A	3308	1/1	0.91	0.13	57,57,57,57	0
58	MG	1A	3892	1/1	0.91	0.12	22,22,22,22	0
58	MG	1A	3288	1/1	0.91	0.12	57,57,57,57	0
58	MG	1A	3370	1/1	0.91	0.09	42,42,42,42	0
58	MG	2A	3316	1/1	0.91	0.09	49,49,49,49	0
58	MG	1a	1676	1/1	0.91	0.13	55,55,55,55	0
58	MG	2A	3624	1/1	0.91	0.11	55,55,55,55	0
58	MG	2a	1628	1/1	0.91	0.10	62,62,62,62	0
58	MG	2A	3632	1/1	0.91	0.13	54,54,54,54	0
58	MG	2A	3319	1/1	0.91	0.10	62,62,62,62	0
58	MG	1A	3477	1/1	0.91	0.11	42,42,42,42	0
58	MG	1A	3151	1/1	0.91	0.21	29,29,29,29	0
58	MG	1A	3052	1/1	0.91	0.09	46,46,46,46	0
58	MG	1A	3002	1/1	0.91	0.07	47,47,47,47	0
58	MG	1B	224	1/1	0.91	0.10	50,50,50,50	0
58	MG	1A	3488	1/1	0.91	0.10	40,40,40,40	0
58	MG	2A	3651	1/1	0.91	0.16	66,66,66,66	0
58	MG	2A	3331	1/1	0.91	0.12	59,59,59,59	0
58	MG	2a	1647	1/1	0.91	0.14	61,61,61,61	0
58	MG	1a	1688	1/1	0.91	0.14	51,51,51,51	0
58	MG	1A	3344	1/1	0.91	0.08	38,38,38,38	0
58	MG	2A	3660	1/1	0.91	0.09	66,66,66,66	0
58	MG	2A	3100	1/1	0.91	0.24	44,44,44,44	0
58	MG	2a	1656	1/1	0.91	0.14	85,85,85,85	0
58	MG	2A	3663	1/1	0.91	0.18	56,56,56,56	0
58	MG	2A	3102	1/1	0.91	0.25	67,67,67,67	0
58	MG	2a	1659	1/1	0.91	0.19	60,60,60,60	0
58	MG	2a	1660	1/1	0.91	0.20	78,78,78,78	0
58	MG	1A	3420	1/1	0.91	0.08	40,40,40,40	0
58	MG	1A	3945	1/1	0.91	0.11	58,58,58,58	0
58	MG	2A	3107	1/1	0.91	0.17	55,55,55,55	0
58	MG	2a	1672	1/1	0.91	0.11	56,56,56,56	0
58	MG	2A	3349	1/1	0.91	0.21	61,61,61,61	0
58	MG	1a	1696	1/1	0.91	0.27	59,59,59,59	0
58	MG	2a	1679	1/1	0.91	0.20	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3650	1/1	0.91	0.09	60,60,60,60	0
58	MG	2A	3673	1/1	0.91	0.08	64,64,64,64	0
58	MG	2A	3356	1/1	0.91	0.30	48,48,48,48	0
58	MG	1A	3506	1/1	0.91	0.14	57,57,57,57	0
58	MG	1a	1705	1/1	0.91	0.24	63,63,63,63	0
58	MG	2A	3124	1/1	0.91	0.26	66,66,66,66	0
58	MG	1a	1706	1/1	0.91	0.24	55,55,55,55	0
58	MG	1A	3653	1/1	0.91	0.09	40,40,40,40	0
58	MG	2A	3685	1/1	0.91	0.19	65,65,65,65	0
58	MG	1a	1717	1/1	0.91	0.09	60,60,60,60	0
58	MG	1E	307	1/1	0.91	0.30	59,59,59,59	0
58	MG	1A	3427	1/1	0.91	0.08	56,56,56,56	0
58	MG	1A	3428	1/1	0.91	0.07	53,53,53,53	0
58	MG	2a	1713	1/1	0.91	0.13	55,55,55,55	0
58	MG	2A	3692	1/1	0.91	0.09	67,67,67,67	0
58	MG	1A	3837	1/1	0.91	0.10	52,52,52,52	0
58	MG	1F	313	1/1	0.91	0.15	50,50,50,50	0
58	MG	1A	3838	1/1	0.91	0.17	61,61,61,61	0
58	MG	2a	1718	1/1	0.91	0.13	74,74,74,74	0
58	MG	1A	3061	1/1	0.91	0.21	43,43,43,43	0
58	MG	2A	3377	1/1	0.91	0.15	58,58,58,58	0
58	MG	1A	3977	1/1	0.91	0.08	67,67,67,67	0
58	MG	1A	3978	1/1	0.91	0.09	57,57,57,57	0
58	MG	2a	1729	1/1	0.91	0.17	61,61,61,61	0
58	MG	1S	201	1/1	0.91	0.25	41,41,41,41	0
58	MG	1A	3312	1/1	0.91	0.06	34,34,34,34	0
58	MG	2A	3178	1/1	0.91	0.11	44,44,44,44	0
58	MG	1a	1757	1/1	0.91	0.18	51,51,51,51	0
58	MG	1W	201	1/1	0.91	0.15	49,49,49,49	0
58	MG	1A	3440	1/1	0.91	0.18	46,46,46,46	0
58	MG	2A	3394	1/1	0.91	0.09	60,60,60,60	0
58	MG	1Y	202	1/1	0.91	0.15	66,66,66,66	0
58	MG	2A	3732	1/1	0.91	0.10	58,58,58,58	0
58	MG	1a	1772	1/1	0.91	0.10	66,66,66,66	0
58	MG	2A	3734	1/1	0.91	0.12	53,53,53,53	0
58	MG	2A	3735	1/1	0.91	0.12	54,54,54,54	0
58	MG	1A	3446	1/1	0.91	0.12	52,52,52,52	0
58	MG	2A	3407	1/1	0.91	0.15	41,41,41,41	0
58	MG	1A	4016	1/1	0.91	0.10	58,58,58,58	0
58	MG	2A	3417	1/1	0.91	0.19	49,49,49,49	0
58	MG	1A	3855	1/1	0.91	0.12	55,55,55,55	0
58	MG	2a	1768	1/1	0.91	0.08	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	3420	1/1	0.91	0.25	64,64,64,64	0
58	MG	1A	3860	1/1	0.91	0.41	40,40,40,40	0
58	MG	2a	1778	1/1	0.91	0.11	52,52,52,52	0
58	MG	13	101	1/1	0.91	0.12	54,54,54,54	0
58	MG	2A	3756	1/1	0.91	0.10	63,63,63,63	0
58	MG	2A	3200	1/1	0.91	0.10	47,47,47,47	0
58	MG	2A	3428	1/1	0.91	0.20	62,62,62,62	0
58	MG	2A	3431	1/1	0.91	0.20	57,57,57,57	0
58	MG	2A	3204	1/1	0.91	0.12	58,58,58,58	0
58	MG	13	103	1/1	0.91	0.10	44,44,44,44	0
58	MG	1A	3862	1/1	0.91	0.11	52,52,52,52	0
58	MG	1A	3095	1/1	0.91	0.09	66,66,66,66	0
58	MG	1A	3728	1/1	0.91	0.16	56,56,56,56	0
58	MG	2A	3214	1/1	0.91	0.09	64,64,64,64	0
58	MG	2A	3786	1/1	0.91	0.10	55,55,55,55	0
58	MG	1a	1603	1/1	0.91	0.15	64,64,64,64	0
58	MG	2A	3794	1/1	0.91	0.21	67,67,67,67	0
58	MG	1a	1607	1/1	0.91	0.14	56,56,56,56	0
58	MG	2a	1811	1/1	0.91	0.07	70,70,70,70	0
58	MG	2A	3802	1/1	0.91	0.11	52,52,52,52	0
58	MG	1A	3743	1/1	0.91	0.09	19,19,19,19	0
58	MG	2A	3225	1/1	0.91	0.23	55,55,55,55	0
58	MG	2A	3460	1/1	0.91	0.10	71,71,71,71	0
58	MG	2A	3465	1/1	0.91	0.18	59,59,59,59	0
58	MG	2a	1819	1/1	0.91	0.17	55,55,55,55	0
58	MG	1a	1611	1/1	0.91	0.21	63,63,63,63	0
58	MG	1a	1613	1/1	0.91	0.13	61,61,61,61	0
58	MG	2A	3830	1/1	0.91	0.09	49,49,49,49	0
58	MG	1w	102	1/1	0.91	0.09	67,67,67,67	0
58	MG	2A	3481	1/1	0.91	0.23	54,54,54,54	0
58	MG	2A	3840	1/1	0.91	0.08	66,66,66,66	0
58	MG	2g	201	1/1	0.91	0.06	71,71,71,71	0
58	MG	2i	201	1/1	0.91	0.14	71,71,71,71	0
58	MG	1a	1615	1/1	0.91	0.11	60,60,60,60	0
58	MG	1a	1616	1/1	0.91	0.13	66,66,66,66	0
58	MG	1A	3456	1/1	0.91	0.07	45,45,45,45	0
58	MG	2A	3244	1/1	0.91	0.13	60,60,60,60	0
58	MG	2l	203	1/1	0.91	0.09	62,62,62,62	0
58	MG	1A	3751	1/1	0.91	0.11	35,35,35,35	0
58	MG	2A	3248	1/1	0.91	0.08	53,53,53,53	0
58	MG	2A	3250	1/1	0.91	0.10	50,50,50,50	0
58	MG	2A	3505	1/1	0.91	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4067	1/1	0.91	0.12	55,55,55,55	0
58	MG	1x	106	1/1	0.91	0.20	56,56,56,56	0
58	MG	1A	3392	1/1	0.91	0.17	51,51,51,51	0
58	MG	2A	3513	1/1	0.91	0.14	56,56,56,56	0
58	MG	2A	3514	1/1	0.91	0.11	46,46,46,46	0
58	MG	2A	3519	1/1	0.91	0.13	51,51,51,51	0
58	MG	2A	3258	1/1	0.91	0.15	57,57,57,57	0
58	MG	2A	3005	1/1	0.91	0.24	58,58,58,58	0
58	MG	2F	302	1/1	0.92	0.08	58,58,58,58	0
58	MG	1A	4056	1/1	0.92	0.12	46,46,46,46	0
58	MG	1A	3331	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3450	1/1	0.92	0.10	56,56,56,56	0
58	MG	1a	1658	1/1	0.92	0.24	65,65,65,65	0
58	MG	2A	3314	1/1	0.92	0.07	49,49,49,49	0
58	MG	2A	3586	1/1	0.92	0.14	52,52,52,52	0
58	MG	2A	3588	1/1	0.92	0.08	47,47,47,47	0
58	MG	2A	3589	1/1	0.92	0.10	64,64,64,64	0
58	MG	1A	3714	1/1	0.92	0.07	63,63,63,63	0
58	MG	2U	201	1/1	0.92	0.28	50,50,50,50	0
58	MG	1A	4071	1/1	0.92	0.10	44,44,44,44	0
58	MG	1A	3266	1/1	0.92	0.28	52,52,52,52	0
58	MG	1a	1667	1/1	0.92	0.14	48,48,48,48	0
58	MG	1A	3867	1/1	0.92	0.07	39,39,39,39	0
58	MG	25	105	1/1	0.92	0.09	48,48,48,48	0
58	MG	2A	3322	1/1	0.92	0.23	55,55,55,55	0
58	MG	2A	3081	1/1	0.92	0.26	55,55,55,55	0
58	MG	1A	3720	1/1	0.92	0.22	58,58,58,58	0
58	MG	1A	3180	1/1	0.92	0.16	52,52,52,52	0
58	MG	2a	1603	1/1	0.92	0.08	68,68,68,68	0
58	MG	2A	3328	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3546	1/1	0.92	0.38	40,40,40,40	0
58	MG	1A	3555	1/1	0.92	0.21	49,49,49,49	0
58	MG	2a	1609	1/1	0.92	0.17	73,73,73,73	0
58	MG	2A	3625	1/1	0.92	0.19	62,62,62,62	0
58	MG	1A	3569	1/1	0.92	0.14	48,48,48,48	0
58	MG	2A	3333	1/1	0.92	0.12	55,55,55,55	0
58	MG	1A	4097	1/1	0.92	0.17	47,47,47,47	0
58	MG	1A	3283	1/1	0.92	0.25	45,45,45,45	0
58	MG	2A	3638	1/1	0.92	0.12	57,57,57,57	0
58	MG	1A	3460	1/1	0.92	0.12	59,59,59,59	0
58	MG	1A	3758	1/1	0.92	0.14	47,47,47,47	0
58	MG	2A	3643	1/1	0.92	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	3185	1/1	0.92	0.07	37,37,37,37	0
58	MG	2A	3345	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3347	1/1	0.92	0.14	61,61,61,61	0
58	MG	2A	3652	1/1	0.92	0.10	75,75,75,75	0
58	MG	1a	1693	1/1	0.92	0.21	55,55,55,55	0
58	MG	1A	3593	1/1	0.92	0.17	48,48,48,48	0
58	MG	1A	3769	1/1	0.92	0.11	36,36,36,36	0
58	MG	2A	3353	1/1	0.92	0.11	61,61,61,61	0
58	MG	1B	223	1/1	0.92	0.16	51,51,51,51	0
58	MG	1A	3114	1/1	0.92	0.06	37,37,37,37	0
58	MG	2a	1640	1/1	0.92	0.15	76,76,76,76	0
58	MG	1a	1699	1/1	0.92	0.10	58,58,58,58	0
58	MG	1A	3776	1/1	0.92	0.08	33,33,33,33	0
58	MG	1A	3895	1/1	0.92	0.17	37,37,37,37	0
58	MG	2A	3361	1/1	0.92	0.14	63,63,63,63	0
58	MG	1A	3777	1/1	0.92	0.07	60,60,60,60	0
58	MG	1a	1713	1/1	0.92	0.23	64,64,64,64	0
58	MG	2A	3129	1/1	0.92	0.10	67,67,67,67	0
58	MG	2A	3132	1/1	0.92	0.08	55,55,55,55	0
58	MG	1B	231	1/1	0.92	0.08	61,61,61,61	0
58	MG	1A	3596	1/1	0.92	0.17	55,55,55,55	0
58	MG	2A	3142	1/1	0.92	0.13	52,52,52,52	0
58	MG	1A	3907	1/1	0.92	0.07	46,46,46,46	0
58	MG	1a	1726	1/1	0.92	0.09	44,44,44,44	0
58	MG	2A	3683	1/1	0.92	0.09	67,67,67,67	0
58	MG	2A	3375	1/1	0.92	0.21	66,66,66,66	0
58	MG	1A	3129	1/1	0.92	0.07	56,56,56,56	0
58	MG	1A	3354	1/1	0.92	0.16	53,53,53,53	0
58	MG	1A	3475	1/1	0.92	0.13	42,42,42,42	0
58	MG	1A	3355	1/1	0.92	0.10	63,63,63,63	0
58	MG	2a	1678	1/1	0.92	0.17	62,62,62,62	0
58	MG	2A	3170	1/1	0.92	0.12	59,59,59,59	0
58	MG	2A	3691	1/1	0.92	0.07	66,66,66,66	0
58	MG	1A	3479	1/1	0.92	0.29	54,54,54,54	0
58	MG	1A	3940	1/1	0.92	0.09	22,22,22,22	0
58	MG	1a	1742	1/1	0.92	0.09	70,70,70,70	0
58	MG	2A	3702	1/1	0.92	0.11	45,45,45,45	0
58	MG	2a	1693	1/1	0.92	0.20	70,70,70,70	0
58	MG	2a	1698	1/1	0.92	0.30	58,58,58,58	0
58	MG	1A	3942	1/1	0.92	0.14	66,66,66,66	0
58	MG	1A	3072	1/1	0.92	0.06	15,15,15,15	0
58	MG	2A	3393	1/1	0.92	0.12	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	3411	1/1	0.92	0.12	47,47,47,47	0
58	MG	2A	3709	1/1	0.92	0.14	51,51,51,51	0
58	MG	1A	3640	1/1	0.92	0.11	57,57,57,57	0
58	MG	1A	3641	1/1	0.92	0.06	22,22,22,22	0
58	MG	2a	1709	1/1	0.92	0.07	73,73,73,73	0
58	MG	2a	1710	1/1	0.92	0.12	75,75,75,75	0
58	MG	1A	3813	1/1	0.92	0.07	45,45,45,45	0
58	MG	1S	202	1/1	0.92	0.12	46,46,46,46	0
58	MG	1a	1762	1/1	0.92	0.12	61,61,61,61	0
58	MG	2A	3725	1/1	0.92	0.16	53,53,53,53	0
58	MG	2A	3415	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3416	1/1	0.92	0.25	59,59,59,59	0
58	MG	2A	3194	1/1	0.92	0.11	55,55,55,55	0
58	MG	2a	1719	1/1	0.92	0.18	63,63,63,63	0
58	MG	1a	1767	1/1	0.92	0.10	55,55,55,55	0
58	MG	2a	1722	1/1	0.92	0.18	64,64,64,64	0
58	MG	2a	1723	1/1	0.92	0.16	64,64,64,64	0
58	MG	2A	3196	1/1	0.92	0.23	65,65,65,65	0
58	MG	1A	3814	1/1	0.92	0.18	48,48,48,48	0
58	MG	1A	3305	1/1	0.92	0.22	53,53,53,53	0
58	MG	1A	3964	1/1	0.92	0.10	30,30,30,30	0
58	MG	1A	3087	1/1	0.92	0.22	36,36,36,36	0
58	MG	2A	3429	1/1	0.92	0.14	39,39,39,39	0
58	MG	2A	3430	1/1	0.92	0.27	60,60,60,60	0
58	MG	1A	3310	1/1	0.92	0.08	49,49,49,49	0
58	MG	1a	1780	1/1	0.92	0.12	47,47,47,47	0
58	MG	2a	1738	1/1	0.92	0.08	48,48,48,48	0
58	MG	1A	3045	1/1	0.92	0.09	37,37,37,37	0
58	MG	2a	1741	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3313	1/1	0.92	0.09	53,53,53,53	0
58	MG	2a	1743	1/1	0.92	0.09	60,60,60,60	0
58	MG	2A	3435	1/1	0.92	0.22	55,55,55,55	0
58	MG	2a	1747	1/1	0.92	0.09	72,72,72,72	0
58	MG	1a	1792	1/1	0.92	0.14	60,60,60,60	0
58	MG	1A	3980	1/1	0.92	0.09	20,20,20,20	0
58	MG	2a	1751	1/1	0.92	0.24	70,70,70,70	0
58	MG	1A	3376	1/1	0.92	0.09	49,49,49,49	0
58	MG	1A	3676	1/1	0.92	0.12	18,18,18,18	0
58	MG	2A	3765	1/1	0.92	0.14	64,64,64,64	0
58	MG	13	104	1/1	0.92	0.10	28,28,28,28	0
58	MG	2a	1758	1/1	0.92	0.07	65,65,65,65	0
58	MG	1A	3678	1/1	0.92	0.06	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	16	101	1/1	0.92	0.20	43,43,43,43	0
58	MG	2A	3778	1/1	0.92	0.09	51,51,51,51	0
58	MG	2a	1767	1/1	0.92	0.10	69,69,69,69	0
58	MG	2A	3459	1/1	0.92	0.11	67,67,67,67	0
58	MG	2A	3780	1/1	0.92	0.10	56,56,56,56	0
58	MG	2a	1773	1/1	0.92	0.20	70,70,70,70	0
58	MG	18	109	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3464	1/1	0.92	0.22	51,51,51,51	0
58	MG	2A	3785	1/1	0.92	0.10	46,46,46,46	0
58	MG	1f	201	1/1	0.92	0.14	49,49,49,49	0
58	MG	2A	3467	1/1	0.92	0.16	56,56,56,56	0
58	MG	1n	101	1/1	0.92	0.14	57,57,57,57	0
58	MG	2A	3242	1/1	0.92	0.31	51,51,51,51	0
58	MG	1A	3997	1/1	0.92	0.11	65,65,65,65	0
58	MG	2A	3473	1/1	0.92	0.14	57,57,57,57	0
58	MG	1v	101	1/1	0.92	0.20	75,75,75,75	0
58	MG	2A	3811	1/1	0.92	0.11	51,51,51,51	0
58	MG	2a	1797	1/1	0.92	0.14	69,69,69,69	0
58	MG	1A	3998	1/1	0.92	0.11	72,72,72,72	0
58	MG	2A	3814	1/1	0.92	0.08	60,60,60,60	0
58	MG	1A	4011	1/1	0.92	0.12	56,56,56,56	0
58	MG	1A	3168	1/1	0.92	0.17	57,57,57,57	0
58	MG	1A	4018	1/1	0.92	0.10	61,61,61,61	0
58	MG	2A	3486	1/1	0.92	0.09	59,59,59,59	0
58	MG	2a	1810	1/1	0.92	0.11	64,64,64,64	0
58	MG	1A	3262	1/1	0.92	0.18	59,59,59,59	0
58	MG	1A	3847	1/1	0.92	0.09	46,46,46,46	0
58	MG	1A	4021	1/1	0.92	0.10	45,45,45,45	0
58	MG	2A	3504	1/1	0.92	0.15	58,58,58,58	0
58	MG	1A	3685	1/1	0.92	0.08	42,42,42,42	0
58	MG	2A	3263	1/1	0.92	0.21	59,59,59,59	0
58	MG	1A	3854	1/1	0.92	0.14	66,66,66,66	0
58	MG	2A	3001	1/1	0.92	0.28	53,53,53,53	0
58	MG	2A	3271	1/1	0.92	0.10	61,61,61,61	0
58	MG	1a	1620	1/1	0.92	0.16	52,52,52,52	0
58	MG	1A	3241	1/1	0.92	0.19	50,50,50,50	0
58	MG	2A	3013	1/1	0.92	0.08	49,49,49,49	0
58	MG	2A	3525	1/1	0.92	0.11	68,68,68,68	0
58	MG	1a	1623	1/1	0.92	0.12	47,47,47,47	0
58	MG	1a	1626	1/1	0.92	0.22	64,64,64,64	0
58	MG	2B	202	1/1	0.92	0.07	65,65,65,65	0
58	MG	2A	3534	1/1	0.92	0.09	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	1627	1/1	0.92	0.19	52,52,52,52	0
58	MG	1A	4035	1/1	0.92	0.07	50,50,50,50	0
58	MG	1a	1630	1/1	0.92	0.20	60,60,60,60	0
58	MG	2A	3547	1/1	0.92	0.08	37,37,37,37	0
58	MG	1A	4039	1/1	0.92	0.10	27,27,27,27	0
58	MG	1a	1632	1/1	0.92	0.22	63,63,63,63	0
58	MG	2A	3041	1/1	0.92	0.23	55,55,55,55	0
58	MG	2B	217	1/1	0.92	0.10	62,62,62,62	0
58	MG	1A	3856	1/1	0.92	0.08	27,27,27,27	0
58	MG	1A	4045	1/1	0.92	0.08	52,52,52,52	0
58	MG	1A	3859	1/1	0.92	0.11	62,62,62,62	0
58	MG	1A	4049	1/1	0.92	0.14	57,57,57,57	0
58	MG	1A	4051	1/1	0.92	0.09	58,58,58,58	0
58	MG	2A	3306	1/1	0.92	0.10	51,51,51,51	0
58	MG	2A	3048	1/1	0.92	0.08	46,46,46,46	0
58	MG	1A	3198	1/1	0.93	0.10	32,32,32,32	0
58	MG	2A	3549	1/1	0.93	0.10	44,44,44,44	0
58	MG	2E	302	1/1	0.93	0.13	58,58,58,58	0
58	MG	1a	1647	1/1	0.93	0.25	54,54,54,54	0
58	MG	2A	3552	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3296	1/1	0.93	0.13	56,56,56,56	0
58	MG	1A	4096	1/1	0.93	0.20	56,56,56,56	0
58	MG	2A	3298	1/1	0.93	0.14	51,51,51,51	0
58	MG	1a	1653	1/1	0.93	0.07	46,46,46,46	0
58	MG	1a	1655	1/1	0.93	0.11	60,60,60,60	0
58	MG	2A	3570	1/1	0.93	0.06	41,41,41,41	0
58	MG	2O	202	1/1	0.93	0.10	55,55,55,55	0
58	MG	2P	201	1/1	0.93	0.10	50,50,50,50	0
58	MG	1A	3803	1/1	0.93	0.10	64,64,64,64	0
58	MG	1A	3909	1/1	0.93	0.20	39,39,39,39	0
58	MG	1B	205	1/1	0.93	0.21	61,61,61,61	0
58	MG	1A	3808	1/1	0.93	0.35	28,28,28,28	0
58	MG	1A	3918	1/1	0.93	0.07	58,58,58,58	0
58	MG	2U	202	1/1	0.93	0.09	60,60,60,60	0
58	MG	1A	3300	1/1	0.93	0.11	37,37,37,37	0
58	MG	2Z	301	1/1	0.93	0.13	78,78,78,78	0
58	MG	2A	3054	1/1	0.93	0.27	60,60,60,60	0
58	MG	1a	1668	1/1	0.93	0.15	51,51,51,51	0
58	MG	2A	3057	1/1	0.93	0.16	72,72,72,72	0
58	MG	25	101	1/1	0.93	0.25	62,62,62,62	0
58	MG	1B	212	1/1	0.93	0.17	64,64,64,64	0
58	MG	2A	3315	1/1	0.93	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3060	1/1	0.93	0.15	55,55,55,55	0
58	MG	1A	3537	1/1	0.93	0.15	52,52,52,52	0
58	MG	1a	1674	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3656	1/1	0.93	0.10	39,39,39,39	0
58	MG	1A	3812	1/1	0.93	0.10	42,42,42,42	0
58	MG	2A	3073	1/1	0.93	0.08	43,43,43,43	0
58	MG	2A	3323	1/1	0.93	0.15	57,57,57,57	0
58	MG	2A	3603	1/1	0.93	0.09	57,57,57,57	0
58	MG	2A	3604	1/1	0.93	0.15	60,60,60,60	0
58	MG	1a	1679	1/1	0.93	0.14	59,59,59,59	0
58	MG	2A	3606	1/1	0.93	0.08	23,23,23,23	0
58	MG	2a	1614	1/1	0.93	0.22	74,74,74,74	0
58	MG	2A	3080	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3349	1/1	0.93	0.13	52,52,52,52	0
58	MG	1A	3665	1/1	0.93	0.06	35,35,35,35	0
58	MG	1B	226	1/1	0.93	0.07	48,48,48,48	0
58	MG	2A	3616	1/1	0.93	0.09	33,33,33,33	0
58	MG	1A	3667	1/1	0.93	0.08	19,19,19,19	0
58	MG	1A	3540	1/1	0.93	0.14	53,53,53,53	0
58	MG	2A	3631	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3301	1/1	0.93	0.31	51,51,51,51	0
58	MG	1a	1689	1/1	0.93	0.30	51,51,51,51	0
58	MG	1B	233	1/1	0.93	0.08	46,46,46,46	0
58	MG	1a	1692	1/1	0.93	0.27	47,47,47,47	0
58	MG	1A	3057	1/1	0.93	0.07	41,41,41,41	0
58	MG	2A	3340	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3205	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3836	1/1	0.93	0.08	36,36,36,36	0
58	MG	1A	3551	1/1	0.93	0.13	24,24,24,24	0
58	MG	1A	3308	1/1	0.93	0.13	47,47,47,47	0
58	MG	1A	3968	1/1	0.93	0.07	68,68,68,68	0
58	MG	1A	3969	1/1	0.93	0.10	60,60,60,60	0
58	MG	2A	3352	1/1	0.93	0.19	62,62,62,62	0
58	MG	2a	1648	1/1	0.93	0.09	60,60,60,60	0
58	MG	1a	1702	1/1	0.93	0.14	53,53,53,53	0
58	MG	2A	3354	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3564	1/1	0.93	0.14	36,36,36,36	0
58	MG	2A	3125	1/1	0.93	0.14	50,50,50,50	0
58	MG	1E	316	1/1	0.93	0.07	36,36,36,36	0
58	MG	1a	1708	1/1	0.93	0.47	69,69,69,69	0
58	MG	1A	3972	1/1	0.93	0.08	40,40,40,40	0
58	MG	1G	201	1/1	0.93	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	3130	1/1	0.93	0.08	47,47,47,47	0
58	MG	2a	1662	1/1	0.93	0.16	69,69,69,69	0
58	MG	1a	1715	1/1	0.93	0.17	53,53,53,53	0
58	MG	2A	3133	1/1	0.93	0.12	80,80,80,80	0
58	MG	2A	3134	1/1	0.93	0.08	40,40,40,40	0
58	MG	2a	1668	1/1	0.93	0.08	67,67,67,67	0
58	MG	2a	1670	1/1	0.93	0.25	66,66,66,66	0
58	MG	2A	3367	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3699	1/1	0.93	0.09	36,36,36,36	0
58	MG	2a	1675	1/1	0.93	0.27	63,63,63,63	0
58	MG	2A	3137	1/1	0.93	0.19	58,58,58,58	0
58	MG	1A	3841	1/1	0.93	0.06	38,38,38,38	0
58	MG	1a	1725	1/1	0.93	0.07	46,46,46,46	0
58	MG	1O	201	1/1	0.93	0.08	54,54,54,54	0
58	MG	2A	3147	1/1	0.93	0.12	48,48,48,48	0
58	MG	2A	3148	1/1	0.93	0.23	52,52,52,52	0
58	MG	1A	3360	1/1	0.93	0.10	37,37,37,37	0
58	MG	2a	1685	1/1	0.93	0.29	68,68,68,68	0
58	MG	2A	3378	1/1	0.93	0.16	62,62,62,62	0
58	MG	2a	1688	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3712	1/1	0.93	0.13	52,52,52,52	0
58	MG	2a	1694	1/1	0.93	0.20	62,62,62,62	0
58	MG	2A	3381	1/1	0.93	0.07	50,50,50,50	0
58	MG	2A	3156	1/1	0.93	0.21	56,56,56,56	0
58	MG	1Q	207	1/1	0.93	0.09	32,32,32,32	0
58	MG	1R	202	1/1	0.93	0.10	49,49,49,49	0
58	MG	2A	3694	1/1	0.93	0.08	19,19,19,19	0
58	MG	1R	204	1/1	0.93	0.11	44,44,44,44	0
58	MG	2A	3388	1/1	0.93	0.12	68,68,68,68	0
58	MG	1A	3473	1/1	0.93	0.14	46,46,46,46	0
58	MG	1a	1741	1/1	0.93	0.10	61,61,61,61	0
58	MG	2A	3172	1/1	0.93	0.16	56,56,56,56	0
58	MG	2A	3392	1/1	0.93	0.22	68,68,68,68	0
58	MG	1A	3987	1/1	0.93	0.08	40,40,40,40	0
58	MG	1U	204	1/1	0.93	0.25	37,37,37,37	0
58	MG	1A	3586	1/1	0.93	0.06	42,42,42,42	0
58	MG	1V	209	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3073	1/1	0.93	0.26	53,53,53,53	0
58	MG	2A	3720	1/1	0.93	0.12	56,56,56,56	0
58	MG	1A	3724	1/1	0.93	0.11	63,63,63,63	0
58	MG	2A	3411	1/1	0.93	0.12	41,41,41,41	0
58	MG	2a	1721	1/1	0.93	0.17	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	3727	1/1	0.93	0.07	68,68,68,68	0
58	MG	1A	3170	1/1	0.93	0.19	39,39,39,39	0
58	MG	1A	3416	1/1	0.93	0.18	48,48,48,48	0
58	MG	1A	3863	1/1	0.93	0.10	54,54,54,54	0
58	MG	1A	3213	1/1	0.93	0.13	50,50,50,50	0
58	MG	10	108	1/1	0.93	0.14	52,52,52,52	0
58	MG	2a	1730	1/1	0.93	0.11	66,66,66,66	0
58	MG	11	104	1/1	0.93	0.10	63,63,63,63	0
58	MG	1A	3225	1/1	0.93	0.07	48,48,48,48	0
58	MG	1A	3230	1/1	0.93	0.09	45,45,45,45	0
58	MG	2A	3736	1/1	0.93	0.07	61,61,61,61	0
58	MG	2A	3426	1/1	0.93	0.11	71,71,71,71	0
58	MG	1A	3025	1/1	0.93	0.07	43,43,43,43	0
58	MG	2a	1739	1/1	0.93	0.35	59,59,59,59	0
58	MG	1a	1782	1/1	0.93	0.06	50,50,50,50	0
58	MG	1a	1783	1/1	0.93	0.07	63,63,63,63	0
58	MG	1A	3608	1/1	0.93	0.07	29,29,29,29	0
58	MG	2A	3744	1/1	0.93	0.16	51,51,51,51	0
58	MG	15	106	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3872	1/1	0.93	0.27	44,44,44,44	0
58	MG	2A	3753	1/1	0.93	0.10	40,40,40,40	0
58	MG	18	102	1/1	0.93	0.15	37,37,37,37	0
58	MG	18	105	1/1	0.93	0.17	40,40,40,40	0
58	MG	18	106	1/1	0.93	0.14	56,56,56,56	0
58	MG	1A	3875	1/1	0.93	0.28	51,51,51,51	0
58	MG	1a	1808	1/1	0.93	0.20	56,56,56,56	0
58	MG	2A	3227	1/1	0.93	0.14	57,57,57,57	0
58	MG	2A	3770	1/1	0.93	0.13	58,58,58,58	0
58	MG	2a	1759	1/1	0.93	0.08	71,71,71,71	0
58	MG	2A	3231	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3774	1/1	0.93	0.13	61,61,61,61	0
58	MG	2a	1765	1/1	0.93	0.06	68,68,68,68	0
58	MG	1A	3182	1/1	0.93	0.09	53,53,53,53	0
58	MG	1A	4040	1/1	0.93	0.06	39,39,39,39	0
58	MG	1A	3617	1/1	0.93	0.12	11,11,11,11	0
58	MG	1A	3620	1/1	0.93	0.09	65,65,65,65	0
58	MG	2A	3240	1/1	0.93	0.09	38,38,38,38	0
58	MG	2a	1775	1/1	0.93	0.13	61,61,61,61	0
58	MG	1A	3149	1/1	0.93	0.32	34,34,34,34	0
58	MG	2A	3466	1/1	0.93	0.16	50,50,50,50	0
58	MG	1A	3883	1/1	0.93	0.07	28,28,28,28	0
58	MG	1A	3053	1/1	0.93	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1785	1/1	0.93	0.11	65,65,65,65	0
58	MG	2A	3791	1/1	0.93	0.11	71,71,71,71	0
58	MG	1a	1614	1/1	0.93	0.19	54,54,54,54	0
58	MG	2A	3245	1/1	0.93	0.12	50,50,50,50	0
58	MG	2A	3800	1/1	0.93	0.11	60,60,60,60	0
58	MG	1A	4053	1/1	0.93	0.18	36,36,36,36	0
58	MG	2A	3475	1/1	0.93	0.14	60,60,60,60	0
58	MG	1A	3630	1/1	0.93	0.06	28,28,28,28	0
58	MG	2A	3808	1/1	0.93	0.14	35,35,35,35	0
58	MG	1A	3162	1/1	0.93	0.11	47,47,47,47	0
58	MG	2a	1799	1/1	0.93	0.13	71,71,71,71	0
58	MG	2A	3251	1/1	0.93	0.22	62,62,62,62	0
58	MG	1A	4062	1/1	0.93	0.09	23,23,23,23	0
58	MG	1A	3516	1/1	0.93	0.11	49,49,49,49	0
58	MG	2a	1803	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3390	1/1	0.93	0.23	36,36,36,36	0
58	MG	2A	3819	1/1	0.93	0.17	63,63,63,63	0
58	MG	2a	1808	1/1	0.93	0.12	74,74,74,74	0
58	MG	2A	3487	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3494	1/1	0.93	0.10	62,62,62,62	0
58	MG	2A	3257	1/1	0.93	0.14	48,48,48,48	0
58	MG	2A	3500	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	4069	1/1	0.93	0.09	45,45,45,45	0
58	MG	2a	1816	1/1	0.93	0.15	68,68,68,68	0
58	MG	1x	107	1/1	0.93	0.24	67,67,67,67	0
58	MG	2A	3503	1/1	0.93	0.13	40,40,40,40	0
58	MG	1A	3519	1/1	0.93	0.06	50,50,50,50	0
58	MG	1x	110	1/1	0.93	0.21	63,63,63,63	0
58	MG	2A	3507	1/1	0.93	0.18	57,57,57,57	0
58	MG	2A	3268	1/1	0.93	0.20	65,65,65,65	0
58	MG	2a	1828	1/1	0.93	0.11	71,71,71,71	0
58	MG	1A	4073	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3793	1/1	0.93	0.10	39,39,39,39	0
58	MG	1A	3523	1/1	0.93	0.22	36,36,36,36	0
58	MG	2f	202	1/1	0.93	0.10	67,67,67,67	0
58	MG	2A	3008	1/1	0.93	0.13	55,55,55,55	0
58	MG	2A	3515	1/1	0.93	0.11	60,60,60,60	0
58	MG	2A	3518	1/1	0.93	0.08	49,49,49,49	0
58	MG	2A	3275	1/1	0.93	0.24	55,55,55,55	0
58	MG	2A	3520	1/1	0.93	0.10	33,33,33,33	0
58	MG	2A	3521	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	4081	1/1	0.93	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3524	1/1	0.93	0.08	40,40,40,40	0
58	MG	2q	201	1/1	0.93	0.08	72,72,72,72	0
58	MG	2A	3277	1/1	0.93	0.10	58,58,58,58	0
58	MG	1A	3339	1/1	0.93	0.08	52,52,52,52	0
58	MG	2A	3529	1/1	0.93	0.10	57,57,57,57	0
58	MG	2B	211	1/1	0.93	0.13	57,57,57,57	0
58	MG	2B	213	1/1	0.93	0.20	62,62,62,62	0
58	MG	2A	3286	1/1	0.93	0.08	47,47,47,47	0
58	MG	1A	3898	1/1	0.93	0.07	54,54,54,54	0
58	MG	2A	3537	1/1	0.93	0.08	35,35,35,35	0
58	MG	1A	4084	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3902	1/1	0.93	0.13	44,44,44,44	0
58	MG	1A	3903	1/1	0.93	0.22	29,29,29,29	0
59	K	1A	3556	1/1	0.93	0.20	72,72,72,72	0
58	MG	2A	3810	1/1	0.94	0.11	59,59,59,59	0
58	MG	1A	4055	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3829	1/1	0.94	0.09	35,35,35,35	0
58	MG	1A	3597	1/1	0.94	0.15	32,32,32,32	0
58	MG	1a	1669	1/1	0.94	0.18	63,63,63,63	0
58	MG	2A	3424	1/1	0.94	0.28	58,58,58,58	0
58	MG	2A	3820	1/1	0.94	0.13	44,44,44,44	0
58	MG	1A	3433	1/1	0.94	0.14	44,44,44,44	0
58	MG	2A	3131	1/1	0.94	0.09	44,44,44,44	0
58	MG	2A	3427	1/1	0.94	0.15	46,46,46,46	0
58	MG	2A	3831	1/1	0.94	0.08	73,73,73,73	0
58	MG	1a	1671	1/1	0.94	0.26	68,68,68,68	0
58	MG	2A	3835	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3064	1/1	0.94	0.11	49,49,49,49	0
58	MG	1A	3605	1/1	0.94	0.07	46,46,46,46	0
58	MG	1a	1675	1/1	0.94	0.16	48,48,48,48	0
58	MG	1A	3606	1/1	0.94	0.12	24,24,24,24	0
58	MG	1A	3439	1/1	0.94	0.20	42,42,42,42	0
58	MG	1A	3242	1/1	0.94	0.06	45,45,45,45	0
58	MG	2A	3145	1/1	0.94	0.16	43,43,43,43	0
58	MG	1A	4074	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3441	1/1	0.94	0.12	37,37,37,37	0
58	MG	1A	3445	1/1	0.94	0.06	52,52,52,52	0
58	MG	2A	3857	1/1	0.94	0.12	53,53,53,53	0
58	MG	1A	4079	1/1	0.94	0.11	55,55,55,55	0
58	MG	2A	3449	1/1	0.94	0.15	50,50,50,50	0
58	MG	2A	3861	1/1	0.94	0.10	54,54,54,54	0
58	MG	1a	1686	1/1	0.94	0.11	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	2A	3452	1/1	0.94	0.10	48,48,48,48	0
58	MG	2B	201	1/1	0.94	0.13	63,63,63,63	0
58	MG	1A	4080	1/1	0.94	0.16	66,66,66,66	0
58	MG	2A	3456	1/1	0.94	0.45	45,45,45,45	0
58	MG	2A	3157	1/1	0.94	0.14	43,43,43,43	0
58	MG	1A	3243	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3161	1/1	0.94	0.17	68,68,68,68	0
58	MG	2A	3462	1/1	0.94	0.14	71,71,71,71	0
58	MG	2A	3163	1/1	0.94	0.20	66,66,66,66	0
58	MG	1A	3853	1/1	0.94	0.16	45,45,45,45	0
58	MG	2A	3166	1/1	0.94	0.11	51,51,51,51	0
58	MG	2A	3167	1/1	0.94	0.11	47,47,47,47	0
58	MG	2B	215	1/1	0.94	0.12	63,63,63,63	0
58	MG	1A	3624	1/1	0.94	0.09	43,43,43,43	0
58	MG	1a	1691	1/1	0.94	0.23	60,60,60,60	0
58	MG	1A	3337	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	4086	1/1	0.94	0.16	50,50,50,50	0
58	MG	1A	3157	1/1	0.94	0.06	51,51,51,51	0
58	MG	1A	4092	1/1	0.94	0.15	55,55,55,55	0
58	MG	2A	3176	1/1	0.94	0.12	73,73,73,73	0
58	MG	2D	307	1/1	0.94	0.09	53,53,53,53	0
58	MG	2E	301	1/1	0.94	0.17	63,63,63,63	0
58	MG	1A	3634	1/1	0.94	0.11	46,46,46,46	0
58	MG	1A	3451	1/1	0.94	0.10	50,50,50,50	0
58	MG	2E	306	1/1	0.94	0.07	30,30,30,30	0
58	MG	2A	3181	1/1	0.94	0.11	47,47,47,47	0
58	MG	2F	301	1/1	0.94	0.20	60,60,60,60	0
58	MG	2A	3182	1/1	0.94	0.18	52,52,52,52	0
58	MG	1a	1698	1/1	0.94	0.19	50,50,50,50	0
58	MG	2A	3488	1/1	0.94	0.15	58,58,58,58	0
58	MG	2F	305	1/1	0.94	0.20	47,47,47,47	0
58	MG	2A	3489	1/1	0.94	0.32	57,57,57,57	0
58	MG	1A	3050	1/1	0.94	0.11	38,38,38,38	0
58	MG	1a	1700	1/1	0.94	0.08	54,54,54,54	0
58	MG	2A	3498	1/1	0.94	0.09	63,63,63,63	0
58	MG	1A	3248	1/1	0.94	0.06	54,54,54,54	0
58	MG	1A	3163	1/1	0.94	0.24	61,61,61,61	0
58	MG	1a	1703	1/1	0.94	0.18	62,62,62,62	0
58	MG	1a	1704	1/1	0.94	0.13	55,55,55,55	0
58	MG	2T	3500	1/1	0.94	0.08	63,63,63,63	0
58	MG	1B	204	1/1	0.94	0.05	35,35,35,35	0
58	MG	1A	3865	1/1	0.94	0.07	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	206	1/1	0.94	0.06	40,40,40,40	0
58	MG	1a	1710	1/1	0.94	0.12	52,52,52,52	0
58	MG	2Y	201	1/1	0.94	0.18	48,48,48,48	0
58	MG	2A	3199	1/1	0.94	0.21	56,56,56,56	0
58	MG	1a	1711	1/1	0.94	0.12	46,46,46,46	0
58	MG	2A	3201	1/1	0.94	0.28	67,67,67,67	0
58	MG	1A	3164	1/1	0.94	0.13	48,48,48,48	0
58	MG	23	101	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	3645	1/1	0.94	0.10	28,28,28,28	0
58	MG	1A	3465	1/1	0.94	0.15	49,49,49,49	0
58	MG	1A	3869	1/1	0.94	0.27	32,32,32,32	0
58	MG	1A	3021	1/1	0.94	0.08	39,39,39,39	0
58	MG	1a	1724	1/1	0.94	0.09	58,58,58,58	0
58	MG	1B	215	1/1	0.94	0.10	53,53,53,53	0
58	MG	1A	3871	1/1	0.94	0.23	38,38,38,38	0
58	MG	2a	1605	1/1	0.94	0.14	58,58,58,58	0
58	MG	2A	3220	1/1	0.94	0.13	48,48,48,48	0
58	MG	1A	3352	1/1	0.94	0.16	37,37,37,37	0
58	MG	2A	3528	1/1	0.94	0.18	58,58,58,58	0
58	MG	1A	3258	1/1	0.94	0.20	50,50,50,50	0
58	MG	1A	3654	1/1	0.94	0.11	40,40,40,40	0
58	MG	2A	3531	1/1	0.94	0.14	42,42,42,42	0
58	MG	1a	1734	1/1	0.94	0.16	51,51,51,51	0
58	MG	1A	3081	1/1	0.94	0.16	36,36,36,36	0
58	MG	2A	3539	1/1	0.94	0.12	39,39,39,39	0
58	MG	2a	1617	1/1	0.94	0.16	49,49,49,49	0
58	MG	2A	3235	1/1	0.94	0.10	41,41,41,41	0
58	MG	2a	1619	1/1	0.94	0.06	43,43,43,43	0
58	MG	1A	3001	1/1	0.94	0.06	39,39,39,39	0
58	MG	1A	3663	1/1	0.94	0.05	23,23,23,23	0
58	MG	1a	1740	1/1	0.94	0.09	56,56,56,56	0
58	MG	1A	3358	1/1	0.94	0.08	47,47,47,47	0
58	MG	1A	3094	1/1	0.94	0.10	43,43,43,43	0
58	MG	2a	1626	1/1	0.94	0.09	65,65,65,65	0
58	MG	1A	3670	1/1	0.94	0.08	27,27,27,27	0
58	MG	1A	3673	1/1	0.94	0.07	20,20,20,20	0
58	MG	2a	1629	1/1	0.94	0.12	64,64,64,64	0
58	MG	1A	3890	1/1	0.94	0.06	25,25,25,25	0
58	MG	1A	3363	1/1	0.94	0.22	42,42,42,42	0
58	MG	2A	3246	1/1	0.94	0.11	62,62,62,62	0
58	MG	2A	3567	1/1	0.94	0.09	64,64,64,64	0
58	MG	2a	1635	1/1	0.94	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1636	1/1	0.94	0.26	59,59,59,59	0
58	MG	1A	3004	1/1	0.94	0.05	24,24,24,24	0
58	MG	1a	1759	1/1	0.94	0.09	56,56,56,56	0
58	MG	2A	3249	1/1	0.94	0.06	63,63,63,63	0
58	MG	1E	310	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3101	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3483	1/1	0.94	0.14	50,50,50,50	0
58	MG	1a	1763	1/1	0.94	0.09	64,64,64,64	0
58	MG	2A	3255	1/1	0.94	0.07	68,68,68,68	0
58	MG	1A	3104	1/1	0.94	0.11	29,29,29,29	0
58	MG	1A	3487	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3583	1/1	0.94	0.06	52,52,52,52	0
58	MG	2a	1651	1/1	0.94	0.05	51,51,51,51	0
58	MG	2a	1652	1/1	0.94	0.27	66,66,66,66	0
58	MG	2A	3584	1/1	0.94	0.08	63,63,63,63	0
58	MG	1a	1769	1/1	0.94	0.12	60,60,60,60	0
58	MG	1F	309	1/1	0.94	0.09	40,40,40,40	0
58	MG	1A	3040	1/1	0.94	0.07	30,30,30,30	0
58	MG	1A	3697	1/1	0.94	0.10	41,41,41,41	0
58	MG	2A	3266	1/1	0.94	0.16	54,54,54,54	0
58	MG	1A	3489	1/1	0.94	0.18	47,47,47,47	0
58	MG	2A	3269	1/1	0.94	0.10	62,62,62,62	0
58	MG	1A	3705	1/1	0.94	0.13	37,37,37,37	0
58	MG	2a	1664	1/1	0.94	0.08	62,62,62,62	0
58	MG	1A	3270	1/1	0.94	0.19	39,39,39,39	0
58	MG	1A	3711	1/1	0.94	0.12	56,56,56,56	0
58	MG	1a	1785	1/1	0.94	0.09	63,63,63,63	0
58	MG	1A	3500	1/1	0.94	0.09	58,58,58,58	0
58	MG	1a	1790	1/1	0.94	0.07	73,73,73,73	0
58	MG	2a	1673	1/1	0.94	0.11	66,66,66,66	0
58	MG	1Q	204	1/1	0.94	0.13	60,60,60,60	0
58	MG	1Q	206	1/1	0.94	0.09	51,51,51,51	0
58	MG	2A	3285	1/1	0.94	0.07	61,61,61,61	0
58	MG	2A	3609	1/1	0.94	0.07	50,50,50,50	0
58	MG	2A	3610	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3271	1/1	0.94	0.07	46,46,46,46	0
58	MG	1a	1794	1/1	0.94	0.13	65,65,65,65	0
58	MG	1A	3922	1/1	0.94	0.07	45,45,45,45	0
58	MG	2a	1683	1/1	0.94	0.08	61,61,61,61	0
58	MG	2A	3617	1/1	0.94	0.11	44,44,44,44	0
58	MG	2A	3623	1/1	0.94	0.07	37,37,37,37	0
58	MG	2a	1686	1/1	0.94	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1796	1/1	0.94	0.09	68,68,68,68	0
58	MG	1a	1797	1/1	0.94	0.06	47,47,47,47	0
58	MG	2a	1689	1/1	0.94	0.23	60,60,60,60	0
58	MG	2a	1690	1/1	0.94	0.15	64,64,64,64	0
58	MG	2a	1691	1/1	0.94	0.27	60,60,60,60	0
58	MG	2A	3627	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3505	1/1	0.94	0.07	46,46,46,46	0
58	MG	2a	1695	1/1	0.94	0.11	76,76,76,76	0
58	MG	2A	3293	1/1	0.94	0.24	56,56,56,56	0
58	MG	2a	1699	1/1	0.94	0.14	57,57,57,57	0
58	MG	1a	1803	1/1	0.94	0.23	58,58,58,58	0
58	MG	1A	3924	1/1	0.94	0.06	40,40,40,40	0
58	MG	1a	1805	1/1	0.94	0.14	53,53,53,53	0
58	MG	1A	3926	1/1	0.94	0.10	45,45,45,45	0
58	MG	1T	202	1/1	0.94	0.10	41,41,41,41	0
58	MG	1U	203	1/1	0.94	0.07	57,57,57,57	0
58	MG	1A	3379	1/1	0.94	0.20	38,38,38,38	0
58	MG	2A	3644	1/1	0.94	0.24	53,53,53,53	0
58	MG	1e	202	1/1	0.94	0.10	54,54,54,54	0
58	MG	1A	3280	1/1	0.94	0.39	33,33,33,33	0
58	MG	1l	202	1/1	0.94	0.06	55,55,55,55	0
58	MG	1A	3508	1/1	0.94	0.12	63,63,63,63	0
58	MG	1A	3281	1/1	0.94	0.07	42,42,42,42	0
58	MG	1A	3941	1/1	0.94	0.08	51,51,51,51	0
58	MG	1A	3734	1/1	0.94	0.11	61,61,61,61	0
58	MG	2A	3659	1/1	0.94	0.13	50,50,50,50	0
58	MG	2A	3311	1/1	0.94	0.11	62,62,62,62	0
58	MG	2A	3312	1/1	0.94	0.11	68,68,68,68	0
58	MG	1A	3943	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3735	1/1	0.94	0.17	57,57,57,57	0
58	MG	1A	3517	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	3747	1/1	0.94	0.17	62,62,62,62	0
58	MG	10	106	1/1	0.94	0.10	64,64,64,64	0
58	MG	1A	3954	1/1	0.94	0.07	44,44,44,44	0
58	MG	1l	101	1/1	0.94	0.30	47,47,47,47	0
58	MG	2A	3671	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3955	1/1	0.94	0.05	34,34,34,34	0
58	MG	2a	1732	1/1	0.94	0.26	59,59,59,59	0
58	MG	1A	3194	1/1	0.94	0.28	36,36,36,36	0
58	MG	1A	3195	1/1	0.94	0.21	47,47,47,47	0
58	MG	1x	111	1/1	0.94	0.21	55,55,55,55	0
58	MG	2a	1736	1/1	0.94	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3115	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3524	1/1	0.94	0.18	47,47,47,47	0
58	MG	15	103	1/1	0.94	0.17	30,30,30,30	0
58	MG	2A	3681	1/1	0.94	0.06	68,68,68,68	0
58	MG	1A	3962	1/1	0.94	0.07	16,16,16,16	0
58	MG	1A	3119	1/1	0.94	0.08	33,33,33,33	0
58	MG	2A	3014	1/1	0.94	0.08	45,45,45,45	0
58	MG	2A	3016	1/1	0.94	0.10	74,74,74,74	0
58	MG	2a	1745	1/1	0.94	0.09	77,77,77,77	0
58	MG	17	102	1/1	0.94	0.10	45,45,45,45	0
58	MG	18	101	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3965	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3033	1/1	0.94	0.20	51,51,51,51	0
58	MG	1A	3296	1/1	0.94	0.30	60,60,60,60	0
58	MG	2A	3341	1/1	0.94	0.16	68,68,68,68	0
58	MG	2A	3695	1/1	0.94	0.10	65,65,65,65	0
58	MG	1A	3763	1/1	0.94	0.07	20,20,20,20	0
58	MG	18	108	1/1	0.94	0.12	48,48,48,48	0
58	MG	2A	3346	1/1	0.94	0.07	55,55,55,55	0
58	MG	1A	3970	1/1	0.94	0.09	62,62,62,62	0
58	MG	1A	3767	1/1	0.94	0.08	25,25,25,25	0
58	MG	2a	1762	1/1	0.94	0.07	56,56,56,56	0
58	MG	1A	3532	1/1	0.94	0.19	57,57,57,57	0
58	MG	2A	3706	1/1	0.94	0.13	53,53,53,53	0
58	MG	2A	3043	1/1	0.94	0.14	67,67,67,67	0
58	MG	2A	3351	1/1	0.94	0.17	64,64,64,64	0
58	MG	2a	1770	1/1	0.94	0.07	79,79,79,79	0
58	MG	1A	3120	1/1	0.94	0.10	33,33,33,33	0
58	MG	1a	1604	1/1	0.94	0.13	64,64,64,64	0
58	MG	1A	3207	1/1	0.94	0.10	52,52,52,52	0
58	MG	1A	3774	1/1	0.94	0.09	20,20,20,20	0
58	MG	1A	3397	1/1	0.94	0.20	31,31,31,31	0
58	MG	1A	3981	1/1	0.94	0.08	39,39,39,39	0
58	MG	1A	3017	1/1	0.94	0.17	34,34,34,34	0
58	MG	1A	3986	1/1	0.94	0.23	41,41,41,41	0
58	MG	2A	3727	1/1	0.94	0.18	48,48,48,48	0
58	MG	1A	3047	1/1	0.94	0.09	19,19,19,19	0
58	MG	1A	3135	1/1	0.94	0.11	31,31,31,31	0
58	MG	1A	3219	1/1	0.94	0.10	42,42,42,42	0
58	MG	2a	1791	1/1	0.94	0.23	71,71,71,71	0
58	MG	1a	1621	1/1	0.94	0.05	46,46,46,46	0
58	MG	2A	3061	1/1	0.94	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	3062	1/1	0.94	0.07	41,41,41,41	0
58	MG	2a	1796	1/1	0.94	0.12	53,53,53,53	0
58	MG	1A	3222	1/1	0.94	0.16	47,47,47,47	0
58	MG	1A	3552	1/1	0.94	0.27	29,29,29,29	0
58	MG	1A	3794	1/1	0.94	0.11	52,52,52,52	0
58	MG	1A	3554	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3373	1/1	0.94	0.11	52,52,52,52	0
58	MG	1A	3223	1/1	0.94	0.12	43,43,43,43	0
58	MG	2A	3741	1/1	0.94	0.06	42,42,42,42	0
58	MG	1A	3142	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3078	1/1	0.94	0.11	50,50,50,50	0
58	MG	1A	3319	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3571	1/1	0.94	0.07	39,39,39,39	0
58	MG	2A	3748	1/1	0.94	0.08	63,63,63,63	0
58	MG	2A	3751	1/1	0.94	0.07	51,51,51,51	0
58	MG	2A	3379	1/1	0.94	0.20	46,46,46,46	0
58	MG	1A	3582	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3085	1/1	0.94	0.14	55,55,55,55	0
58	MG	2A	3383	1/1	0.94	0.28	58,58,58,58	0
58	MG	1A	3583	1/1	0.94	0.08	38,38,38,38	0
58	MG	2A	3762	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	4032	1/1	0.94	0.09	33,33,33,33	0
58	MG	2a	1822	1/1	0.94	0.23	64,64,64,64	0
58	MG	2a	1824	1/1	0.94	0.16	61,61,61,61	0
58	MG	1A	3227	1/1	0.94	0.11	28,28,28,28	0
58	MG	2A	3768	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3585	1/1	0.94	0.12	35,35,35,35	0
58	MG	2A	3093	1/1	0.94	0.06	42,42,42,42	0
58	MG	2d	301	1/1	0.94	0.40	60,60,60,60	0
58	MG	1a	1643	1/1	0.94	0.13	50,50,50,50	0
58	MG	1A	3419	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3322	1/1	0.94	0.12	56,56,56,56	0
58	MG	1A	4042	1/1	0.94	0.07	37,37,37,37	0
58	MG	1A	3324	1/1	0.94	0.11	45,45,45,45	0
58	MG	2A	3105	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3781	1/1	0.94	0.14	74,74,74,74	0
58	MG	1a	1654	1/1	0.94	0.15	60,60,60,60	0
58	MG	2A	3396	1/1	0.94	0.08	52,52,52,52	0
58	MG	1A	3147	1/1	0.94	0.09	30,30,30,30	0
58	MG	1A	3062	1/1	0.94	0.21	40,40,40,40	0
58	MG	2A	3789	1/1	0.94	0.08	52,52,52,52	0
58	MG	1a	1657	1/1	0.94	0.10	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	3410	1/1	0.94	0.10	42,42,42,42	0
58	MG	1A	3823	1/1	0.94	0.08	23,23,23,23	0
58	MG	2A	3795	1/1	0.94	0.09	40,40,40,40	0
58	MG	1A	3432	1/1	0.94	0.13	39,39,39,39	0
58	MG	2A	3413	1/1	0.94	0.28	52,52,52,52	0
58	MG	2x	101	1/1	0.94	0.08	56,56,56,56	0
58	MG	2A	3414	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3119	1/1	0.94	0.18	57,57,57,57	0
58	MG	2A	3806	1/1	0.94	0.07	37,37,37,37	0
58	MG	2A	3807	1/1	0.94	0.08	52,52,52,52	0
58	MG	1A	3827	1/1	0.94	0.08	37,37,37,37	0
58	MG	1a	1663	1/1	0.94	0.11	54,54,54,54	0
58	MG	2A	3446	1/1	0.95	0.28	48,48,48,48	0
58	MG	2A	3828	1/1	0.95	0.07	56,56,56,56	0
58	MG	1B	228	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3164	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3425	1/1	0.95	0.12	50,50,50,50	0
58	MG	2A	3834	1/1	0.95	0.13	55,55,55,55	0
58	MG	1A	3900	1/1	0.95	0.08	44,44,44,44	0
58	MG	2A	3453	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3158	1/1	0.95	0.12	27,27,27,27	0
58	MG	2A	3455	1/1	0.95	0.17	45,45,45,45	0
58	MG	2A	3843	1/1	0.95	0.09	52,52,52,52	0
58	MG	1a	1707	1/1	0.95	0.18	41,41,41,41	0
58	MG	1A	3713	1/1	0.95	0.14	52,52,52,52	0
58	MG	2A	3847	1/1	0.95	0.06	66,66,66,66	0
58	MG	1A	3272	1/1	0.95	0.26	47,47,47,47	0
58	MG	1A	3274	1/1	0.95	0.09	41,41,41,41	0
58	MG	2A	3851	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3542	1/1	0.95	0.09	61,61,61,61	0
58	MG	2A	3174	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3346	1/1	0.95	0.07	39,39,39,39	0
58	MG	1E	304	1/1	0.95	0.12	35,35,35,35	0
58	MG	1A	3915	1/1	0.95	0.16	28,28,28,28	0
58	MG	2A	3468	1/1	0.95	0.14	48,48,48,48	0
58	MG	1E	308	1/1	0.95	0.08	40,40,40,40	0
58	MG	1a	1720	1/1	0.95	0.10	49,49,49,49	0
58	MG	2A	3471	1/1	0.95	0.09	37,37,37,37	0
58	MG	1a	1721	1/1	0.95	0.17	54,54,54,54	0
58	MG	1A	3278	1/1	0.95	0.14	28,28,28,28	0
58	MG	1A	3919	1/1	0.95	0.07	31,31,31,31	0
58	MG	2A	3476	1/1	0.95	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2B	205	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3477	1/1	0.95	0.06	61,61,61,61	0
58	MG	2B	207	1/1	0.95	0.07	62,62,62,62	0
58	MG	2A	3480	1/1	0.95	0.12	37,37,37,37	0
58	MG	1A	3920	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3921	1/1	0.95	0.12	69,69,69,69	0
58	MG	1E	315	1/1	0.95	0.05	45,45,45,45	0
58	MG	2B	212	1/1	0.95	0.25	62,62,62,62	0
58	MG	1a	1732	1/1	0.95	0.08	52,52,52,52	0
58	MG	1A	3545	1/1	0.95	0.18	60,60,60,60	0
58	MG	1F	303	1/1	0.95	0.12	29,29,29,29	0
58	MG	1A	3434	1/1	0.95	0.10	52,52,52,52	0
58	MG	1F	310	1/1	0.95	0.14	47,47,47,47	0
58	MG	1F	311	1/1	0.95	0.17	40,40,40,40	0
58	MG	2A	3493	1/1	0.95	0.18	44,44,44,44	0
58	MG	1A	3016	1/1	0.95	0.14	61,61,61,61	0
58	MG	1A	3736	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3737	1/1	0.95	0.07	64,64,64,64	0
58	MG	1G	204	1/1	0.95	0.12	52,52,52,52	0
58	MG	1A	3111	1/1	0.95	0.17	39,39,39,39	0
58	MG	1a	1749	1/1	0.95	0.14	53,53,53,53	0
58	MG	2A	3207	1/1	0.95	0.08	55,55,55,55	0
58	MG	2E	304	1/1	0.95	0.08	61,61,61,61	0
58	MG	2A	3208	1/1	0.95	0.08	42,42,42,42	0
58	MG	1a	1752	1/1	0.95	0.09	48,48,48,48	0
58	MG	1a	1753	1/1	0.95	0.19	58,58,58,58	0
58	MG	1H	201	1/1	0.95	0.09	36,36,36,36	0
58	MG	2A	3215	1/1	0.95	0.10	67,67,67,67	0
58	MG	1I	201	1/1	0.95	0.08	59,59,59,59	0
58	MG	2A	3217	1/1	0.95	0.14	44,44,44,44	0
58	MG	2F	306	1/1	0.95	0.34	50,50,50,50	0
58	MG	1N	201	1/1	0.95	0.08	39,39,39,39	0
58	MG	2A	3219	1/1	0.95	0.15	46,46,46,46	0
58	MG	2A	3516	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3076	1/1	0.95	0.22	51,51,51,51	0
58	MG	2A	3222	1/1	0.95	0.17	50,50,50,50	0
58	MG	2A	3223	1/1	0.95	0.20	52,52,52,52	0
58	MG	2Q	201	1/1	0.95	0.08	56,56,56,56	0
58	MG	1O	202	1/1	0.95	0.17	55,55,55,55	0
58	MG	1A	3748	1/1	0.95	0.07	49,49,49,49	0
58	MG	1P	204	1/1	0.95	0.36	57,57,57,57	0
58	MG	2A	3228	1/1	0.95	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2T	3502	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3229	1/1	0.95	0.07	67,67,67,67	0
58	MG	2A	3527	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3230	1/1	0.95	0.07	31,31,31,31	0
58	MG	1A	3353	1/1	0.95	0.18	54,54,54,54	0
58	MG	1a	1765	1/1	0.95	0.07	60,60,60,60	0
58	MG	1Q	202	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3532	1/1	0.95	0.14	52,52,52,52	0
58	MG	1Q	203	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3557	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3538	1/1	0.95	0.08	49,49,49,49	0
58	MG	25	102	1/1	0.95	0.20	39,39,39,39	0
58	MG	1a	1771	1/1	0.95	0.09	66,66,66,66	0
58	MG	2A	3239	1/1	0.95	0.10	63,63,63,63	0
58	MG	1A	3563	1/1	0.95	0.23	58,58,58,58	0
58	MG	1A	3442	1/1	0.95	0.28	44,44,44,44	0
58	MG	1A	3286	1/1	0.95	0.12	52,52,52,52	0
58	MG	1a	1775	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3550	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3950	1/1	0.95	0.07	45,45,45,45	0
58	MG	1a	1779	1/1	0.95	0.09	69,69,69,69	0
58	MG	2A	3553	1/1	0.95	0.07	29,29,29,29	0
58	MG	1A	3570	1/1	0.95	0.20	32,32,32,32	0
58	MG	2A	3560	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3953	1/1	0.95	0.06	43,43,43,43	0
58	MG	1S	203	1/1	0.95	0.11	61,61,61,61	0
58	MG	1A	3761	1/1	0.95	0.13	45,45,45,45	0
58	MG	2A	3565	1/1	0.95	0.16	54,54,54,54	0
58	MG	2A	3566	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3027	1/1	0.95	0.20	27,27,27,27	0
58	MG	1A	3764	1/1	0.95	0.06	25,25,25,25	0
58	MG	1U	205	1/1	0.95	0.09	31,31,31,31	0
58	MG	1U	206	1/1	0.95	0.32	30,30,30,30	0
58	MG	1A	3573	1/1	0.95	0.14	40,40,40,40	0
58	MG	1V	208	1/1	0.95	0.08	51,51,51,51	0
58	MG	1A	3577	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3959	1/1	0.95	0.10	49,49,49,49	0
58	MG	2A	3577	1/1	0.95	0.10	53,53,53,53	0
58	MG	1W	202	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3262	1/1	0.95	0.28	58,58,58,58	0
58	MG	1a	1798	1/1	0.95	0.08	66,66,66,66	0
58	MG	1A	3580	1/1	0.95	0.12	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3356	1/1	0.95	0.09	43,43,43,43	0
58	MG	1A	3449	1/1	0.95	0.12	47,47,47,47	0
58	MG	2a	1634	1/1	0.95	0.14	64,64,64,64	0
58	MG	1A	3116	1/1	0.95	0.07	41,41,41,41	0
58	MG	1a	1807	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3967	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3591	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3592	1/1	0.95	0.14	53,53,53,53	0
58	MG	2A	3593	1/1	0.95	0.10	58,58,58,58	0
58	MG	1A	3085	1/1	0.95	0.14	31,31,31,31	0
58	MG	2A	3595	1/1	0.95	0.14	62,62,62,62	0
58	MG	1A	3453	1/1	0.95	0.09	41,41,41,41	0
58	MG	2a	1646	1/1	0.95	0.08	61,61,61,61	0
58	MG	2A	3597	1/1	0.95	0.13	53,53,53,53	0
58	MG	1A	3588	1/1	0.95	0.12	50,50,50,50	0
58	MG	10	109	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3240	1/1	0.95	0.20	34,34,34,34	0
58	MG	1l	201	1/1	0.95	0.05	76,76,76,76	0
58	MG	2A	3602	1/1	0.95	0.11	54,54,54,54	0
58	MG	2A	3281	1/1	0.95	0.08	47,47,47,47	0
58	MG	2a	1654	1/1	0.95	0.06	58,58,58,58	0
58	MG	2A	3282	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3284	1/1	0.95	0.11	71,71,71,71	0
58	MG	1A	3788	1/1	0.95	0.08	58,58,58,58	0
58	MG	1l	105	1/1	0.95	0.07	42,42,42,42	0
58	MG	1n	102	1/1	0.95	0.26	59,59,59,59	0
58	MG	1p	101	1/1	0.95	0.11	51,51,51,51	0
58	MG	2a	1661	1/1	0.95	0.12	70,70,70,70	0
58	MG	2A	3289	1/1	0.95	0.12	58,58,58,58	0
58	MG	2A	3612	1/1	0.95	0.15	37,37,37,37	0
58	MG	1A	3591	1/1	0.95	0.12	53,53,53,53	0
58	MG	13	102	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3361	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3297	1/1	0.95	0.11	35,35,35,35	0
58	MG	2A	3619	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3621	1/1	0.95	0.13	38,38,38,38	0
58	MG	2A	3294	1/1	0.95	0.09	61,61,61,61	0
58	MG	1A	3795	1/1	0.95	0.06	23,23,23,23	0
58	MG	1A	3594	1/1	0.95	0.16	52,52,52,52	0
58	MG	15	105	1/1	0.95	0.16	38,38,38,38	0
58	MG	1A	3982	1/1	0.95	0.11	35,35,35,35	0
58	MG	2A	3299	1/1	0.95	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3459	1/1	0.95	0.09	31,31,31,31	0
58	MG	1A	3179	1/1	0.95	0.13	23,23,23,23	0
58	MG	1A	3461	1/1	0.95	0.15	37,37,37,37	0
58	MG	1A	3598	1/1	0.95	0.11	37,37,37,37	0
58	MG	2A	3639	1/1	0.95	0.15	54,54,54,54	0
58	MG	1A	3993	1/1	0.95	0.05	16,16,16,16	0
58	MG	1A	3464	1/1	0.95	0.08	54,54,54,54	0
58	MG	18	107	1/1	0.95	0.10	58,58,58,58	0
58	MG	2A	3002	1/1	0.95	0.27	49,49,49,49	0
58	MG	1A	3368	1/1	0.95	0.12	53,53,53,53	0
58	MG	1A	3033	1/1	0.95	0.17	30,30,30,30	0
58	MG	2A	3650	1/1	0.95	0.18	60,60,60,60	0
58	MG	2a	1692	1/1	0.95	0.12	82,82,82,82	0
58	MG	1A	4000	1/1	0.95	0.14	39,39,39,39	0
58	MG	1A	4002	1/1	0.95	0.07	24,24,24,24	0
58	MG	1A	3467	1/1	0.95	0.20	47,47,47,47	0
58	MG	2a	1696	1/1	0.95	0.18	60,60,60,60	0
58	MG	2A	3015	1/1	0.95	0.09	48,48,48,48	0
58	MG	1A	4015	1/1	0.95	0.13	58,58,58,58	0
58	MG	2A	3658	1/1	0.95	0.05	48,48,48,48	0
58	MG	2A	3020	1/1	0.95	0.08	56,56,56,56	0
58	MG	1a	1605	1/1	0.95	0.10	47,47,47,47	0
58	MG	2a	1703	1/1	0.95	0.12	59,59,59,59	0
58	MG	1a	1606	1/1	0.95	0.12	65,65,65,65	0
58	MG	2A	3025	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3026	1/1	0.95	0.16	46,46,46,46	0
58	MG	2A	3028	1/1	0.95	0.13	58,58,58,58	0
58	MG	1A	3181	1/1	0.95	0.10	48,48,48,48	0
58	MG	2A	3030	1/1	0.95	0.12	44,44,44,44	0
58	MG	1A	3304	1/1	0.95	0.23	56,56,56,56	0
58	MG	1A	3373	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3124	1/1	0.95	0.27	32,32,32,32	0
58	MG	1A	3183	1/1	0.95	0.14	67,67,67,67	0
58	MG	1A	4022	1/1	0.95	0.07	49,49,49,49	0
58	MG	1A	3307	1/1	0.95	0.09	57,57,57,57	0
58	MG	1A	3128	1/1	0.95	0.11	33,33,33,33	0
58	MG	2A	3677	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	4031	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	3826	1/1	0.95	0.06	33,33,33,33	0
58	MG	2A	3336	1/1	0.95	0.17	59,59,59,59	0
58	MG	1A	3309	1/1	0.95	0.13	45,45,45,45	0
58	MG	1A	3828	1/1	0.95	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1624	1/1	0.95	0.27	54,54,54,54	0
58	MG	2a	1726	1/1	0.95	0.25	63,63,63,63	0
58	MG	2a	1727	1/1	0.95	0.17	62,62,62,62	0
58	MG	1A	4036	1/1	0.95	0.06	37,37,37,37	0
58	MG	2A	3342	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3343	1/1	0.95	0.20	52,52,52,52	0
58	MG	2A	3688	1/1	0.95	0.06	69,69,69,69	0
58	MG	2A	3050	1/1	0.95	0.11	47,47,47,47	0
58	MG	1A	3632	1/1	0.95	0.06	30,30,30,30	0
58	MG	1A	3088	1/1	0.95	0.09	38,38,38,38	0
58	MG	1A	3835	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3693	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3636	1/1	0.95	0.06	20,20,20,20	0
58	MG	1A	3090	1/1	0.95	0.08	39,39,39,39	0
58	MG	1a	1634	1/1	0.95	0.28	74,74,74,74	0
58	MG	2A	3697	1/1	0.95	0.27	61,61,61,61	0
58	MG	2A	3698	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3699	1/1	0.95	0.12	44,44,44,44	0
58	MG	1A	3484	1/1	0.95	0.22	52,52,52,52	0
58	MG	1A	4048	1/1	0.95	0.11	53,53,53,53	0
58	MG	1A	3389	1/1	0.95	0.28	46,46,46,46	0
58	MG	2a	1746	1/1	0.95	0.17	63,63,63,63	0
58	MG	1A	4050	1/1	0.95	0.06	39,39,39,39	0
58	MG	1a	1640	1/1	0.95	0.17	56,56,56,56	0
58	MG	1A	3091	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	3315	1/1	0.95	0.06	26,26,26,26	0
58	MG	2A	3068	1/1	0.95	0.18	52,52,52,52	0
58	MG	2A	3070	1/1	0.95	0.05	34,34,34,34	0
58	MG	2A	3711	1/1	0.95	0.10	54,54,54,54	0
58	MG	2A	3712	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3714	1/1	0.95	0.08	40,40,40,40	0
58	MG	2A	3072	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3718	1/1	0.95	0.15	58,58,58,58	0
58	MG	1A	3843	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3644	1/1	0.95	0.06	61,61,61,61	0
58	MG	2a	1763	1/1	0.95	0.15	55,55,55,55	0
58	MG	2a	1764	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3076	1/1	0.95	0.10	48,48,48,48	0
58	MG	1a	1650	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	4058	1/1	0.95	0.09	43,43,43,43	0
58	MG	1a	1652	1/1	0.95	0.19	56,56,56,56	0
58	MG	2a	1769	1/1	0.95	0.07	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3082	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3256	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3495	1/1	0.95	0.23	45,45,45,45	0
58	MG	1A	3648	1/1	0.95	0.06	26,26,26,26	0
58	MG	1A	3649	1/1	0.95	0.05	29,29,29,29	0
58	MG	2a	1777	1/1	0.95	0.14	64,64,64,64	0
58	MG	1A	3137	1/1	0.95	0.33	34,34,34,34	0
58	MG	1A	3499	1/1	0.95	0.13	57,57,57,57	0
58	MG	2a	1783	1/1	0.95	0.19	58,58,58,58	0
58	MG	1A	3858	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3094	1/1	0.95	0.14	52,52,52,52	0
58	MG	1A	3092	1/1	0.95	0.10	47,47,47,47	0
58	MG	1A	3006	1/1	0.95	0.11	40,40,40,40	0
58	MG	2A	3099	1/1	0.95	0.11	55,55,55,55	0
58	MG	1A	3861	1/1	0.95	0.06	45,45,45,45	0
58	MG	2A	3101	1/1	0.95	0.23	59,59,59,59	0
58	MG	1a	1665	1/1	0.95	0.21	56,56,56,56	0
58	MG	1A	3399	1/1	0.95	0.13	40,40,40,40	0
58	MG	2A	3104	1/1	0.95	0.10	34,34,34,34	0
58	MG	1A	3657	1/1	0.95	0.06	31,31,31,31	0
58	MG	2A	3747	1/1	0.95	0.10	53,53,53,53	0
58	MG	1A	3148	1/1	0.95	0.18	43,43,43,43	0
58	MG	1A	3327	1/1	0.95	0.23	48,48,48,48	0
58	MG	2A	3108	1/1	0.95	0.11	62,62,62,62	0
58	MG	1A	3664	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3111	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3328	1/1	0.95	0.21	52,52,52,52	0
58	MG	2a	1804	1/1	0.95	0.24	53,53,53,53	0
58	MG	1a	1673	1/1	0.95	0.14	48,48,48,48	0
58	MG	2A	3760	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3206	1/1	0.95	0.07	33,33,33,33	0
58	MG	2a	1809	1/1	0.95	0.18	63,63,63,63	0
58	MG	2A	3399	1/1	0.95	0.17	39,39,39,39	0
58	MG	2A	3400	1/1	0.95	0.10	39,39,39,39	0
58	MG	1A	4087	1/1	0.95	0.10	47,47,47,47	0
58	MG	2A	3403	1/1	0.95	0.19	49,49,49,49	0
58	MG	2A	3120	1/1	0.95	0.08	42,42,42,42	0
58	MG	2A	3123	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3409	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3024	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	4090	1/1	0.95	0.13	58,58,58,58	0
58	MG	1a	1678	1/1	0.95	0.08	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	3671	1/1	0.95	0.09	40,40,40,40	0
58	MG	2a	1823	1/1	0.95	0.18	59,59,59,59	0
58	MG	1A	3100	1/1	0.95	0.17	49,49,49,49	0
58	MG	1A	3333	1/1	0.95	0.06	48,48,48,48	0
58	MG	1A	3873	1/1	0.95	0.19	34,34,34,34	0
58	MG	2a	1827	1/1	0.95	0.14	63,63,63,63	0
58	MG	1A	3520	1/1	0.95	0.09	45,45,45,45	0
58	MG	1B	201	1/1	0.95	0.06	42,42,42,42	0
58	MG	2a	1830	1/1	0.95	0.11	65,65,65,65	0
58	MG	1A	3521	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3421	1/1	0.95	0.17	47,47,47,47	0
58	MG	1A	3334	1/1	0.95	0.11	56,56,56,56	0
58	MG	2A	3793	1/1	0.95	0.07	60,60,60,60	0
58	MG	2A	3135	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3152	1/1	0.95	0.23	40,40,40,40	0
58	MG	2A	3797	1/1	0.95	0.13	65,65,65,65	0
58	MG	2A	3798	1/1	0.95	0.06	43,43,43,43	0
58	MG	1A	3336	1/1	0.95	0.06	57,57,57,57	0
58	MG	1A	3691	1/1	0.95	0.08	17,17,17,17	0
58	MG	1A	3527	1/1	0.95	0.11	44,44,44,44	0
58	MG	2l	204	1/1	0.95	0.05	61,61,61,61	0
58	MG	2A	3803	1/1	0.95	0.06	41,41,41,41	0
58	MG	1A	3528	1/1	0.95	0.19	49,49,49,49	0
58	MG	2q	202	1/1	0.95	0.09	65,65,65,65	0
58	MG	1A	3698	1/1	0.95	0.06	28,28,28,28	0
58	MG	1A	3529	1/1	0.95	0.21	38,38,38,38	0
58	MG	1A	3700	1/1	0.95	0.07	28,28,28,28	0
58	MG	1B	221	1/1	0.95	0.10	60,60,60,60	0
58	MG	1A	3701	1/1	0.95	0.04	25,25,25,25	0
58	MG	2A	3155	1/1	0.95	0.16	57,57,57,57	0
58	MG	1A	3055	1/1	0.95	0.14	37,37,37,37	0
58	MG	1A	3422	1/1	0.95	0.10	40,40,40,40	0
58	MG	2A	3440	1/1	0.95	0.07	47,47,47,47	0
58	MG	2x	104	1/1	0.95	0.26	55,55,55,55	0
58	MG	1A	3709	1/1	0.95	0.14	37,37,37,37	0
58	MG	2A	3442	1/1	0.95	0.06	54,54,54,54	0
58	MG	2A	3823	1/1	0.95	0.09	60,60,60,60	0
58	MG	1A	3710	1/1	0.95	0.08	42,42,42,42	0
58	MG	1A	4095	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3579	1/1	0.96	0.07	34,34,34,34	0
58	MG	2A	3562	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	3381	1/1	0.96	0.17	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1644	1/1	0.96	0.18	38,38,38,38	0
58	MG	1A	3904	1/1	0.96	0.11	53,53,53,53	0
58	MG	1A	3320	1/1	0.96	0.16	46,46,46,46	0
58	MG	1A	3742	1/1	0.96	0.05	54,54,54,54	0
58	MG	1A	3067	1/1	0.96	0.13	45,45,45,45	0
58	MG	1A	3469	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3914	1/1	0.96	0.06	27,27,27,27	0
58	MG	1B	209	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3138	1/1	0.96	0.10	41,41,41,41	0
58	MG	2A	3049	1/1	0.96	0.12	33,33,33,33	0
58	MG	1A	3916	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3917	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3471	1/1	0.96	0.20	51,51,51,51	0
58	MG	2A	3579	1/1	0.96	0.11	55,55,55,55	0
58	MG	2A	3053	1/1	0.96	0.12	66,66,66,66	0
58	MG	2A	3305	1/1	0.96	0.31	60,60,60,60	0
58	MG	1A	3323	1/1	0.96	0.13	51,51,51,51	0
58	MG	1a	1660	1/1	0.96	0.12	67,67,67,67	0
58	MG	2A	3056	1/1	0.96	0.09	48,48,48,48	0
58	MG	1B	219	1/1	0.96	0.09	38,38,38,38	0
58	MG	2P	203	1/1	0.96	0.08	55,55,55,55	0
58	MG	1A	3210	1/1	0.96	0.11	41,41,41,41	0
58	MG	2A	3059	1/1	0.96	0.15	49,49,49,49	0
58	MG	1A	3754	1/1	0.96	0.09	44,44,44,44	0
58	MG	1A	3264	1/1	0.96	0.21	45,45,45,45	0
58	MG	1a	1666	1/1	0.96	0.23	63,63,63,63	0
58	MG	1A	3476	1/1	0.96	0.11	41,41,41,41	0
58	MG	2A	3064	1/1	0.96	0.10	68,68,68,68	0
58	MG	1A	3759	1/1	0.96	0.08	43,43,43,43	0
58	MG	2V	201	1/1	0.96	0.23	52,52,52,52	0
58	MG	2A	3318	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3169	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3044	1/1	0.96	0.05	30,30,30,30	0
58	MG	1A	3215	1/1	0.96	0.15	40,40,40,40	0
58	MG	2A	3069	1/1	0.96	0.06	43,43,43,43	0
58	MG	1A	3395	1/1	0.96	0.25	43,43,43,43	0
58	MG	2A	3071	1/1	0.96	0.13	50,50,50,50	0
58	MG	23	102	1/1	0.96	0.07	57,57,57,57	0
58	MG	23	103	1/1	0.96	0.08	59,59,59,59	0
58	MG	1A	3482	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3330	1/1	0.96	0.13	43,43,43,43	0
58	MG	2A	3074	1/1	0.96	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	27	102	1/1	0.96	0.07	53,53,53,53	0
58	MG	1A	3269	1/1	0.96	0.12	44,44,44,44	0
58	MG	2A	3330	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3600	1/1	0.96	0.11	37,37,37,37	0
58	MG	1B	236	1/1	0.96	0.10	44,44,44,44	0
58	MG	1D	302	1/1	0.96	0.18	36,36,36,36	0
58	MG	2a	1604	1/1	0.96	0.10	52,52,52,52	0
58	MG	1D	308	1/1	0.96	0.06	37,37,37,37	0
58	MG	1D	310	1/1	0.96	0.27	27,27,27,27	0
58	MG	1D	311	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3216	1/1	0.96	0.10	40,40,40,40	0
58	MG	2A	3618	1/1	0.96	0.15	51,51,51,51	0
58	MG	2A	3086	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3620	1/1	0.96	0.11	51,51,51,51	0
58	MG	2A	3087	1/1	0.96	0.06	44,44,44,44	0
58	MG	2a	1613	1/1	0.96	0.10	46,46,46,46	0
58	MG	1E	301	1/1	0.96	0.28	37,37,37,37	0
58	MG	1A	3602	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3949	1/1	0.96	0.06	49,49,49,49	0
58	MG	1E	306	1/1	0.96	0.14	29,29,29,29	0
58	MG	2A	3628	1/1	0.96	0.18	54,54,54,54	0
58	MG	2a	1620	1/1	0.96	0.07	62,62,62,62	0
58	MG	1A	3603	1/1	0.96	0.08	24,24,24,24	0
58	MG	1A	3217	1/1	0.96	0.13	38,38,38,38	0
58	MG	2A	3095	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3096	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3176	1/1	0.96	0.04	26,26,26,26	0
58	MG	1A	3220	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3786	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3640	1/1	0.96	0.10	32,32,32,32	0
58	MG	1A	3609	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3790	1/1	0.96	0.06	34,34,34,34	0
58	MG	1A	3490	1/1	0.96	0.06	47,47,47,47	0
58	MG	1F	301	1/1	0.96	0.15	40,40,40,40	0
58	MG	1A	3792	1/1	0.96	0.09	58,58,58,58	0
58	MG	1F	307	1/1	0.96	0.15	25,25,25,25	0
58	MG	1A	3493	1/1	0.96	0.18	36,36,36,36	0
58	MG	1A	3619	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3360	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3963	1/1	0.96	0.08	47,47,47,47	0
58	MG	2A	3109	1/1	0.96	0.16	50,50,50,50	0
58	MG	2A	3655	1/1	0.96	0.10	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	3656	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3177	1/1	0.96	0.04	22,22,22,22	0
58	MG	2a	1643	1/1	0.96	0.28	63,63,63,63	0
58	MG	1A	3408	1/1	0.96	0.09	46,46,46,46	0
58	MG	2a	1645	1/1	0.96	0.08	66,66,66,66	0
58	MG	1A	3497	1/1	0.96	0.04	28,28,28,28	0
58	MG	1A	3498	1/1	0.96	0.07	39,39,39,39	0
58	MG	1A	3627	1/1	0.96	0.05	21,21,21,21	0
58	MG	2A	3118	1/1	0.96	0.17	48,48,48,48	0
58	MG	1A	3629	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3409	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3121	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3122	1/1	0.96	0.09	69,69,69,69	0
58	MG	1A	3026	1/1	0.96	0.19	69,69,69,69	0
58	MG	1N	202	1/1	0.96	0.05	35,35,35,35	0
58	MG	1N	204	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3973	1/1	0.96	0.05	59,59,59,59	0
58	MG	1a	1716	1/1	0.96	0.13	67,67,67,67	0
58	MG	2A	3674	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3501	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3976	1/1	0.96	0.09	58,58,58,58	0
58	MG	2A	3382	1/1	0.96	0.08	59,59,59,59	0
58	MG	1P	202	1/1	0.96	0.17	28,28,28,28	0
58	MG	1A	3412	1/1	0.96	0.15	44,44,44,44	0
58	MG	1A	3413	1/1	0.96	0.05	50,50,50,50	0
58	MG	1A	3015	1/1	0.96	0.10	49,49,49,49	0
58	MG	2a	1667	1/1	0.96	0.12	44,44,44,44	0
58	MG	1A	3415	1/1	0.96	0.33	44,44,44,44	0
58	MG	2a	1669	1/1	0.96	0.07	56,56,56,56	0
58	MG	1a	1727	1/1	0.96	0.11	33,33,33,33	0
58	MG	1a	1729	1/1	0.96	0.08	51,51,51,51	0
58	MG	1A	3079	1/1	0.96	0.07	57,57,57,57	0
58	MG	2A	3138	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3509	1/1	0.96	0.14	37,37,37,37	0
58	MG	1A	3511	1/1	0.96	0.23	26,26,26,26	0
58	MG	2A	3144	1/1	0.96	0.11	47,47,47,47	0
58	MG	1A	3514	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3988	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3515	1/1	0.96	0.06	49,49,49,49	0
58	MG	1A	3340	1/1	0.96	0.18	48,48,48,48	0
58	MG	2A	3150	1/1	0.96	0.09	61,61,61,61	0
58	MG	2A	3402	1/1	0.96	0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3994	1/1	0.96	0.09	27,27,27,27	0
58	MG	1A	3341	1/1	0.96	0.18	36,36,36,36	0
58	MG	2A	3405	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3996	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3408	1/1	0.96	0.22	51,51,51,51	0
58	MG	1A	3150	1/1	0.96	0.21	37,37,37,37	0
58	MG	1A	3231	1/1	0.96	0.05	50,50,50,50	0
58	MG	1a	1745	1/1	0.96	0.12	44,44,44,44	0
58	MG	2A	3160	1/1	0.96	0.08	63,63,63,63	0
58	MG	1a	1746	1/1	0.96	0.14	47,47,47,47	0
58	MG	1A	3999	1/1	0.96	0.06	61,61,61,61	0
58	MG	1A	3834	1/1	0.96	0.09	48,48,48,48	0
58	MG	1V	202	1/1	0.96	0.23	28,28,28,28	0
58	MG	1V	206	1/1	0.96	0.17	43,43,43,43	0
58	MG	2A	3713	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	3347	1/1	0.96	0.08	34,34,34,34	0
58	MG	2A	3419	1/1	0.96	0.22	45,45,45,45	0
58	MG	1A	4004	1/1	0.96	0.06	35,35,35,35	0
58	MG	1a	1756	1/1	0.96	0.05	47,47,47,47	0
58	MG	1A	4005	1/1	0.96	0.07	25,25,25,25	0
58	MG	1a	1758	1/1	0.96	0.12	63,63,63,63	0
58	MG	1A	3426	1/1	0.96	0.17	57,57,57,57	0
58	MG	1A	4012	1/1	0.96	0.15	68,68,68,68	0
58	MG	1X	101	1/1	0.96	0.34	34,34,34,34	0
58	MG	1X	102	1/1	0.96	0.09	39,39,39,39	0
58	MG	1A	3290	1/1	0.96	0.13	36,36,36,36	0
58	MG	1A	3291	1/1	0.96	0.07	37,37,37,37	0
58	MG	2A	3180	1/1	0.96	0.05	59,59,59,59	0
58	MG	1A	4017	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3659	1/1	0.96	0.08	28,28,28,28	0
58	MG	2A	3183	1/1	0.96	0.11	57,57,57,57	0
58	MG	10	101	1/1	0.96	0.08	34,34,34,34	0
58	MG	2A	3186	1/1	0.96	0.14	67,67,67,67	0
58	MG	2A	3436	1/1	0.96	0.12	41,41,41,41	0
58	MG	10	102	1/1	0.96	0.10	44,44,44,44	0
58	MG	10	104	1/1	0.96	0.12	36,36,36,36	0
58	MG	1A	3660	1/1	0.96	0.05	29,29,29,29	0
58	MG	1A	3232	1/1	0.96	0.15	41,41,41,41	0
58	MG	2A	3443	1/1	0.96	0.12	58,58,58,58	0
58	MG	10	107	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3445	1/1	0.96	0.11	52,52,52,52	0
58	MG	1A	3526	1/1	0.96	0.16	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1777	1/1	0.96	0.10	49,49,49,49	0
58	MG	1a	1778	1/1	0.96	0.06	46,46,46,46	0
58	MG	2A	3750	1/1	0.96	0.08	54,54,54,54	0
58	MG	1A	3430	1/1	0.96	0.05	42,42,42,42	0
58	MG	2A	3752	1/1	0.96	0.12	57,57,57,57	0
58	MG	1A	3846	1/1	0.96	0.11	44,44,44,44	0
58	MG	11	102	1/1	0.96	0.08	43,43,43,43	0
58	MG	11	103	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	4029	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3202	1/1	0.96	0.14	50,50,50,50	0
58	MG	2A	3759	1/1	0.96	0.14	56,56,56,56	0
58	MG	2A	3203	1/1	0.96	0.12	55,55,55,55	0
58	MG	2A	3458	1/1	0.96	0.07	57,57,57,57	0
58	MG	1A	3431	1/1	0.96	0.10	39,39,39,39	0
58	MG	2A	3764	1/1	0.96	0.09	57,57,57,57	0
58	MG	1A	3351	1/1	0.96	0.11	55,55,55,55	0
58	MG	2A	3767	1/1	0.96	0.12	59,59,59,59	0
58	MG	1A	3530	1/1	0.96	0.12	39,39,39,39	0
58	MG	2A	3769	1/1	0.96	0.07	48,48,48,48	0
58	MG	1A	4033	1/1	0.96	0.07	29,29,29,29	0
58	MG	2A	3771	1/1	0.96	0.05	69,69,69,69	0
58	MG	1A	3049	1/1	0.96	0.05	23,23,23,23	0
58	MG	2a	1753	1/1	0.96	0.07	56,56,56,56	0
58	MG	2A	3209	1/1	0.96	0.08	47,47,47,47	0
58	MG	13	105	1/1	0.96	0.05	31,31,31,31	0
58	MG	1A	3238	1/1	0.96	0.10	36,36,36,36	0
58	MG	2A	3777	1/1	0.96	0.06	48,48,48,48	0
58	MG	15	101	1/1	0.96	0.30	35,35,35,35	0
58	MG	15	102	1/1	0.96	0.14	33,33,33,33	0
58	MG	1A	3534	1/1	0.96	0.09	25,25,25,25	0
58	MG	1A	3857	1/1	0.96	0.11	22,22,22,22	0
58	MG	1A	3127	1/1	0.96	0.15	45,45,45,45	0
58	MG	1A	3153	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3784	1/1	0.96	0.11	48,48,48,48	0
58	MG	16	102	1/1	0.96	0.06	54,54,54,54	0
58	MG	2A	3221	1/1	0.96	0.20	60,60,60,60	0
58	MG	2A	3787	1/1	0.96	0.10	52,52,52,52	0
58	MG	2A	3479	1/1	0.96	0.10	43,43,43,43	0
58	MG	2A	3790	1/1	0.96	0.08	58,58,58,58	0
58	MG	2a	1771	1/1	0.96	0.10	63,63,63,63	0
58	MG	1A	3682	1/1	0.96	0.04	27,27,27,27	0
58	MG	17	104	1/1	0.96	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	17	105	1/1	0.96	0.07	28,28,28,28	0
58	MG	1a	1810	1/1	0.96	0.14	56,56,56,56	0
58	MG	17	106	1/1	0.96	0.11	54,54,54,54	0
58	MG	2A	3796	1/1	0.96	0.10	52,52,52,52	0
58	MG	2a	1780	1/1	0.96	0.10	56,56,56,56	0
58	MG	1A	3189	1/1	0.96	0.09	35,35,35,35	0
58	MG	2a	1782	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3019	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3799	1/1	0.96	0.07	47,47,47,47	0
58	MG	18	103	1/1	0.96	0.07	35,35,35,35	0
58	MG	2a	1786	1/1	0.96	0.08	54,54,54,54	0
58	MG	1A	3541	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3690	1/1	0.96	0.06	35,35,35,35	0
58	MG	2A	3491	1/1	0.96	0.13	49,49,49,49	0
58	MG	1m	3001	1/1	0.96	0.05	59,59,59,59	0
58	MG	1A	3103	1/1	0.96	0.12	28,28,28,28	0
58	MG	1A	3161	1/1	0.96	0.37	35,35,35,35	0
58	MG	2a	1793	1/1	0.96	0.06	65,65,65,65	0
58	MG	1A	3694	1/1	0.96	0.08	69,69,69,69	0
58	MG	2A	3499	1/1	0.96	0.07	63,63,63,63	0
58	MG	1A	3246	1/1	0.96	0.05	46,46,46,46	0
58	MG	1A	3447	1/1	0.96	0.21	35,35,35,35	0
58	MG	1A	3196	1/1	0.96	0.04	30,30,30,30	0
58	MG	1A	3365	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3197	1/1	0.96	0.21	32,32,32,32	0
58	MG	1A	4063	1/1	0.96	0.05	36,36,36,36	0
58	MG	2A	3506	1/1	0.96	0.10	28,28,28,28	0
58	MG	2A	3821	1/1	0.96	0.08	51,51,51,51	0
58	MG	2A	3822	1/1	0.96	0.10	47,47,47,47	0
58	MG	1A	3703	1/1	0.96	0.06	17,17,17,17	0
58	MG	2A	3824	1/1	0.96	0.07	46,46,46,46	0
58	MG	1x	103	1/1	0.96	0.18	53,53,53,53	0
58	MG	1A	3039	1/1	0.96	0.07	49,49,49,49	0
58	MG	1A	3009	1/1	0.96	0.07	28,28,28,28	0
58	MG	2A	3512	1/1	0.96	0.09	64,64,64,64	0
58	MG	1a	1612	1/1	0.96	0.10	26,26,26,26	0
58	MG	2a	1813	1/1	0.96	0.05	63,63,63,63	0
58	MG	2A	3832	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	4070	1/1	0.96	0.06	32,32,32,32	0
58	MG	1x	108	1/1	0.96	0.06	26,26,26,26	0
58	MG	1A	3311	1/1	0.96	0.21	44,44,44,44	0
58	MG	1A	3879	1/1	0.96	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3838	1/1	0.96	0.07	40,40,40,40	0
58	MG	2a	1820	1/1	0.96	0.14	61,61,61,61	0
58	MG	1A	3562	1/1	0.96	0.08	57,57,57,57	0
58	MG	1a	1617	1/1	0.96	0.05	52,52,52,52	0
58	MG	2A	3842	1/1	0.96	0.07	46,46,46,46	0
58	MG	1A	3371	1/1	0.96	0.29	47,47,47,47	0
58	MG	2A	3844	1/1	0.96	0.09	45,45,45,45	0
58	MG	1A	3255	1/1	0.96	0.09	22,22,22,22	0
58	MG	2A	3523	1/1	0.96	0.05	47,47,47,47	0
58	MG	2A	3259	1/1	0.96	0.09	53,53,53,53	0
58	MG	2A	3006	1/1	0.96	0.23	55,55,55,55	0
58	MG	1A	3884	1/1	0.96	0.12	30,30,30,30	0
58	MG	1A	3203	1/1	0.96	0.14	21,21,21,21	0
58	MG	2A	3009	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3010	1/1	0.96	0.09	61,61,61,61	0
58	MG	1A	3314	1/1	0.96	0.17	53,53,53,53	0
58	MG	1A	3136	1/1	0.96	0.14	22,22,22,22	0
58	MG	2A	3858	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3717	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3533	1/1	0.96	0.20	60,60,60,60	0
58	MG	1A	3719	1/1	0.96	0.06	47,47,47,47	0
58	MG	2A	3536	1/1	0.96	0.09	55,55,55,55	0
58	MG	2A	3863	1/1	0.96	0.08	58,58,58,58	0
58	MG	2A	3017	1/1	0.96	0.07	40,40,40,40	0
58	MG	2A	3018	1/1	0.96	0.17	49,49,49,49	0
58	MG	1A	4085	1/1	0.96	0.11	39,39,39,39	0
58	MG	1A	3572	1/1	0.96	0.05	35,35,35,35	0
58	MG	1A	3316	1/1	0.96	0.21	31,31,31,31	0
58	MG	2A	3278	1/1	0.96	0.08	60,60,60,60	0
58	MG	2A	3543	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3544	1/1	0.96	0.06	37,37,37,37	0
58	MG	1A	4088	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3725	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3574	1/1	0.96	0.11	40,40,40,40	0
58	MG	1A	3575	1/1	0.96	0.12	45,45,45,45	0
58	MG	1A	3729	1/1	0.96	0.08	63,63,63,63	0
58	MG	2A	3031	1/1	0.96	0.08	48,48,48,48	0
58	MG	1A	3165	1/1	0.96	0.16	35,35,35,35	0
58	MG	2A	3556	1/1	0.96	0.06	41,41,41,41	0
58	MG	2A	3557	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3558	1/1	0.96	0.08	62,62,62,62	0
59	K	2A	3448	1/1	0.96	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	ZN	14	102	1/1	0.96	0.10	112,112,112,112	0
58	MG	1A	3398	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3071	1/1	0.97	0.15	28,28,28,28	0
58	MG	1A	3400	1/1	0.97	0.06	36,36,36,36	0
58	MG	1B	207	1/1	0.97	0.15	46,46,46,46	0
58	MG	2A	3326	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3204	1/1	0.97	0.10	27,27,27,27	0
58	MG	1A	3263	1/1	0.97	0.23	46,46,46,46	0
58	MG	2Q	202	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3730	1/1	0.97	0.07	47,47,47,47	0
58	MG	1A	3005	1/1	0.97	0.05	26,26,26,26	0
58	MG	1A	3901	1/1	0.97	0.10	33,33,33,33	0
58	MG	2A	3611	1/1	0.97	0.08	36,36,36,36	0
58	MG	1a	1662	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	3107	1/1	0.97	0.21	31,31,31,31	0
58	MG	2A	3614	1/1	0.97	0.08	45,45,45,45	0
58	MG	1B	214	1/1	0.97	0.19	51,51,51,51	0
58	MG	2V	202	1/1	0.97	0.05	51,51,51,51	0
58	MG	1A	3406	1/1	0.97	0.09	42,42,42,42	0
58	MG	2X	101	1/1	0.97	0.07	64,64,64,64	0
58	MG	1B	218	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3034	1/1	0.97	0.06	45,45,45,45	0
58	MG	20	101	1/1	0.97	0.16	64,64,64,64	0
58	MG	1B	220	1/1	0.97	0.08	31,31,31,31	0
58	MG	2A	3339	1/1	0.97	0.05	51,51,51,51	0
58	MG	2A	3077	1/1	0.97	0.09	37,37,37,37	0
58	MG	2A	3622	1/1	0.97	0.10	51,51,51,51	0
58	MG	1A	3738	1/1	0.97	0.09	58,58,58,58	0
58	MG	2A	3079	1/1	0.97	0.07	24,24,24,24	0
58	MG	1A	3739	1/1	0.97	0.07	37,37,37,37	0
58	MG	2A	3626	1/1	0.97	0.07	41,41,41,41	0
58	MG	25	103	1/1	0.97	0.08	47,47,47,47	0
58	MG	1A	3908	1/1	0.97	0.10	33,33,33,33	0
58	MG	27	101	1/1	0.97	0.16	51,51,51,51	0
58	MG	1A	3741	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3629	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3910	1/1	0.97	0.14	32,32,32,32	0
58	MG	2A	3084	1/1	0.97	0.06	43,43,43,43	0
58	MG	2A	3633	1/1	0.97	0.08	52,52,52,52	0
58	MG	1A	3912	1/1	0.97	0.03	26,26,26,26	0
58	MG	1B	227	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3154	1/1	0.97	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3088	1/1	0.97	0.06	50,50,50,50	0
58	MG	1A	3268	1/1	0.97	0.23	40,40,40,40	0
58	MG	1A	3745	1/1	0.97	0.06	42,42,42,42	0
58	MG	1A	3491	1/1	0.97	0.12	46,46,46,46	0
58	MG	1A	3492	1/1	0.97	0.10	36,36,36,36	0
58	MG	1A	3209	1/1	0.97	0.06	36,36,36,36	0
58	MG	1a	1682	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3645	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3494	1/1	0.97	0.09	45,45,45,45	0
58	MG	2a	1615	1/1	0.97	0.07	67,67,67,67	0
58	MG	1A	3112	1/1	0.97	0.10	32,32,32,32	0
58	MG	1a	1685	1/1	0.97	0.12	55,55,55,55	0
58	MG	1A	3753	1/1	0.97	0.04	38,38,38,38	0
58	MG	1D	303	1/1	0.97	0.14	40,40,40,40	0
58	MG	1A	3113	1/1	0.97	0.08	33,33,33,33	0
58	MG	1D	309	1/1	0.97	0.04	32,32,32,32	0
58	MG	1A	3755	1/1	0.97	0.07	32,32,32,32	0
58	MG	1A	3756	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3925	1/1	0.97	0.07	49,49,49,49	0
58	MG	1D	313	1/1	0.97	0.10	31,31,31,31	0
58	MG	1A	3010	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3273	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3928	1/1	0.97	0.04	17,17,17,17	0
58	MG	1A	3932	1/1	0.97	0.04	33,33,33,33	0
58	MG	1A	3933	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3018	1/1	0.97	0.14	39,39,39,39	0
58	MG	1A	3417	1/1	0.97	0.10	37,37,37,37	0
58	MG	1A	3607	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3342	1/1	0.97	0.22	37,37,37,37	0
58	MG	2A	3116	1/1	0.97	0.25	56,56,56,56	0
58	MG	1A	3276	1/1	0.97	0.09	29,29,29,29	0
58	MG	1A	3765	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	3766	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3503	1/1	0.97	0.05	36,36,36,36	0
58	MG	1F	302	1/1	0.97	0.18	32,32,32,32	0
58	MG	1A	3947	1/1	0.97	0.07	57,57,57,57	0
58	MG	1a	1709	1/1	0.97	0.13	45,45,45,45	0
58	MG	1F	304	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3948	1/1	0.97	0.09	47,47,47,47	0
58	MG	1a	1712	1/1	0.97	0.20	55,55,55,55	0
58	MG	1F	308	1/1	0.97	0.17	29,29,29,29	0
58	MG	2A	3682	1/1	0.97	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3616	1/1	0.97	0.04	36,36,36,36	0
58	MG	1A	3345	1/1	0.97	0.16	33,33,33,33	0
58	MG	1A	3770	1/1	0.97	0.13	25,25,25,25	0
58	MG	1F	312	1/1	0.97	0.05	48,48,48,48	0
58	MG	1A	3952	1/1	0.97	0.07	55,55,55,55	0
58	MG	1a	1719	1/1	0.97	0.10	52,52,52,52	0
58	MG	1A	3771	1/1	0.97	0.05	23,23,23,23	0
58	MG	1G	202	1/1	0.97	0.20	50,50,50,50	0
58	MG	1a	1722	1/1	0.97	0.08	45,45,45,45	0
58	MG	1a	1723	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3421	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3773	1/1	0.97	0.04	45,45,45,45	0
58	MG	2A	3143	1/1	0.97	0.17	41,41,41,41	0
58	MG	1A	3277	1/1	0.97	0.32	44,44,44,44	0
58	MG	1A	3423	1/1	0.97	0.06	42,42,42,42	0
58	MG	1A	3424	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3779	1/1	0.97	0.06	21,21,21,21	0
58	MG	1A	3780	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	3510	1/1	0.97	0.29	31,31,31,31	0
58	MG	1A	3782	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3041	1/1	0.97	0.16	28,28,28,28	0
58	MG	1a	1735	1/1	0.97	0.10	45,45,45,45	0
58	MG	1O	203	1/1	0.97	0.07	52,52,52,52	0
58	MG	2a	1671	1/1	0.97	0.11	53,53,53,53	0
58	MG	1A	3784	1/1	0.97	0.05	17,17,17,17	0
58	MG	2A	3158	1/1	0.97	0.11	47,47,47,47	0
58	MG	1P	201	1/1	0.97	0.14	23,23,23,23	0
58	MG	1A	3628	1/1	0.97	0.07	53,53,53,53	0
58	MG	2a	1676	1/1	0.97	0.09	51,51,51,51	0
58	MG	1A	3513	1/1	0.97	0.10	24,24,24,24	0
58	MG	1P	205	1/1	0.97	0.04	33,33,33,33	0
58	MG	1A	3787	1/1	0.97	0.03	23,23,23,23	0
58	MG	2A	3715	1/1	0.97	0.10	50,50,50,50	0
58	MG	1Q	201	1/1	0.97	0.23	32,32,32,32	0
58	MG	1A	3082	1/1	0.97	0.21	32,32,32,32	0
58	MG	1A	3083	1/1	0.97	0.12	35,35,35,35	0
58	MG	1A	3633	1/1	0.97	0.05	20,20,20,20	0
58	MG	1a	1750	1/1	0.97	0.08	59,59,59,59	0
58	MG	1a	1751	1/1	0.97	0.05	54,54,54,54	0
58	MG	1A	3166	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3122	1/1	0.97	0.12	29,29,29,29	0
58	MG	1A	3637	1/1	0.97	0.07	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	3287	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3797	1/1	0.97	0.07	16,16,16,16	0
58	MG	1A	3979	1/1	0.97	0.12	46,46,46,46	0
58	MG	1A	3123	1/1	0.97	0.12	35,35,35,35	0
58	MG	1T	201	1/1	0.97	0.12	46,46,46,46	0
58	MG	1A	3224	1/1	0.97	0.08	48,48,48,48	0
58	MG	1A	3084	1/1	0.97	0.14	32,32,32,32	0
58	MG	2a	1697	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3802	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3184	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3642	1/1	0.97	0.04	15,15,15,15	0
58	MG	1A	3804	1/1	0.97	0.05	23,23,23,23	0
58	MG	1a	1766	1/1	0.97	0.08	66,66,66,66	0
58	MG	2A	3189	1/1	0.97	0.06	63,63,63,63	0
58	MG	1A	3805	1/1	0.97	0.07	22,22,22,22	0
58	MG	1V	201	1/1	0.97	0.17	23,23,23,23	0
58	MG	1A	3226	1/1	0.97	0.11	32,32,32,32	0
58	MG	1A	3125	1/1	0.97	0.15	35,35,35,35	0
58	MG	1A	3438	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3229	1/1	0.97	0.08	36,36,36,36	0
58	MG	2A	3749	1/1	0.97	0.05	45,45,45,45	0
58	MG	2a	1712	1/1	0.97	0.14	57,57,57,57	0
58	MG	1A	3171	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3175	1/1	0.97	0.09	29,29,29,29	0
58	MG	1W	203	1/1	0.97	0.09	38,38,38,38	0
58	MG	1W	206	1/1	0.97	0.12	26,26,26,26	0
58	MG	2A	3754	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3126	1/1	0.97	0.20	32,32,32,32	0
58	MG	2A	3463	1/1	0.97	0.11	62,62,62,62	0
58	MG	1A	3443	1/1	0.97	0.11	28,28,28,28	0
58	MG	1A	3816	1/1	0.97	0.05	24,24,24,24	0
58	MG	1a	1781	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3652	1/1	0.97	0.08	34,34,34,34	0
58	MG	1A	4003	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3818	1/1	0.97	0.30	29,29,29,29	0
58	MG	1a	1786	1/1	0.97	0.10	52,52,52,52	0
58	MG	1A	3444	1/1	0.97	0.08	32,32,32,32	0
58	MG	2A	3766	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	4008	1/1	0.97	0.05	37,37,37,37	0
58	MG	2A	3210	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3474	1/1	0.97	0.04	45,45,45,45	0
58	MG	2A	3211	1/1	0.97	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4009	1/1	0.97	0.06	29,29,29,29	0
58	MG	1A	4010	1/1	0.97	0.04	37,37,37,37	0
58	MG	1A	3822	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3364	1/1	0.97	0.18	32,32,32,32	0
58	MG	1A	4013	1/1	0.97	0.07	66,66,66,66	0
58	MG	1A	3533	1/1	0.97	0.26	39,39,39,39	0
58	MG	1A	3233	1/1	0.97	0.07	62,62,62,62	0
58	MG	1A	3658	1/1	0.97	0.12	55,55,55,55	0
58	MG	1a	1800	1/1	0.97	0.06	60,60,60,60	0
58	MG	1a	1801	1/1	0.97	0.21	48,48,48,48	0
58	MG	1A	3535	1/1	0.97	0.20	41,41,41,41	0
58	MG	1A	3366	1/1	0.97	0.24	37,37,37,37	0
58	MG	1A	3830	1/1	0.97	0.09	29,29,29,29	0
58	MG	1A	3831	1/1	0.97	0.08	48,48,48,48	0
58	MG	2A	3226	1/1	0.97	0.08	42,42,42,42	0
58	MG	2a	1748	1/1	0.97	0.04	58,58,58,58	0
58	MG	12	101	1/1	0.97	0.08	42,42,42,42	0
58	MG	2A	3788	1/1	0.97	0.06	62,62,62,62	0
58	MG	1A	3832	1/1	0.97	0.06	45,45,45,45	0
58	MG	2A	3497	1/1	0.97	0.09	52,52,52,52	0
58	MG	1A	4023	1/1	0.97	0.07	62,62,62,62	0
58	MG	1A	4024	1/1	0.97	0.09	30,30,30,30	0
58	MG	1A	3234	1/1	0.97	0.26	37,37,37,37	0
58	MG	1A	4028	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3233	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3662	1/1	0.97	0.04	22,22,22,22	0
58	MG	1A	3043	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3237	1/1	0.97	0.19	28,28,28,28	0
58	MG	1A	3058	1/1	0.97	0.10	47,47,47,47	0
58	MG	15	104	1/1	0.97	0.27	26,26,26,26	0
58	MG	1A	3014	1/1	0.97	0.11	37,37,37,37	0
58	MG	1A	3668	1/1	0.97	0.05	19,19,19,19	0
58	MG	1A	3455	1/1	0.97	0.19	38,38,38,38	0
58	MG	1A	3130	1/1	0.97	0.13	43,43,43,43	0
58	MG	2A	3805	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	4038	1/1	0.97	0.08	26,26,26,26	0
58	MG	1A	3842	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3008	1/1	0.97	0.04	30,30,30,30	0
58	MG	1A	3675	1/1	0.97	0.05	17,17,17,17	0
58	MG	2A	3517	1/1	0.97	0.06	53,53,53,53	0
58	MG	2a	1774	1/1	0.97	0.07	64,64,64,64	0
58	MG	1A	3845	1/1	0.97	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4044	1/1	0.97	0.05	28,28,28,28	0
58	MG	1A	3132	1/1	0.97	0.21	31,31,31,31	0
58	MG	2A	3816	1/1	0.97	0.05	46,46,46,46	0
58	MG	2a	1779	1/1	0.97	0.05	46,46,46,46	0
58	MG	18	104	1/1	0.97	0.14	33,33,33,33	0
58	MG	2A	3252	1/1	0.97	0.12	61,61,61,61	0
58	MG	1A	3547	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3548	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3849	1/1	0.97	0.13	41,41,41,41	0
58	MG	1A	3851	1/1	0.97	0.17	31,31,31,31	0
58	MG	1A	3852	1/1	0.97	0.06	16,16,16,16	0
58	MG	1A	3681	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3550	1/1	0.97	0.18	33,33,33,33	0
58	MG	1A	3134	1/1	0.97	0.08	27,27,27,27	0
58	MG	1A	3046	1/1	0.97	0.13	28,28,28,28	0
58	MG	2A	3003	1/1	0.97	0.28	55,55,55,55	0
58	MG	2A	3004	1/1	0.97	0.26	44,44,44,44	0
58	MG	2A	3265	1/1	0.97	0.14	47,47,47,47	0
58	MG	2A	3535	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	4059	1/1	0.97	0.09	15,15,15,15	0
58	MG	2A	3836	1/1	0.97	0.09	44,44,44,44	0
58	MG	2A	3267	1/1	0.97	0.07	50,50,50,50	0
58	MG	1A	3686	1/1	0.97	0.05	29,29,29,29	0
58	MG	2A	3839	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3553	1/1	0.97	0.14	34,34,34,34	0
58	MG	1A	3689	1/1	0.97	0.04	22,22,22,22	0
58	MG	1a	1609	1/1	0.97	0.07	54,54,54,54	0
58	MG	1a	1610	1/1	0.97	0.19	48,48,48,48	0
58	MG	2A	3011	1/1	0.97	0.11	53,53,53,53	0
58	MG	2A	3274	1/1	0.97	0.08	62,62,62,62	0
58	MG	2A	3545	1/1	0.97	0.04	44,44,44,44	0
58	MG	2a	1807	1/1	0.97	0.20	51,51,51,51	0
58	MG	2A	3012	1/1	0.97	0.04	37,37,37,37	0
58	MG	1A	4066	1/1	0.97	0.12	47,47,47,47	0
58	MG	1A	3188	1/1	0.97	0.11	39,39,39,39	0
58	MG	1A	3463	1/1	0.97	0.12	40,40,40,40	0
58	MG	2A	3279	1/1	0.97	0.09	48,48,48,48	0
58	MG	1A	3247	1/1	0.97	0.19	36,36,36,36	0
58	MG	1A	3693	1/1	0.97	0.04	26,26,26,26	0
58	MG	2A	3555	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3559	1/1	0.97	0.14	26,26,26,26	0
58	MG	2A	3019	1/1	0.97	0.08	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	1A	4072	1/1	0.97	0.08	38,38,38,38	0
58	MG	2A	3559	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3560	1/1	0.97	0.06	22,22,22,22	0
58	MG	1a	1619	1/1	0.97	0.05	57,57,57,57	0
58	MG	1A	3063	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3384	1/1	0.97	0.26	43,43,43,43	0
58	MG	2A	3027	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	4077	1/1	0.97	0.13	44,44,44,44	0
58	MG	1A	3318	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3566	1/1	0.97	0.26	36,36,36,36	0
58	MG	1a	1625	1/1	0.97	0.12	58,58,58,58	0
58	MG	2A	3569	1/1	0.97	0.10	43,43,43,43	0
58	MG	2A	3032	1/1	0.97	0.05	51,51,51,51	0
58	MG	1A	3028	1/1	0.97	0.12	34,34,34,34	0
58	MG	1A	3193	1/1	0.97	0.11	25,25,25,25	0
58	MG	1A	3706	1/1	0.97	0.04	25,25,25,25	0
58	MG	2f	201	1/1	0.97	0.09	49,49,49,49	0
58	MG	1a	1629	1/1	0.97	0.18	43,43,43,43	0
58	MG	2A	3575	1/1	0.97	0.04	27,27,27,27	0
58	MG	1A	3065	1/1	0.97	0.08	29,29,29,29	0
58	MG	2A	3040	1/1	0.97	0.17	51,51,51,51	0
58	MG	1A	3099	1/1	0.97	0.04	38,38,38,38	0
58	MG	1A	3145	1/1	0.97	0.10	27,27,27,27	0
58	MG	1A	3031	1/1	0.97	0.11	23,23,23,23	0
58	MG	1A	3474	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3880	1/1	0.97	0.05	55,55,55,55	0
58	MG	2D	301	1/1	0.97	0.06	39,39,39,39	0
58	MG	2D	302	1/1	0.97	0.22	43,43,43,43	0
58	MG	1A	3576	1/1	0.97	0.09	36,36,36,36	0
58	MG	2r	101	1/1	0.97	0.12	50,50,50,50	0
58	MG	2D	304	1/1	0.97	0.07	34,34,34,34	0
58	MG	1a	1638	1/1	0.97	0.15	57,57,57,57	0
58	MG	1A	3325	1/1	0.97	0.14	30,30,30,30	0
58	MG	1A	4091	1/1	0.97	0.06	47,47,47,47	0
58	MG	1a	1641	1/1	0.97	0.10	70,70,70,70	0
58	MG	2A	3590	1/1	0.97	0.06	47,47,47,47	0
58	MG	1A	3578	1/1	0.97	0.12	49,49,49,49	0
58	MG	1A	3069	1/1	0.97	0.07	16,16,16,16	0
58	MG	1A	3886	1/1	0.97	0.07	48,48,48,48	0
58	MG	1a	1645	1/1	0.97	0.12	44,44,44,44	0
58	MG	1A	3718	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3102	1/1	0.97	0.13	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	1649	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3478	1/1	0.97	0.05	60,60,60,60	0
58	MG	1A	3722	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3723	1/1	0.97	0.05	22,22,22,22	0
60	ZN	24	501	1/1	0.97	0.12	124,124,124,124	0
61	SF4	2d	303	8/8	0.97	0.05	77,84,90,103	0
58	MG	1A	3695	1/1	0.98	0.07	23,23,23,23	0
58	MG	1A	3587	1/1	0.98	0.21	29,29,29,29	0
58	MG	2A	3112	1/1	0.98	0.10	45,45,45,45	0
58	MG	1B	202	1/1	0.98	0.13	43,43,43,43	0
58	MG	1a	1764	1/1	0.98	0.05	57,57,57,57	0
58	MG	1A	3174	1/1	0.98	0.10	24,24,24,24	0
58	MG	17	103	1/1	0.98	0.13	25,25,25,25	0
58	MG	2A	3117	1/1	0.98	0.26	62,62,62,62	0
58	MG	1A	3819	1/1	0.98	0.03	21,21,21,21	0
58	MG	1A	3589	1/1	0.98	0.09	40,40,40,40	0
58	MG	1A	3821	1/1	0.98	0.03	21,21,21,21	0
58	MG	1A	3105	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3106	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3702	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3825	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3020	1/1	0.98	0.04	21,21,21,21	0
58	MG	1A	3704	1/1	0.98	0.04	15,15,15,15	0
58	MG	2A	3761	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3108	1/1	0.98	0.15	34,34,34,34	0
58	MG	1A	3504	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3110	1/1	0.98	0.04	35,35,35,35	0
58	MG	1B	217	1/1	0.98	0.09	45,45,45,45	0
58	MG	1A	3961	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3708	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3293	1/1	0.98	0.07	54,54,54,54	0
58	MG	1a	1784	1/1	0.98	0.06	41,41,41,41	0
58	MG	2A	3546	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3139	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3772	1/1	0.98	0.06	56,56,56,56	0
58	MG	2A	3548	1/1	0.98	0.11	36,36,36,36	0
58	MG	1A	3359	1/1	0.98	0.07	49,49,49,49	0
58	MG	1A	3966	1/1	0.98	0.06	41,41,41,41	0
58	MG	1a	1789	1/1	0.98	0.04	52,52,52,52	0
58	MG	2A	3139	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3140	1/1	0.98	0.06	29,29,29,29	0
58	MG	2A	3141	1/1	0.98	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3235	1/1	0.98	0.15	23,23,23,23	0
58	MG	1A	3362	1/1	0.98	0.11	46,46,46,46	0
58	MG	1A	3512	1/1	0.98	0.23	25,25,25,25	0
58	MG	1A	3716	1/1	0.98	0.03	12,12,12,12	0
58	MG	1A	3141	1/1	0.98	0.09	17,17,17,17	0
58	MG	1A	3604	1/1	0.98	0.09	43,43,43,43	0
58	MG	1A	3007	1/1	0.98	0.10	35,35,35,35	0
58	MG	1B	232	1/1	0.98	0.04	46,46,46,46	0
58	MG	1a	1799	1/1	0.98	0.09	51,51,51,51	0
58	MG	1A	3436	1/1	0.98	0.08	42,42,42,42	0
58	MG	2A	3154	1/1	0.98	0.11	41,41,41,41	0
58	MG	1A	3437	1/1	0.98	0.20	33,33,33,33	0
58	MG	1A	3143	1/1	0.98	0.09	54,54,54,54	0
58	MG	1A	3303	1/1	0.98	0.04	29,29,29,29	0
58	MG	1B	237	1/1	0.98	0.03	27,27,27,27	0
58	MG	1D	301	1/1	0.98	0.19	42,42,42,42	0
58	MG	1a	1806	1/1	0.98	0.10	56,56,56,56	0
58	MG	1A	3239	1/1	0.98	0.20	33,33,33,33	0
58	MG	2A	3162	1/1	0.98	0.15	39,39,39,39	0
58	MG	1A	3726	1/1	0.98	0.13	56,56,56,56	0
58	MG	1D	305	1/1	0.98	0.08	33,33,33,33	0
58	MG	1D	306	1/1	0.98	0.14	35,35,35,35	0
58	MG	1A	3611	1/1	0.98	0.09	47,47,47,47	0
58	MG	1A	3983	1/1	0.98	0.04	18,18,18,18	0
58	MG	1e	201	1/1	0.98	0.03	49,49,49,49	0
58	MG	2A	3169	1/1	0.98	0.08	54,54,54,54	0
58	MG	2A	3581	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3984	1/1	0.98	0.06	28,28,28,28	0
58	MG	2A	3369	1/1	0.98	0.15	40,40,40,40	0
58	MG	1A	3850	1/1	0.98	0.07	49,49,49,49	0
58	MG	1k	201	1/1	0.98	0.13	45,45,45,45	0
58	MG	1A	3612	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3613	1/1	0.98	0.08	36,36,36,36	0
58	MG	1A	3615	1/1	0.98	0.06	19,19,19,19	0
58	MG	2a	1705	1/1	0.98	0.10	60,60,60,60	0
58	MG	1A	3989	1/1	0.98	0.04	40,40,40,40	0
58	MG	2A	3177	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3818	1/1	0.98	0.10	69,69,69,69	0
58	MG	1E	303	1/1	0.98	0.15	44,44,44,44	0
58	MG	1A	3991	1/1	0.98	0.05	33,33,33,33	0
58	MG	1E	305	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3731	1/1	0.98	0.04	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3732	1/1	0.98	0.03	27,27,27,27	0
58	MG	1A	3733	1/1	0.98	0.05	20,20,20,20	0
58	MG	1E	309	1/1	0.98	0.09	49,49,49,49	0
58	MG	1A	3144	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	3054	1/1	0.98	0.09	29,29,29,29	0
58	MG	2A	3829	1/1	0.98	0.04	66,66,66,66	0
58	MG	1A	3522	1/1	0.98	0.04	35,35,35,35	0
58	MG	2A	3188	1/1	0.98	0.07	46,46,46,46	0
58	MG	1A	3190	1/1	0.98	0.21	31,31,31,31	0
58	MG	1A	3146	1/1	0.98	0.12	26,26,26,26	0
58	MG	1A	3622	1/1	0.98	0.08	24,24,24,24	0
58	MG	1A	3740	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3192	1/1	0.98	0.21	29,29,29,29	0
58	MG	1A	3086	1/1	0.98	0.18	25,25,25,25	0
58	MG	1A	3374	1/1	0.98	0.09	36,36,36,36	0
58	MG	1F	305	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	4006	1/1	0.98	0.03	38,38,38,38	0
58	MG	2A	3397	1/1	0.98	0.15	42,42,42,42	0
58	MG	2A	3398	1/1	0.98	0.11	48,48,48,48	0
58	MG	1A	4007	1/1	0.98	0.04	44,44,44,44	0
58	MG	1A	3068	1/1	0.98	0.10	31,31,31,31	0
58	MG	1A	3035	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3377	1/1	0.98	0.07	41,41,41,41	0
58	MG	1A	3631	1/1	0.98	0.04	16,16,16,16	0
58	MG	1A	3378	1/1	0.98	0.13	24,24,24,24	0
58	MG	1A	3452	1/1	0.98	0.05	45,45,45,45	0
58	MG	2A	3850	1/1	0.98	0.09	53,53,53,53	0
58	MG	2A	3406	1/1	0.98	0.19	38,38,38,38	0
58	MG	1A	4014	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3089	1/1	0.98	0.07	32,32,32,32	0
58	MG	2A	3855	1/1	0.98	0.04	64,64,64,64	0
58	MG	1A	3874	1/1	0.98	0.23	29,29,29,29	0
58	MG	1A	3454	1/1	0.98	0.17	50,50,50,50	0
58	MG	1A	3876	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3249	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3250	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3382	1/1	0.98	0.04	33,33,33,33	0
58	MG	2A	3630	1/1	0.98	0.07	46,46,46,46	0
58	MG	1N	203	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3538	1/1	0.98	0.14	37,37,37,37	0
58	MG	1N	205	1/1	0.98	0.04	36,36,36,36	0
58	MG	1A	3117	1/1	0.98	0.11	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1755	1/1	0.98	0.04	64,64,64,64	0
58	MG	2A	3021	1/1	0.98	0.06	30,30,30,30	0
58	MG	2A	3022	1/1	0.98	0.09	42,42,42,42	0
58	MG	2A	3637	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3317	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3385	1/1	0.98	0.30	25,25,25,25	0
58	MG	1A	3118	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3885	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3387	1/1	0.98	0.16	21,21,21,21	0
58	MG	1P	203	1/1	0.98	0.17	32,32,32,32	0
58	MG	1A	3199	1/1	0.98	0.10	23,23,23,23	0
58	MG	1A	3647	1/1	0.98	0.06	27,27,27,27	0
58	MG	1A	3201	1/1	0.98	0.12	31,31,31,31	0
58	MG	2A	3647	1/1	0.98	0.15	55,55,55,55	0
58	MG	2A	3648	1/1	0.98	0.12	63,63,63,63	0
58	MG	1A	3037	1/1	0.98	0.09	34,34,34,34	0
58	MG	1A	3257	1/1	0.98	0.11	38,38,38,38	0
58	MG	2A	3034	1/1	0.98	0.06	49,49,49,49	0
58	MG	1A	3038	1/1	0.98	0.21	31,31,31,31	0
58	MG	1A	4037	1/1	0.98	0.10	26,26,26,26	0
58	MG	2A	3037	1/1	0.98	0.15	44,44,44,44	0
58	MG	2A	3234	1/1	0.98	0.27	37,37,37,37	0
58	MG	1Q	205	1/1	0.98	0.04	45,45,45,45	0
58	MG	2D	305	1/1	0.98	0.24	39,39,39,39	0
58	MG	2A	3438	1/1	0.98	0.16	46,46,46,46	0
58	MG	2A	3439	1/1	0.98	0.23	53,53,53,53	0
58	MG	1A	3155	1/1	0.98	0.13	27,27,27,27	0
58	MG	1A	3156	1/1	0.98	0.04	30,30,30,30	0
58	MG	2A	3661	1/1	0.98	0.08	38,38,38,38	0
58	MG	1R	201	1/1	0.98	0.08	30,30,30,30	0
58	MG	2E	305	1/1	0.98	0.08	35,35,35,35	0
58	MG	1A	3121	1/1	0.98	0.16	29,29,29,29	0
58	MG	1A	4041	1/1	0.98	0.09	36,36,36,36	0
58	MG	2A	3665	1/1	0.98	0.17	41,41,41,41	0
58	MG	1A	3896	1/1	0.98	0.06	41,41,41,41	0
58	MG	1A	3396	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3775	1/1	0.98	0.06	20,20,20,20	0
58	MG	1A	3899	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	4046	1/1	0.98	0.06	42,42,42,42	0
58	MG	1U	201	1/1	0.98	0.10	30,30,30,30	0
58	MG	1A	3048	1/1	0.98	0.08	25,25,25,25	0
58	MG	1A	3159	1/1	0.98	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3778	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3074	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3558	1/1	0.98	0.06	28,28,28,28	0
58	MG	1U	209	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	4052	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3060	1/1	0.98	0.10	49,49,49,49	0
58	MG	2A	3461	1/1	0.98	0.08	51,51,51,51	0
58	MG	1V	204	1/1	0.98	0.19	30,30,30,30	0
58	MG	1V	205	1/1	0.98	0.18	29,29,29,29	0
58	MG	1A	3906	1/1	0.98	0.07	36,36,36,36	0
58	MG	1V	207	1/1	0.98	0.03	36,36,36,36	0
58	MG	1A	3211	1/1	0.98	0.15	33,33,33,33	0
58	MG	1A	4057	1/1	0.98	0.03	43,43,43,43	0
58	MG	2A	3261	1/1	0.98	0.05	53,53,53,53	0
58	MG	1A	3402	1/1	0.98	0.07	39,39,39,39	0
58	MG	1A	3096	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3097	1/1	0.98	0.07	33,33,33,33	0
58	MG	1W	204	1/1	0.98	0.09	30,30,30,30	0
58	MG	1W	205	1/1	0.98	0.10	32,32,32,32	0
58	MG	1A	3565	1/1	0.98	0.27	38,38,38,38	0
58	MG	1A	3214	1/1	0.98	0.12	34,34,34,34	0
58	MG	1A	3669	1/1	0.98	0.04	18,18,18,18	0
58	MG	1A	3789	1/1	0.98	0.04	45,45,45,45	0
58	MG	2A	3478	1/1	0.98	0.06	48,48,48,48	0
58	MG	1X	103	1/1	0.98	0.23	43,43,43,43	0
58	MG	1X	104	1/1	0.98	0.10	33,33,33,33	0
58	MG	23	104	1/1	0.98	0.07	49,49,49,49	0
58	MG	1X	105	1/1	0.98	0.04	47,47,47,47	0
58	MG	1Y	201	1/1	0.98	0.05	41,41,41,41	0
58	MG	1A	3568	1/1	0.98	0.18	35,35,35,35	0
58	MG	1a	1728	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3077	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3078	1/1	0.98	0.10	26,26,26,26	0
58	MG	1A	3674	1/1	0.98	0.08	24,24,24,24	0
58	MG	1A	3029	1/1	0.98	0.14	22,22,22,22	0
58	MG	1A	3485	1/1	0.98	0.07	36,36,36,36	0
58	MG	2A	3490	1/1	0.98	0.14	33,33,33,33	0
58	MG	10	103	1/1	0.98	0.05	35,35,35,35	0
58	MG	2A	3283	1/1	0.98	0.25	52,52,52,52	0
58	MG	1A	3218	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	4075	1/1	0.98	0.13	46,46,46,46	0
58	MG	1A	3410	1/1	0.98	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3717	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3080	1/1	0.98	0.17	29,29,29,29	0
58	MG	1A	3275	1/1	0.98	0.13	21,21,21,21	0
58	MG	1A	3012	1/1	0.98	0.14	30,30,30,30	0
58	MG	1A	3684	1/1	0.98	0.05	22,22,22,22	0
58	MG	2A	3722	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3221	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3724	1/1	0.98	0.10	50,50,50,50	0
58	MG	1a	1744	1/1	0.98	0.14	38,38,38,38	0
58	MG	1A	3929	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3930	1/1	0.98	0.04	58,58,58,58	0
58	MG	1A	3931	1/1	0.98	0.05	29,29,29,29	0
58	MG	1a	1748	1/1	0.98	0.10	61,61,61,61	0
58	MG	2A	3730	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3032	1/1	0.98	0.25	29,29,29,29	0
58	MG	1A	3133	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3688	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3937	1/1	0.98	0.11	46,46,46,46	0
58	MG	1A	3938	1/1	0.98	0.03	36,36,36,36	0
58	MG	1A	3581	1/1	0.98	0.03	37,37,37,37	0
58	MG	1A	3172	1/1	0.98	0.13	40,40,40,40	0
58	MG	1A	3282	1/1	0.98	0.12	39,39,39,39	0
58	MG	1A	3173	1/1	0.98	0.22	31,31,31,31	0
58	MG	1A	3284	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3944	1/1	0.98	0.07	40,40,40,40	0
60	ZN	2Y	202	1/1	0.98	0.04	96,96,96,96	0
58	MG	2A	3742	1/1	0.98	0.04	49,49,49,49	0
60	ZN	25	106	1/1	0.98	0.03	67,67,67,67	0
60	ZN	29	501	1/1	0.98	0.04	62,62,62,62	0
60	ZN	2n	102	1/1	0.98	0.05	92,92,92,92	0
61	SF4	1d	302	8/8	0.98	0.06	62,67,71,80	0
58	MG	1A	3285	1/1	0.98	0.23	46,46,46,46	0
58	MG	2A	3365	1/1	0.99	0.08	37,37,37,37	0
58	MG	1A	3066	1/1	0.99	0.02	27,27,27,27	0
58	MG	1A	3696	1/1	0.99	0.03	37,37,37,37	0
58	MG	1A	3036	1/1	0.99	0.10	24,24,24,24	0
58	MG	1A	3623	1/1	0.99	0.05	22,22,22,22	0
58	MG	1A	3561	1/1	0.99	0.23	30,30,30,30	0
58	MG	1A	3625	1/1	0.99	0.07	51,51,51,51	0
58	MG	2A	3450	1/1	0.99	0.15	26,26,26,26	0
58	MG	1F	306	1/1	0.99	0.06	42,42,42,42	0
58	MG	1A	3935	1/1	0.99	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3936	1/1	0.99	0.03	40,40,40,40	0
58	MG	1A	3990	1/1	0.99	0.05	44,44,44,44	0
58	MG	1A	3022	1/1	0.99	0.04	16,16,16,16	0
58	MG	1A	3252	1/1	0.99	0.04	26,26,26,26	0
58	MG	2A	3149	1/1	0.99	0.06	36,36,36,36	0
58	MG	1A	3744	1/1	0.99	0.07	20,20,20,20	0
58	MG	2A	3151	1/1	0.99	0.04	37,37,37,37	0
58	MG	1A	3298	1/1	0.99	0.09	23,23,23,23	0
58	MG	1B	216	1/1	0.99	0.04	43,43,43,43	0
58	MG	2A	3708	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3746	1/1	0.99	0.03	11,11,11,11	0
58	MG	1A	3160	1/1	0.99	0.05	24,24,24,24	0
58	MG	1A	4054	1/1	0.99	0.06	22,22,22,22	0
58	MG	1a	1770	1/1	0.99	0.03	39,39,39,39	0
58	MG	1A	3013	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	3666	1/1	0.99	0.03	36,36,36,36	0
58	MG	1A	3750	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	3796	1/1	0.99	0.09	21,21,21,21	0
58	MG	1A	4001	1/1	0.99	0.03	30,30,30,30	0
58	MG	1A	3567	1/1	0.99	0.19	39,39,39,39	0
58	MG	1A	3070	1/1	0.99	0.05	28,28,28,28	0
58	MG	1A	3302	1/1	0.99	0.04	32,32,32,32	0
58	MG	1a	1633	1/1	0.99	0.11	28,28,28,28	0
58	MG	1A	4064	1/1	0.99	0.04	31,31,31,31	0
58	MG	1A	3800	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3178	1/1	0.99	0.09	33,33,33,33	0
58	MG	1A	3635	1/1	0.99	0.05	27,27,27,27	0
58	MG	1A	3672	1/1	0.99	0.06	30,30,30,30	0
58	MG	1A	3093	1/1	0.99	0.06	17,17,17,17	0
58	MG	1A	3279	1/1	0.99	0.12	28,28,28,28	0
58	MG	1A	3806	1/1	0.99	0.03	32,32,32,32	0
58	MG	2A	3813	1/1	0.99	0.06	32,32,32,32	0
58	MG	12	102	1/1	0.99	0.06	39,39,39,39	0
58	MG	2A	3815	1/1	0.99	0.04	43,43,43,43	0
58	MG	1A	3807	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3011	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3462	1/1	0.99	0.10	35,35,35,35	0
58	MG	1A	3677	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3762	1/1	0.99	0.07	35,35,35,35	0
58	MG	1a	1648	1/1	0.99	0.03	49,49,49,49	0
58	MG	1D	304	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3003	1/1	0.99	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3492	1/1	0.99	0.11	25,25,25,25	0
58	MG	2A	3825	1/1	0.99	0.07	20,20,20,20	0
58	MG	1A	3911	1/1	0.99	0.03	23,23,23,23	0
58	MG	1D	307	1/1	0.99	0.12	28,28,28,28	0
58	MG	1A	3679	1/1	0.99	0.02	27,27,27,27	0
58	MG	2A	3496	1/1	0.99	0.03	61,61,61,61	0
58	MG	1A	3200	1/1	0.99	0.03	30,30,30,30	0
58	MG	1R	203	1/1	0.99	0.12	34,34,34,34	0
58	MG	1A	3721	1/1	0.99	0.04	40,40,40,40	0
58	MG	1A	3109	1/1	0.99	0.13	28,28,28,28	0
58	MG	17	101	1/1	0.99	0.05	29,29,29,29	0
58	MG	1A	3030	1/1	0.99	0.14	23,23,23,23	0
58	MG	1A	3184	1/1	0.99	0.04	35,35,35,35	0
58	MG	2W	202	1/1	0.99	0.15	37,37,37,37	0
58	MG	1A	4025	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	4026	1/1	0.99	0.03	41,41,41,41	0
58	MG	2A	3587	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	3549	1/1	0.99	0.17	36,36,36,36	0
58	MG	1a	1736	1/1	0.99	0.08	41,41,41,41	0
58	MG	1U	202	1/1	0.99	0.15	36,36,36,36	0
58	MG	1A	3056	1/1	0.99	0.05	29,29,29,29	0
58	MG	1A	3186	1/1	0.99	0.11	34,34,34,34	0
58	MG	2A	3511	1/1	0.99	0.07	38,38,38,38	0
58	MG	1A	3098	1/1	0.99	0.11	16,16,16,16	0
58	MG	1A	3614	1/1	0.99	0.05	34,34,34,34	0
58	MG	1U	207	1/1	0.99	0.13	26,26,26,26	0
58	MG	1A	3975	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3289	1/1	0.99	0.09	24,24,24,24	0
58	MG	25	104	1/1	0.99	0.05	52,52,52,52	0
60	ZN	1Y	204	1/1	0.99	0.03	70,70,70,70	0
58	MG	1A	3075	1/1	0.99	0.02	33,33,33,33	0
60	ZN	19	501	1/1	0.99	0.11	60,60,60,60	0
60	ZN	1n	103	1/1	0.99	0.02	65,65,65,65	0
58	MG	1A	3042	1/1	0.99	0.20	33,33,33,33	0
58	MG	1V	203	1/1	0.99	0.04	34,34,34,34	0
58	MG	2A	3854	1/1	0.99	0.13	39,39,39,39	0
60	ZN	26	501	1/1	0.99	0.05	61,61,61,61	0
58	MG	1E	312	1/1	0.99	0.11	21,21,21,21	0
58	MG	1A	3343	1/1	0.99	0.11	34,34,34,34	0
58	MG	1A	3228	1/1	0.99	0.15	33,33,33,33	0
58	MG	1A	3655	1/1	0.99	0.06	30,30,30,30	0
58	MG	1a	1787	1/1	1.00	0.02	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4065	1/1	1.00	0.04	22,22,22,22	0
58	MG	1A	3295	1/1	1.00	0.02	28,28,28,28	0
58	MG	1A	4060	1/1	1.00	0.04	21,21,21,21	0
60	ZN	15	107	1/1	1.00	0.01	38,38,38,38	0
60	ZN	16	103	1/1	1.00	0.02	39,39,39,39	0
58	MG	1A	3618	1/1	1.00	0.05	31,31,31,31	0
58	MG	2A	3700	1/1	1.00	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.