



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 11:15 PM UTC

PDB ID : 9D7T / pdb_00009d7t
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with Api137 antimicrobial peptide, mRNA, A-site release factor 1, and deacylated P-site and E-site tRNA^{phe} at 2.70Å resolution
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Deposited on : 2024-08-17
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<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

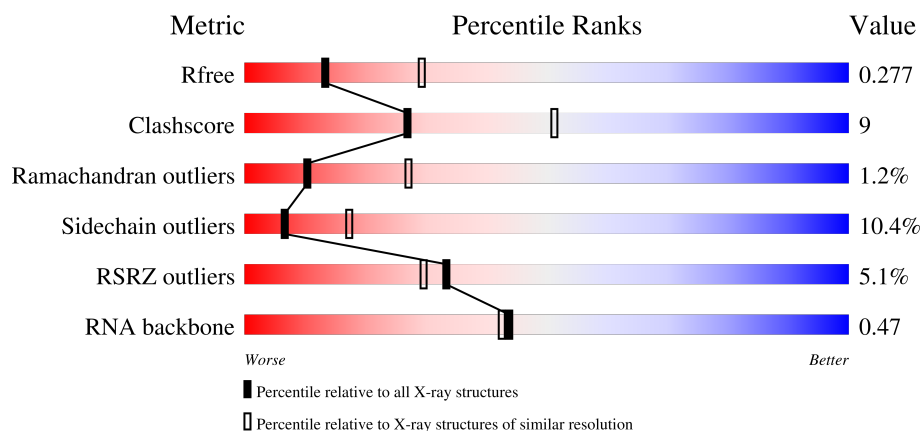
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	 3% 62% 30% 7% .
1	2A	2915	 3% 55% 35% 6% .
2	1B	121	 69% 27% ..

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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	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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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	354	
54	2w	354	
55	1x	76	
55	1y	76	
55	2x	76	
55	2y	76	
56	1z	18	
56	2z	18	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3634	-	-	-	X
57	MG	2A	3116	-	-	-	X
59	SF4	1d	302	-	-	X	-

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 299179 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
			2576	1146	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	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
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	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
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	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
			877	553	175	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
			746	485	134	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
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	183	Total	C	N	O	S	0	0	0
			1437	919	256	260	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1451	928	256	265	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			548	347	99	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	68	Total	C	N	O	S	0	0	0
			517	330	92	90	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
			511	328	99	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
			1554	977	302	274	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
			1659	1040	326	286	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
			1130	714	214	199	3			

- 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	513	143	151	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	123	Total	C	N	O	0	0	0
			940	593	185	162			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	98	Total	C	N	O	0	0	0
			721	449	140	132			
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	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	115	Total	C	N	O	S	0	0	0
			889	546	183	158	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
			486	309	101	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
			551	353	108	90				

- 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 PHE-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			
53	2v	13	Total	C	N	O	P	0	0	0
			274	124	48	89	13			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1954	1208	361	377	8			

- Molecule 55 is a RNA chain called P-site and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	1y	74	Total	C	N	O	P	S	0	0	0
			1590	712	285	517	74	2			
55	2x	75	Total	C	N	O	P	S	0	0	0
			1612	722	288	525	75	2			
55	2y	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			

- Molecule 56 is a protein called Api137 Antimicrobial Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	1z	14	Total	C	N	O	0	0	0
			121	80	25	16			
56	2z	14	Total	C	N	O	0	0	0
			121	80	25	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	807	Total	Mg	0	0
			807	807		
57	1B	20	Total	Mg	0	0
			20	20		
57	1D	6	Total	Mg	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1E	7	Total 7	Mg 7	0	0
57	1F	8	Total 8	Mg 8	0	0
57	1G	3	Total 3	Mg 3	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	2	Total 2	Mg 2	0	0
57	1P	4	Total 4	Mg 4	0	0
57	1Q	5	Total 5	Mg 5	0	0
57	1R	2	Total 2	Mg 2	0	0
57	1T	1	Total 1	Mg 1	0	0
57	1U	6	Total 6	Mg 6	0	0
57	1V	5	Total 5	Mg 5	0	0
57	1W	4	Total 4	Mg 4	0	0
57	1X	3	Total 3	Mg 3	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	5	Total 5	Mg 5	0	0
57	11	4	Total 4	Mg 4	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	1	Total 1	Mg 1	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	4	Total 4	Mg 4	0	0
57	16	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	17	7	Total 7	Mg 7	0	0
57	18	2	Total 2	Mg 2	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	187	Total 187	Mg 187	0	0
57	1c	1	Total 1	Mg 1	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	1	Total 1	Mg 1	0	0
57	1v	3	Total 3	Mg 3	0	0
57	1w	4	Total 4	Mg 4	0	0
57	1x	8	Total 8	Mg 8	0	0
57	1y	2	Total 2	Mg 2	0	0
57	2A	665	Total 665	Mg 665	0	0
57	2B	11	Total 11	Mg 11	0	0
57	2D	9	Total 9	Mg 9	0	0
57	2E	5	Total 5	Mg 5	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2Q	3	Total 3	Mg 3	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2U	1	Total 1	Mg 1	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	4	Total 4	Mg 4	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	20	2	Total 2	Mg 2	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	1	Total 1	Mg 1	0	0
57	28	3	Total 3	Mg 3	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	172	Total 172	Mg 172	0	0
57	2d	1	Total 1	Mg 1	0	0
57	2e	2	Total 2	Mg 2	0	0
57	2f	1	Total 1	Mg 1	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2u	1	Total 1	Mg 1	0	0

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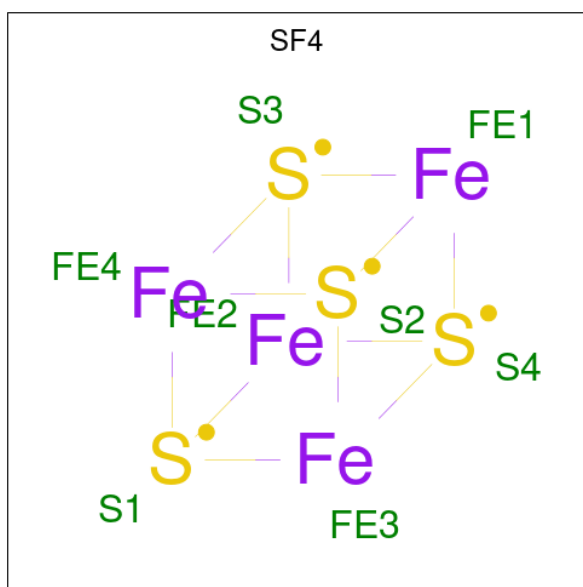
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2v	2	Total 2	Mg 2	0	0
57	2w	2	Total 2	Mg 2	0	0
57	2x	9	Total 9	Mg 9	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total 1	Zn 1	0	0
58	14	1	Total 1	Zn 1	0	0
58	15	1	Total 1	Zn 1	0	0
58	16	1	Total 1	Zn 1	0	0
58	19	1	Total 1	Zn 1	0	0
58	1n	1	Total 1	Zn 1	0	0
58	2Y	1	Total 1	Zn 1	0	0
58	24	1	Total 1	Zn 1	0	0
58	25	1	Total 1	Zn 1	0	0
58	26	1	Total 1	Zn 1	0	0
58	29	1	Total 1	Zn 1	0	0
58	2n	1	Total 1	Zn 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1394	Total	O	0	0
			1394	1394		
60	1B	31	Total	O	0	0
			31	31		
60	1D	15	Total	O	0	0
			15	15		
60	1E	12	Total	O	0	0
			12	12		
60	1F	6	Total	O	0	0
			6	6		
60	1G	1	Total	O	0	0
			1	1		
60	1N	3	Total	O	0	0
			3	3		
60	1O	3	Total	O	0	0
			3	3		
60	1P	15	Total	O	0	0
			15	15		
60	1Q	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1R	2	Total 2	O 2	0	0
60	1T	1	Total 1	O 1	0	0
60	1U	5	Total 5	O 5	0	0
60	1V	1	Total 1	O 1	0	0
60	1W	2	Total 2	O 2	0	0
60	1X	4	Total 4	O 4	0	0
60	10	1	Total 1	O 1	0	0
60	11	3	Total 3	O 3	0	0
60	13	2	Total 2	O 2	0	0
60	15	5	Total 5	O 5	0	0
60	16	1	Total 1	O 1	0	0
60	17	2	Total 2	O 2	0	0
60	18	7	Total 7	O 7	0	0
60	1a	194	Total 194	O 194	0	0
60	1d	1	Total 1	O 1	0	0
60	1l	1	Total 1	O 1	0	0
60	1p	1	Total 1	O 1	0	0
60	1v	3	Total 3	O 3	0	0
60	1w	5	Total 5	O 5	0	0
60	1x	22	Total 22	O 22	0	0
60	1y	1	Total 1	O 1	0	0

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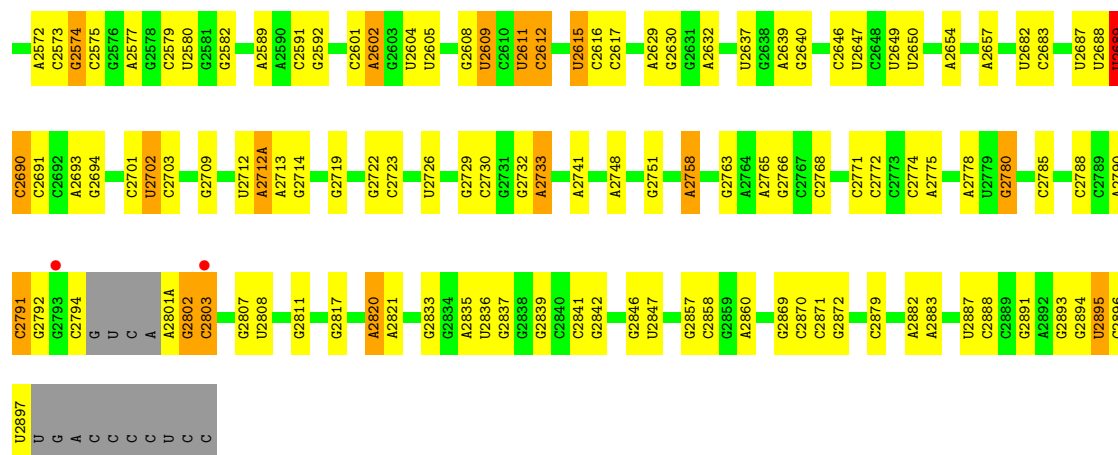
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1z	4	Total 4	O 4	0	0
60	2A	997	Total 997	O 997	0	0
60	2B	7	Total 7	O 7	0	0
60	2D	16	Total 16	O 16	0	0
60	2E	11	Total 11	O 11	0	0
60	2F	5	Total 5	O 5	0	0
60	2N	1	Total 1	O 1	0	0
60	2O	1	Total 1	O 1	0	0
60	2P	12	Total 12	O 12	0	0
60	2Q	1	Total 1	O 1	0	0
60	2R	3	Total 3	O 3	0	0
60	2T	1	Total 1	O 1	0	0
60	2U	2	Total 2	O 2	0	0
60	2W	1	Total 1	O 1	0	0
60	2X	2	Total 2	O 2	0	0
60	2Y	2	Total 2	O 2	0	0
60	20	6	Total 6	O 6	0	0
60	21	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	25	1	Total 1	O 1	0	0
60	27	3	Total 3	O 3	0	0

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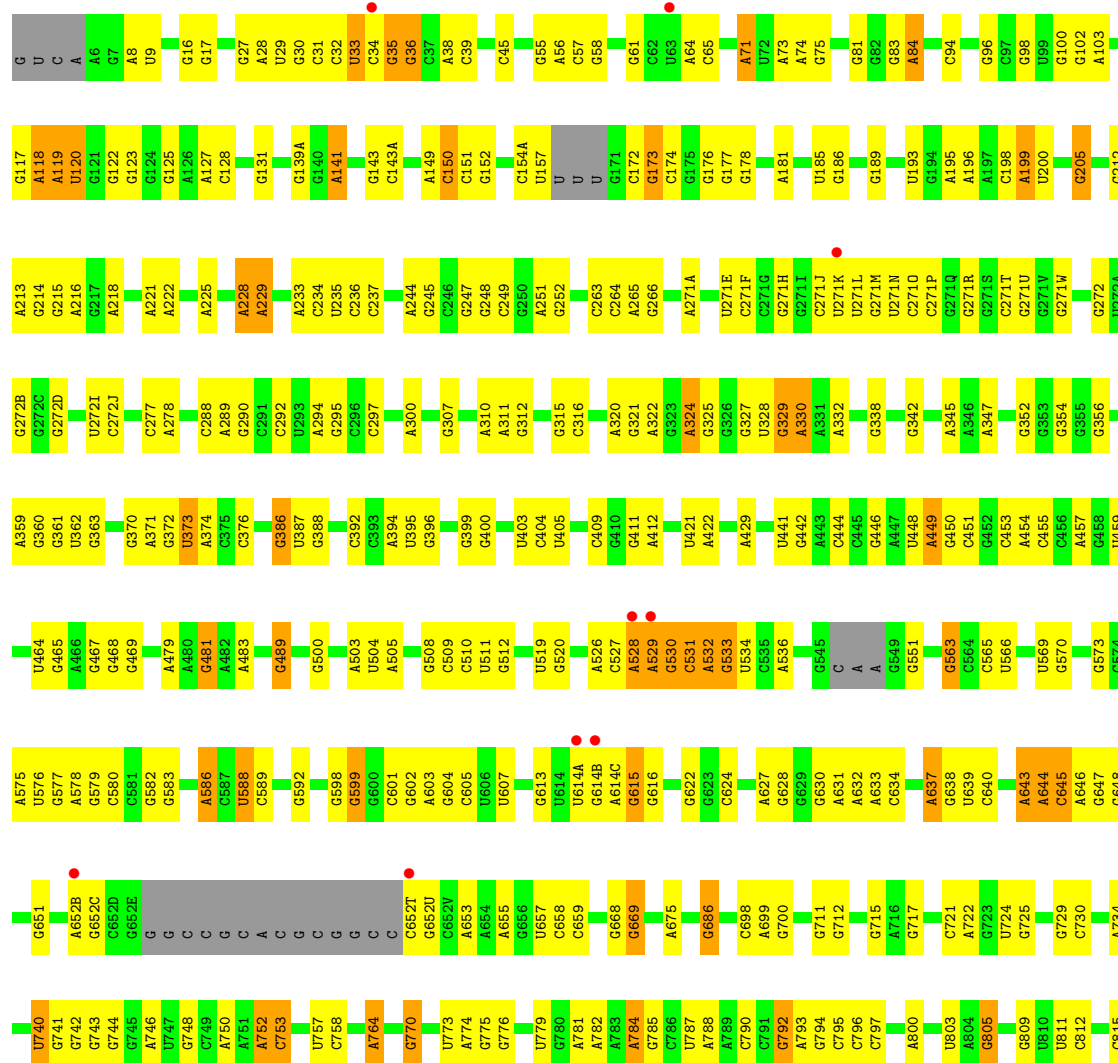
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	28	3	Total 3	O 3	0	0
60	2a	154	Total 154	O 154	0	0
60	2d	1	Total 1	O 1	0	0
60	2j	1	Total 1	O 1	0	0
60	2t	2	Total 2	O 2	0	0
60	2v	2	Total 2	O 2	0	0
60	2w	2	Total 2	O 2	0	0
60	2x	13	Total 13	O 13	0	0

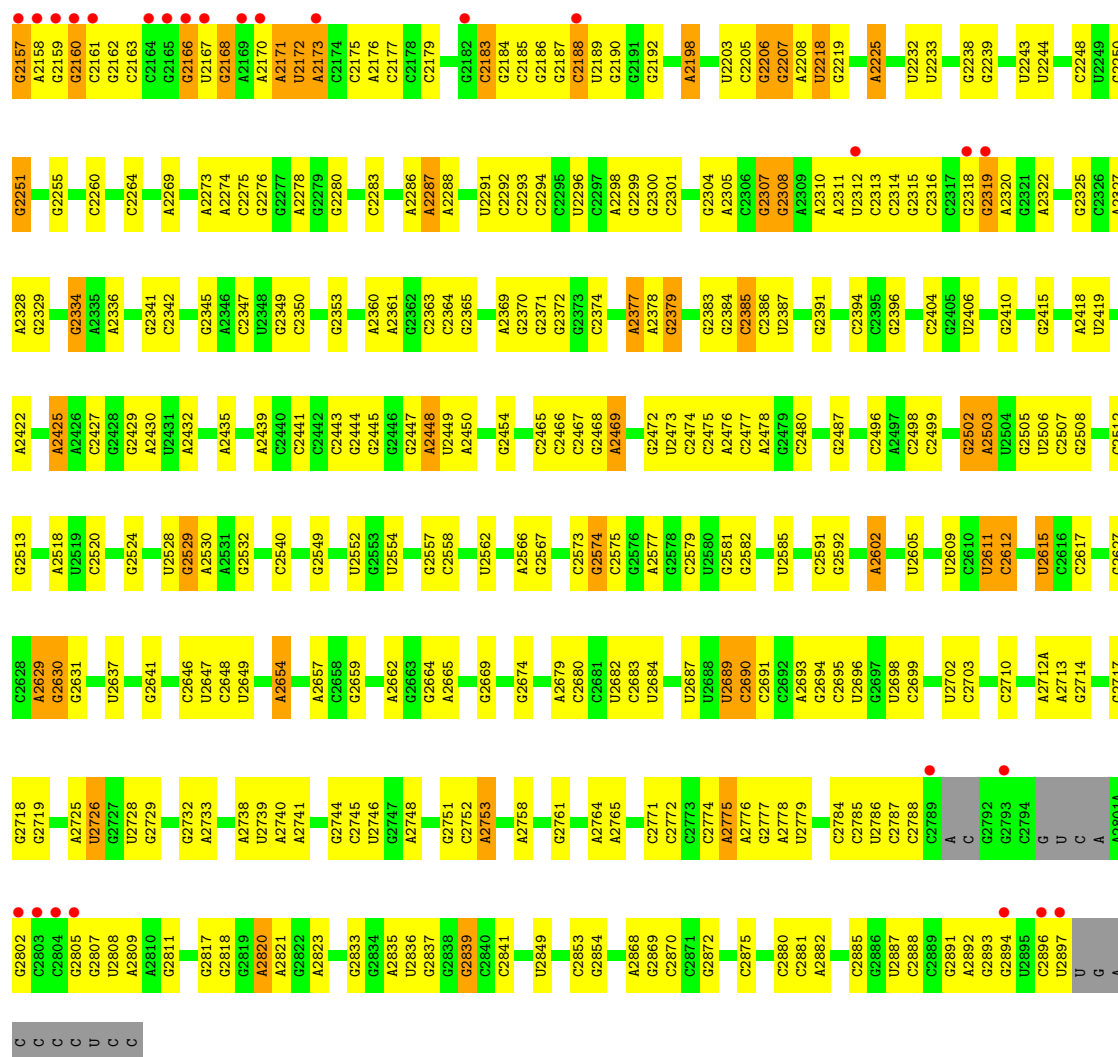
C2471	C2472	A2476	C2477	A2478	C2483	G2484	G2487	G2491	G2494	A2497	C2498	C2499	G2502	A2503	G2504	G2505	G2506	G2507	G2508	A2518	G2519	C2520	G2529	G2532	A2533	A2534	G2535	G2536	C2537	C2538	A2541	G2543	G2544	G2552	G2553	G2554	G2555	G2557	G2563	A2564	A2565	A2566	G2567	C2568																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G2370	G2371	A2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	A2388	G2389	G2390	G2391	C2402	C2403	G2404	G2405	G2406	G2407	G2410	A2422	G2423	G2424	A2425	G2428	G2429	A2430	A2431	A2432	A2435	G2436	A2438	A2439	C2440	C2441	G2445	A2448	G2452	G2458	A2459	U2460	G2461	U2462	G2468	A2469	G2470																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G2277	A2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	A2286	A2287	A2288	G2289	G2290	U2291	G2292	U2296	G2297	A2298	G2299	A2305	G2308	C2313	G2319	A2320	G2325	C2326	A2327	A2328	G2329	G2330	G2331	G2334	A2335	A2336	G2345	A2346	C2347	U2348	G2349	C2350	G2354	C2355	C2356	U2357	C2364	C2365	A2366																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
U2172	A2173	C2174	A2176	C2177	C2178	C2179	U2180	G2181	G2182	G2183	G2184	C2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	A2198	U2203	C2205	G2206	G2207	A2208	G2224	A2225	C2226	U2233	G2234	G2238	U2243	U2244	A2247	G2251	C2254	C2255	C2256	C2260	U2261	A2266	A2267	A2268	A2269	A2273	A2274																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	A2125	C2126	C2127	C2128	C2129	U2130	G2131	U2132	G2133	G2134	A2135	C2136	C2137	C2138	G2139	C2140	G2141	C2142	C2143	U2144	C2145	C2146	G2147	G2148	U2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	G2159	G2160	C2161	G2162	C2163	C2164	G2165	G2166	U2167	G2168	A2169	C2170	A2171																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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• Molecule 1: 23S Ribosomal RNA

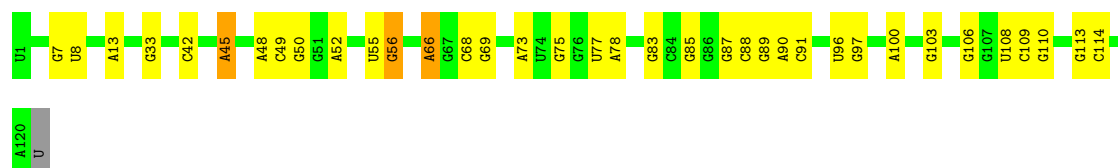


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U2108	G2024	G1922	C1797	A1668	A1569	A1379	A1272	G1170	A	A1022	A916	A916
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●	U2076	C1979	G1883	A1762	A1632	C1531	A1349	A1237	G	A	A999	A999
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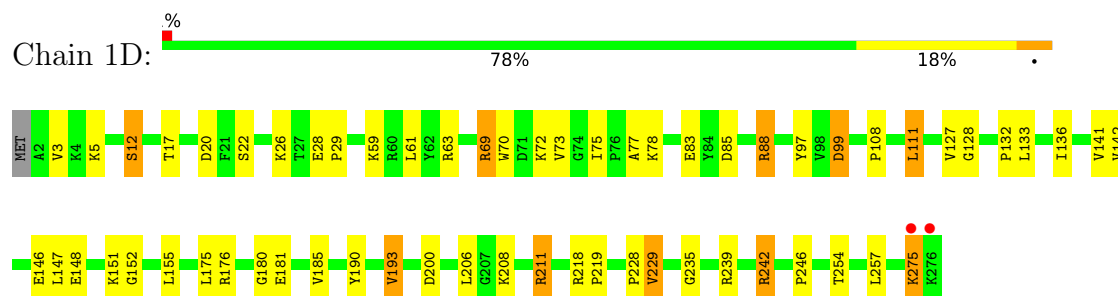


• Molecule 2: 5S Ribosomal RNA

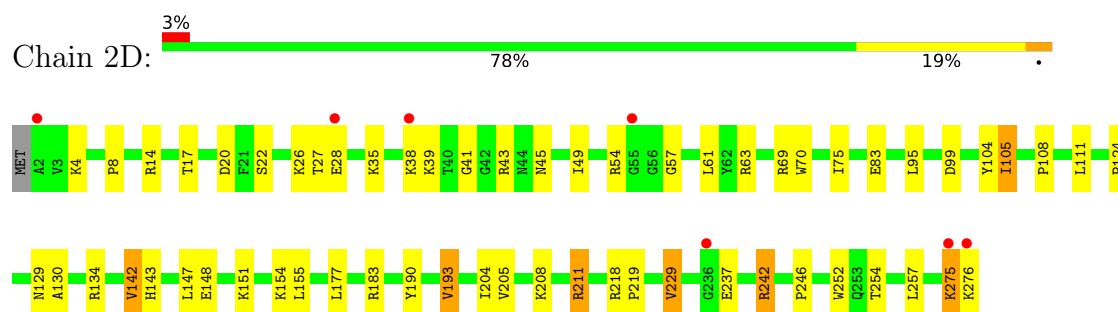
Chain 1B: 69% 27%



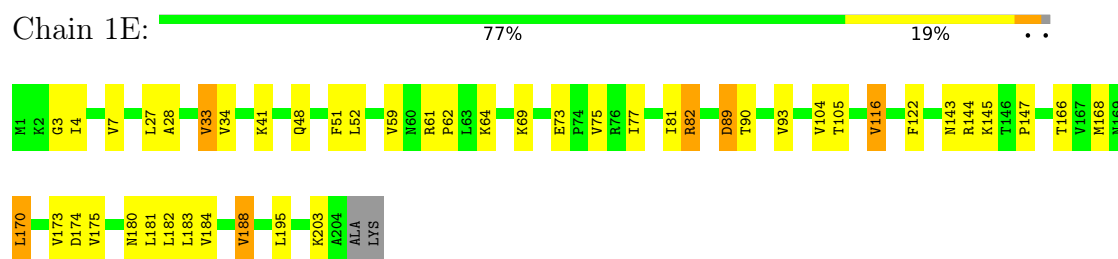
- Molecule 3: 50S ribosomal protein L2



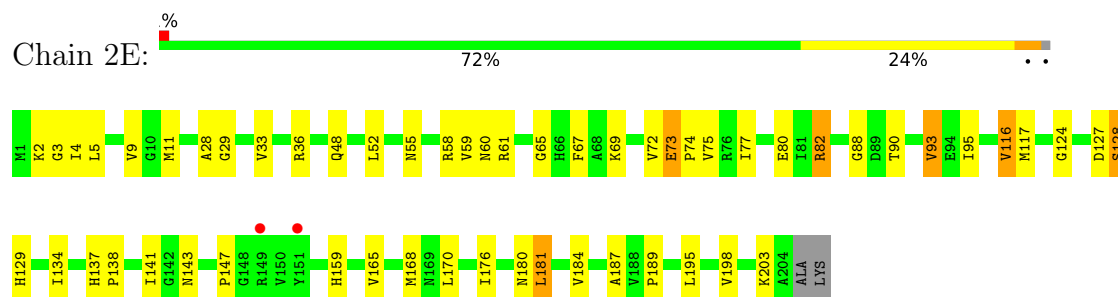
- Molecule 3: 50S ribosomal protein L2



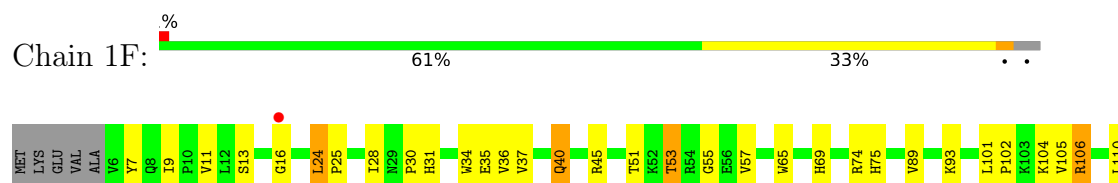
- Molecule 4: 50S ribosomal protein L3

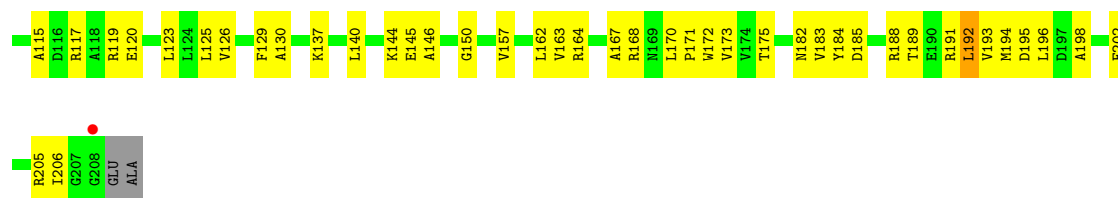


- Molecule 4: 50S ribosomal protein L3



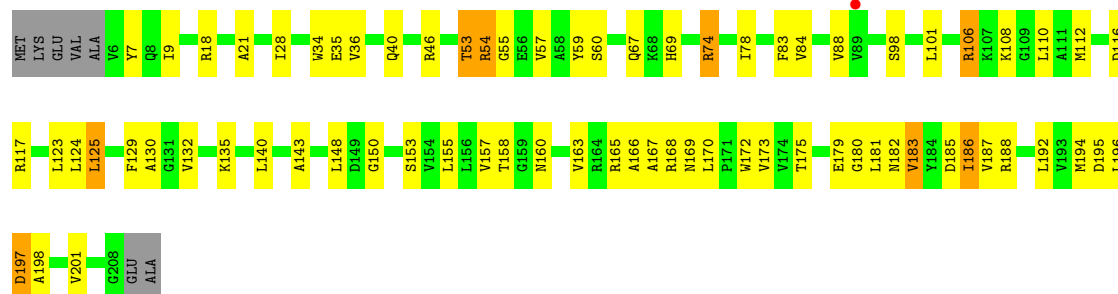
- Molecule 5: 50S ribosomal protein L4





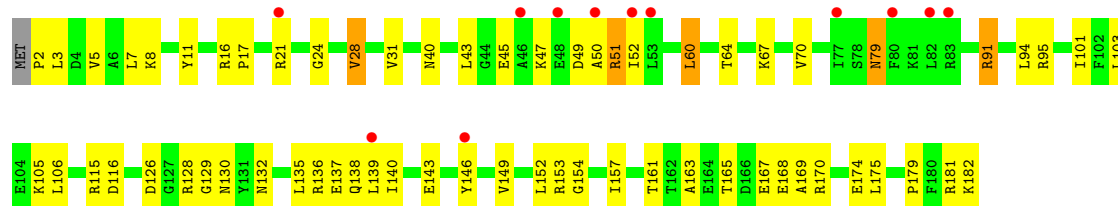
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 62% 31%



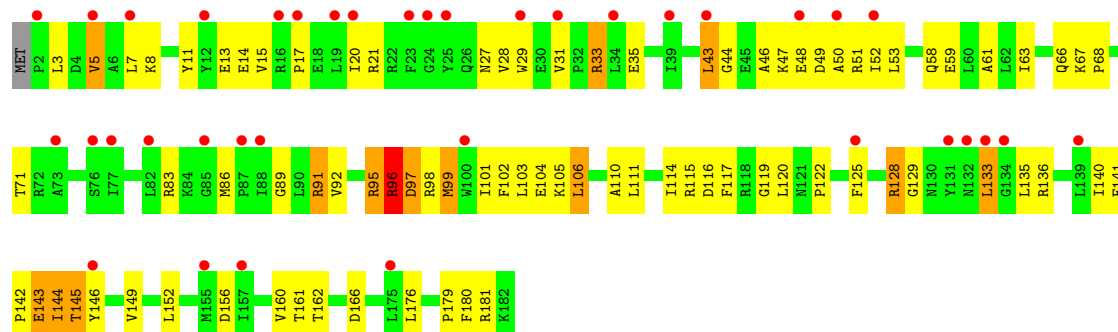
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 7% 64% 32%



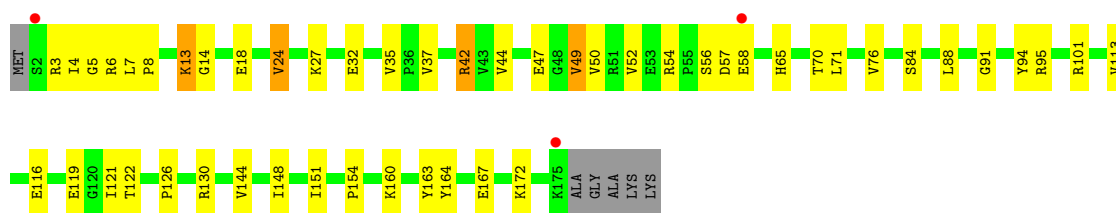
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 20% 53% 38% 7%

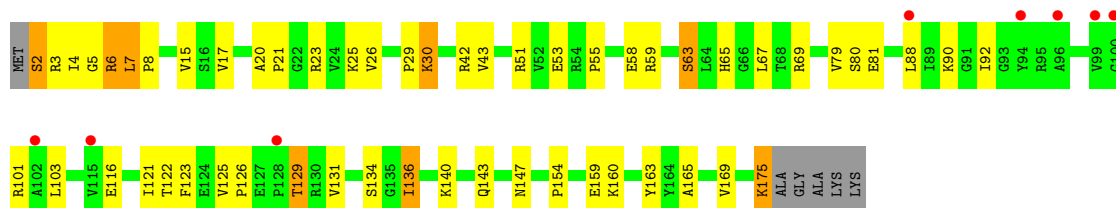


• Molecule 7: 50S ribosomal protein L6

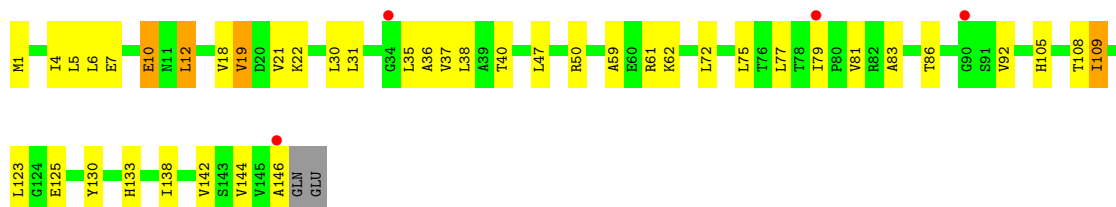
Chain 1H: 2% 69% 26%



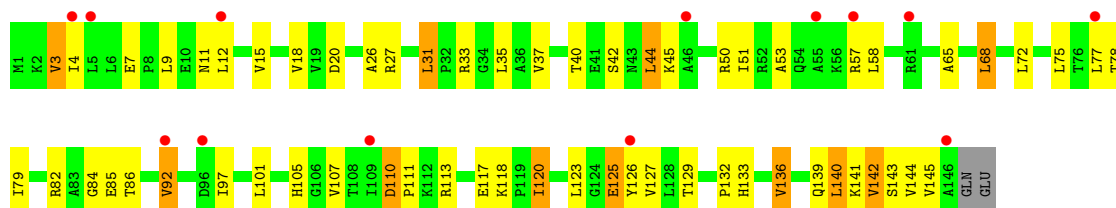
• Molecule 7: 50S ribosomal protein L6



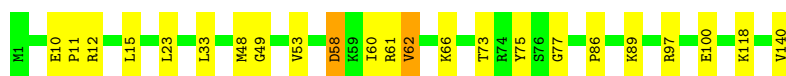
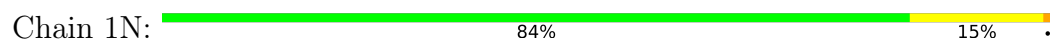
• Molecule 8: 50S ribosomal protein L9



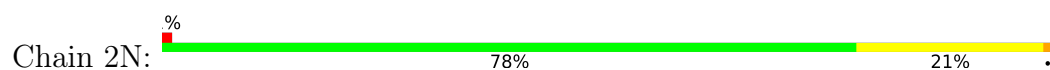
• Molecule 8: 50S ribosomal protein L9

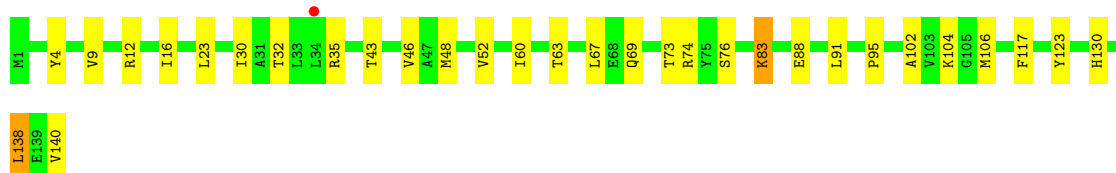


• Molecule 9: 50S ribosomal protein L13



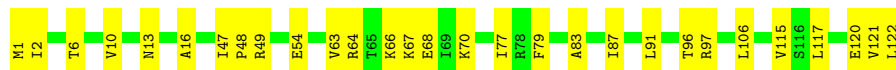
• Molecule 9: 50S ribosomal protein L13





- Molecule 10: 50S ribosomal protein L14

Chain 10: 76% 24%



- Molecule 10: 50S ribosomal protein L14

Chain 20: 71% 28%



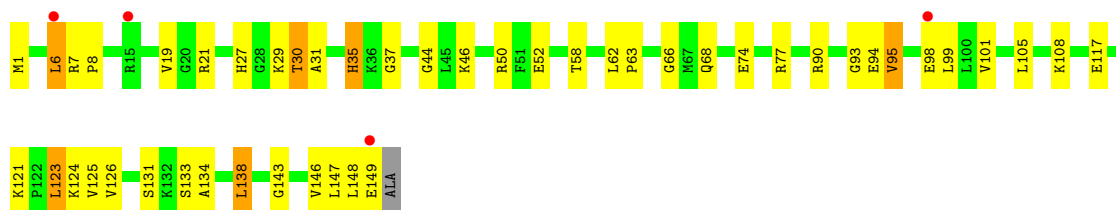
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 73% 25%



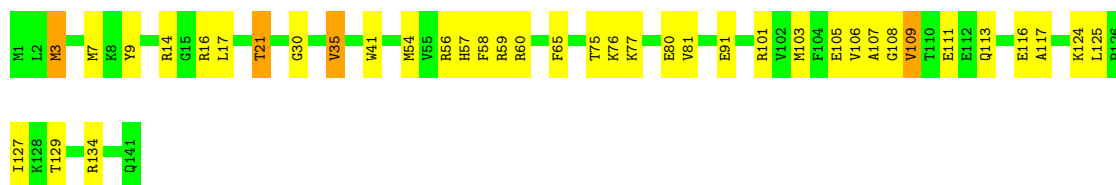
- Molecule 11: 50S ribosomal protein L15

Chain 2P: 68% 27%

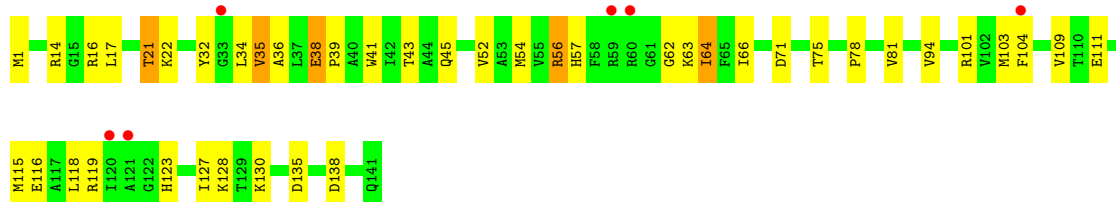


- Molecule 12: 50S ribosomal protein L16

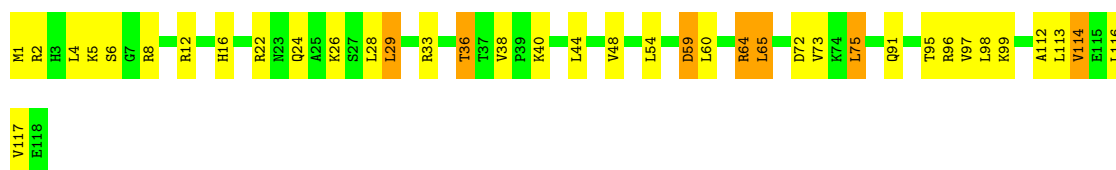
Chain 1Q: 72% 25%



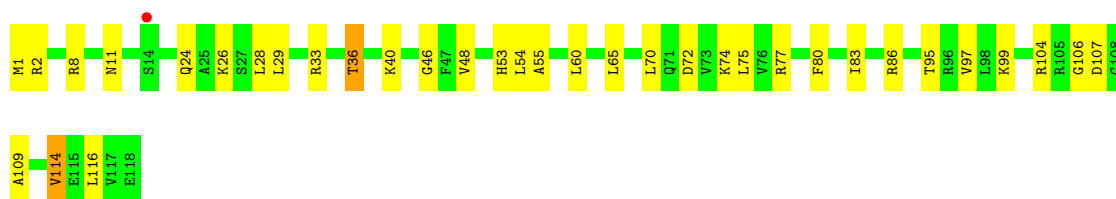
- Molecule 12: 50S ribosomal protein L16



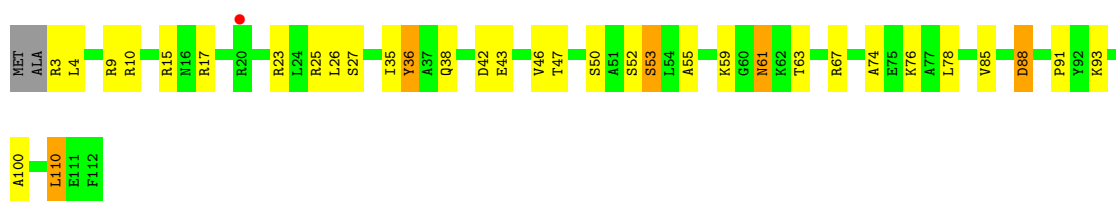
- Molecule 13: 50S ribosomal protein L17



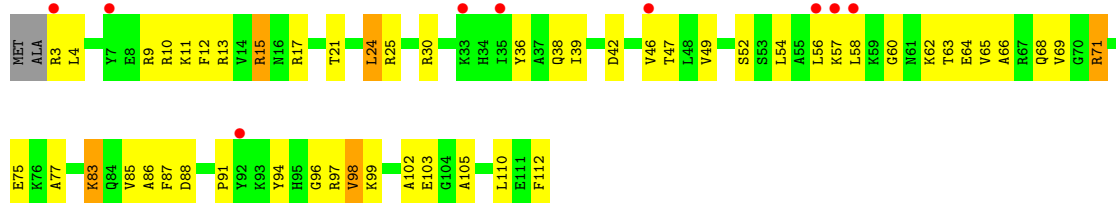
- Molecule 13: 50S ribosomal protein L17



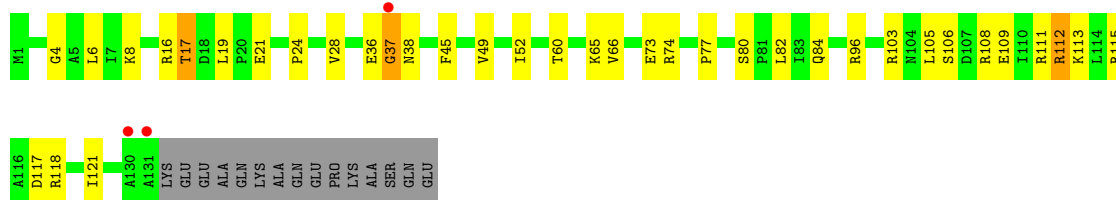
- Molecule 14: 50S ribosomal protein L18



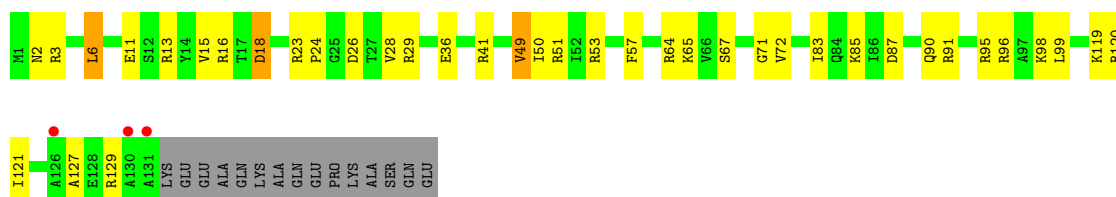
- Molecule 14: 50S ribosomal protein L18



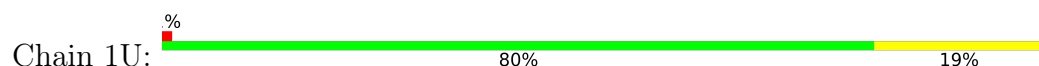
- Molecule 15: 50S ribosomal protein L19



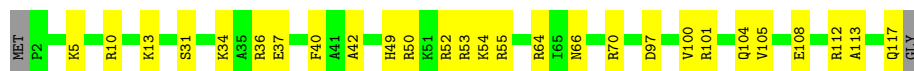
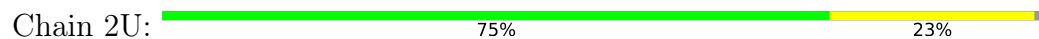
- Molecule 15: 50S ribosomal protein L19



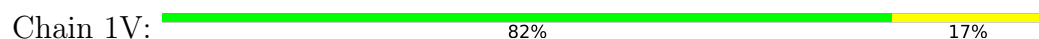
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



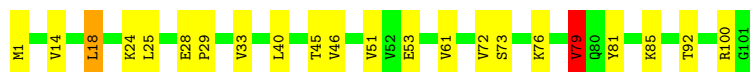
- Molecule 17: 50S ribosomal protein L21





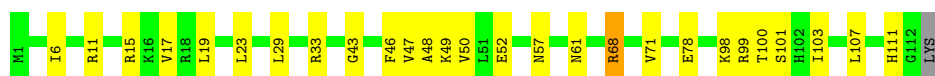
- Molecule 17: 50S ribosomal protein L21

Chain 2V: 78% 20% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 75% 23% ..



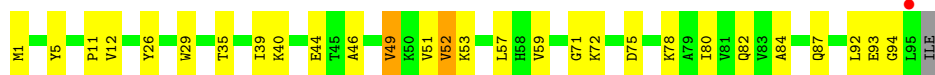
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 75% 24% .



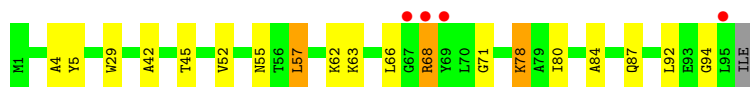
- Molecule 19: 50S ribosomal protein L23

Chain 1X: 70% 27% ..



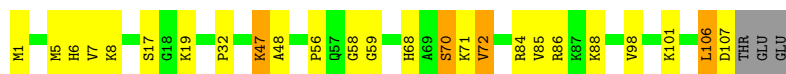
- Molecule 19: 50S ribosomal protein L23

Chain 2X: 79% 17% ..



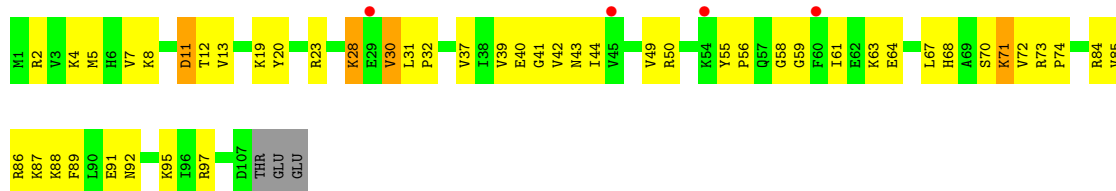
- Molecule 20: 50S ribosomal protein L24

Chain 1Y: 75% 19% .

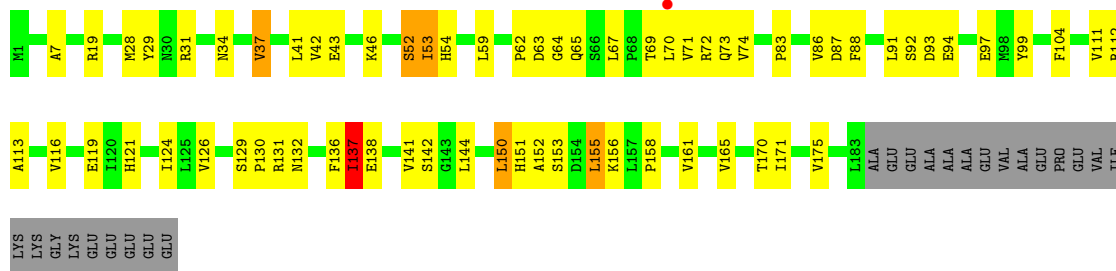


- Molecule 20: 50S ribosomal protein L24

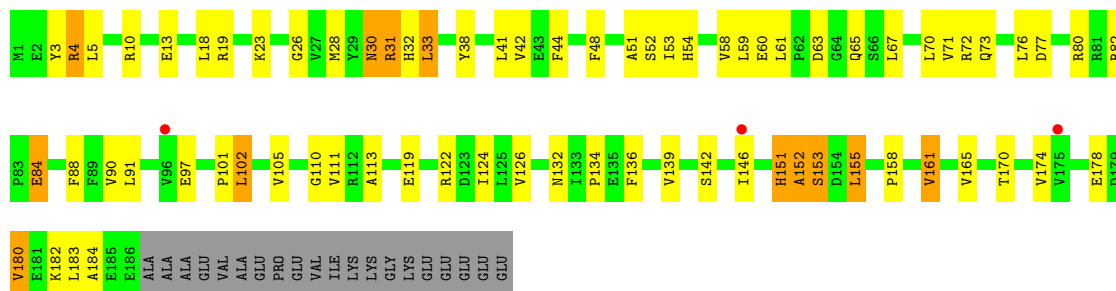
Chain 2Y: 54% 40% .



- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25



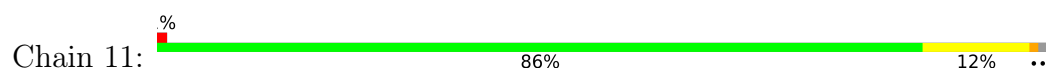
- Molecule 22: 50S ribosomal protein L27



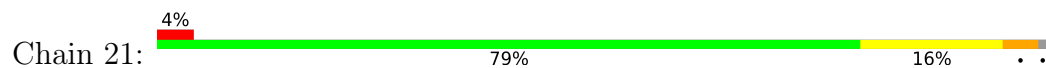
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



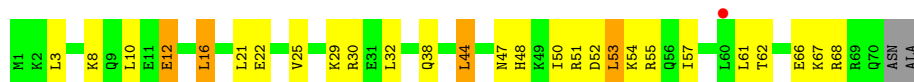
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



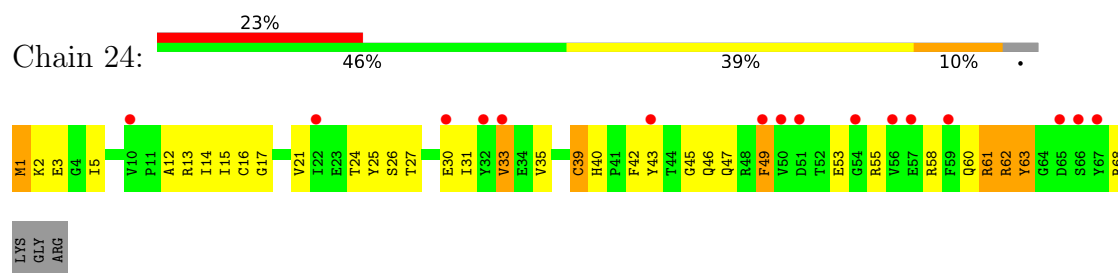
- Molecule 25: 50S ribosomal protein L30



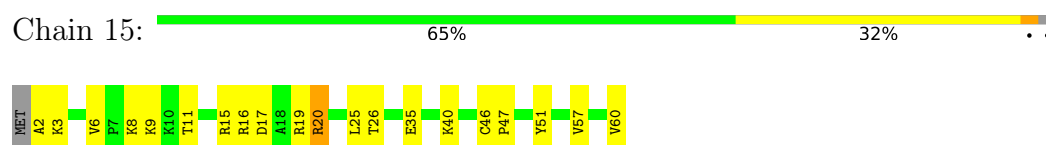
- Molecule 26: 50S ribosomal protein L31



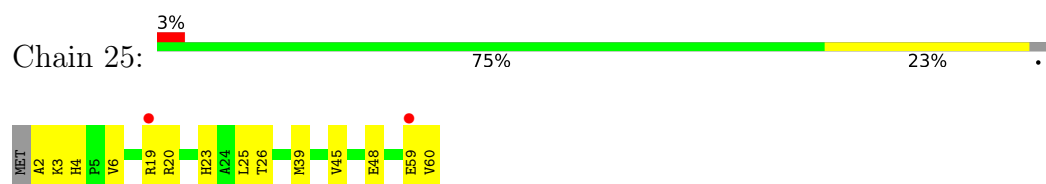
- Molecule 26: 50S ribosomal protein L31



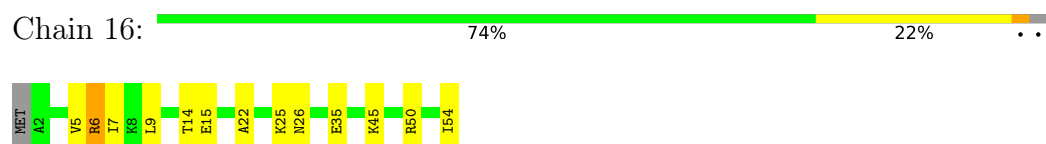
- Molecule 27: 50S ribosomal protein L32



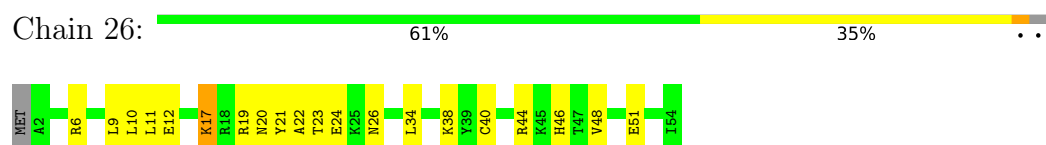
- Molecule 27: 50S ribosomal protein L32



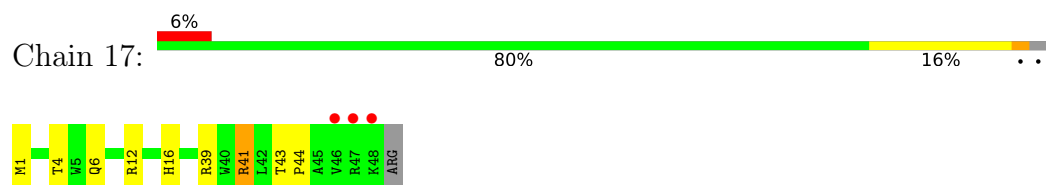
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

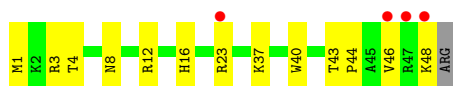


- Molecule 29: 50S ribosomal protein L34

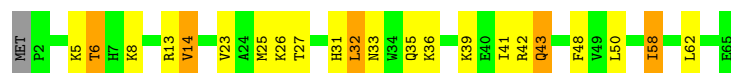


- Molecule 29: 50S ribosomal protein L34

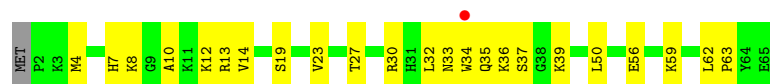




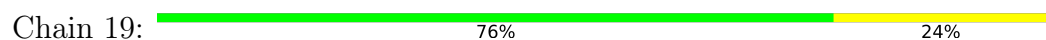
- Molecule 30: 50S ribosomal protein L35



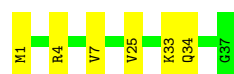
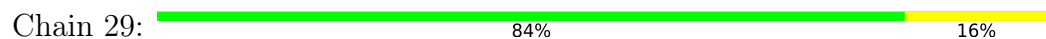
- Molecule 30: 50S ribosomal protein L35



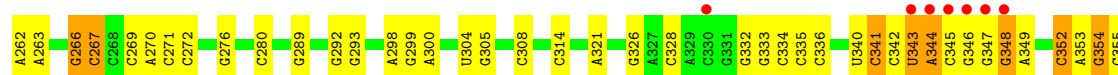
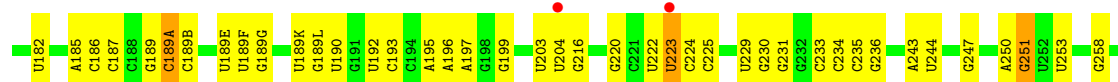
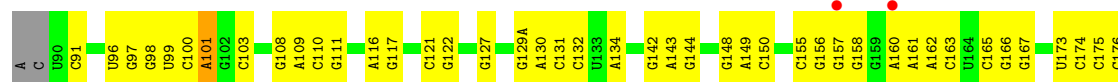
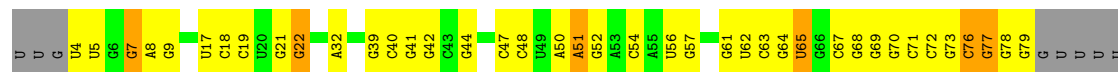
- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36

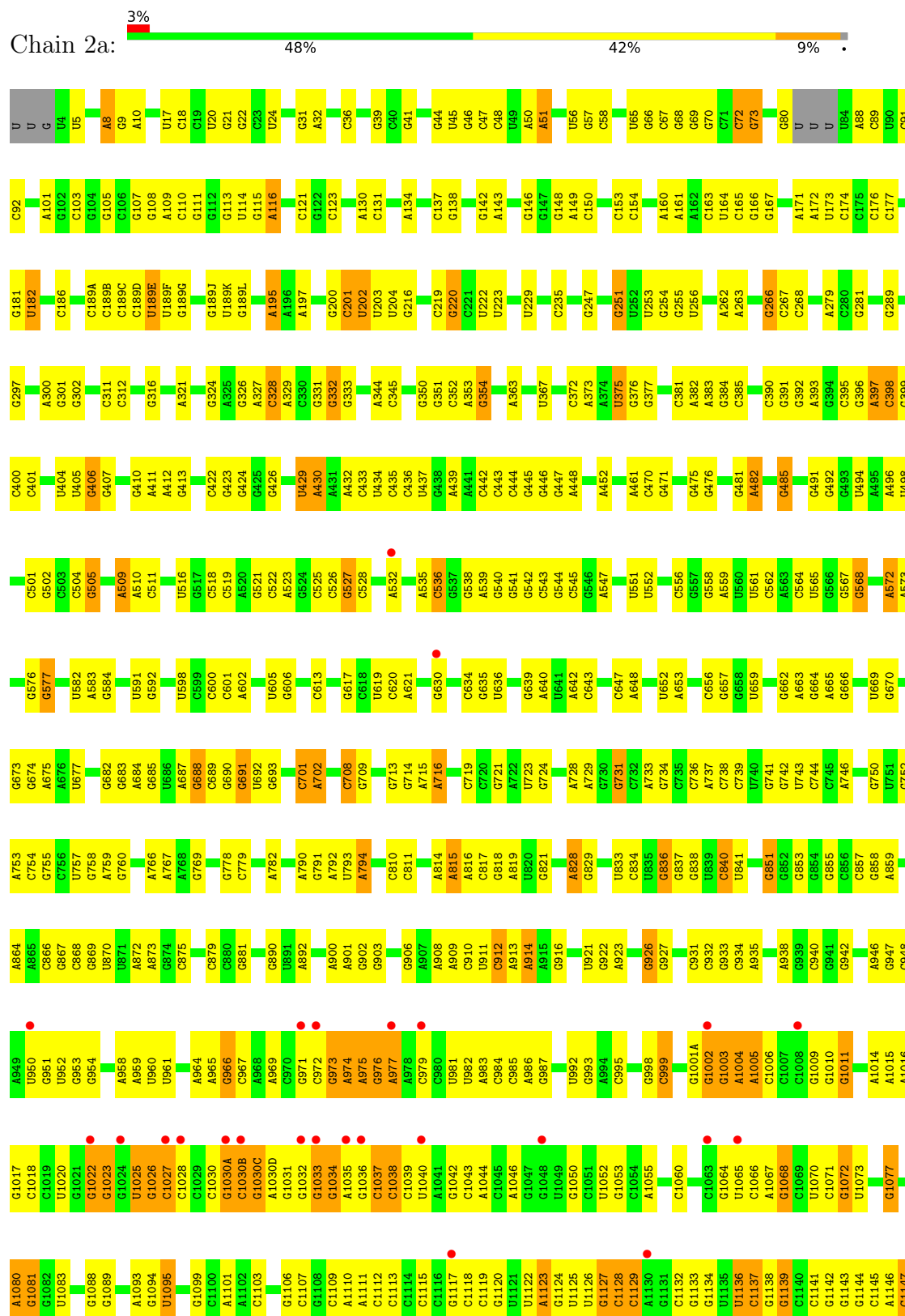


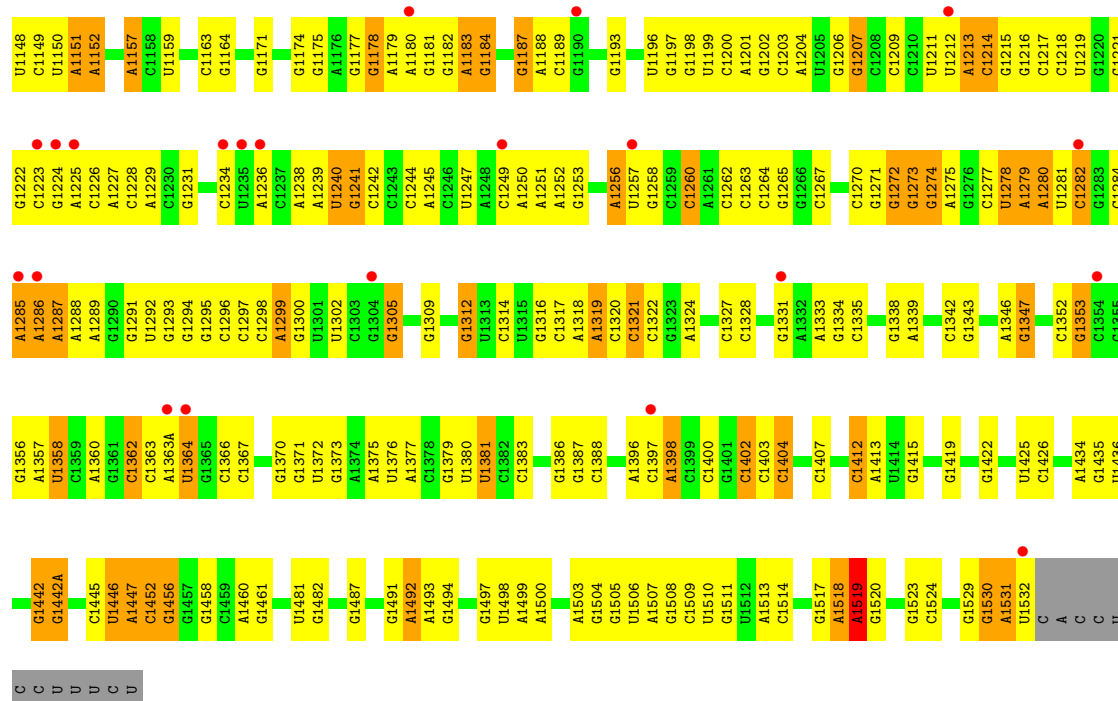
- Molecule 32: 16S Ribosomal RNA



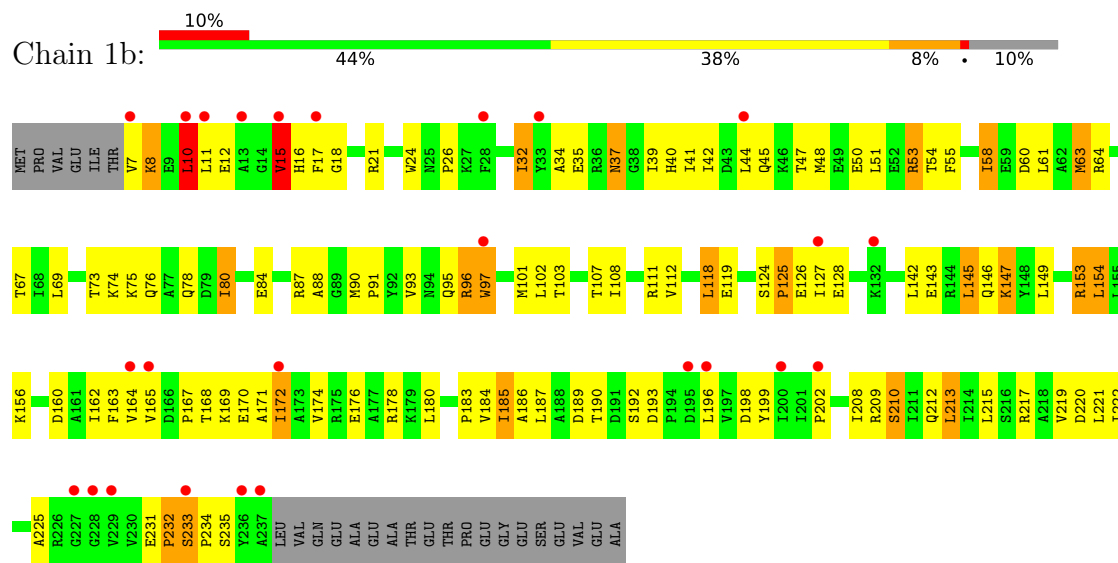


● Molecule 32: 16S Ribosomal RNA

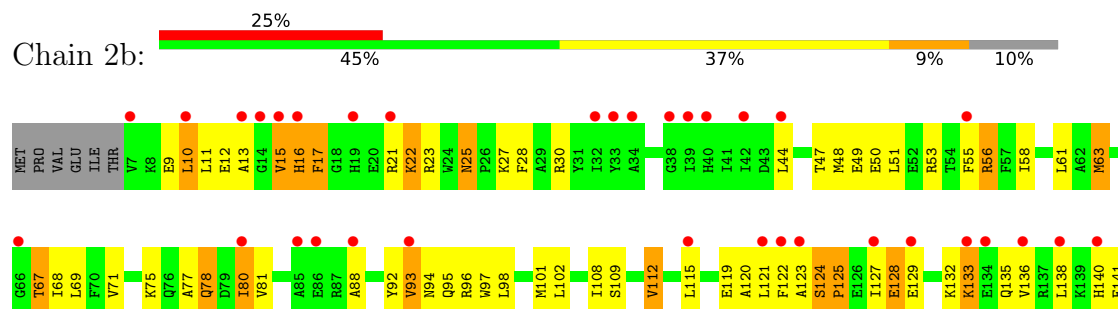


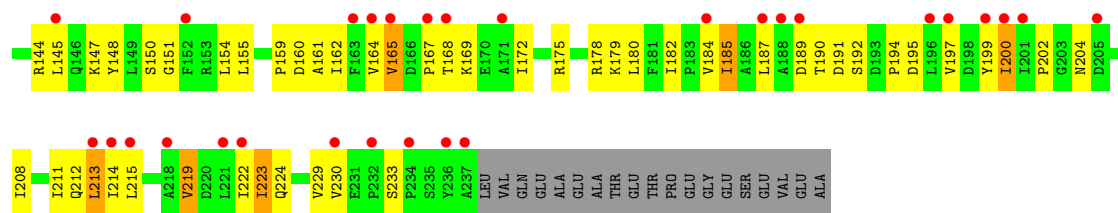


• Molecule 33: 30S ribosomal protein S2

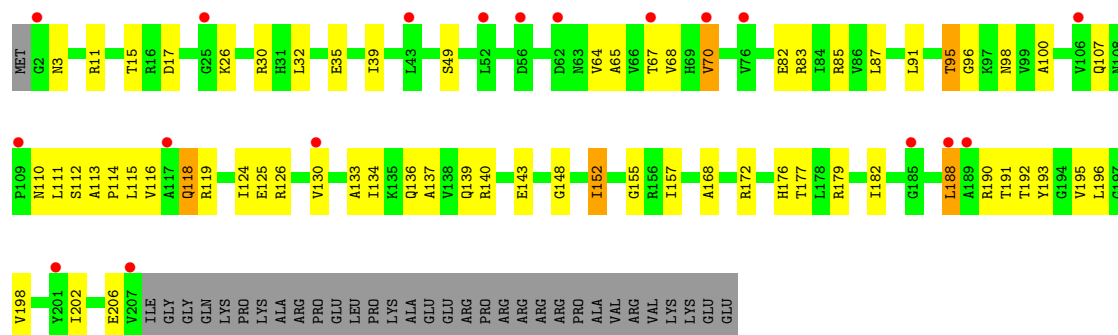


• Molecule 33: 30S ribosomal protein S2

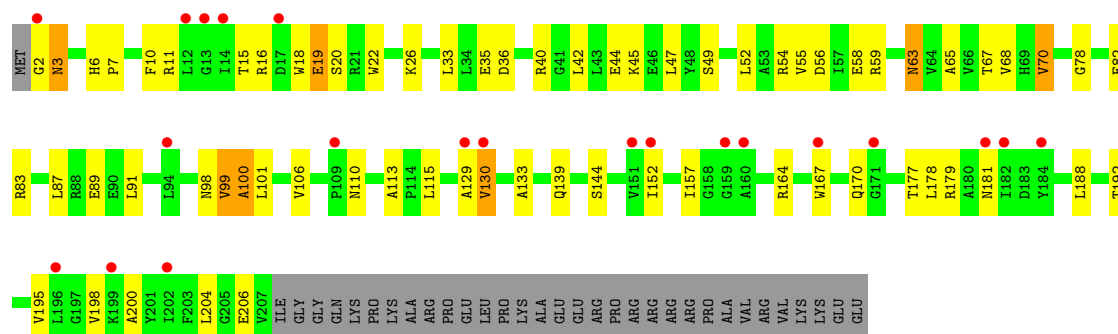




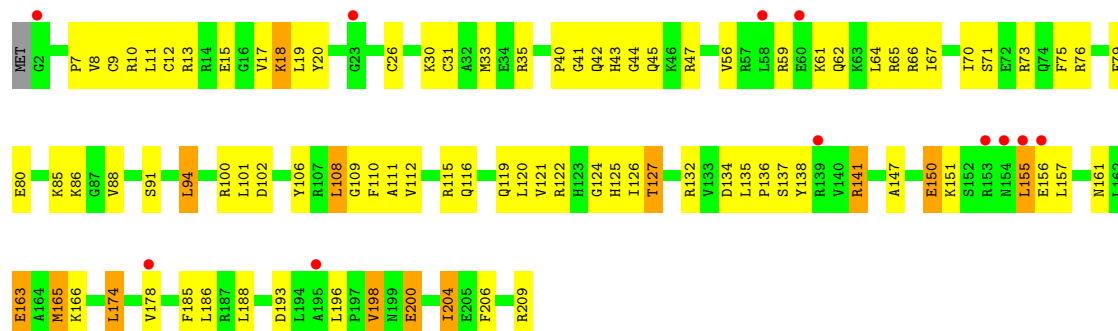
• Molecule 34: 30S ribosomal protein S3



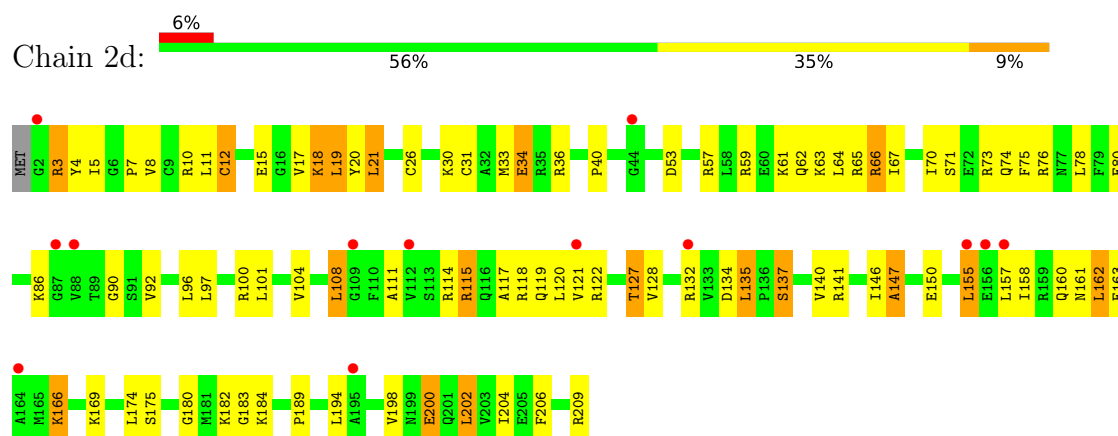
• Molecule 34: 30S ribosomal protein S3



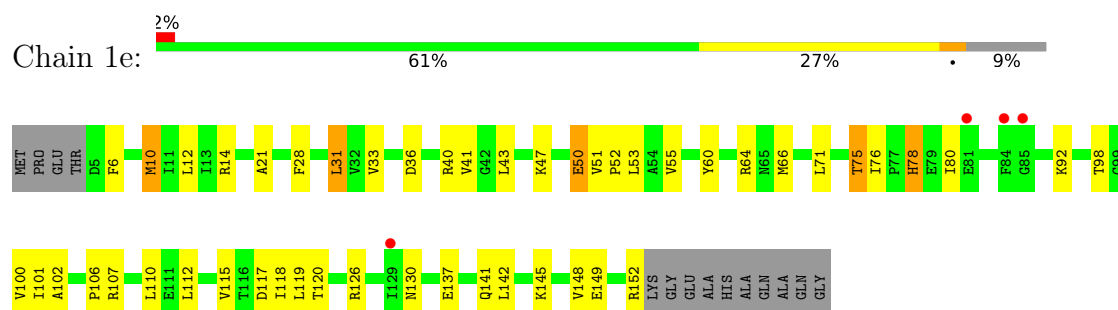
• Molecule 35: 30S ribosomal protein S4



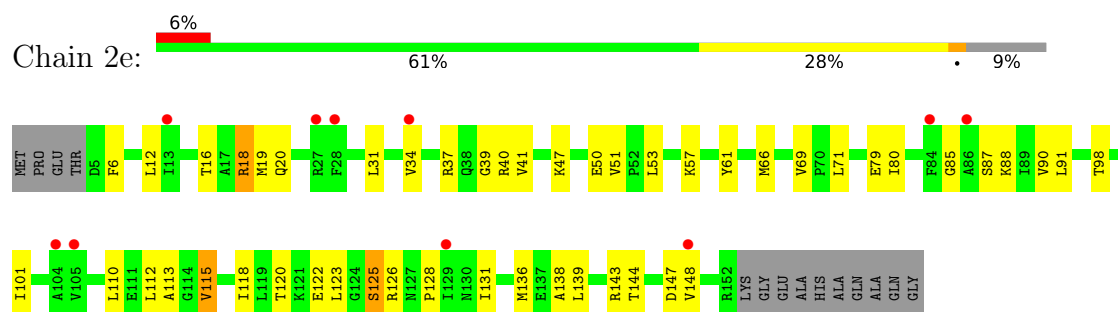
- Molecule 35: 30S ribosomal protein S4



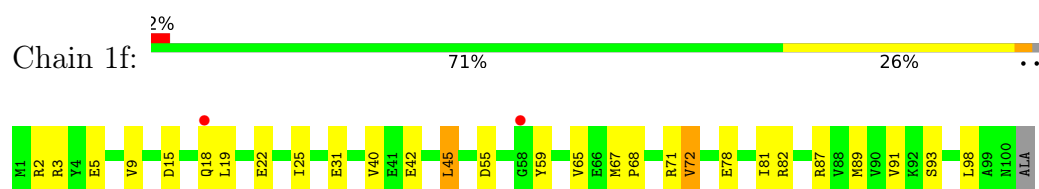
- Molecule 36: 30S ribosomal protein S5



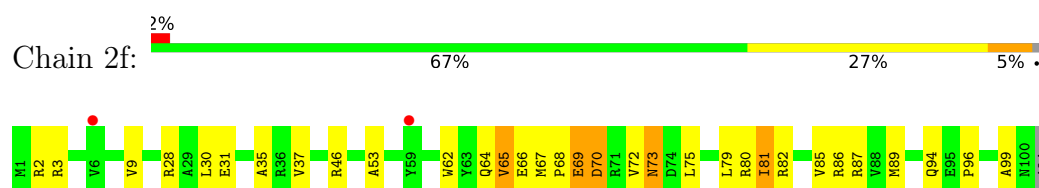
- Molecule 36: 30S ribosomal protein S5



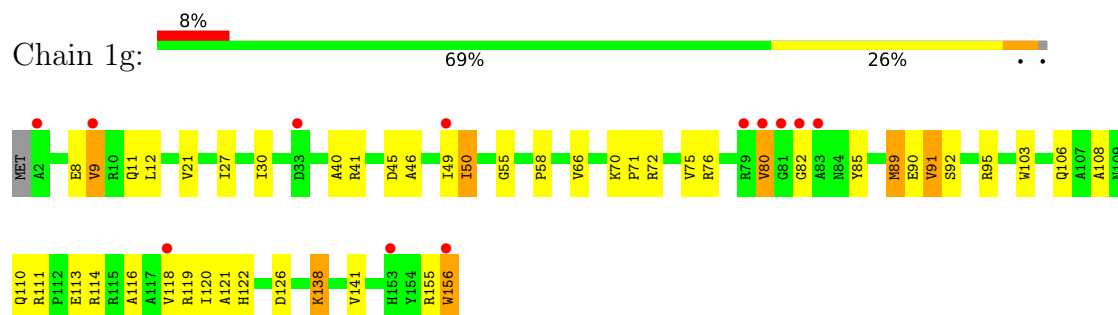
- Molecule 37: 30S ribosomal protein S6



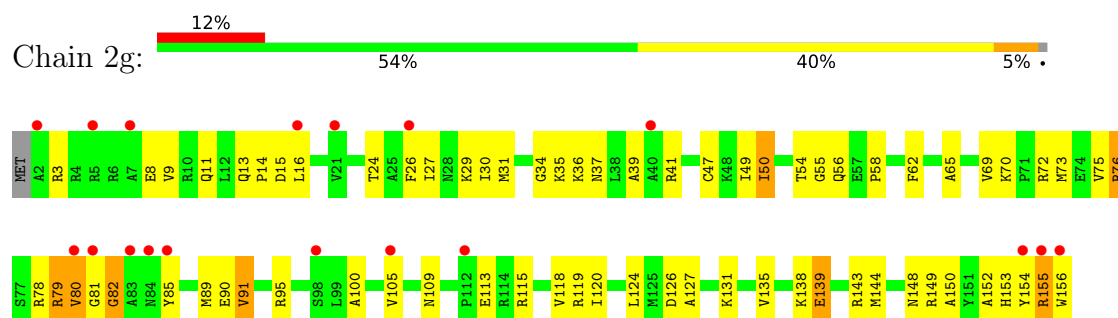
- Molecule 37: 30S ribosomal protein S6



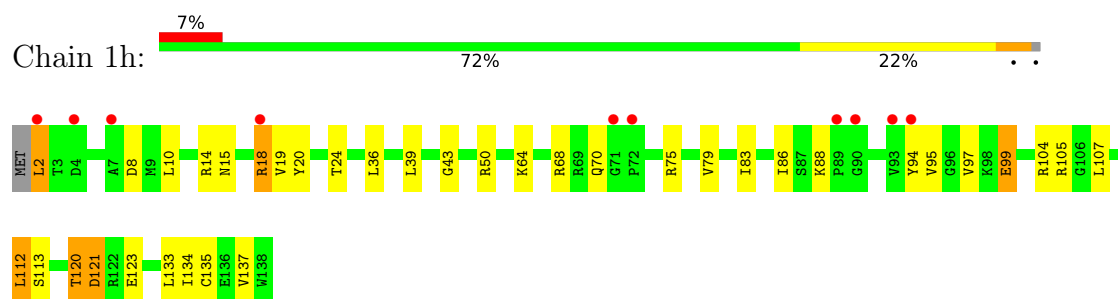
- Molecule 38: 30S ribosomal protein S7



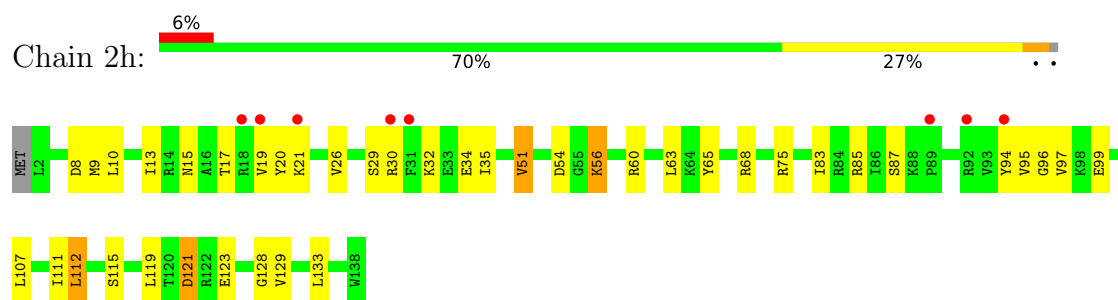
- Molecule 38: 30S ribosomal protein S7



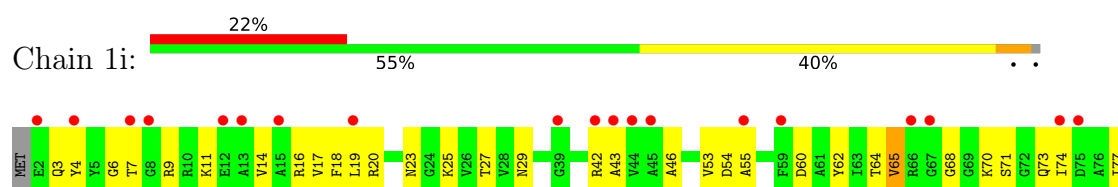
- Molecule 39: 30S ribosomal protein S8

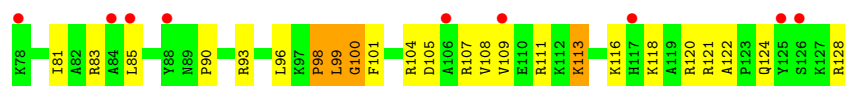


- Molecule 39: 30S ribosomal protein S8

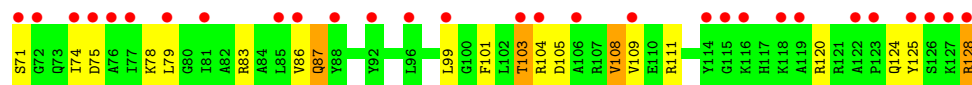
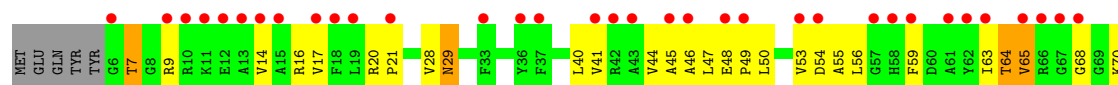


- Molecule 40: 30S ribosomal protein S9

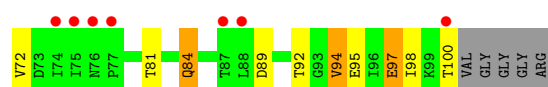
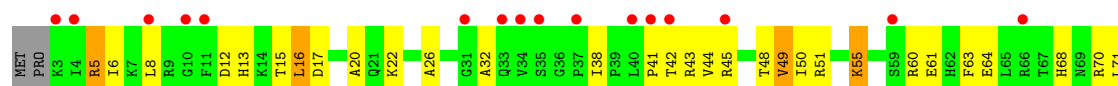




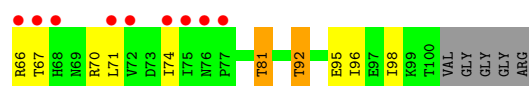
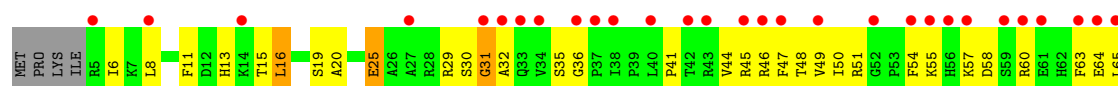
- Molecule 40: 30S ribosomal protein S9



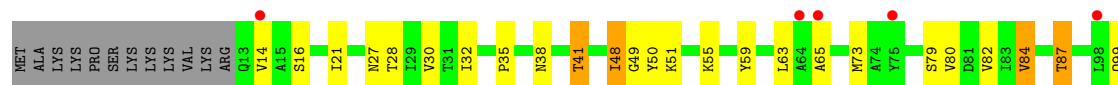
- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

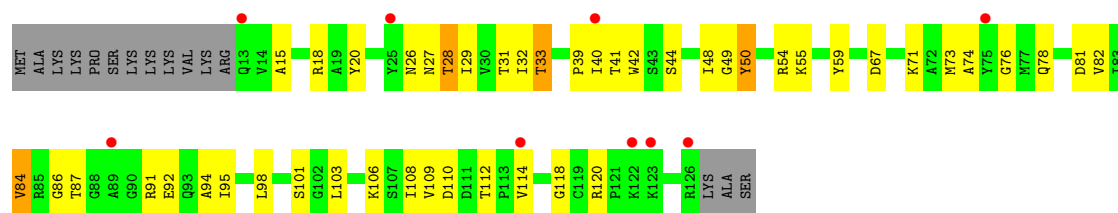


- Molecule 42: 30S ribosomal protein S11

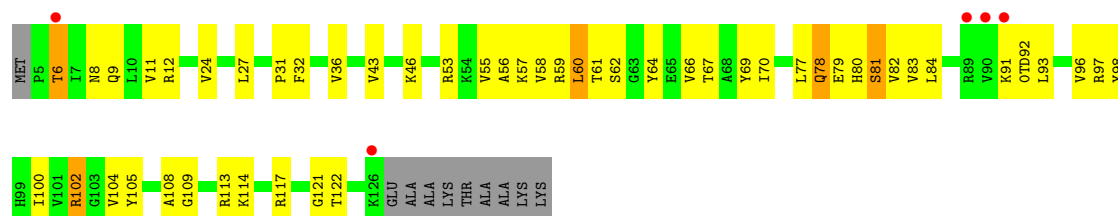


- Molecule 42: 30S ribosomal protein S11

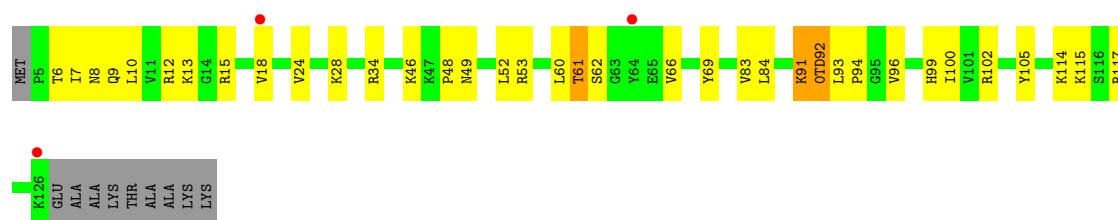




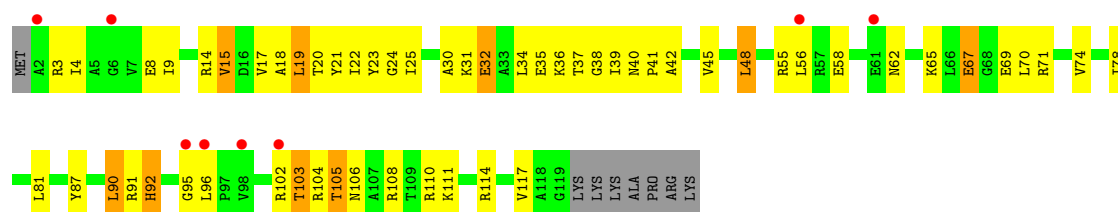
• Molecule 43: 30S ribosomal protein S12



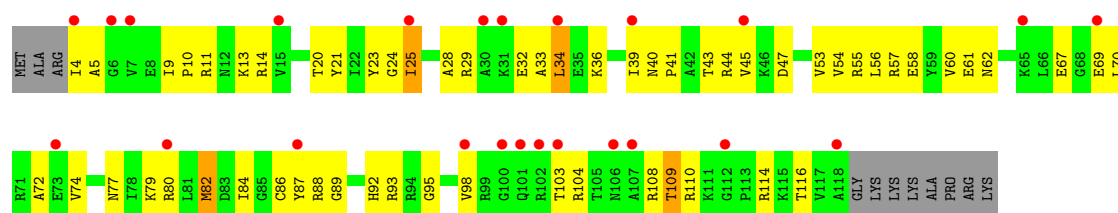
• Molecule 43: 30S ribosomal protein S12



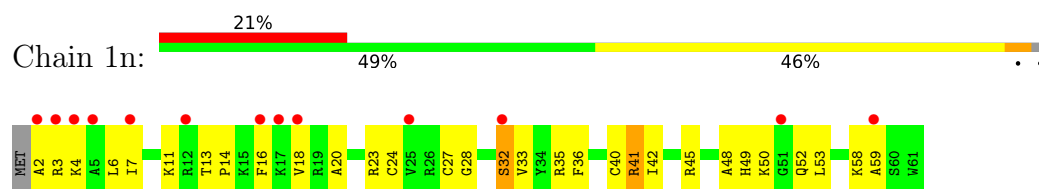
• Molecule 44: 30S ribosomal protein S13



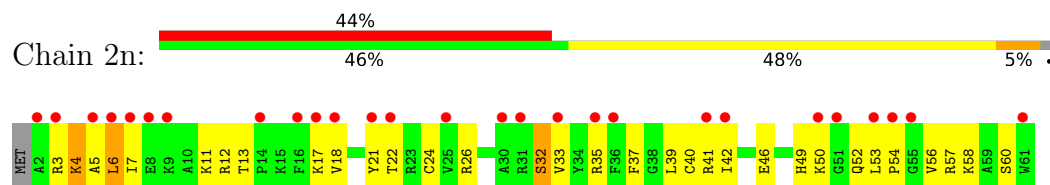
• Molecule 44: 30S ribosomal protein S13



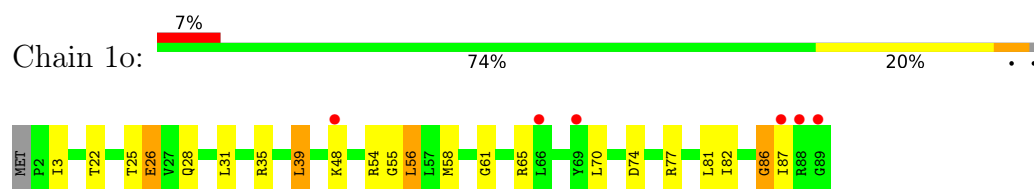
- Molecule 45: 30S ribosomal protein S14 type Z



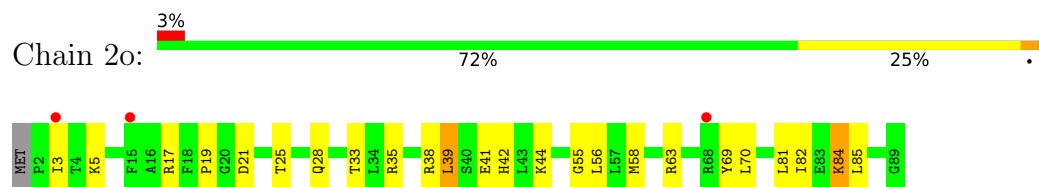
- Molecule 45: 30S ribosomal protein S14 type Z



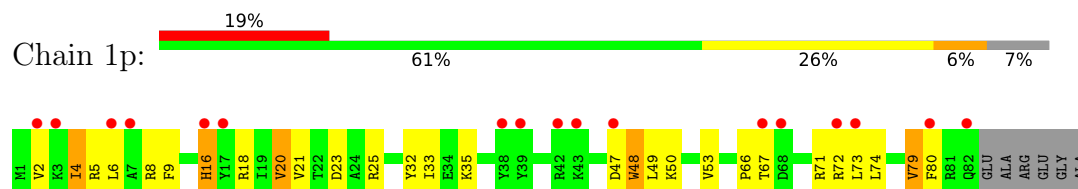
- Molecule 46: 30S ribosomal protein S15



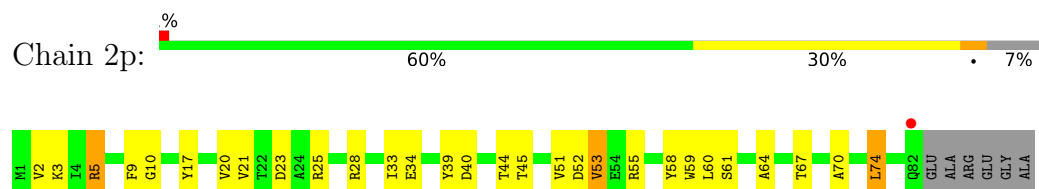
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

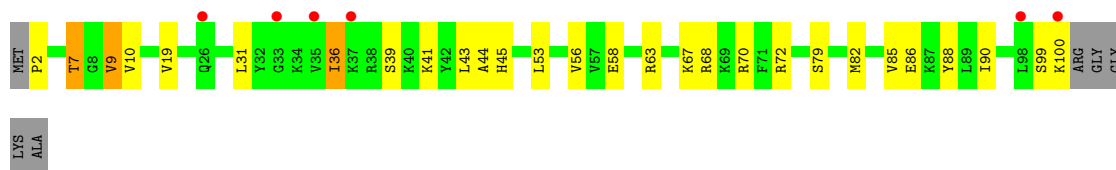


- Molecule 47: 30S ribosomal protein S16

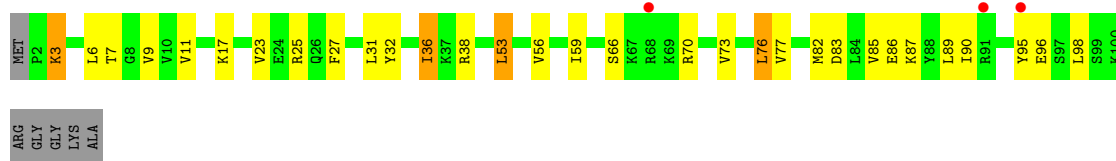


- Molecule 48: 30S ribosomal protein S17

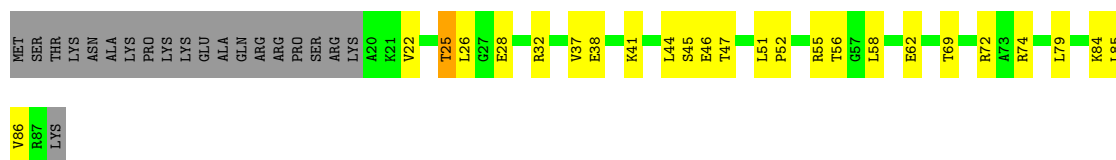




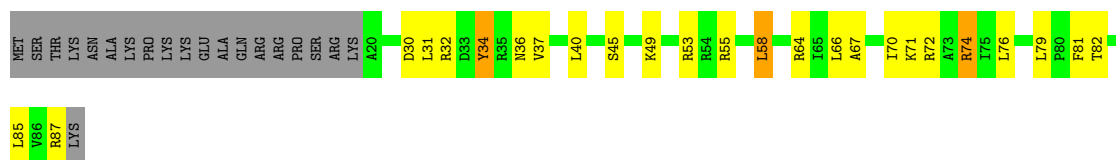
- Molecule 48: 30S ribosomal protein S17



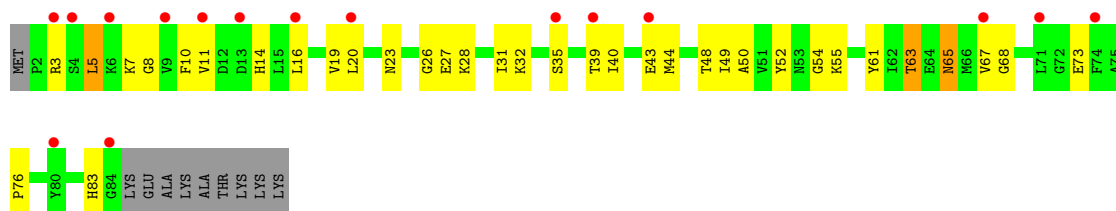
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

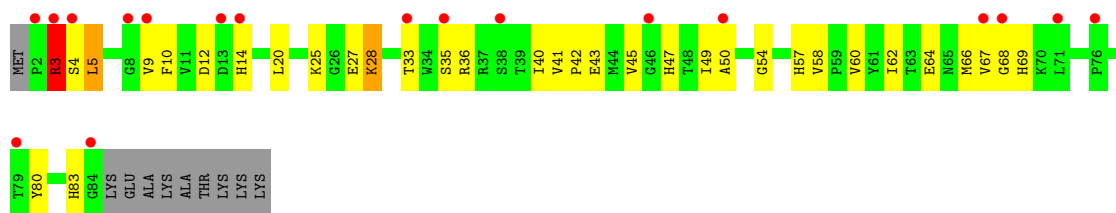


- Molecule 50: 30S ribosomal protein S19

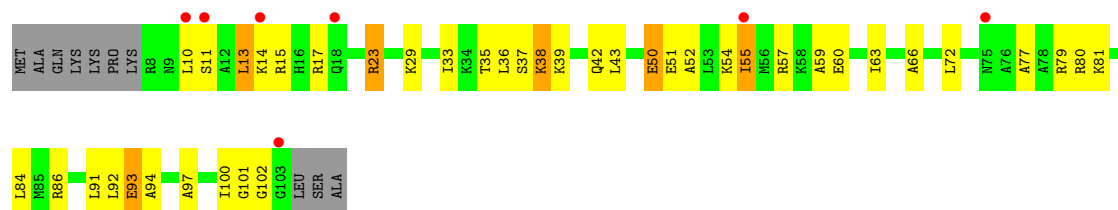


- Molecule 50: 30S ribosomal protein S19

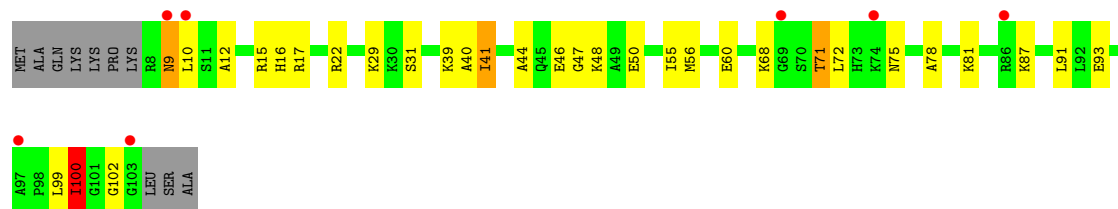




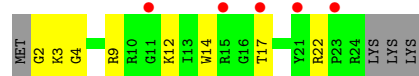
- Molecule 51: 30S ribosomal protein S20



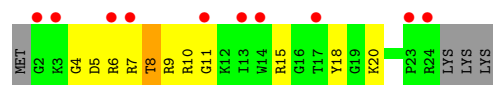
- Molecule 51: 30S ribosomal protein S20



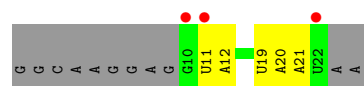
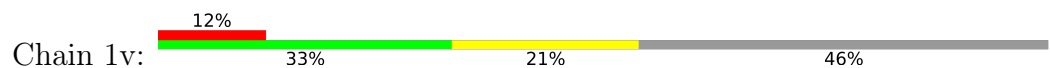
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: PHE-Stop mRNA



Chain 2v:

Category	Value (%)
G	33%
U10	21%
U11	17%
A12	46%
A13	.
A14	.
U22	.
A	.

[illegible]

Chain 2w:

3% 43% 25% 29%

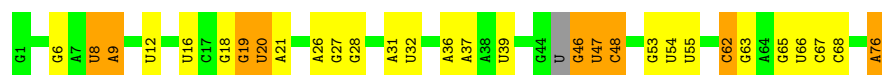
MET LEU ASP SER GLU

ALA SER LEU ASP ASP PRG LEU LYS TYR MET ARG LEU GLU ALA LEU ARG LYS PRO GLU VAL LEU LYS ASP LYS GLY ARG TYR GLN ASP LYS ALA ASP MET GLY VAL ILE GLY LEU ILE ARG TYR ARG LYS VAL LEU GLU ASP LEU GLU

F140 E143 E144 E145 D146 S147 H148 P149 T150 D151 K157 K158 V159 E161 V162 R163 A167 Y168 K172 S175 G176 V177 H178 R179 R182 R183 P184 V185 T186 E187 T188 Q189 G190 R191 H192 H193 T194 S195 T196 A197 T198 V201 L202 P203 K204 E207 D208 E209 F210 N213 M214 D215 E216 W222 S225 G226 P227 G228 G229 Q230 G231 V232 T235 A238 P245 T248 R249 V250 Q253 S257 Q258 T259 R262 E263 K264 A265 L266 M267 T268 S271 R278 R284 L290 T293 G294 T295 R298 S299 E300 K301 L302 R303 T304 R306 F307 P308 R311 V312 T313 D314 H315 R316 T321 E325 G326 V327 L328 L332 T333 L336 L339 K340 E345 A349 A350 L351 A352 E353 G354

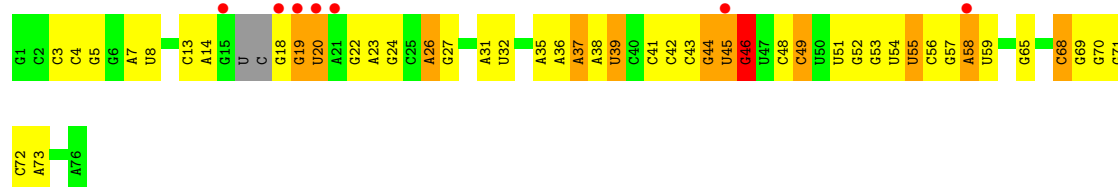
WORLD WIDE
PDB
PROTEIN DATA BANK

Chain 1x: 



• Molecule 55: P-site and E-site Deacylated tRNA^{phe}

Chain 1y: 



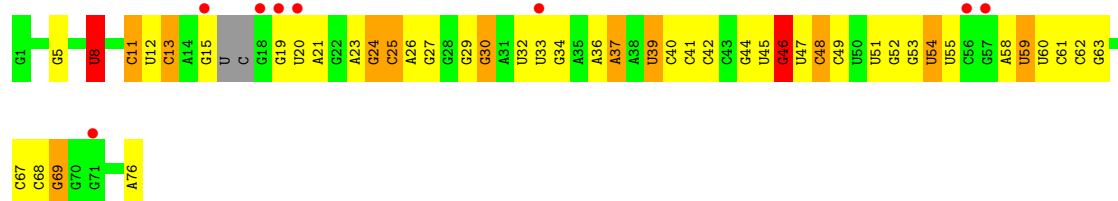
• Molecule 55: P-site and E-site Deacylated tRNA^{phe}

Chain 2x: 



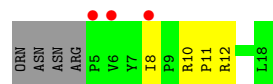
• Molecule 55: P-site and E-site Deacylated tRNA^{phe}

Chain 2y: 



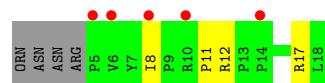
• Molecule 56: Api137 Antimicrobial Peptide

Chain 1z: 



• Molecule 56: Api137 Antimicrobial Peptide

Chain 2z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.60Å 450.81Å 624.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.87 – 2.70 152.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (152.87-2.70) 99.1 (152.87-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.227 , 0.278 0.229 , 0.277	Depositor DCC
R_{free} test set	79249 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299179	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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: MIA, 4OC, UR3, MEQ, 0TD, 2MA, SF4, OMU, M2G, MG, ZN, 5MU, PSU, 4SU, 2MG, OMG, OMC, 5MC, G7M, MA6

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	0/69011	0.47	2/107720 (0.0%)
1	2A	0.22	0/67295	0.40	1/105042 (0.0%)
2	1B	0.23	0/2881	0.40	0/4494
2	2B	0.19	0/2881	0.35	0/4494
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.30	0/1592	0.54	1/2149 (0.0%)
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.26	1/1615 (0.1%)	0.44	0/2188
6	1G	0.22	0/1450	0.47	0/1959
6	2G	0.21	0/1449	0.45	0/1958
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.41	0/1834
8	1I	0.21	0/1100	0.43	0/1501
8	2I	0.19	0/1076	0.43	0/1471
9	1N	0.27	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.40	0/1543
10	1O	0.27	0/943	0.50	0/1269
10	2O	0.21	0/943	0.44	0/1269
11	1P	0.28	0/1152	0.55	0/1533
11	2P	0.22	0/1152	0.47	0/1533
12	1Q	0.28	0/1143	0.51	0/1527
12	2Q	0.20	0/1143	0.41	0/1527
13	1R	0.29	0/982	0.52	0/1312
13	2R	0.21	0/982	0.44	0/1312
14	1S	0.22	0/887	0.52	0/1180
14	2S	0.21	0/880	0.47	0/1172
15	1T	0.26	0/1105	0.49	0/1477
15	2T	0.22	0/1097	0.44	0/1468
16	1U	0.32	0/977	0.48	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.32	0/782	0.48	0/1049
17	2V	0.19	0/782	0.41	0/1049
18	1W	0.31	0/897	0.50	0/1205
18	2W	0.21	0/897	0.43	0/1205
19	1X	0.28	0/764	0.54	1/1025 (0.1%)
19	2X	0.20	0/760	0.35	0/1021
20	1Y	0.26	0/819	0.50	0/1095
20	2Y	0.21	0/823	0.46	0/1100
21	1Z	0.22	0/1469	0.48	0/1998
21	2Z	0.20	0/1483	0.47	0/2018
22	10	0.28	0/612	0.53	0/816
22	20	0.22	0/616	0.51	0/821
23	11	0.26	0/762	0.45	0/1014
23	21	0.22	0/762	0.44	0/1014
24	12	0.24	0/590	0.44	0/781
24	22	0.19	0/590	0.43	0/781
25	13	0.27	0/474	0.47	0/635
25	23	0.21	0/469	0.38	0/630
26	14	0.24	0/561	0.52	0/756
26	24	0.30	0/530	0.58	0/719
27	15	0.31	0/469	0.54	0/635
27	25	0.23	0/469	0.48	0/635
28	16	0.27	0/460	0.49	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.32	0/426	0.48	0/561
29	27	0.25	0/426	0.46	0/561
30	18	0.30	0/519	0.48	0/684
30	28	0.21	0/525	0.42	0/691
31	19	0.27	0/310	0.66	1/407 (0.2%)
31	29	0.22	0/310	0.49	0/407
32	1a	0.20	1/35795 (0.0%)	0.38	1/55864 (0.0%)
32	2a	0.20	2/35886 (0.0%)	0.38	0/56005
33	1b	0.23	0/1881	0.50	0/2542
33	2b	0.30	0/1860	0.54	0/2518
34	1c	0.20	0/1578	0.39	0/2133
34	2c	0.21	0/1566	0.44	0/2119
35	1d	0.20	0/1689	0.49	0/2267
35	2d	0.21	0/1704	0.46	0/2284
36	1e	0.21	0/1145	0.48	0/1543
36	2e	0.20	0/1146	0.45	0/1545
37	1f	0.21	0/823	0.43	0/1116
37	2f	0.18	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.21	0/1250	0.42	0/1679
38	2g	0.21	0/1254	0.43	0/1683
39	1h	0.20	0/1108	0.44	0/1494
39	2h	0.22	0/1108	0.50	1/1494 (0.1%)
40	1i	0.22	0/1002	0.49	0/1346
40	2i	0.26	0/957	0.50	1/1288 (0.1%)
41	1j	0.21	0/734	0.42	0/997
41	2j	0.24	0/727	0.46	0/988
42	1k	0.19	0/844	0.39	0/1145
42	2k	0.20	0/848	0.43	0/1149
43	1l	0.21	0/937	0.43	0/1260
43	2l	0.20	0/937	0.42	0/1260
44	1m	0.22	0/933	0.48	0/1254
44	2m	0.23	0/899	0.51	0/1212
45	1n	0.19	0/501	0.47	0/664
45	2n	0.20	0/495	0.45	0/657
46	1o	0.22	0/739	0.40	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.22	0/697	0.51	0/939
47	2p	0.21	0/693	0.48	0/935
48	1q	0.19	0/836	0.40	0/1117
48	2q	0.22	0/836	0.45	0/1117
49	1r	0.21	0/560	0.43	0/746
49	2r	0.20	0/556	0.44	0/741
50	1s	0.32	1/667 (0.1%)	0.48	0/900
50	2s	0.19	0/661	0.42	0/893
51	1t	0.21	0/730	0.46	0/965
51	2t	0.19	0/729	0.42	0/965
52	1u	0.20	0/203	0.42	0/266
52	2u	0.19	0/203	0.46	0/266
53	1v	0.23	0/306	0.42	0/473
53	2v	0.21	0/306	0.40	0/473
54	1w	0.20	0/1956	0.40	0/2634
54	2w	0.21	0/1971	0.44	1/2654 (0.0%)
55	1x	0.28	1/1629 (0.1%)	0.41	0/2535
55	1y	0.30	2/1602 (0.1%)	0.42	0/2488
55	2x	0.25	0/1629	0.36	0/2535
55	2y	0.31	1/1606 (0.1%)	0.36	0/2497
56	1z	0.27	0/128	0.49	0/175
56	2z	0.20	0/128	0.44	0/175
All	All	0.24	9/317654 (0.0%)	0.43	10/474763 (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
11	2P	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2y	46	G7M	O3'-P	5.99	1.62	1.56
50	1s	65	ASN	CA-C	5.90	1.60	1.52
32	1a	527	G7M	O3'-P	5.39	1.61	1.56
32	2a	527	G7M	O3'-P	5.29	1.61	1.56
55	1y	46	G7M	O3'-P	5.14	1.61	1.56

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	345	GLU	N-CA-C	-9.54	103.75	114.62
39	2h	19	VAL	N-CA-C	-8.59	104.22	112.29
31	19	10	ILE	N-CA-C	-6.55	106.41	112.96
1	2A	1992	G	C2'-C3'-O3'	5.88	118.33	109.50
1	1A	2689	U	C4'-C3'-O3'	5.55	117.72	109.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	2P	35	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	627	1
1	2A	60322	0	30426	720	0
2	1B	2576	0	1305	24	0
2	2B	2576	0	1305	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	40	0
4	1E	1559	0	1618	25	0
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	51	0
5	2F	1580	0	1619	51	0
6	1G	1425	0	1443	31	1
6	2G	1424	0	1434	61	0
7	1H	1330	0	1407	29	0
7	2H	1330	0	1407	30	0
8	1I	1085	0	1114	25	0
8	2I	1061	0	1080	33	0
9	1N	1117	0	1184	12	0
9	2N	1117	0	1184	18	0
10	1O	933	0	996	19	0
10	2O	933	0	996	26	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1178	23	0
12	2Q	1122	0	1179	30	0
13	1R	968	0	1033	23	0
13	2R	968	0	1033	28	0
14	1S	877	0	938	22	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	17	0
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	10	0
16	2U	959	0	1019	18	0
17	1V	771	0	829	10	0
17	2V	771	0	829	11	0
18	1W	886	0	940	15	0
18	2W	886	0	940	16	0
19	1X	750	0	814	19	0
19	2X	746	0	803	13	0
20	1Y	806	0	881	14	0
20	2Y	810	0	887	31	0
21	1Z	1437	0	1446	43	0
21	2Z	1451	0	1450	47	0
22	10	604	0	619	8	0
22	20	608	0	622	20	0
23	11	755	0	825	9	0
23	21	755	0	826	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	14	0
24	22	588	0	643	19	0
25	13	469	0	518	14	0
25	23	464	0	514	11	0
26	14	548	0	529	16	0
26	24	517	0	479	27	0
27	15	455	0	465	16	0
27	25	455	0	465	10	0
28	16	453	0	472	7	0
28	26	449	0	469	13	0
29	17	418	0	467	7	0
29	27	418	0	467	9	0
30	18	511	0	571	16	0
30	28	517	0	582	16	0
31	19	307	0	335	4	0
31	29	307	0	335	3	0
32	1a	32246	0	16295	488	0
32	2a	32327	0	16338	508	0
33	1b	1846	0	1867	77	0
33	2b	1825	0	1828	76	0
34	1c	1554	0	1551	38	0
34	2c	1542	0	1517	42	0
35	1d	1659	0	1676	63	0
35	2d	1674	0	1714	70	0
36	1e	1129	0	1185	41	0
36	2e	1130	0	1184	26	0
37	1f	810	0	797	15	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	22	0
38	2g	1235	0	1249	45	0
39	1h	1088	0	1126	28	0
39	2h	1088	0	1126	23	0
40	1i	983	0	986	42	0
40	2i	940	0	938	39	0
41	1j	721	0	672	33	0
41	2j	714	0	672	30	0
42	1k	829	0	825	23	0
42	2k	833	0	836	32	0
43	1l	932	0	979	32	0
43	2l	932	0	980	26	0
44	1m	923	0	962	41	0
44	2m	889	0	901	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	492	0	529	22	0
45	2n	486	0	518	28	0
46	1o	728	0	760	16	0
46	2o	728	0	760	16	0
47	1p	681	0	697	21	0
47	2p	677	0	686	22	0
48	1q	823	0	891	16	0
48	2q	823	0	891	14	0
49	1r	555	0	618	12	0
49	2r	551	0	614	17	0
50	1s	652	0	662	29	0
50	2s	646	0	644	23	0
51	1t	728	0	798	25	0
51	2t	727	0	796	21	0
52	1u	199	0	208	9	0
52	2u	199	0	208	8	0
53	1v	274	0	139	2	0
53	2v	274	0	139	4	0
54	1w	1939	0	1925	60	0
54	2w	1954	0	1930	54	0
55	1x	1612	0	829	13	0
55	1y	1590	0	815	25	0
55	2x	1612	0	829	15	0
55	2y	1592	0	818	27	0
56	1z	121	0	128	2	0
56	2z	121	0	128	2	0
57	10	5	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	1	0	0	0	0
57	14	1	0	0	0	0
57	15	4	0	0	0	0
57	16	1	0	0	0	0
57	17	7	0	0	0	0
57	18	2	0	0	0	0
57	19	1	0	0	0	0
57	1A	807	0	0	0	0
57	1B	20	0	0	0	0
57	1D	6	0	0	0	0
57	1E	7	0	0	0	0
57	1F	8	0	0	0	0
57	1G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1N	4	0	0	0	0
57	1O	2	0	0	0	0
57	1P	4	0	0	0	0
57	1Q	5	0	0	0	0
57	1R	2	0	0	0	0
57	1T	1	0	0	0	0
57	1U	6	0	0	0	0
57	1V	5	0	0	0	0
57	1W	4	0	0	0	0
57	1X	3	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	187	0	0	0	0
57	1c	1	0	0	0	0
57	1d	1	0	0	0	0
57	1f	1	0	0	0	0
57	1k	1	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1v	3	0	0	0	0
57	1w	4	0	0	0	0
57	1x	8	0	0	0	0
57	1y	2	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	2	0	0	0	0
57	25	1	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	665	0	0	0	0
57	2B	11	0	0	0	0
57	2D	9	0	0	0	0
57	2E	5	0	0	0	0
57	2F	6	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	1	0	0	0	0
57	2U	1	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	4	0	0	0	0
57	2Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2a	172	0	0	0	0
57	2d	1	0	0	0	0
57	2e	2	0	0	0	0
57	2f	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	2	0	0	0	0
57	2t	1	0	0	0	0
57	2u	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	2	0	0	0	0
57	2x	9	0	0	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	2	0
59	2d	8	0	0	1	0
60	10	1	0	0	0	0
60	11	3	0	0	0	0
60	13	2	0	0	0	0
60	15	5	0	0	0	0
60	16	1	0	0	1	0
60	17	2	0	0	0	0
60	18	7	0	0	1	0
60	1A	1394	0	0	75	0
60	1B	31	0	0	1	0
60	1D	15	0	0	1	0
60	1E	12	0	0	0	0
60	1F	6	0	0	2	0
60	1G	1	0	0	0	0
60	1N	3	0	0	1	0
60	1O	3	0	0	1	0
60	1P	15	0	0	1	0
60	1Q	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1R	2	0	0	0	0
60	1T	1	0	0	0	0
60	1U	5	0	0	0	0
60	1V	1	0	0	0	0
60	1W	2	0	0	0	0
60	1X	4	0	0	0	0
60	1a	194	0	0	23	0
60	1d	1	0	0	0	0
60	1l	1	0	0	0	0
60	1p	1	0	0	0	0
60	1v	3	0	0	1	0
60	1w	5	0	0	0	0
60	1x	22	0	0	2	0
60	1y	1	0	0	1	0
60	1z	4	0	0	0	0
60	20	6	0	0	0	0
60	21	2	0	0	0	0
60	23	2	0	0	1	0
60	25	1	0	0	0	0
60	27	3	0	0	0	0
60	28	3	0	0	0	0
60	2A	997	0	0	97	0
60	2B	7	0	0	0	0
60	2D	16	0	0	0	0
60	2E	11	0	0	2	0
60	2F	5	0	0	0	0
60	2N	1	0	0	0	0
60	2O	1	0	0	0	0
60	2P	12	0	0	1	0
60	2Q	1	0	0	0	0
60	2R	3	0	0	1	0
60	2T	1	0	0	0	0
60	2U	2	0	0	0	0
60	2W	1	0	0	0	0
60	2X	2	0	0	0	0
60	2Y	2	0	0	0	0
60	2a	154	0	0	12	0
60	2d	1	0	0	0	0
60	2j	1	0	0	0	0
60	2t	2	0	0	0	0
60	2v	2	0	0	0	0
60	2w	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2x	13	0	0	1	0
All	All	299179	0	199300	4441	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 4441 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:2124:G:H1	1:1A:2174:C:H42	1.01	0.97
1:2A:2129:C:N4	1:2A:2159:G:H1	1.66	0.94
1:1A:1057:A:N6	1:1A:1081:U:H3	1.66	0.94
1:1A:2124:G:H1	1:1A:2174:C:N4	1.68	0.91
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.36	0.91

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1472:A:O2'	6:1G:21:ARG:NH1[1_455]	2.19	0.01

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%)	254 (93%)	19 (7%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	48
4	2E	202/206 (98%)	184 (91%)	17 (8%)	1 (0%)	24	48
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	2F	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	8	22
6	1G	179/182 (98%)	155 (87%)	19 (11%)	5 (3%)	4	9
6	2G	179/182 (98%)	155 (87%)	22 (12%)	2 (1%)	11	29
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	44
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	7	19
8	1I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	23
8	2I	144/148 (97%)	122 (85%)	20 (14%)	2 (1%)	9	23
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
11	1P	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9	23
11	2P	147/150 (98%)	127 (86%)	19 (13%)	1 (1%)	18	41
12	1Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	41
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
14	2S	108/112 (96%)	91 (84%)	11 (10%)	6 (6%)	1	2
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	37
15	2T	129/146 (88%)	117 (91%)	12 (9%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	32
17	2V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	16
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	1 (1%)	2 (2%)	5	14
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	32
20	2Y	105/110 (96%)	88 (84%)	17 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	1Z	181/206 (88%)	159 (88%)	19 (10%)	3 (2%)	7	19
21	2Z	184/206 (89%)	159 (86%)	21 (11%)	4 (2%)	5	14
22	10	74/85 (87%)	70 (95%)	3 (4%)	1 (1%)	9	23
22	20	75/85 (88%)	67 (89%)	8 (11%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	29
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	29
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	18
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	48 (72%)	11 (16%)	8 (12%)	0	0
26	24	66/71 (93%)	43 (65%)	18 (27%)	5 (8%)	1	1
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%)	46 (90%)	5 (10%)	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%)	57 (92%)	5 (8%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	29 (13%)	7 (3%)	3	8
33	2b	229/256 (90%)	193 (84%)	24 (10%)	12 (5%)	1	3
34	1c	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	12	32
34	2c	204/239 (85%)	166 (81%)	36 (18%)	2 (1%)	12	32
35	1d	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	12	32
35	2d	206/209 (99%)	177 (86%)	27 (13%)	2 (1%)	12	32
36	1e	146/162 (90%)	129 (88%)	17 (12%)	0	100	100
36	2e	146/162 (90%)	124 (85%)	19 (13%)	3 (2%)	5	15
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	2f	98/101 (97%)	85 (87%)	12 (12%)	1 (1%)	12	32
38	1g	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	4	11
38	2g	153/156 (98%)	135 (88%)	13 (8%)	5 (3%)	3	7
39	1h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	18	41
39	2h	135/138 (98%)	123 (91%)	11 (8%)	1 (1%)	18	41
40	1i	125/128 (98%)	103 (82%)	18 (14%)	4 (3%)	3	7
40	2i	121/128 (94%)	99 (82%)	20 (16%)	2 (2%)	7	19
41	1j	96/105 (91%)	88 (92%)	7 (7%)	1 (1%)	12	32
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	5	15
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6	18
42	2k	112/129 (87%)	96 (86%)	15 (13%)	1 (1%)	14	35
43	1l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
43	2l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
44	1m	116/126 (92%)	102 (88%)	13 (11%)	1 (1%)	14	35
44	2m	113/126 (90%)	96 (85%)	14 (12%)	3 (3%)	4	10
45	1n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	19
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	27
46	2o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10	27
47	1p	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	9	25
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	8	22
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10	27
50	2s	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	4	11
51	1t	94/106 (89%)	80 (85%)	10 (11%)	4 (4%)	2	4
51	2t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2	4
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	1w	246/354 (70%)	228 (93%)	13 (5%)	5 (2%)	6	16
54	2w	250/354 (71%)	235 (94%)	14 (6%)	1 (0%)	30	54
56	1z	12/18 (67%)	11 (92%)	1 (8%)	0	100	100
56	2z	12/18 (67%)	10 (83%)	2 (17%)	0	100	100
All	All	11922/12872 (93%)	10772 (90%)	1007 (8%)	143 (1%)	10	27

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	50	ALA
8	1I	10	GLU
17	1V	79	VAL
23	11	3	LYS

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%)	199 (93%)	16 (7%)	13	32
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	34
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9	22
4	2E	164/166 (99%)	149 (91%)	15 (9%)	9	22
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	27
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	14
6	1G	143/156 (92%)	122 (85%)	21 (15%)	3	8
6	2G	142/156 (91%)	122 (86%)	20 (14%)	3	9
7	1H	144/148 (97%)	128 (89%)	16 (11%)	6	15
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	15
8	1I	110/124 (89%)	94 (86%)	16 (14%)	3	8
8	2I	104/124 (84%)	76 (73%)	28 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	42
9	2N	118/119 (99%)	112 (95%)	6 (5%)	21	48
10	1O	100/100 (100%)	98 (98%)	2 (2%)	48	76
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	76
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	47
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	29
12	1Q	111/111 (100%)	99 (89%)	12 (11%)	6	16
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	19
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4	10
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	42
14	1S	87/88 (99%)	72 (83%)	15 (17%)	2	6
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	10
15	1T	115/127 (91%)	104 (90%)	11 (10%)	8	20
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	39
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	37
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	64
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	48
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	14
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	44
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	44
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	57
19	2X	76/78 (97%)	71 (93%)	5 (7%)	15	36
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	17
20	2Y	86/91 (94%)	75 (87%)	11 (13%)	4	11
21	1Z	155/179 (87%)	141 (91%)	14 (9%)	9	23
21	2Z	155/179 (87%)	137 (88%)	18 (12%)	5	13
22	10	61/67 (91%)	56 (92%)	5 (8%)	10	27
22	20	61/67 (91%)	54 (88%)	7 (12%)	5	14
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	48
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	31
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	22	65/67 (97%)	58 (89%)	7 (11%)	6	16
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	57
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	41
26	14	58/63 (92%)	52 (90%)	6 (10%)	7	18
26	24	51/63 (81%)	41 (80%)	10 (20%)	1	4
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	41
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	41
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	29
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	19
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	49
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	49
30	18	53/55 (96%)	45 (85%)	8 (15%)	3	7
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	44
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	67
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	67
33	1b	192/220 (87%)	156 (81%)	36 (19%)	1	4
33	2b	187/220 (85%)	154 (82%)	33 (18%)	2	5
34	1c	144/188 (77%)	127 (88%)	17 (12%)	5	13
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3	8
35	1d	170/181 (94%)	142 (84%)	28 (16%)	2	6
35	2d	173/181 (96%)	148 (86%)	25 (14%)	3	8
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	39
36	2e	113/123 (92%)	103 (91%)	10 (9%)	9	23
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	20
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	27
38	1g	119/127 (94%)	104 (87%)	15 (13%)	4	11
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8	22
39	1h	114/119 (96%)	102 (90%)	12 (10%)	6	17
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	28
40	1i	90/99 (91%)	83 (92%)	7 (8%)	11	29
40	2i	86/99 (87%)	72 (84%)	14 (16%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	68/92 (74%)	56 (82%)	12 (18%)	2	5
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	8
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	15
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	20
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	17
43	2l	96/108 (89%)	88 (92%)	8 (8%)	10	26
44	1m	90/101 (89%)	78 (87%)	12 (13%)	4	10
44	2m	85/101 (84%)	79 (93%)	6 (7%)	13	33
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	12
45	2n	48/50 (96%)	38 (79%)	10 (21%)	1	3
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	38
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	38
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	10
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	18
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	20
48	2q	94/97 (97%)	80 (85%)	14 (15%)	3	8
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	9
49	2r	58/77 (75%)	48 (83%)	10 (17%)	2	6
50	1s	69/80 (86%)	64 (93%)	5 (7%)	13	32
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	8
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	10
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	25
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	44
54	1w	203/298 (68%)	177 (87%)	26 (13%)	4	11
54	2w	202/298 (68%)	167 (83%)	35 (17%)	2	5
56	1z	14/17 (82%)	12 (86%)	2 (14%)	3	8
56	2z	14/17 (82%)	12 (86%)	2 (14%)	3	8
All	All	9747/10694 (91%)	8729 (90%)	1018 (10%)	7	17

5 of 1018 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	1t	55	ILE
41	2j	13	HIS
7	2H	122	THR
40	2i	64	THR
48	2q	76	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	42	GLN
35	2d	119	GLN
40	2i	87	GLN
40	1i	31	GLN
39	1h	82	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	468 (16%)	28 (0%)
1	2A	2791/2915 (95%)	490 (17%)	25 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1497/1521 (98%)	318 (21%)	0
32	2a	1501/1521 (98%)	323 (21%)	0
53	1v	10/24 (41%)	3 (30%)	0
53	2v	10/24 (41%)	2 (20%)	0
55	1x	73/76 (96%)	13 (17%)	0
55	1y	71/76 (93%)	22 (30%)	0
55	2x	73/76 (96%)	12 (16%)	0
55	2y	72/76 (94%)	26 (36%)	0
All	All	9200/9466 (97%)	1706 (18%)	53 (0%)

5 of 1706 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	34	C
1	1A	45	C

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	34	C
1	2A	746	A
1	2A	2119	A
1	2A	196	A
1	2A	271(M)	G

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

78 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	PSU	1y	39	55	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
55	4SU	1x	8	55	18,21,22	1.78	5 (27%)	25,30,33	2.16	5 (20%)
1	2MA	1A	2503	57,1	22,25,26	1.51	4 (18%)	32,37,40	2.32	7 (21%)
43	0TD	1l	92	43	8,9,10	4.34	1 (12%)	6,11,13	7.76	1 (16%)
55	PSU	2y	39	55	18,21,22	1.42	2 (11%)	21,30,33	1.66	3 (14%)
1	PSU	2A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	2.10	5 (23%)
55	PSU	1y	32	55	18,21,22	1.40	3 (16%)	21,30,33	1.94	3 (14%)
55	5MU	1y	54	55	19,22,23	1.43	4 (21%)	27,32,35	1.68	6 (22%)
55	G7M	2y	46	55	23,26,27	1.55	4 (17%)	34,39,42	1.78	5 (14%)
55	PSU	2x	32	55	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
32	PSU	1a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	2.00	5 (23%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.06	9 (27%)
55	PSU	1x	39	55	18,21,22	1.42	2 (11%)	21,30,33	1.86	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.11	8 (24%)
32	PSU	2a	516	57,32	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)
55	MIA	2x	37	55	28,31,32	2.41	5 (17%)	38,44,47	2.70	14 (36%)
55	G7M	2x	46	55	23,26,27	1.51	3 (13%)	34,39,42	1.75	5 (14%)
32	4OC	1a	1402	57,32	20,23,24	0.80	1 (5%)	25,32,35	0.96	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	MIA	1x	37	55	28,31,32	2.36	7 (25%)	38,44,47	2.62	13 (34%)
32	G7M	1a	527	57,32	23,26,27	1.56	3 (13%)	34,39,42	1.73	5 (14%)
32	5MC	2a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.24	4 (15%)
32	UR3	2a	1498	57,32	19,22,23	0.96	0	26,32,35	1.70	2 (7%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	1.96	9 (27%)
55	5MU	1x	54	55	19,22,23	1.40	4 (21%)	27,32,35	1.78	7 (25%)
55	4SU	1y	8	55	18,21,22	1.74	4 (22%)	25,30,33	2.46	6 (24%)
1	2MA	2A	2503	57,1	22,25,26	1.48	4 (18%)	32,37,40	2.24	9 (28%)
1	OMG	1A	2251	55,57,1	23,26,27	1.25	3 (13%)	32,38,41	2.09	7 (21%)
1	5MU	2A	1915	57,1	19,22,23	1.44	5 (26%)	27,32,35	2.14	6 (22%)
1	5MU	1A	1939	57,1	19,22,23	1.46	6 (31%)	27,32,35	2.30	6 (22%)
32	2MG	2a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.21	8 (24%)
54	MEQ	1w	230	54	8,9,10	1.00	0	5,10,12	0.78	0
1	PSU	1A	2605	57,1	18,21,22	1.49	4 (22%)	21,30,33	1.99	4 (19%)
1	OMG	2A	2251	55,57,1	23,26,27	1.29	3 (13%)	32,38,41	1.93	6 (18%)
1	OMC	2A	1920	57,1	19,22,23	0.82	0	25,31,34	0.89	0
32	5MC	1a	1400	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
55	PSU	1x	32	55	18,21,22	1.38	3 (16%)	21,30,33	2.09	5 (23%)
1	5MU	2A	1939	57,1	19,22,23	1.48	6 (31%)	27,32,35	2.15	6 (22%)
1	PSU	2A	1917	1	18,21,22	1.36	3 (16%)	21,30,33	2.09	4 (19%)
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	21,30,33	2.08	3 (14%)
55	PSU	2y	55	55	18,21,22	1.37	3 (16%)	21,30,33	1.98	3 (14%)
32	2MG	1a	1207	32	23,26,27	1.24	4 (17%)	33,38,41	2.20	8 (24%)
55	MIA	2y	37	55	28,31,32	2.45	6 (21%)	38,44,47	2.81	13 (34%)
1	5MU	1A	1915	57,1	19,22,23	1.48	5 (26%)	27,32,35	2.11	6 (22%)
55	G7M	1y	46	55	23,26,27	1.55	4 (17%)	34,39,42	1.81	5 (14%)
32	5MC	2a	967	32	19,22,23	1.61	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.60	2 (10%)	26,32,35	1.16	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.21	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.12	5 (23%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	1.03	2 (8%)
32	M2G	2a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.88	6 (18%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
55	4SU	2y	8	55	18,21,22	1.83	6 (33%)	25,30,33	1.67	5 (20%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.14	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1A	2552	57,1	19,22,23	1.27	3 (15%)	25,31,34	1.93	5 (20%)
55	5MU	2y	54	55	19,22,23	1.44	5 (26%)	27,32,35	2.15	8 (29%)
1	5MC	1A	1942	1	19,22,23	1.50	3 (15%)	26,32,35	1.14	3 (11%)
1	OMU	2A	2552	57,1	19,22,23	1.25	3 (15%)	25,31,34	1.90	5 (20%)
55	PSU	1y	55	55	18,21,22	1.41	2 (11%)	21,30,33	1.91	3 (14%)
55	MIA	1y	37	55	28,31,32	2.36	5 (17%)	38,44,47	2.53	12 (31%)
1	5MC	1A	1962	57,1	19,22,23	1.55	3 (15%)	26,32,35	1.11	2 (7%)
55	PSU	2x	39	55	18,21,22	1.40	2 (11%)	21,30,33	1.86	3 (14%)
32	4OC	2a	1402	57,32	20,23,24	0.79	0	25,32,35	0.92	0
55	G7M	1x	46	55	23,26,27	1.55	4 (17%)	34,39,42	1.78	4 (11%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	2.14	10 (30%)
1	5MC	2A	1962	57,1	19,22,23	1.57	3 (15%)	26,32,35	1.14	2 (7%)
54	MEQ	2w	230	54	8,9,10	0.91	0	5,10,12	0.50	0
55	PSU	2y	32	55	18,21,22	1.40	2 (11%)	21,30,33	1.90	3 (14%)
32	5MC	1a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.10	2 (7%)
32	M2G	1a	966	32	24,27,28	1.31	3 (12%)	33,40,43	1.92	7 (21%)
32	G7M	2a	527	32	23,26,27	1.49	3 (13%)	34,39,42	1.71	5 (14%)
32	UR3	1a	1498	32	19,22,23	1.08	2 (10%)	26,32,35	1.66	4 (15%)
32	5MC	1a	967	32	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
43	0TD	2l	92	43	8,9,10	4.44	2 (25%)	6,11,13	5.67	1 (16%)
55	4SU	2x	8	55	18,21,22	1.87	5 (27%)	25,30,33	2.04	5 (20%)
1	PSU	1A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	2.12	5 (23%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	27,32,35	1.80	6 (22%)
32	5MC	1a	1407	32	19,22,23	1.43	2 (10%)	26,32,35	1.06	2 (7%)
55	PSU	1x	55	55	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)

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	PSU	1y	39	55	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	2/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
55	PSU	2y	39	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	PSU	1y	32	55	-	0/7/25/26	0/2/2/2
55	5MU	1y	54	55	-	0/7/25/26	0/2/2/2
55	G7M	2y	46	55	-	2/7/25/26	0/3/3/3
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	PSU	2a	516	57,32	-	0/7/25/26	0/2/2/2
55	MIA	2x	37	55	-	3/15/33/34	0/3/3/3
55	G7M	2x	46	55	-	3/7/25/26	0/3/3/3
32	4OC	1a	1402	57,32	-	2/9/29/30	0/2/2/2
55	MIA	1x	37	55	-	5/15/33/34	0/3/3/3
32	G7M	1a	527	57,32	-	2/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	57,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
55	4SU	1y	8	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	2/7/25/26	0/3/3/3
1	OMG	1A	2251	55,57,1	-	0/9/27/28	0/3/3/3
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
54	MEQ	1w	230	54	-	3/8/9/11	-
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,57,1	-	0/9/27/28	0/3/3/3
1	OMC	2A	1920	57,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	PSU	2y	55	55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
55	MIA	2y	37	55	-	3/15/33/34	0/3/3/3
1	5MU	1A	1915	57,1	-	0/7/25/26	0/2/2/2
55	G7M	1y	46	55	-	3/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	3/9/27/28	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2y	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
55	5MU	2y	54	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
55	PSU	1y	55	55	-	0/7/25/26	0/2/2/2
55	MIA	1y	37	55	-	4/15/33/34	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	57,32	-	2/9/29/30	0/2/2/2
55	G7M	1x	46	55	-	3/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	5MC	2A	1962	57,1	-	2/7/25/26	0/2/2/2
54	MEQ	2w	230	54	-	2/8/9/11	-
55	PSU	2y	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	5/7/12/14	-
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.01	1.70	1.82
43	1l	92	0TD	CB-SB	-11.84	1.70	1.82
55	2y	37	MIA	C2-S10	-7.45	1.69	1.75
55	1x	37	MIA	C2-S10	-7.12	1.69	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	37	MIA	C13-C14	7.06	1.53	1.32

The worst 5 of 372 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	18.90	136.33	102.36
43	2l	92	0TD	CSB-SB-CB	13.78	127.14	102.36
55	2y	37	MIA	C12-C13-C14	-8.81	111.21	127.01
1	1A	2503	2MA	C5-C4-N3	-8.24	118.50	127.18
55	1x	37	MIA	C12-C13-C14	-8.09	112.49	127.01

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	230	MEQ	C-CA-CB-CG
55	1x	37	MIA	C12-C13-C14-C15
55	1x	37	MIA	C12-C13-C14-C16
55	1x	46	G7M	C4'-C5'-O5'-P

There are no ring outliers.

35 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1y	39	PSU	1	0
55	1x	8	4SU	1	0
1	1A	2503	2MA	2	0
55	2y	39	PSU	1	0
55	2y	46	G7M	1	0
32	2a	1518	MA6	1	0
32	2a	1519	MA6	2	0
32	1a	1402	4OC	2	0
32	1a	1518	MA6	2	0
1	2A	2503	2MA	1	0
1	1A	2251	OMG	1	0
1	1A	1939	5MU	1	0
32	2a	1207	2MG	1	0
1	2A	2251	OMG	1	0
1	2A	1917	PSU	1	0
32	1a	1207	2MG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2y	37	MIA	1	0
55	1y	46	G7M	2	0
32	2a	1404	5MC	1	0
1	1A	1920	OMC	1	0
55	2y	8	4SU	4	0
1	1A	2552	OMU	1	0
55	2y	54	5MU	1	0
55	1y	55	PSU	1	0
55	1y	37	MIA	3	0
32	2a	1402	4OC	2	0
55	1x	46	G7M	1	0
32	1a	1519	MA6	3	0
54	2w	230	MEQ	1	0
32	1a	966	M2G	1	0
32	2a	527	G7M	1	0
32	1a	967	5MC	1	0
43	2l	92	0TD	2	0
55	2x	8	4SU	1	0
1	1A	1917	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2056 ligands modelled in this entry, 2054 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	$\# Z > 2$
59	SF4	1d	302	35	0,12,12	-	-	-		
59	SF4	2d	302	35	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1d	302	SF4	2	0
59	2d	302	SF4	1	0

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%)	-0.51	91 (3%)	50	46	16, 33, 90, 104	0
1	2A	2789/2915 (95%)	-0.02	78 (2%)	55	51	29, 56, 89, 104	0
2	1B	120/121 (99%)	-0.44	0	100	100	25, 48, 61, 77	0
2	2B	120/121 (99%)	0.66	6 (5%)	34	30	59, 79, 88, 98	0
3	1D	275/276 (99%)	-0.18	2 (0%)	84	83	17, 35, 51, 75	0
3	2D	275/276 (99%)	0.41	7 (2%)	58	55	31, 50, 64, 77	0
4	1E	204/206 (99%)	-0.15	0	100	100	17, 36, 55, 67	0
4	2E	204/206 (99%)	0.38	2 (0%)	79	78	35, 56, 69, 77	0
5	1F	203/210 (96%)	-0.15	2 (0%)	79	78	18, 38, 65, 82	0
5	2F	203/210 (96%)	0.48	1 (0%)	87	86	36, 63, 76, 89	0
6	1G	181/182 (99%)	0.59	12 (6%)	24	21	43, 56, 71, 84	0
6	2G	181/182 (99%)	1.35	37 (20%)	3	2	63, 79, 85, 89	0
7	1H	174/180 (96%)	0.17	3 (1%)	69	67	34, 51, 65, 69	0
7	2H	174/180 (96%)	0.91	8 (4%)	37	34	64, 77, 84, 91	0
8	1I	146/148 (98%)	0.51	4 (2%)	56	53	42, 67, 76, 80	0
8	2I	146/148 (98%)	1.01	13 (8%)	15	13	55, 72, 79, 83	0
9	1N	140/140 (100%)	-0.31	0	100	100	21, 32, 54, 61	0
9	2N	140/140 (100%)	0.44	1 (0%)	84	83	45, 61, 72, 80	0
10	1O	122/122 (100%)	-0.13	0	100	100	27, 38, 54, 60	0
10	2O	122/122 (100%)	0.09	0	100	100	38, 53, 63, 73	0
11	1P	149/150 (99%)	0.03	2 (1%)	75	73	15, 39, 59, 67	0
11	2P	149/150 (99%)	0.61	4 (2%)	56	53	37, 65, 77, 88	0
12	1Q	141/141 (100%)	-0.11	0	100	100	23, 37, 52, 71	0
12	2Q	141/141 (100%)	0.60	6 (4%)	40	36	48, 60, 70, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.22	0 100 100	21, 31, 44, 57	0
13	2R	118/118 (100%)	0.33	1 (0%) 82 81	38, 53, 64, 71	0
14	1S	110/112 (98%)	0.11	1 (0%) 81 80	37, 47, 60, 64	0
14	2S	110/112 (98%)	1.05	9 (8%) 17 15	62, 71, 76, 81	0
15	1T	131/146 (89%)	-0.00	3 (2%) 61 58	29, 41, 66, 81	0
15	2T	131/146 (89%)	0.47	3 (2%) 61 58	46, 56, 72, 83	0
16	1U	116/118 (98%)	-0.27	1 (0%) 81 80	18, 26, 39, 58	0
16	2U	116/118 (98%)	0.32	0 100 100	41, 57, 70, 76	0
17	1V	101/101 (100%)	-0.26	0 100 100	18, 35, 52, 58	0
17	2V	101/101 (100%)	0.46	0 100 100	40, 65, 75, 81	0
18	1W	112/113 (99%)	-0.37	0 100 100	21, 27, 42, 81	0
18	2W	112/113 (99%)	0.15	0 100 100	40, 50, 66, 84	0
19	1X	95/96 (98%)	-0.08	1 (1%) 78 76	24, 35, 54, 68	0
19	2X	95/96 (98%)	0.74	4 (4%) 40 37	49, 61, 69, 80	0
20	1Y	107/110 (97%)	0.15	0 100 100	27, 44, 63, 74	0
20	2Y	107/110 (97%)	0.78	4 (3%) 45 41	56, 69, 77, 82	0
21	1Z	183/206 (88%)	0.30	1 (0%) 87 86	35, 54, 69, 74	0
21	2Z	186/206 (90%)	0.69	3 (1%) 70 68	59, 73, 80, 89	0
22	10	76/85 (89%)	-0.08	0 100 100	25, 35, 48, 61	0
22	20	77/85 (90%)	1.02	9 (11%) 9 7	50, 62, 70, 77	0
23	11	97/98 (98%)	0.09	1 (1%) 79 78	26, 40, 66, 70	0
23	21	97/98 (98%)	0.63	4 (4%) 41 37	41, 58, 74, 79	0
24	12	70/72 (97%)	0.12	3 (4%) 40 36	34, 46, 58, 74	0
24	22	70/72 (97%)	0.41	1 (1%) 73 72	57, 67, 73, 78	0
25	13	59/60 (98%)	-0.27	0 100 100	20, 31, 55, 72	0
25	23	59/60 (98%)	0.40	1 (1%) 69 67	50, 58, 71, 78	0
26	14	69/71 (97%)	0.93	9 (13%) 7 6	53, 73, 86, 88	0
26	24	68/71 (95%)	1.29	16 (23%) 2 1	76, 84, 89, 94	0
27	15	59/60 (98%)	-0.46	0 100 100	16, 28, 45, 55	0
27	25	59/60 (98%)	0.37	2 (3%) 48 44	34, 50, 66, 82	0
28	16	53/54 (98%)	-0.14	0 100 100	30, 40, 54, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.56	0 100 100	54, 61, 68, 73	0
29	17	48/49 (97%)	-0.10	3 (6%) 26 23	21, 26, 64, 66	0
29	27	48/49 (97%)	0.31	4 (8%) 17 14	36, 44, 65, 79	0
30	18	64/65 (98%)	0.04	0 100 100	24, 30, 37, 46	0
30	28	64/65 (98%)	0.52	1 (1%) 70 68	43, 51, 60, 62	0
31	19	37/37 (100%)	0.00	0 100 100	27, 39, 52, 57	0
31	29	37/37 (100%)	0.71	0 100 100	56, 64, 73, 76	0
32	1a	1488/1521 (97%)	0.45	56 (3%) 44 40	35, 71, 92, 103	0
32	2a	1491/1521 (98%)	0.50	46 (3%) 51 48	44, 74, 92, 104	0
33	1b	231/256 (90%)	1.02	25 (10%) 11 9	63, 75, 85, 90	0
33	2b	231/256 (90%)	1.43	63 (27%) 1 1	63, 79, 87, 96	0
34	1c	206/239 (86%)	1.07	18 (8%) 16 13	63, 77, 84, 91	0
34	2c	206/239 (86%)	1.07	21 (10%) 12 10	67, 78, 84, 87	0
35	1d	208/209 (99%)	0.99	11 (5%) 32 28	53, 72, 79, 89	0
35	2d	208/209 (99%)	0.86	13 (6%) 26 23	53, 68, 76, 86	0
36	1e	148/162 (91%)	0.64	4 (2%) 56 53	53, 64, 73, 81	0
36	2e	148/162 (91%)	0.89	10 (6%) 23 20	58, 70, 76, 88	0
37	1f	100/101 (99%)	0.62	2 (2%) 65 62	55, 68, 75, 80	0
37	2f	100/101 (99%)	0.75	2 (2%) 65 62	57, 70, 76, 79	0
38	1g	155/156 (99%)	0.85	12 (7%) 19 17	60, 73, 82, 90	0
38	2g	155/156 (99%)	1.03	18 (11%) 9 8	66, 79, 85, 91	0
39	1h	137/138 (99%)	0.59	10 (7%) 21 18	56, 65, 73, 76	0
39	2h	137/138 (99%)	0.87	8 (5%) 29 25	59, 70, 77, 83	0
40	1i	127/128 (99%)	1.40	28 (22%) 2 2	60, 77, 83, 89	0
40	2i	123/128 (96%)	2.11	63 (51%) 0 0	70, 82, 87, 91	0
41	1j	98/105 (93%)	1.46	23 (23%) 2 1	63, 79, 85, 89	0
41	2j	96/105 (91%)	1.94	38 (39%) 1 0	72, 82, 88, 91	0
42	1k	114/129 (88%)	0.57	5 (4%) 39 35	45, 65, 75, 78	0
42	2k	114/129 (88%)	0.92	9 (7%) 18 16	62, 73, 80, 85	0
43	1l	121/132 (91%)	0.52	5 (4%) 41 37	47, 59, 70, 73	0
43	2l	121/132 (91%)	0.57	3 (2%) 58 55	49, 61, 69, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	1.16	8 (6%) 23 20	60, 73, 78, 84	0
44	2m	115/126 (91%)	1.49	24 (20%) 2 2	69, 81, 87, 88	0
45	1n	60/61 (98%)	1.43	13 (21%) 2 2	67, 74, 80, 81	0
45	2n	60/61 (98%)	2.25	27 (45%) 0 0	72, 80, 86, 92	0
46	1o	88/89 (98%)	0.72	6 (6%) 23 20	49, 63, 73, 79	0
46	2o	88/89 (98%)	0.85	3 (3%) 48 44	60, 69, 77, 81	0
47	1p	82/88 (93%)	1.35	17 (20%) 2 2	58, 71, 80, 82	0
47	2p	82/88 (93%)	0.85	1 (1%) 76 75	56, 67, 74, 78	0
48	1q	99/105 (94%)	0.70	6 (6%) 27 24	50, 63, 71, 75	0
48	2q	99/105 (94%)	0.67	3 (3%) 52 49	57, 67, 74, 78	0
49	1r	68/88 (77%)	0.44	0 100 100	53, 64, 74, 80	0
49	2r	68/88 (77%)	0.80	0 100 100	61, 71, 76, 80	0
50	1s	83/93 (89%)	1.43	16 (19%) 3 3	66, 76, 81, 83	0
50	2s	83/93 (89%)	1.46	18 (21%) 2 2	74, 82, 88, 90	0
51	1t	96/106 (90%)	0.88	7 (7%) 21 18	54, 67, 78, 83	0
51	2t	96/106 (90%)	0.81	7 (7%) 21 18	56, 68, 78, 83	0
52	1u	23/27 (85%)	1.53	5 (21%) 2 2	65, 71, 74, 79	0
52	2u	23/27 (85%)	1.81	10 (43%) 0 0	72, 82, 85, 86	0
53	1v	13/24 (54%)	0.72	3 (23%) 2 2	52, 64, 92, 92	0
53	2v	13/24 (54%)	1.44	5 (38%) 1 0	68, 75, 98, 100	0
54	1w	248/354 (70%)	0.29	8 (3%) 50 46	29, 65, 79, 87	0
54	2w	252/354 (71%)	0.69	12 (4%) 35 32	48, 73, 83, 88	0
55	1x	68/76 (89%)	-0.20	0 100 100	27, 59, 73, 82	0
55	1y	67/76 (88%)	0.81	7 (10%) 11 10	41, 91, 97, 99	0
55	2x	68/76 (89%)	0.22	0 100 100	48, 74, 82, 94	0
55	2y	67/76 (88%)	1.26	8 (11%) 9 7	61, 97, 101, 103	0
56	1z	14/18 (77%)	1.19	3 (21%) 2 2	31, 49, 71, 80	0
56	2z	14/18 (77%)	1.77	5 (35%) 1 0	52, 65, 77, 82	0
All	All	21290/22338 (95%)	0.34	1079 (5%) 33 29	15, 62, 86, 104	0

The worst 5 of 1079 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	7.6
23	11	2	SER	6.3
44	1m	2	ALA	5.9
40	2i	14	VAL	5.9
1	1A	1088	A	5.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MIA	2y	37	29/30	0.56	0.18	82,91,98,107	0
55	PSU	2y	32	20/21	0.61	0.15	86,94,101,104	0
55	G7M	2y	46	24/25	0.61	0.13	85,97,109,126	0
55	4SU	2y	8	20/21	0.62	0.13	94,98,108,118	0
55	5MU	1y	54	21/22	0.63	0.12	82,90,99,103	0
55	PSU	2y	55	20/21	0.63	0.16	88,99,107,107	0
55	5MU	2y	54	21/22	0.65	0.14	89,97,103,117	0
55	PSU	1y	55	20/21	0.66	0.13	82,96,103,107	0
55	PSU	2y	39	20/21	0.68	0.13	87,96,107,118	0
55	G7M	1y	46	24/25	0.69	0.14	79,92,98,111	0
55	MIA	1y	37	29/30	0.71	0.16	73,88,99,113	0
55	4SU	1y	8	20/21	0.75	0.12	80,92,98,103	0
55	PSU	1y	32	20/21	0.81	0.12	72,83,91,96	0
55	PSU	1y	39	20/21	0.81	0.09	76,87,94,98	0
32	2MG	2a	1207	24/25	0.83	0.13	72,83,87,87	0
55	G7M	2x	46	24/25	0.85	0.12	65,73,81,100	0
43	0TD	1l	92	10/11	0.86	0.15	60,63,67,79	0
55	PSU	2x	32	20/21	0.86	0.13	72,79,86,86	0
55	MIA	2x	37	29/30	0.88	0.15	65,76,83,102	0
55	G7M	1x	46	24/25	0.88	0.10	50,60,73,97	0
32	2MG	1a	1207	24/25	0.88	0.11	73,78,83,84	0
55	PSU	2x	55	20/21	0.89	0.09	70,76,82,90	0
32	PSU	2a	516	20/21	0.90	0.10	69,77,84,86	0
32	5MC	2a	967	21/22	0.90	0.15	63,69,76,76	0
32	5MC	2a	1400	21/22	0.91	0.14	57,73,74,79	0
55	5MU	1x	54	21/22	0.92	0.09	58,64,70,73	0
55	4SU	2x	8	20/21	0.92	0.09	60,70,77,78	0
32	G7M	2a	527	24/25	0.92	0.11	60,68,71,73	0
32	M2G	2a	966	25/26	0.92	0.13	61,67,78,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	MIA	1x	37	29/30	0.92	0.11	43,58,65,90	0
55	5MU	2x	54	21/22	0.92	0.09	62,70,78,80	0
1	5MU	2A	1915	21/22	0.92	0.09	62,68,75,79	0
32	M2G	1a	966	25/26	0.93	0.12	49,61,69,75	0
55	PSU	1x	32	20/21	0.93	0.10	52,61,71,71	0
32	PSU	1a	516	20/21	0.93	0.10	51,67,75,75	0
55	PSU	2x	39	20/21	0.93	0.09	56,72,78,78	0
55	PSU	1x	39	20/21	0.93	0.09	54,59,63,69	0
32	MA6	2a	1518	24/25	0.93	0.13	51,57,62,63	0
43	0TD	2l	92	10/11	0.93	0.11	52,64,68,81	0
1	5MU	1A	1915	21/22	0.94	0.10	46,51,58,62	0
1	PSU	2A	1917	20/21	0.94	0.09	59,63,67,68	0
32	5MC	1a	1400	21/22	0.94	0.11	47,60,68,73	0
32	4OC	2a	1402	22/23	0.94	0.12	54,61,65,66	0
32	5MC	1a	967	21/22	0.94	0.10	55,62,67,69	0
1	PSU	2A	1911	20/21	0.94	0.09	52,61,66,68	0
54	MEQ	2w	230	10/11	0.94	0.12	52,54,56,57	0
32	G7M	1a	527	24/25	0.95	0.10	51,62,71,74	0
32	5MC	2a	1404	21/22	0.95	0.10	49,58,65,67	0
32	5MC	2a	1407	21/22	0.95	0.10	47,56,61,64	0
55	PSU	1x	55	20/21	0.95	0.08	55,60,64,71	0
1	PSU	1A	1917	20/21	0.96	0.07	42,48,53,54	0
1	5MC	1A	1962	21/22	0.96	0.09	22,29,36,37	0
32	4OC	1a	1402	22/23	0.96	0.09	41,47,53,54	0
32	5MC	1a	1404	21/22	0.96	0.09	40,46,52,59	0
32	5MC	1a	1407	21/22	0.96	0.09	36,42,48,50	0
32	MA6	1a	1518	24/25	0.96	0.10	36,43,48,60	0
1	PSU	1A	1911	20/21	0.96	0.09	36,47,55,55	0
55	4SU	1x	8	20/21	0.96	0.07	39,48,55,59	0
1	OMC	2A	1920	21/22	0.96	0.09	53,57,62,63	0
32	UR3	2a	1498	21/22	0.96	0.10	48,53,62,68	0
1	5MC	2A	1962	21/22	0.96	0.09	37,43,47,57	0
32	MA6	2a	1519	24/25	0.96	0.11	51,57,62,63	0
1	OMG	2A	2251	24/25	0.96	0.09	24,39,45,50	0
1	2MA	2A	2503	23/24	0.96	0.07	31,35,41,42	0
1	OMU	2A	2552	21/22	0.97	0.08	30,36,41,48	0
1	PSU	2A	2605	20/21	0.97	0.07	33,39,46,49	0
32	MA6	1a	1519	24/25	0.97	0.09	38,42,48,50	0
1	OMU	1A	2552	21/22	0.97	0.08	19,26,30,35	0
54	MEQ	1w	230	10/11	0.97	0.07	25,30,33,33	0
1	5MU	2A	1939	21/22	0.97	0.08	36,41,46,48	0
1	5MC	2A	1942	21/22	0.97	0.07	44,52,56,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PSU	1A	2605	20/21	0.97	0.07	20,25,35,36	0
1	5MC	1A	1942	21/22	0.97	0.07	30,33,39,45	0
1	OMC	1A	1920	21/22	0.97	0.08	34,43,46,50	0
1	OMG	1A	2251	24/25	0.98	0.06	19,23,26,29	0
1	5MU	1A	1939	21/22	0.98	0.07	18,26,30,31	0
32	UR3	1a	1498	21/22	0.98	0.07	38,45,50,53	0
1	2MA	1A	2503	23/24	0.99	0.05	14,19,22,22	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
57	MG	1A	3634	1/1	0.56	0.58	60,60,60,60	0
57	MG	1A	3490	1/1	0.58	0.20	75,75,75,75	0
57	MG	1A	3658	1/1	0.59	0.22	68,68,68,68	0
57	MG	1A	3726	1/1	0.64	0.14	46,46,46,46	0
57	MG	2A	3148	1/1	0.66	0.26	69,69,69,69	0
57	MG	2A	3116	1/1	0.67	0.42	81,81,81,81	0
57	MG	2a	1694	1/1	0.67	0.26	78,78,78,78	0
57	MG	1A	3650	1/1	0.68	0.20	54,54,54,54	0
57	MG	2A	3638	1/1	0.70	0.17	65,65,65,65	0
57	MG	1A	3641	1/1	0.70	0.10	42,42,42,42	0
57	MG	1a	1638	1/1	0.71	0.32	79,79,79,79	0
57	MG	2A	3511	1/1	0.71	0.17	77,77,77,77	0
57	MG	2A	3110	1/1	0.72	0.13	75,75,75,75	0
57	MG	2A	3598	1/1	0.72	0.19	82,82,82,82	0
57	MG	2A	3379	1/1	0.72	0.14	67,67,67,67	0
57	MG	2a	1602	1/1	0.72	0.14	68,68,68,68	0
57	MG	2A	3410	1/1	0.72	0.20	69,69,69,69	0
57	MG	2A	3431	1/1	0.73	0.20	50,50,50,50	0
57	MG	1w	404	1/1	0.73	0.18	69,69,69,69	0
57	MG	2A	3182	1/1	0.73	0.23	65,65,65,65	0
57	MG	1A	3336	1/1	0.74	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3624	1/1	0.74	0.30	72,72,72,72	0
57	MG	1a	1738	1/1	0.74	0.22	64,64,64,64	0
57	MG	2A	3535	1/1	0.74	0.23	67,67,67,67	0
57	MG	2A	3262	1/1	0.75	0.28	68,68,68,68	0
57	MG	2A	3486	1/1	0.75	0.14	65,65,65,65	0
57	MG	2A	3648	1/1	0.75	0.15	77,77,77,77	0
57	MG	1A	3644	1/1	0.75	0.18	32,32,32,32	0
57	MG	2A	3144	1/1	0.75	0.16	71,71,71,71	0
57	MG	2a	1759	1/1	0.75	0.14	78,78,78,78	0
57	MG	2A	3578	1/1	0.76	0.12	54,54,54,54	0
57	MG	2a	1752	1/1	0.76	0.25	69,69,69,69	0
57	MG	2A	3639	1/1	0.76	0.15	78,78,78,78	0
57	MG	2A	3348	1/1	0.77	0.13	56,56,56,56	0
57	MG	1a	1707	1/1	0.77	0.23	71,71,71,71	0
57	MG	2a	1720	1/1	0.77	0.20	76,76,76,76	0
57	MG	2A	3055	1/1	0.77	0.20	64,64,64,64	0
57	MG	2A	3662	1/1	0.77	0.29	73,73,73,73	0
57	MG	2e	201	1/1	0.77	0.11	70,70,70,70	0
57	MG	1A	3771	1/1	0.78	0.16	66,66,66,66	0
57	MG	2A	3481	1/1	0.78	0.19	60,60,60,60	0
57	MG	1O	202	1/1	0.78	0.16	67,67,67,67	0
57	MG	2X	104	1/1	0.78	0.15	83,83,83,83	0
57	MG	2A	3137	1/1	0.78	0.15	69,69,69,69	0
57	MG	2A	3532	1/1	0.78	0.19	68,68,68,68	0
57	MG	2A	3354	1/1	0.78	0.18	72,72,72,72	0
57	MG	1A	3664	1/1	0.78	0.11	45,45,45,45	0
57	MG	2a	1758	1/1	0.78	0.24	69,69,69,69	0
57	MG	1a	1669	1/1	0.78	0.29	59,59,59,59	0
57	MG	2A	3422	1/1	0.78	0.22	47,47,47,47	0
57	MG	2A	3665	1/1	0.79	0.12	63,63,63,63	0
57	MG	1A	3371	1/1	0.79	0.13	66,66,66,66	0
57	MG	1A	3219	1/1	0.79	0.18	69,69,69,69	0
57	MG	2a	1665	1/1	0.79	0.39	68,68,68,68	0
57	MG	2A	3256	1/1	0.79	0.14	53,53,53,53	0
57	MG	1E	307	1/1	0.79	0.19	31,31,31,31	0
57	MG	2A	3434	1/1	0.79	0.15	57,57,57,57	0
57	MG	2A	3284	1/1	0.79	0.23	49,49,49,49	0
57	MG	1A	3021	1/1	0.79	0.16	56,56,56,56	0
57	MG	1a	1612	1/1	0.79	0.22	54,54,54,54	0
57	MG	1A	3516	1/1	0.80	0.23	54,54,54,54	0
57	MG	2A	3603	1/1	0.80	0.13	69,69,69,69	0
57	MG	2a	1643	1/1	0.80	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3618	1/1	0.80	0.14	58,58,58,58	0
57	MG	2A	3105	1/1	0.80	0.32	67,67,67,67	0
57	MG	1c	301	1/1	0.80	0.28	71,71,71,71	0
57	MG	2a	1735	1/1	0.80	0.17	65,65,65,65	0
57	MG	2A	3647	1/1	0.80	0.16	67,67,67,67	0
57	MG	2A	3572	1/1	0.80	0.19	75,75,75,75	0
57	MG	1A	3690	1/1	0.80	0.18	58,58,58,58	0
57	MG	2A	3580	1/1	0.80	0.19	61,61,61,61	0
57	MG	2x	108	1/1	0.80	0.29	77,77,77,77	0
57	MG	1a	1771	1/1	0.81	0.13	60,60,60,60	0
57	MG	1a	1783	1/1	0.81	0.25	60,60,60,60	0
57	MG	2A	3505	1/1	0.81	0.14	70,70,70,70	0
57	MG	1A	3455	1/1	0.81	0.14	16,16,16,16	0
57	MG	1A	3314	1/1	0.81	0.14	39,39,39,39	0
57	MG	2A	3305	1/1	0.81	0.23	67,67,67,67	0
57	MG	2a	1657	1/1	0.81	0.16	72,72,72,72	0
57	MG	1A	3328	1/1	0.81	0.21	51,51,51,51	0
57	MG	1a	1683	1/1	0.81	0.18	63,63,63,63	0
57	MG	2A	3359	1/1	0.81	0.22	60,60,60,60	0
57	MG	1a	1688	1/1	0.81	0.18	57,57,57,57	0
57	MG	1A	3596	1/1	0.81	0.17	62,62,62,62	0
57	MG	2A	3416	1/1	0.81	0.32	59,59,59,59	0
57	MG	1a	1718	1/1	0.81	0.20	69,69,69,69	0
57	MG	2a	1769	1/1	0.81	0.33	77,77,77,77	0
57	MG	1a	1733	1/1	0.81	0.25	62,62,62,62	0
57	MG	2x	101	1/1	0.81	0.20	72,72,72,72	0
57	MG	1l	103	1/1	0.81	0.26	52,52,52,52	0
57	MG	1a	1756	1/1	0.82	0.17	63,63,63,63	0
57	MG	2A	3374	1/1	0.82	0.17	63,63,63,63	0
57	MG	2A	3195	1/1	0.82	0.23	60,60,60,60	0
57	MG	2A	3201	1/1	0.82	0.13	57,57,57,57	0
57	MG	2A	3211	1/1	0.82	0.10	81,81,81,81	0
57	MG	2a	1668	1/1	0.82	0.34	70,70,70,70	0
57	MG	2A	3589	1/1	0.82	0.26	70,70,70,70	0
57	MG	2a	1708	1/1	0.82	0.22	66,66,66,66	0
57	MG	1A	3674	1/1	0.82	0.13	54,54,54,54	0
57	MG	1A	3746	1/1	0.82	0.14	25,25,25,25	0
57	MG	1A	3102	1/1	0.82	0.23	52,52,52,52	0
57	MG	2A	3472	1/1	0.82	0.18	65,65,65,65	0
57	MG	2A	3473	1/1	0.82	0.21	71,71,71,71	0
57	MG	2A	3288	1/1	0.82	0.13	61,61,61,61	0
57	MG	2a	1771	1/1	0.82	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3807	1/1	0.82	0.19	49,49,49,49	0
57	MG	2A	3037	1/1	0.82	0.23	59,59,59,59	0
57	MG	2A	3048	1/1	0.82	0.30	61,61,61,61	0
57	MG	2A	3652	1/1	0.83	0.15	49,49,49,49	0
57	MG	2A	3655	1/1	0.83	0.19	70,70,70,70	0
57	MG	2A	3369	1/1	0.83	0.14	66,66,66,66	0
57	MG	2A	3513	1/1	0.83	0.13	60,60,60,60	0
57	MG	2B	206	1/1	0.83	0.37	69,69,69,69	0
57	MG	2A	3523	1/1	0.83	0.14	62,62,62,62	0
57	MG	1A	3362	1/1	0.83	0.09	39,39,39,39	0
57	MG	1A	3753	1/1	0.83	0.10	50,50,50,50	0
57	MG	2a	1652	1/1	0.83	0.17	67,67,67,67	0
57	MG	2A	3555	1/1	0.83	0.19	59,59,59,59	0
57	MG	2A	3556	1/1	0.83	0.27	61,61,61,61	0
57	MG	2A	3244	1/1	0.83	0.30	79,79,79,79	0
57	MG	2a	1674	1/1	0.83	0.23	65,65,65,65	0
57	MG	2a	1684	1/1	0.83	0.19	61,61,61,61	0
57	MG	2A	3129	1/1	0.83	0.30	64,64,64,64	0
57	MG	2a	1701	1/1	0.83	0.18	82,82,82,82	0
57	MG	1A	3049	1/1	0.83	0.28	63,63,63,63	0
57	MG	2A	3584	1/1	0.83	0.14	81,81,81,81	0
57	MG	2A	3138	1/1	0.83	0.14	71,71,71,71	0
57	MG	1A	3524	1/1	0.83	0.11	49,49,49,49	0
57	MG	1a	1750	1/1	0.83	0.24	66,66,66,66	0
57	MG	2A	3610	1/1	0.83	0.16	41,41,41,41	0
57	MG	2A	3314	1/1	0.83	0.12	64,64,64,64	0
57	MG	2A	3173	1/1	0.83	0.18	65,65,65,65	0
57	MG	1A	3153	1/1	0.83	0.09	76,76,76,76	0
57	MG	2A	3503	1/1	0.83	0.11	54,54,54,54	0
57	MG	1A	3604	1/1	0.83	0.09	23,23,23,23	0
57	MG	1A	3274	1/1	0.84	0.23	43,43,43,43	0
57	MG	2A	3461	1/1	0.84	0.20	46,46,46,46	0
57	MG	1A	3589	1/1	0.84	0.09	21,21,21,21	0
57	MG	2A	3025	1/1	0.84	0.25	67,67,67,67	0
57	MG	1A	3020	1/1	0.84	0.24	65,65,65,65	0
57	MG	1a	1725	1/1	0.84	0.26	53,53,53,53	0
57	MG	2A	3501	1/1	0.84	0.28	70,70,70,70	0
57	MG	1A	3404	1/1	0.84	0.16	37,37,37,37	0
57	MG	2A	3617	1/1	0.84	0.25	57,57,57,57	0
57	MG	1A	3775	1/1	0.84	0.19	59,59,59,59	0
57	MG	2A	3622	1/1	0.84	0.15	81,81,81,81	0
57	MG	2A	3626	1/1	0.84	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
57	MG	1a	1652	1/1	0.84	0.22	76,76,76,76	0
57	MG	2A	3405	1/1	0.84	0.14	63,63,63,63	0
57	MG	1a	1661	1/1	0.84	0.24	56,56,56,56	0
57	MG	1a	1767	1/1	0.84	0.25	52,52,52,52	0
57	MG	1A	3798	1/1	0.84	0.19	64,64,64,64	0
57	MG	2A	3537	1/1	0.84	0.17	75,75,75,75	0
57	MG	2A	3656	1/1	0.84	0.11	45,45,45,45	0
57	MG	2A	3543	1/1	0.84	0.13	71,71,71,71	0
57	MG	2A	3423	1/1	0.84	0.23	61,61,61,61	0
57	MG	1A	3646	1/1	0.84	0.15	46,46,46,46	0
57	MG	1B	212	1/1	0.85	0.29	67,67,67,67	0
57	MG	1a	1702	1/1	0.85	0.21	57,57,57,57	0
57	MG	2A	3274	1/1	0.85	0.11	44,44,44,44	0
57	MG	2A	3046	1/1	0.85	0.15	61,61,61,61	0
57	MG	1A	3286	1/1	0.85	0.13	60,60,60,60	0
57	MG	2A	3661	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3491	1/1	0.85	0.17	49,49,49,49	0
57	MG	2A	3071	1/1	0.85	0.10	44,44,44,44	0
57	MG	2B	205	1/1	0.85	0.16	61,61,61,61	0
57	MG	1A	3496	1/1	0.85	0.12	32,32,32,32	0
57	MG	1a	1731	1/1	0.85	0.10	54,54,54,54	0
57	MG	2A	3536	1/1	0.85	0.19	72,72,72,72	0
57	MG	2a	1605	1/1	0.85	0.17	66,66,66,66	0
57	MG	1a	1611	1/1	0.85	0.23	68,68,68,68	0
57	MG	2a	1648	1/1	0.85	0.16	51,51,51,51	0
57	MG	1A	3761	1/1	0.85	0.15	45,45,45,45	0
57	MG	1a	1623	1/1	0.85	0.15	58,58,58,58	0
57	MG	2a	1658	1/1	0.85	0.22	59,59,59,59	0
57	MG	1a	1633	1/1	0.85	0.18	57,57,57,57	0
57	MG	2A	3564	1/1	0.85	0.19	65,65,65,65	0
57	MG	2A	3401	1/1	0.85	0.11	39,39,39,39	0
57	MG	1A	3610	1/1	0.85	0.11	53,53,53,53	0
57	MG	1a	1769	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3583	1/1	0.85	0.26	73,73,73,73	0
57	MG	1A	3423	1/1	0.85	0.09	18,18,18,18	0
57	MG	2a	1713	1/1	0.85	0.11	63,63,63,63	0
57	MG	1a	1782	1/1	0.85	0.12	58,58,58,58	0
57	MG	1A	3105	1/1	0.85	0.18	50,50,50,50	0
57	MG	2A	3197	1/1	0.85	0.19	64,64,64,64	0
57	MG	1A	3571	1/1	0.85	0.11	37,37,37,37	0
57	MG	2A	3443	1/1	0.85	0.14	65,65,65,65	0
57	MG	2A	3448	1/1	0.85	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1w	402	1/1	0.85	0.21	44,44,44,44	0
57	MG	2A	3227	1/1	0.85	0.24	54,54,54,54	0
57	MG	2A	3240	1/1	0.85	0.13	47,47,47,47	0
57	MG	1B	211	1/1	0.85	0.21	57,57,57,57	0
57	MG	2A	3482	1/1	0.86	0.11	41,41,41,41	0
57	MG	1a	1626	1/1	0.86	0.33	70,70,70,70	0
57	MG	2A	3500	1/1	0.86	0.11	54,54,54,54	0
57	MG	1A	3370	1/1	0.86	0.20	66,66,66,66	0
57	MG	1A	3492	1/1	0.86	0.13	52,52,52,52	0
57	MG	2A	3319	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3339	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3341	1/1	0.86	0.16	60,60,60,60	0
57	MG	1a	1648	1/1	0.86	0.21	54,54,54,54	0
57	MG	1A	3661	1/1	0.86	0.12	52,52,52,52	0
57	MG	1a	1656	1/1	0.86	0.24	53,53,53,53	0
57	MG	20	101	1/1	0.86	0.10	77,77,77,77	0
57	MG	21	101	1/1	0.86	0.13	57,57,57,57	0
57	MG	1a	1659	1/1	0.86	0.18	56,56,56,56	0
57	MG	2A	3161	1/1	0.86	0.29	59,59,59,59	0
57	MG	2a	1626	1/1	0.86	0.26	60,60,60,60	0
57	MG	2a	1632	1/1	0.86	0.20	69,69,69,69	0
57	MG	2A	3171	1/1	0.86	0.25	53,53,53,53	0
57	MG	2A	3397	1/1	0.86	0.14	49,49,49,49	0
57	MG	2A	3399	1/1	0.86	0.29	68,68,68,68	0
57	MG	1a	1778	1/1	0.86	0.17	58,58,58,58	0
57	MG	1A	3175	1/1	0.86	0.28	43,43,43,43	0
57	MG	1A	3615	1/1	0.86	0.21	47,47,47,47	0
57	MG	1A	3466	1/1	0.86	0.11	25,25,25,25	0
57	MG	2A	3418	1/1	0.86	0.18	60,60,60,60	0
57	MG	1A	3716	1/1	0.86	0.12	50,50,50,50	0
57	MG	1a	1693	1/1	0.86	0.20	66,66,66,66	0
57	MG	2A	3591	1/1	0.86	0.26	57,57,57,57	0
57	MG	1a	1701	1/1	0.86	0.09	62,62,62,62	0
57	MG	2A	3601	1/1	0.86	0.12	52,52,52,52	0
57	MG	1A	3470	1/1	0.86	0.18	60,60,60,60	0
57	MG	1A	3544	1/1	0.86	0.14	37,37,37,37	0
57	MG	2a	1744	1/1	0.86	0.24	67,67,67,67	0
57	MG	2A	3611	1/1	0.86	0.13	66,66,66,66	0
57	MG	2a	1756	1/1	0.86	0.17	47,47,47,47	0
57	MG	2A	3613	1/1	0.86	0.11	43,43,43,43	0
57	MG	1A	3749	1/1	0.86	0.13	30,30,30,30	0
57	MG	1a	1721	1/1	0.86	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3468	1/1	0.86	0.13	54,54,54,54	0
57	MG	1A	3488	1/1	0.86	0.22	62,62,62,62	0
57	MG	2A	3281	1/1	0.86	0.12	65,65,65,65	0
57	MG	1A	3045	1/1	0.86	0.12	30,30,30,30	0
57	MG	1B	201	1/1	0.87	0.08	56,56,56,56	0
57	MG	2A	3072	1/1	0.87	0.17	57,57,57,57	0
57	MG	2A	3081	1/1	0.87	0.16	59,59,59,59	0
57	MG	1A	3594	1/1	0.87	0.10	33,33,33,33	0
57	MG	2A	3383	1/1	0.87	0.21	57,57,57,57	0
57	MG	2A	3612	1/1	0.87	0.15	54,54,54,54	0
57	MG	2A	3393	1/1	0.87	0.12	58,58,58,58	0
57	MG	1A	3281	1/1	0.87	0.14	50,50,50,50	0
57	MG	2A	3112	1/1	0.87	0.24	60,60,60,60	0
57	MG	1A	3346	1/1	0.87	0.12	49,49,49,49	0
57	MG	2A	3126	1/1	0.87	0.24	55,55,55,55	0
57	MG	2A	3634	1/1	0.87	0.07	57,57,57,57	0
57	MG	2A	3406	1/1	0.87	0.13	51,51,51,51	0
57	MG	1A	3503	1/1	0.87	0.11	52,52,52,52	0
57	MG	1A	3613	1/1	0.87	0.47	30,30,30,30	0
57	MG	18	101	1/1	0.87	0.24	64,64,64,64	0
57	MG	1A	3350	1/1	0.87	0.12	56,56,56,56	0
57	MG	2A	3654	1/1	0.87	0.25	56,56,56,56	0
57	MG	2A	3147	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3059	1/1	0.87	0.17	35,35,35,35	0
57	MG	2A	3151	1/1	0.87	0.20	53,53,53,53	0
57	MG	2A	3159	1/1	0.87	0.14	53,53,53,53	0
57	MG	1a	1617	1/1	0.87	0.16	59,59,59,59	0
57	MG	2A	3455	1/1	0.87	0.12	56,56,56,56	0
57	MG	2A	3168	1/1	0.87	0.31	64,64,64,64	0
57	MG	2X	102	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3467	1/1	0.87	0.18	54,54,54,54	0
57	MG	1a	1740	1/1	0.87	0.20	73,73,73,73	0
57	MG	1A	3736	1/1	0.87	0.23	30,30,30,30	0
57	MG	1A	3629	1/1	0.87	0.11	34,34,34,34	0
57	MG	1a	1758	1/1	0.87	0.23	73,73,73,73	0
57	MG	1a	1759	1/1	0.87	0.09	63,63,63,63	0
57	MG	1A	3543	1/1	0.87	0.12	17,17,17,17	0
57	MG	2a	1636	1/1	0.87	0.18	65,65,65,65	0
57	MG	2A	3210	1/1	0.87	0.10	57,57,57,57	0
57	MG	1A	3636	1/1	0.87	0.29	41,41,41,41	0
57	MG	1A	3758	1/1	0.87	0.10	51,51,51,51	0
57	MG	1a	1773	1/1	0.87	0.14	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3302	1/1	0.87	0.34	34,34,34,34	0
57	MG	1A	3765	1/1	0.87	0.15	49,49,49,49	0
57	MG	1a	1657	1/1	0.87	0.20	57,57,57,57	0
57	MG	2A	3526	1/1	0.87	0.27	67,67,67,67	0
57	MG	2a	1677	1/1	0.87	0.25	65,65,65,65	0
57	MG	2A	3531	1/1	0.87	0.18	64,64,64,64	0
57	MG	1A	3770	1/1	0.87	0.38	43,43,43,43	0
57	MG	1v	101	1/1	0.87	0.12	71,71,71,71	0
57	MG	1A	3552	1/1	0.87	0.09	16,16,16,16	0
57	MG	1a	1667	1/1	0.87	0.39	64,64,64,64	0
57	MG	2a	1717	1/1	0.87	0.20	73,73,73,73	0
57	MG	2A	3542	1/1	0.87	0.14	58,58,58,58	0
57	MG	2a	1728	1/1	0.87	0.24	49,49,49,49	0
57	MG	2A	3295	1/1	0.87	0.11	74,74,74,74	0
57	MG	2A	3298	1/1	0.87	0.19	50,50,50,50	0
57	MG	1y	101	1/1	0.87	0.22	77,77,77,77	0
57	MG	1A	3122	1/1	0.87	0.21	56,56,56,56	0
57	MG	1a	1673	1/1	0.87	0.29	66,66,66,66	0
57	MG	2A	3335	1/1	0.87	0.17	59,59,59,59	0
57	MG	2a	1761	1/1	0.87	0.11	59,59,59,59	0
57	MG	1A	3647	1/1	0.87	0.18	54,54,54,54	0
57	MG	1a	1686	1/1	0.87	0.10	75,75,75,75	0
57	MG	2A	3347	1/1	0.87	0.14	40,40,40,40	0
57	MG	2j	201	1/1	0.87	0.15	74,74,74,74	0
57	MG	1A	3016	1/1	0.87	0.19	40,40,40,40	0
57	MG	2x	102	1/1	0.87	0.24	68,68,68,68	0
57	MG	2A	3059	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3186	1/1	0.88	0.12	54,54,54,54	0
57	MG	2A	3194	1/1	0.88	0.35	65,65,65,65	0
57	MG	2A	3390	1/1	0.88	0.21	64,64,64,64	0
57	MG	2B	209	1/1	0.88	0.31	63,63,63,63	0
57	MG	2D	306	1/1	0.88	0.12	54,54,54,54	0
57	MG	1A	3108	1/1	0.88	0.18	44,44,44,44	0
57	MG	1a	1668	1/1	0.88	0.29	60,60,60,60	0
57	MG	2A	3198	1/1	0.88	0.14	45,45,45,45	0
57	MG	1A	3645	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3538	1/1	0.88	0.20	41,41,41,41	0
57	MG	1a	1679	1/1	0.88	0.16	42,42,42,42	0
57	MG	2a	1612	1/1	0.88	0.11	50,50,50,50	0
57	MG	2a	1624	1/1	0.88	0.22	61,61,61,61	0
57	MG	1B	210	1/1	0.88	0.28	59,59,59,59	0
57	MG	1a	1624	1/1	0.88	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3579	1/1	0.88	0.20	53,53,53,53	0
57	MG	1A	3111	1/1	0.88	0.16	42,42,42,42	0
57	MG	2A	3248	1/1	0.88	0.10	38,38,38,38	0
57	MG	2a	1650	1/1	0.88	0.33	57,57,57,57	0
57	MG	2A	3250	1/1	0.88	0.26	67,67,67,67	0
57	MG	2A	3588	1/1	0.88	0.20	64,64,64,64	0
57	MG	2A	3428	1/1	0.88	0.09	42,42,42,42	0
57	MG	2a	1659	1/1	0.88	0.12	48,48,48,48	0
57	MG	2A	3115	1/1	0.88	0.32	61,61,61,61	0
57	MG	1A	3477	1/1	0.88	0.08	31,31,31,31	0
57	MG	2a	1671	1/1	0.88	0.29	53,53,53,53	0
57	MG	1a	1634	1/1	0.88	0.34	62,62,62,62	0
57	MG	2A	3602	1/1	0.88	0.17	44,44,44,44	0
57	MG	2a	1680	1/1	0.88	0.20	50,50,50,50	0
57	MG	1a	1779	1/1	0.88	0.18	56,56,56,56	0
57	MG	2A	3134	1/1	0.88	0.19	46,46,46,46	0
57	MG	1A	3375	1/1	0.88	0.09	31,31,31,31	0
57	MG	2A	3292	1/1	0.88	0.14	66,66,66,66	0
57	MG	1a	1703	1/1	0.88	0.15	64,64,64,64	0
57	MG	2A	3140	1/1	0.88	0.11	64,64,64,64	0
57	MG	2A	3141	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3620	1/1	0.88	0.13	46,46,46,46	0
57	MG	2A	3476	1/1	0.88	0.23	52,52,52,52	0
57	MG	1A	3741	1/1	0.88	0.25	68,68,68,68	0
57	MG	2A	3629	1/1	0.88	0.20	70,70,70,70	0
57	MG	1a	1649	1/1	0.88	0.12	58,58,58,58	0
57	MG	1Z	301	1/1	0.88	0.17	53,53,53,53	0
57	MG	1A	3459	1/1	0.88	0.20	58,58,58,58	0
57	MG	2A	3340	1/1	0.88	0.13	47,47,47,47	0
57	MG	2a	1763	1/1	0.88	0.15	64,64,64,64	0
57	MG	2a	1764	1/1	0.88	0.11	51,51,51,51	0
57	MG	1a	1729	1/1	0.88	0.20	58,58,58,58	0
57	MG	14	502	1/1	0.88	0.28	69,69,69,69	0
57	MG	2A	3164	1/1	0.88	0.15	56,56,56,56	0
57	MG	2f	201	1/1	0.88	0.19	59,59,59,59	0
57	MG	1A	3796	1/1	0.88	0.25	69,69,69,69	0
57	MG	2t	201	1/1	0.88	0.21	54,54,54,54	0
57	MG	2A	3039	1/1	0.88	0.11	51,51,51,51	0
57	MG	1a	1734	1/1	0.88	0.26	71,71,71,71	0
57	MG	1a	1605	1/1	0.88	0.35	54,54,54,54	0
57	MG	2A	3346	1/1	0.89	0.11	58,58,58,58	0
57	MG	2A	3029	1/1	0.89	0.20	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3033	1/1	0.89	0.20	69,69,69,69	0
57	MG	2A	3352	1/1	0.89	0.18	54,54,54,54	0
57	MG	2F	303	1/1	0.89	0.11	64,64,64,64	0
57	MG	2Q	203	1/1	0.89	0.28	56,56,56,56	0
57	MG	1A	3744	1/1	0.89	0.12	40,40,40,40	0
57	MG	2A	3356	1/1	0.89	0.13	65,65,65,65	0
57	MG	1a	1732	1/1	0.89	0.24	56,56,56,56	0
57	MG	2A	3362	1/1	0.89	0.13	48,48,48,48	0
57	MG	28	101	1/1	0.89	0.19	63,63,63,63	0
57	MG	1A	3195	1/1	0.89	0.16	42,42,42,42	0
57	MG	1A	3518	1/1	0.89	0.12	39,39,39,39	0
57	MG	2a	1610	1/1	0.89	0.17	64,64,64,64	0
57	MG	2A	3544	1/1	0.89	0.13	67,67,67,67	0
57	MG	2a	1620	1/1	0.89	0.19	59,59,59,59	0
57	MG	2A	3546	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3751	1/1	0.89	0.12	56,56,56,56	0
57	MG	2a	1630	1/1	0.89	0.15	60,60,60,60	0
57	MG	1A	3648	1/1	0.89	0.15	47,47,47,47	0
57	MG	1a	1744	1/1	0.89	0.27	74,74,74,74	0
57	MG	2A	3570	1/1	0.89	0.17	50,50,50,50	0
57	MG	2a	1645	1/1	0.89	0.16	59,59,59,59	0
57	MG	1a	1665	1/1	0.89	0.15	66,66,66,66	0
57	MG	2A	3074	1/1	0.89	0.22	62,62,62,62	0
57	MG	2A	3207	1/1	0.89	0.15	39,39,39,39	0
57	MG	2a	1653	1/1	0.89	0.14	61,61,61,61	0
57	MG	2A	3075	1/1	0.89	0.16	59,59,59,59	0
57	MG	1A	3064	1/1	0.89	0.18	40,40,40,40	0
57	MG	2A	3212	1/1	0.89	0.09	58,58,58,58	0
57	MG	2A	3587	1/1	0.89	0.12	73,73,73,73	0
57	MG	2A	3407	1/1	0.89	0.15	43,43,43,43	0
57	MG	2A	3083	1/1	0.89	0.23	53,53,53,53	0
57	MG	2A	3413	1/1	0.89	0.15	50,50,50,50	0
57	MG	2A	3233	1/1	0.89	0.13	62,62,62,62	0
57	MG	2A	3239	1/1	0.89	0.20	63,63,63,63	0
57	MG	2A	3419	1/1	0.89	0.18	65,65,65,65	0
57	MG	2a	1685	1/1	0.89	0.28	65,65,65,65	0
57	MG	2a	1688	1/1	0.89	0.28	64,64,64,64	0
57	MG	1A	3267	1/1	0.89	0.23	48,48,48,48	0
57	MG	1A	3085	1/1	0.89	0.26	51,51,51,51	0
57	MG	1A	3767	1/1	0.89	0.23	29,29,29,29	0
57	MG	1A	3626	1/1	0.89	0.12	35,35,35,35	0
57	MG	1A	3670	1/1	0.89	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3261	1/1	0.89	0.12	57,57,57,57	0
57	MG	2a	1727	1/1	0.89	0.20	76,76,76,76	0
57	MG	1a	1620	1/1	0.89	0.10	49,49,49,49	0
57	MG	2a	1730	1/1	0.89	0.19	71,71,71,71	0
57	MG	1A	3030	1/1	0.89	0.11	43,43,43,43	0
57	MG	2A	3621	1/1	0.89	0.12	48,48,48,48	0
57	MG	2a	1747	1/1	0.89	0.16	64,64,64,64	0
57	MG	2a	1748	1/1	0.89	0.22	62,62,62,62	0
57	MG	1A	3683	1/1	0.89	0.16	46,46,46,46	0
57	MG	2A	3135	1/1	0.89	0.28	53,53,53,53	0
57	MG	1A	3188	1/1	0.89	0.24	51,51,51,51	0
57	MG	1A	3802	1/1	0.89	0.07	20,20,20,20	0
57	MG	2a	1760	1/1	0.89	0.15	65,65,65,65	0
57	MG	1A	3355	1/1	0.89	0.11	45,45,45,45	0
57	MG	1A	3288	1/1	0.89	0.40	40,40,40,40	0
57	MG	1a	1639	1/1	0.89	0.22	62,62,62,62	0
57	MG	2a	1768	1/1	0.89	0.20	73,73,73,73	0
57	MG	1a	1647	1/1	0.89	0.20	60,60,60,60	0
57	MG	1x	107	1/1	0.89	0.07	43,43,43,43	0
57	MG	2A	3493	1/1	0.89	0.18	57,57,57,57	0
57	MG	2A	3322	1/1	0.89	0.17	46,46,46,46	0
57	MG	1A	3514	1/1	0.89	0.08	31,31,31,31	0
57	MG	2k	201	1/1	0.89	0.27	68,68,68,68	0
57	MG	2A	3019	1/1	0.89	0.25	40,40,40,40	0
57	MG	1A	3515	1/1	0.89	0.09	29,29,29,29	0
57	MG	2A	3162	1/1	0.89	0.23	45,45,45,45	0
57	MG	2x	105	1/1	0.89	0.14	40,40,40,40	0
57	MG	2B	204	1/1	0.89	0.23	56,56,56,56	0
57	MG	1a	1685	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3738	1/1	0.90	0.16	63,63,63,63	0
57	MG	2A	3027	1/1	0.90	0.35	51,51,51,51	0
57	MG	1A	3247	1/1	0.90	0.16	54,54,54,54	0
57	MG	2A	3214	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3463	1/1	0.90	0.30	48,48,48,48	0
57	MG	1A	3424	1/1	0.90	0.10	17,17,17,17	0
57	MG	1a	1609	1/1	0.90	0.20	65,65,65,65	0
57	MG	2B	202	1/1	0.90	0.19	70,70,70,70	0
57	MG	2A	3470	1/1	0.90	0.11	43,43,43,43	0
57	MG	1A	3431	1/1	0.90	0.07	16,16,16,16	0
57	MG	1A	3452	1/1	0.90	0.12	35,35,35,35	0
57	MG	2A	3474	1/1	0.90	0.15	52,52,52,52	0
57	MG	2D	301	1/1	0.90	0.25	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1614	1/1	0.90	0.12	74,74,74,74	0
57	MG	2A	3478	1/1	0.90	0.17	70,70,70,70	0
57	MG	2Q	201	1/1	0.90	0.27	61,61,61,61	0
57	MG	1a	1711	1/1	0.90	0.16	76,76,76,76	0
57	MG	2R	201	1/1	0.90	0.13	66,66,66,66	0
57	MG	2V	202	1/1	0.90	0.19	49,49,49,49	0
57	MG	2A	3058	1/1	0.90	0.15	61,61,61,61	0
57	MG	1a	1717	1/1	0.90	0.15	51,51,51,51	0
57	MG	2A	3490	1/1	0.90	0.17	75,75,75,75	0
57	MG	1A	3750	1/1	0.90	0.14	32,32,32,32	0
57	MG	2A	3495	1/1	0.90	0.10	54,54,54,54	0
57	MG	1A	3261	1/1	0.90	0.10	52,52,52,52	0
57	MG	1a	1724	1/1	0.90	0.21	51,51,51,51	0
57	MG	2A	3278	1/1	0.90	0.15	49,49,49,49	0
57	MG	2A	3504	1/1	0.90	0.16	64,64,64,64	0
57	MG	2a	1613	1/1	0.90	0.24	56,56,56,56	0
57	MG	2A	3279	1/1	0.90	0.13	61,61,61,61	0
57	MG	1a	1622	1/1	0.90	0.26	55,55,55,55	0
57	MG	1A	3642	1/1	0.90	0.07	19,19,19,19	0
57	MG	2a	1629	1/1	0.90	0.13	67,67,67,67	0
57	MG	2A	3082	1/1	0.90	0.15	48,48,48,48	0
57	MG	1a	1730	1/1	0.90	0.15	46,46,46,46	0
57	MG	2A	3528	1/1	0.90	0.12	68,68,68,68	0
57	MG	2a	1639	1/1	0.90	0.14	44,44,44,44	0
57	MG	2A	3096	1/1	0.90	0.13	48,48,48,48	0
57	MG	1A	3542	1/1	0.90	0.13	30,30,30,30	0
57	MG	2a	1646	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3533	1/1	0.90	0.11	65,65,65,65	0
57	MG	1A	3156	1/1	0.90	0.09	54,54,54,54	0
57	MG	1A	3028	1/1	0.90	0.17	52,52,52,52	0
57	MG	1A	3546	1/1	0.90	0.08	36,36,36,36	0
57	MG	1A	3467	1/1	0.90	0.12	25,25,25,25	0
57	MG	2A	3334	1/1	0.90	0.10	35,35,35,35	0
57	MG	1A	3275	1/1	0.90	0.18	65,65,65,65	0
57	MG	2A	3127	1/1	0.90	0.16	54,54,54,54	0
57	MG	2A	3554	1/1	0.90	0.13	65,65,65,65	0
57	MG	1a	1743	1/1	0.90	0.14	51,51,51,51	0
57	MG	2A	3131	1/1	0.90	0.11	50,50,50,50	0
57	MG	2a	1675	1/1	0.90	0.11	59,59,59,59	0
57	MG	1a	1646	1/1	0.90	0.18	66,66,66,66	0
57	MG	2A	3566	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3568	1/1	0.90	0.09	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3583	1/1	0.90	0.11	19,19,19,19	0
57	MG	1a	1753	1/1	0.90	0.19	58,58,58,58	0
57	MG	2a	1691	1/1	0.90	0.15	39,39,39,39	0
57	MG	1A	3279	1/1	0.90	0.26	56,56,56,56	0
57	MG	1A	3361	1/1	0.90	0.09	40,40,40,40	0
57	MG	1a	1651	1/1	0.90	0.25	36,36,36,36	0
57	MG	2a	1711	1/1	0.90	0.14	52,52,52,52	0
57	MG	2A	3143	1/1	0.90	0.25	56,56,56,56	0
57	MG	1a	1762	1/1	0.90	0.14	50,50,50,50	0
57	MG	1A	3019	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	3368	1/1	0.90	0.10	10,10,10,10	0
57	MG	1A	3677	1/1	0.90	0.11	71,71,71,71	0
57	MG	2A	3590	1/1	0.90	0.20	48,48,48,48	0
57	MG	2A	3153	1/1	0.90	0.14	60,60,60,60	0
57	MG	2a	1742	1/1	0.90	0.17	50,50,50,50	0
57	MG	1A	3191	1/1	0.90	0.10	35,35,35,35	0
57	MG	1a	1775	1/1	0.90	0.12	71,71,71,71	0
57	MG	1a	1660	1/1	0.90	0.12	48,48,48,48	0
57	MG	2A	3163	1/1	0.90	0.23	62,62,62,62	0
57	MG	2a	1754	1/1	0.90	0.23	67,67,67,67	0
57	MG	1A	3287	1/1	0.90	0.23	49,49,49,49	0
57	MG	1A	3709	1/1	0.90	0.13	55,55,55,55	0
57	MG	1E	303	1/1	0.90	0.11	42,42,42,42	0
57	MG	1a	1787	1/1	0.90	0.16	49,49,49,49	0
57	MG	2A	3409	1/1	0.90	0.14	76,76,76,76	0
57	MG	1A	3103	1/1	0.90	0.25	53,53,53,53	0
57	MG	1N	203	1/1	0.90	0.08	36,36,36,36	0
57	MG	2A	3191	1/1	0.90	0.12	45,45,45,45	0
57	MG	1a	1671	1/1	0.90	0.33	71,71,71,71	0
57	MG	2A	3624	1/1	0.90	0.27	66,66,66,66	0
57	MG	1A	3619	1/1	0.90	0.11	47,47,47,47	0
57	MG	2e	202	1/1	0.90	0.13	60,60,60,60	0
57	MG	1A	3731	1/1	0.90	0.26	32,32,32,32	0
57	MG	2A	3632	1/1	0.90	0.24	53,53,53,53	0
57	MG	2A	3633	1/1	0.90	0.08	67,67,67,67	0
57	MG	1A	3077	1/1	0.90	0.16	51,51,51,51	0
57	MG	2A	3200	1/1	0.90	0.18	57,57,57,57	0
57	MG	2A	3002	1/1	0.90	0.18	57,57,57,57	0
57	MG	2A	3645	1/1	0.90	0.41	69,69,69,69	0
57	MG	2A	3433	1/1	0.90	0.12	40,40,40,40	0
57	MG	2A	3636	1/1	0.91	0.10	49,49,49,49	0
57	MG	2A	3157	1/1	0.91	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3068	1/1	0.91	0.30	54,54,54,54	0
57	MG	2A	3640	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1642	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	3003	1/1	0.91	0.07	21,21,21,21	0
57	MG	1a	1772	1/1	0.91	0.19	76,76,76,76	0
57	MG	2A	3420	1/1	0.91	0.19	48,48,48,48	0
57	MG	1A	3224	1/1	0.91	0.11	35,35,35,35	0
57	MG	1A	3461	1/1	0.91	0.07	24,24,24,24	0
57	MG	1A	3364	1/1	0.91	0.11	29,29,29,29	0
57	MG	2A	3657	1/1	0.91	0.15	48,48,48,48	0
57	MG	2A	3658	1/1	0.91	0.13	52,52,52,52	0
57	MG	2A	3659	1/1	0.91	0.25	63,63,63,63	0
57	MG	1A	3230	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3176	1/1	0.91	0.08	40,40,40,40	0
57	MG	2A	3177	1/1	0.91	0.22	52,52,52,52	0
57	MG	2A	3438	1/1	0.91	0.09	32,32,32,32	0
57	MG	2A	3178	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3553	1/1	0.91	0.11	19,19,19,19	0
57	MG	1A	3173	1/1	0.91	0.07	43,43,43,43	0
57	MG	2A	3458	1/1	0.91	0.21	57,57,57,57	0
57	MG	2B	210	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3776	1/1	0.91	0.09	29,29,29,29	0
57	MG	1A	3780	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3781	1/1	0.91	0.11	43,43,43,43	0
57	MG	1w	401	1/1	0.91	0.41	46,46,46,46	0
57	MG	1A	3785	1/1	0.91	0.14	45,45,45,45	0
57	MG	1A	3651	1/1	0.91	0.15	40,40,40,40	0
57	MG	2U	201	1/1	0.91	0.09	48,48,48,48	0
57	MG	1A	3580	1/1	0.91	0.07	32,32,32,32	0
57	MG	1A	3253	1/1	0.91	0.10	73,73,73,73	0
57	MG	1A	3585	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3005	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3006	1/1	0.91	0.22	54,54,54,54	0
57	MG	23	101	1/1	0.91	0.14	51,51,51,51	0
57	MG	1A	3668	1/1	0.91	0.08	46,46,46,46	0
57	MG	2A	3484	1/1	0.91	0.14	43,43,43,43	0
57	MG	2a	1604	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3216	1/1	0.91	0.24	53,53,53,53	0
57	MG	2A	3221	1/1	0.91	0.32	66,66,66,66	0
57	MG	2a	1611	1/1	0.91	0.14	54,54,54,54	0
57	MG	1B	209	1/1	0.91	0.23	58,58,58,58	0
57	MG	2A	3026	1/1	0.91	0.25	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3259	1/1	0.91	0.09	57,57,57,57	0
57	MG	1A	3671	1/1	0.91	0.16	49,49,49,49	0
57	MG	2a	1625	1/1	0.91	0.09	51,51,51,51	0
57	MG	2A	3032	1/1	0.91	0.16	48,48,48,48	0
57	MG	2A	3245	1/1	0.91	0.11	62,62,62,62	0
57	MG	1A	3592	1/1	0.91	0.09	18,18,18,18	0
57	MG	1B	219	1/1	0.91	0.19	57,57,57,57	0
57	MG	2a	1634	1/1	0.91	0.22	50,50,50,50	0
57	MG	1A	3377	1/1	0.91	0.07	29,29,29,29	0
57	MG	2A	3514	1/1	0.91	0.09	59,59,59,59	0
57	MG	2a	1640	1/1	0.91	0.20	49,49,49,49	0
57	MG	2a	1642	1/1	0.91	0.22	60,60,60,60	0
57	MG	1a	1692	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	3678	1/1	0.91	0.07	43,43,43,43	0
57	MG	2A	3266	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3529	1/1	0.91	0.09	40,40,40,40	0
57	MG	2A	3051	1/1	0.91	0.21	67,67,67,67	0
57	MG	1N	202	1/1	0.91	0.06	40,40,40,40	0
57	MG	1A	3393	1/1	0.91	0.15	42,42,42,42	0
57	MG	1A	3689	1/1	0.91	0.17	61,61,61,61	0
57	MG	1a	1706	1/1	0.91	0.13	70,70,70,70	0
57	MG	2A	3285	1/1	0.91	0.10	33,33,33,33	0
57	MG	2a	1663	1/1	0.91	0.31	54,54,54,54	0
57	MG	1P	204	1/1	0.91	0.14	42,42,42,42	0
57	MG	2a	1666	1/1	0.91	0.11	62,62,62,62	0
57	MG	1A	3599	1/1	0.91	0.11	31,31,31,31	0
57	MG	1a	1712	1/1	0.91	0.25	64,64,64,64	0
57	MG	2a	1673	1/1	0.91	0.14	80,80,80,80	0
57	MG	2A	3296	1/1	0.91	0.12	40,40,40,40	0
57	MG	2A	3548	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3553	1/1	0.91	0.22	65,65,65,65	0
57	MG	2a	1679	1/1	0.91	0.13	73,73,73,73	0
57	MG	1A	3695	1/1	0.91	0.10	30,30,30,30	0
57	MG	2A	3303	1/1	0.91	0.06	55,55,55,55	0
57	MG	12	101	1/1	0.91	0.12	36,36,36,36	0
57	MG	2A	3557	1/1	0.91	0.10	46,46,46,46	0
57	MG	2A	3307	1/1	0.91	0.11	47,47,47,47	0
57	MG	2A	3565	1/1	0.91	0.20	61,61,61,61	0
57	MG	2a	1698	1/1	0.91	0.21	73,73,73,73	0
57	MG	1a	1720	1/1	0.91	0.22	64,64,64,64	0
57	MG	2A	3084	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3320	1/1	0.91	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3086	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3092	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3706	1/1	0.91	0.13	49,49,49,49	0
57	MG	2A	3104	1/1	0.91	0.18	55,55,55,55	0
57	MG	15	101	1/1	0.91	0.20	38,38,38,38	0
57	MG	2A	3108	1/1	0.91	0.33	48,48,48,48	0
57	MG	2a	1734	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3585	1/1	0.91	0.09	60,60,60,60	0
57	MG	2a	1736	1/1	0.91	0.13	63,63,63,63	0
57	MG	2a	1738	1/1	0.91	0.18	49,49,49,49	0
57	MG	1A	3707	1/1	0.91	0.08	42,42,42,42	0
57	MG	1A	3603	1/1	0.91	0.09	44,44,44,44	0
57	MG	1a	1607	1/1	0.91	0.07	67,67,67,67	0
57	MG	1A	3710	1/1	0.91	0.09	23,23,23,23	0
57	MG	2A	3120	1/1	0.91	0.24	55,55,55,55	0
57	MG	1A	3395	1/1	0.91	0.09	34,34,34,34	0
57	MG	2A	3358	1/1	0.91	0.19	56,56,56,56	0
57	MG	1A	3401	1/1	0.91	0.15	46,46,46,46	0
57	MG	1A	3730	1/1	0.91	0.16	29,29,29,29	0
57	MG	2A	3606	1/1	0.91	0.20	69,69,69,69	0
57	MG	2A	3608	1/1	0.91	0.08	67,67,67,67	0
57	MG	2A	3368	1/1	0.91	0.11	55,55,55,55	0
57	MG	1A	3061	1/1	0.91	0.23	57,57,57,57	0
57	MG	2a	1766	1/1	0.91	0.15	48,48,48,48	0
57	MG	1a	1618	1/1	0.91	0.25	53,53,53,53	0
57	MG	1a	1741	1/1	0.91	0.14	71,71,71,71	0
57	MG	1A	3504	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3508	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3406	1/1	0.91	0.07	22,22,22,22	0
57	MG	2A	3395	1/1	0.91	0.18	68,68,68,68	0
57	MG	1A	3086	1/1	0.91	0.10	27,27,27,27	0
57	MG	1a	1754	1/1	0.91	0.14	41,41,41,41	0
57	MG	1A	3031	1/1	0.91	0.34	38,38,38,38	0
57	MG	2v	101	1/1	0.91	0.16	63,63,63,63	0
57	MG	1A	3194	1/1	0.91	0.19	37,37,37,37	0
57	MG	1A	3635	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3441	1/1	0.91	0.07	19,19,19,19	0
57	MG	1a	1763	1/1	0.91	0.15	69,69,69,69	0
57	MG	2A	3192	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3618	1/1	0.92	0.12	41,41,41,41	0
57	MG	2A	3021	1/1	0.92	0.12	56,56,56,56	0
57	MG	2A	3196	1/1	0.92	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1E	306	1/1	0.92	0.12	24,24,24,24	0
57	MG	1A	3278	1/1	0.92	0.32	56,56,56,56	0
57	MG	2A	3450	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3199	1/1	0.92	0.20	57,57,57,57	0
57	MG	1a	1687	1/1	0.92	0.19	60,60,60,60	0
57	MG	1A	3622	1/1	0.92	0.14	32,32,32,32	0
57	MG	1a	1691	1/1	0.92	0.19	52,52,52,52	0
57	MG	2A	3466	1/1	0.92	0.16	46,46,46,46	0
57	MG	1A	3159	1/1	0.92	0.11	34,34,34,34	0
57	MG	2A	3034	1/1	0.92	0.20	44,44,44,44	0
57	MG	2A	3036	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3471	1/1	0.92	0.16	58,58,58,58	0
57	MG	1A	3522	1/1	0.92	0.09	47,47,47,47	0
57	MG	1a	1698	1/1	0.92	0.19	65,65,65,65	0
57	MG	2A	3220	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3040	1/1	0.92	0.10	54,54,54,54	0
57	MG	2A	3225	1/1	0.92	0.18	46,46,46,46	0
57	MG	2V	201	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3479	1/1	0.92	0.13	60,60,60,60	0
57	MG	1P	201	1/1	0.92	0.27	28,28,28,28	0
57	MG	1A	3433	1/1	0.92	0.17	38,38,38,38	0
57	MG	2A	3236	1/1	0.92	0.18	60,60,60,60	0
57	MG	2A	3049	1/1	0.92	0.15	62,62,62,62	0
57	MG	1Q	205	1/1	0.92	0.10	42,42,42,42	0
57	MG	2A	3491	1/1	0.92	0.11	46,46,46,46	0
57	MG	29	101	1/1	0.92	0.21	64,64,64,64	0
57	MG	2A	3241	1/1	0.92	0.09	64,64,64,64	0
57	MG	2a	1603	1/1	0.92	0.19	64,64,64,64	0
57	MG	2A	3052	1/1	0.92	0.13	46,46,46,46	0
57	MG	1U	201	1/1	0.92	0.16	33,33,33,33	0
57	MG	1A	3537	1/1	0.92	0.10	22,22,22,22	0
57	MG	1A	3360	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3060	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3257	1/1	0.92	0.13	42,42,42,42	0
57	MG	2a	1614	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3509	1/1	0.92	0.15	56,56,56,56	0
57	MG	2a	1623	1/1	0.92	0.18	54,54,54,54	0
57	MG	2A	3258	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3512	1/1	0.92	0.10	61,61,61,61	0
57	MG	1A	3739	1/1	0.92	0.08	38,38,38,38	0
57	MG	1A	3539	1/1	0.92	0.10	31,31,31,31	0
57	MG	2A	3518	1/1	0.92	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3519	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3442	1/1	0.92	0.08	43,43,43,43	0
57	MG	2A	3267	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3052	1/1	0.92	0.10	32,32,32,32	0
57	MG	2A	3076	1/1	0.92	0.17	52,52,52,52	0
57	MG	1a	1603	1/1	0.92	0.23	57,57,57,57	0
57	MG	1A	3282	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3076	1/1	0.92	0.10	28,28,28,28	0
57	MG	1A	3248	1/1	0.92	0.10	41,41,41,41	0
57	MG	2A	3286	1/1	0.92	0.17	63,63,63,63	0
57	MG	2a	1649	1/1	0.92	0.17	59,59,59,59	0
57	MG	2A	3287	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3540	1/1	0.92	0.08	51,51,51,51	0
57	MG	1A	3187	1/1	0.92	0.28	32,32,32,32	0
57	MG	1A	3754	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3555	1/1	0.92	0.08	39,39,39,39	0
57	MG	1A	3007	1/1	0.92	0.07	33,33,33,33	0
57	MG	2a	1660	1/1	0.92	0.18	63,63,63,63	0
57	MG	2a	1661	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3763	1/1	0.92	0.18	59,59,59,59	0
57	MG	2a	1664	1/1	0.92	0.24	52,52,52,52	0
57	MG	2A	3552	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3129	1/1	0.92	0.28	36,36,36,36	0
57	MG	2a	1667	1/1	0.92	0.14	69,69,69,69	0
57	MG	1A	3315	1/1	0.92	0.11	35,35,35,35	0
57	MG	2a	1669	1/1	0.92	0.15	64,64,64,64	0
57	MG	1A	3485	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3380	1/1	0.92	0.15	31,31,31,31	0
57	MG	2A	3317	1/1	0.92	0.15	32,32,32,32	0
57	MG	2A	3559	1/1	0.92	0.10	48,48,48,48	0
57	MG	2a	1676	1/1	0.92	0.39	57,57,57,57	0
57	MG	1A	3591	1/1	0.92	0.11	28,28,28,28	0
57	MG	2A	3118	1/1	0.92	0.08	53,53,53,53	0
57	MG	2A	3321	1/1	0.92	0.13	37,37,37,37	0
57	MG	2a	1683	1/1	0.92	0.15	55,55,55,55	0
57	MG	1a	1627	1/1	0.92	0.34	65,65,65,65	0
57	MG	2A	3323	1/1	0.92	0.10	40,40,40,40	0
57	MG	2a	1687	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3121	1/1	0.92	0.21	55,55,55,55	0
57	MG	2a	1689	1/1	0.92	0.12	61,61,61,61	0
57	MG	1a	1628	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3669	1/1	0.92	0.28	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3778	1/1	0.92	0.09	40,40,40,40	0
57	MG	2A	3130	1/1	0.92	0.23	59,59,59,59	0
57	MG	2a	1703	1/1	0.92	0.22	56,56,56,56	0
57	MG	1a	1757	1/1	0.92	0.10	70,70,70,70	0
57	MG	1A	3386	1/1	0.92	0.09	34,34,34,34	0
57	MG	1A	3325	1/1	0.92	0.17	45,45,45,45	0
57	MG	2a	1715	1/1	0.92	0.09	70,70,70,70	0
57	MG	1a	1760	1/1	0.92	0.18	71,71,71,71	0
57	MG	1a	1761	1/1	0.92	0.15	66,66,66,66	0
57	MG	2a	1722	1/1	0.92	0.22	51,51,51,51	0
57	MG	2a	1723	1/1	0.92	0.14	67,67,67,67	0
57	MG	1A	3783	1/1	0.92	0.11	43,43,43,43	0
57	MG	1A	3133	1/1	0.92	0.07	30,30,30,30	0
57	MG	2a	1729	1/1	0.92	0.21	62,62,62,62	0
57	MG	2A	3142	1/1	0.92	0.26	48,48,48,48	0
57	MG	1A	3789	1/1	0.92	0.22	57,57,57,57	0
57	MG	2A	3366	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3791	1/1	0.92	0.12	20,20,20,20	0
57	MG	1A	3794	1/1	0.92	0.10	45,45,45,45	0
57	MG	2a	1741	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3370	1/1	0.92	0.23	48,48,48,48	0
57	MG	1A	3399	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3329	1/1	0.92	0.06	21,21,21,21	0
57	MG	2A	3152	1/1	0.92	0.14	52,52,52,52	0
57	MG	1a	1653	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3615	1/1	0.92	0.26	49,49,49,49	0
57	MG	1A	3066	1/1	0.92	0.30	46,46,46,46	0
57	MG	1A	3337	1/1	0.92	0.12	37,37,37,37	0
57	MG	2A	3396	1/1	0.92	0.12	49,49,49,49	0
57	MG	2A	3160	1/1	0.92	0.20	65,65,65,65	0
57	MG	1a	1658	1/1	0.92	0.15	62,62,62,62	0
57	MG	2a	1762	1/1	0.92	0.18	65,65,65,65	0
57	MG	1A	3411	1/1	0.92	0.08	39,39,39,39	0
57	MG	1B	202	1/1	0.92	0.20	44,44,44,44	0
57	MG	1B	205	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3107	1/1	0.92	0.23	55,55,55,55	0
57	MG	1A	3700	1/1	0.92	0.23	57,57,57,57	0
57	MG	2a	1770	1/1	0.92	0.22	67,67,67,67	0
57	MG	1A	3703	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3635	1/1	0.92	0.08	49,49,49,49	0
57	MG	2A	3412	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3616	1/1	0.92	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
57	MG	1a	1670	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3617	1/1	0.92	0.16	49,49,49,49	0
57	MG	2A	3641	1/1	0.92	0.07	44,44,44,44	0
57	MG	1D	305	1/1	0.92	0.11	38,38,38,38	0
57	MG	2v	102	1/1	0.92	0.19	59,59,59,59	0
57	MG	2A	3183	1/1	0.92	0.10	37,37,37,37	0
57	MG	2A	3184	1/1	0.92	0.12	51,51,51,51	0
57	MG	1E	302	1/1	0.92	0.09	17,17,17,17	0
57	MG	1a	1680	1/1	0.92	0.12	51,51,51,51	0
57	MG	1A	3523	1/1	0.93	0.16	42,42,42,42	0
57	MG	1A	3095	1/1	0.93	0.11	35,35,35,35	0
57	MG	2A	3172	1/1	0.93	0.09	33,33,33,33	0
57	MG	1a	1784	1/1	0.93	0.20	51,51,51,51	0
57	MG	2A	3174	1/1	0.93	0.16	71,71,71,71	0
57	MG	1A	3533	1/1	0.93	0.06	19,19,19,19	0
57	MG	1a	1650	1/1	0.93	0.13	54,54,54,54	0
57	MG	1A	3407	1/1	0.93	0.07	21,21,21,21	0
57	MG	1v	103	1/1	0.93	0.15	78,78,78,78	0
57	MG	2A	3424	1/1	0.93	0.07	36,36,36,36	0
57	MG	2A	3426	1/1	0.93	0.17	61,61,61,61	0
57	MG	2B	201	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3250	1/1	0.93	0.08	33,33,33,33	0
57	MG	1A	3100	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3341	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3344	1/1	0.93	0.21	43,43,43,43	0
57	MG	2B	208	1/1	0.93	0.21	47,47,47,47	0
57	MG	1A	3432	1/1	0.93	0.09	36,36,36,36	0
57	MG	2A	3193	1/1	0.93	0.10	68,68,68,68	0
57	MG	2B	211	1/1	0.93	0.12	47,47,47,47	0
57	MG	1y	102	1/1	0.93	0.12	73,73,73,73	0
57	MG	2A	3001	1/1	0.93	0.18	59,59,59,59	0
57	MG	2D	307	1/1	0.93	0.10	60,60,60,60	0
57	MG	2A	3451	1/1	0.93	0.10	38,38,38,38	0
57	MG	2F	304	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3453	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3545	1/1	0.93	0.10	19,19,19,19	0
57	MG	2A	3457	1/1	0.93	0.14	54,54,54,54	0
57	MG	1A	3804	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3806	1/1	0.93	0.07	34,34,34,34	0
57	MG	2A	3007	1/1	0.93	0.08	39,39,39,39	0
57	MG	2W	201	1/1	0.93	0.10	52,52,52,52	0
57	MG	2X	101	1/1	0.93	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3013	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3181	1/1	0.93	0.08	36,36,36,36	0
57	MG	2A	3205	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3469	1/1	0.93	0.22	59,59,59,59	0
57	MG	1A	3435	1/1	0.93	0.16	70,70,70,70	0
57	MG	2A	3209	1/1	0.93	0.11	63,63,63,63	0
57	MG	2A	3024	1/1	0.93	0.11	39,39,39,39	0
57	MG	1A	3123	1/1	0.93	0.06	32,32,32,32	0
57	MG	1B	203	1/1	0.93	0.15	50,50,50,50	0
57	MG	1A	3263	1/1	0.93	0.14	39,39,39,39	0
57	MG	1A	3447	1/1	0.93	0.09	17,17,17,17	0
57	MG	2A	3219	1/1	0.93	0.15	46,46,46,46	0
57	MG	2A	3480	1/1	0.93	0.16	48,48,48,48	0
57	MG	2A	3031	1/1	0.93	0.05	47,47,47,47	0
57	MG	1a	1672	1/1	0.93	0.13	56,56,56,56	0
57	MG	1A	3449	1/1	0.93	0.13	55,55,55,55	0
57	MG	2a	1615	1/1	0.93	0.15	59,59,59,59	0
57	MG	1a	1675	1/1	0.93	0.17	59,59,59,59	0
57	MG	2a	1622	1/1	0.93	0.18	58,58,58,58	0
57	MG	2A	3489	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3229	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3035	1/1	0.93	0.10	68,68,68,68	0
57	MG	1A	3679	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3358	1/1	0.93	0.18	40,40,40,40	0
57	MG	2A	3497	1/1	0.93	0.07	63,63,63,63	0
57	MG	2a	1631	1/1	0.93	0.22	63,63,63,63	0
57	MG	2A	3498	1/1	0.93	0.10	57,57,57,57	0
57	MG	1a	1681	1/1	0.93	0.18	66,66,66,66	0
57	MG	1A	3359	1/1	0.93	0.07	38,38,38,38	0
57	MG	2a	1637	1/1	0.93	0.20	49,49,49,49	0
57	MG	1A	3456	1/1	0.93	0.08	32,32,32,32	0
57	MG	1A	3017	1/1	0.93	0.10	41,41,41,41	0
57	MG	1A	3190	1/1	0.93	0.22	54,54,54,54	0
57	MG	2A	3508	1/1	0.93	0.22	55,55,55,55	0
57	MG	2a	1644	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3701	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3032	1/1	0.93	0.15	34,34,34,34	0
57	MG	2A	3053	1/1	0.93	0.21	65,65,65,65	0
57	MG	1A	3595	1/1	0.93	0.05	38,38,38,38	0
57	MG	2A	3260	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3138	1/1	0.93	0.19	30,30,30,30	0
57	MG	1A	3468	1/1	0.93	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3520	1/1	0.93	0.18	47,47,47,47	0
57	MG	2A	3263	1/1	0.93	0.11	66,66,66,66	0
57	MG	2A	3524	1/1	0.93	0.08	40,40,40,40	0
57	MG	2A	3264	1/1	0.93	0.07	47,47,47,47	0
57	MG	1A	3602	1/1	0.93	0.12	62,62,62,62	0
57	MG	2A	3065	1/1	0.93	0.14	46,46,46,46	0
57	MG	2A	3066	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3276	1/1	0.93	0.09	33,33,33,33	0
57	MG	2A	3277	1/1	0.93	0.23	67,67,67,67	0
57	MG	2A	3067	1/1	0.93	0.13	42,42,42,42	0
57	MG	1P	202	1/1	0.93	0.24	24,24,24,24	0
57	MG	1A	3140	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3538	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	3471	1/1	0.93	0.11	50,50,50,50	0
57	MG	1A	3727	1/1	0.93	0.35	21,21,21,21	0
57	MG	1U	203	1/1	0.93	0.07	27,27,27,27	0
57	MG	1A	3606	1/1	0.93	0.07	44,44,44,44	0
57	MG	1a	1714	1/1	0.93	0.14	62,62,62,62	0
57	MG	10	102	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3474	1/1	0.93	0.07	59,59,59,59	0
57	MG	1A	3733	1/1	0.93	0.23	34,34,34,34	0
57	MG	1A	3196	1/1	0.93	0.23	52,52,52,52	0
57	MG	2A	3093	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3095	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3152	1/1	0.93	0.13	30,30,30,30	0
57	MG	1A	3221	1/1	0.93	0.07	30,30,30,30	0
57	MG	2A	3316	1/1	0.93	0.11	46,46,46,46	0
57	MG	2a	1693	1/1	0.93	0.19	47,47,47,47	0
57	MG	1a	1601	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3106	1/1	0.93	0.10	46,46,46,46	0
57	MG	2a	1700	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3740	1/1	0.93	0.17	32,32,32,32	0
57	MG	2A	3569	1/1	0.93	0.11	47,47,47,47	0
57	MG	2a	1706	1/1	0.93	0.25	69,69,69,69	0
57	MG	2a	1707	1/1	0.93	0.17	60,60,60,60	0
57	MG	1a	1604	1/1	0.93	0.09	69,69,69,69	0
57	MG	1A	3011	1/1	0.93	0.16	43,43,43,43	0
57	MG	1A	3378	1/1	0.93	0.06	23,23,23,23	0
57	MG	2a	1714	1/1	0.93	0.16	52,52,52,52	0
57	MG	2A	3324	1/1	0.93	0.09	29,29,29,29	0
57	MG	2a	1716	1/1	0.93	0.12	65,65,65,65	0
57	MG	2A	3326	1/1	0.93	0.16	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3327	1/1	0.93	0.15	50,50,50,50	0
57	MG	1a	1608	1/1	0.93	0.12	52,52,52,52	0
57	MG	1a	1735	1/1	0.93	0.09	54,54,54,54	0
57	MG	2a	1724	1/1	0.93	0.12	55,55,55,55	0
57	MG	2a	1726	1/1	0.93	0.08	58,58,58,58	0
57	MG	2A	3119	1/1	0.93	0.08	58,58,58,58	0
57	MG	1A	3379	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3621	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3343	1/1	0.93	0.08	61,61,61,61	0
57	MG	2a	1731	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	3494	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3593	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3595	1/1	0.93	0.28	63,63,63,63	0
57	MG	1A	3623	1/1	0.93	0.12	51,51,51,51	0
57	MG	2a	1740	1/1	0.93	0.15	64,64,64,64	0
57	MG	2A	3600	1/1	0.93	0.10	54,54,54,54	0
57	MG	1a	1616	1/1	0.93	0.19	55,55,55,55	0
57	MG	1a	1748	1/1	0.93	0.18	42,42,42,42	0
57	MG	1A	3227	1/1	0.93	0.16	36,36,36,36	0
57	MG	1A	3293	1/1	0.93	0.13	48,48,48,48	0
57	MG	1A	3757	1/1	0.93	0.09	41,41,41,41	0
57	MG	2a	1753	1/1	0.93	0.19	56,56,56,56	0
57	MG	1A	3388	1/1	0.93	0.11	44,44,44,44	0
57	MG	1A	3633	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3229	1/1	0.93	0.08	34,34,34,34	0
57	MG	1a	1625	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3764	1/1	0.93	0.07	50,50,50,50	0
57	MG	1A	3001	1/1	0.93	0.09	26,26,26,26	0
57	MG	1A	3232	1/1	0.93	0.14	25,25,25,25	0
57	MG	1a	1632	1/1	0.93	0.26	55,55,55,55	0
57	MG	2A	3380	1/1	0.93	0.17	58,58,58,58	0
57	MG	1a	1764	1/1	0.93	0.19	69,69,69,69	0
57	MG	2a	1767	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3623	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3384	1/1	0.93	0.13	56,56,56,56	0
57	MG	2A	3387	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3627	1/1	0.93	0.09	61,61,61,61	0
57	MG	1A	3637	1/1	0.93	0.24	49,49,49,49	0
57	MG	1A	3638	1/1	0.93	0.32	26,26,26,26	0
57	MG	1a	1637	1/1	0.93	0.15	58,58,58,58	0
57	MG	2A	3155	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3773	1/1	0.93	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3236	1/1	0.93	0.28	35,35,35,35	0
57	MG	2u	101	1/1	0.93	0.19	66,66,66,66	0
57	MG	1a	1774	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3404	1/1	0.93	0.13	58,58,58,58	0
57	MG	1A	3402	1/1	0.93	0.07	26,26,26,26	0
57	MG	1a	1645	1/1	0.93	0.29	55,55,55,55	0
57	MG	1A	3050	1/1	0.93	0.06	26,26,26,26	0
57	MG	2x	106	1/1	0.93	0.18	65,65,65,65	0
57	MG	1a	1781	1/1	0.93	0.16	73,73,73,73	0
57	MG	2A	3337	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3182	1/1	0.94	0.32	29,29,29,29	0
57	MG	2A	3078	1/1	0.94	0.07	51,51,51,51	0
57	MG	2A	3079	1/1	0.94	0.06	30,30,30,30	0
57	MG	1A	3390	1/1	0.94	0.20	42,42,42,42	0
57	MG	1A	3277	1/1	0.94	0.12	28,28,28,28	0
57	MG	1B	206	1/1	0.94	0.13	30,30,30,30	0
57	MG	2A	3628	1/1	0.94	0.08	54,54,54,54	0
57	MG	1a	1689	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3631	1/1	0.94	0.09	56,56,56,56	0
57	MG	2A	3085	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3667	1/1	0.94	0.09	36,36,36,36	0
57	MG	2A	3090	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3394	1/1	0.94	0.11	48,48,48,48	0
57	MG	1A	3117	1/1	0.94	0.07	36,36,36,36	0
57	MG	1a	1694	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3119	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3099	1/1	0.94	0.10	53,53,53,53	0
57	MG	1B	214	1/1	0.94	0.06	42,42,42,42	0
57	MG	1B	215	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3189	1/1	0.94	0.25	45,45,45,45	0
57	MG	1a	1704	1/1	0.94	0.07	64,64,64,64	0
57	MG	2A	3651	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3109	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3381	1/1	0.94	0.06	36,36,36,36	0
57	MG	1A	3089	1/1	0.94	0.27	48,48,48,48	0
57	MG	1A	3675	1/1	0.94	0.06	60,60,60,60	0
57	MG	1A	3403	1/1	0.94	0.07	14,14,14,14	0
57	MG	2A	3389	1/1	0.94	0.08	64,64,64,64	0
57	MG	1A	3283	1/1	0.94	0.24	51,51,51,51	0
57	MG	1A	3284	1/1	0.94	0.07	20,20,20,20	0
57	MG	1F	308	1/1	0.94	0.11	53,53,53,53	0
57	MG	1N	201	1/1	0.94	0.24	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3682	1/1	0.94	0.14	26,26,26,26	0
57	MG	1A	3090	1/1	0.94	0.22	34,34,34,34	0
57	MG	1a	1722	1/1	0.94	0.16	66,66,66,66	0
57	MG	2A	3128	1/1	0.94	0.28	53,53,53,53	0
57	MG	1N	204	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	3687	1/1	0.94	0.21	42,42,42,42	0
57	MG	1a	1726	1/1	0.94	0.17	49,49,49,49	0
57	MG	1A	3688	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3550	1/1	0.94	0.08	23,23,23,23	0
57	MG	2A	3411	1/1	0.94	0.17	45,45,45,45	0
57	MG	2D	304	1/1	0.94	0.51	46,46,46,46	0
57	MG	2A	3136	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3192	1/1	0.94	0.21	30,30,30,30	0
57	MG	2D	308	1/1	0.94	0.09	54,54,54,54	0
57	MG	2D	309	1/1	0.94	0.10	64,64,64,64	0
57	MG	2A	3414	1/1	0.94	0.14	36,36,36,36	0
57	MG	1Q	201	1/1	0.94	0.21	38,38,38,38	0
57	MG	2O	3700	1/1	0.94	0.15	45,45,45,45	0
57	MG	1A	3193	1/1	0.94	0.07	26,26,26,26	0
57	MG	1A	3699	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3124	1/1	0.94	0.19	36,36,36,36	0
57	MG	1V	204	1/1	0.94	0.18	44,44,44,44	0
57	MG	1W	202	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3094	1/1	0.94	0.16	40,40,40,40	0
57	MG	1A	3303	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3581	1/1	0.94	0.09	22,22,22,22	0
57	MG	2A	3430	1/1	0.94	0.21	53,53,53,53	0
57	MG	1a	1746	1/1	0.94	0.09	49,49,49,49	0
57	MG	2Y	201	1/1	0.94	0.09	55,55,55,55	0
57	MG	1a	1747	1/1	0.94	0.20	41,41,41,41	0
57	MG	1A	3582	1/1	0.94	0.18	55,55,55,55	0
57	MG	12	102	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3440	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3441	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3442	1/1	0.94	0.07	34,34,34,34	0
57	MG	1a	1752	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3310	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3132	1/1	0.94	0.22	28,28,28,28	0
57	MG	2a	1606	1/1	0.94	0.16	52,52,52,52	0
57	MG	2a	1608	1/1	0.94	0.12	63,63,63,63	0
57	MG	15	102	1/1	0.94	0.20	27,27,27,27	0
57	MG	2A	3452	1/1	0.94	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	15	103	1/1	0.94	0.13	43,43,43,43	0
57	MG	15	104	1/1	0.94	0.15	29,29,29,29	0
57	MG	2A	3456	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3165	1/1	0.94	0.20	42,42,42,42	0
57	MG	2a	1616	1/1	0.94	0.21	61,61,61,61	0
57	MG	2a	1618	1/1	0.94	0.12	56,56,56,56	0
57	MG	16	101	1/1	0.94	0.09	46,46,46,46	0
57	MG	2a	1621	1/1	0.94	0.25	50,50,50,50	0
57	MG	17	105	1/1	0.94	0.11	30,30,30,30	0
57	MG	1A	3712	1/1	0.94	0.10	46,46,46,46	0
57	MG	2A	3464	1/1	0.94	0.25	58,58,58,58	0
57	MG	18	102	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3715	1/1	0.94	0.18	60,60,60,60	0
57	MG	1A	3587	1/1	0.94	0.06	16,16,16,16	0
57	MG	1A	3717	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3720	1/1	0.94	0.07	39,39,39,39	0
57	MG	1a	1770	1/1	0.94	0.11	42,42,42,42	0
57	MG	1A	3723	1/1	0.94	0.06	43,43,43,43	0
57	MG	2a	1635	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3724	1/1	0.94	0.13	22,22,22,22	0
57	MG	2A	3185	1/1	0.94	0.19	53,53,53,53	0
57	MG	1A	3439	1/1	0.94	0.16	52,52,52,52	0
57	MG	2A	3477	1/1	0.94	0.11	42,42,42,42	0
57	MG	2a	1641	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3189	1/1	0.94	0.27	61,61,61,61	0
57	MG	1A	3590	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3198	1/1	0.94	0.08	48,48,48,48	0
57	MG	1a	1776	1/1	0.94	0.19	56,56,56,56	0
57	MG	1a	1777	1/1	0.94	0.15	57,57,57,57	0
57	MG	2a	1647	1/1	0.94	0.13	63,63,63,63	0
57	MG	1a	1613	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3485	1/1	0.94	0.13	62,62,62,62	0
57	MG	1A	3317	1/1	0.94	0.18	61,61,61,61	0
57	MG	1a	1780	1/1	0.94	0.06	43,43,43,43	0
57	MG	1A	3593	1/1	0.94	0.07	16,16,16,16	0
57	MG	2a	1656	1/1	0.94	0.23	51,51,51,51	0
57	MG	1A	3324	1/1	0.94	0.09	26,26,26,26	0
57	MG	1A	3211	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3212	1/1	0.94	0.15	45,45,45,45	0
57	MG	1A	3454	1/1	0.94	0.07	28,28,28,28	0
57	MG	2A	3206	1/1	0.94	0.19	55,55,55,55	0
57	MG	2a	1662	1/1	0.94	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3499	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3048	1/1	0.94	0.13	35,35,35,35	0
57	MG	1n	101	1/1	0.94	0.17	62,62,62,62	0
57	MG	2A	3502	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3335	1/1	0.94	0.08	39,39,39,39	0
57	MG	1v	102	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3457	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3458	1/1	0.94	0.08	24,24,24,24	0
57	MG	1A	3607	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3218	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3036	1/1	0.94	0.33	30,30,30,30	0
57	MG	1x	103	1/1	0.94	0.12	60,60,60,60	0
57	MG	1a	1630	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3752	1/1	0.94	0.12	58,58,58,58	0
57	MG	1A	3222	1/1	0.94	0.10	36,36,36,36	0
57	MG	2a	1681	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	3101	1/1	0.94	0.15	45,45,45,45	0
57	MG	2A	3230	1/1	0.94	0.52	47,47,47,47	0
57	MG	2A	3232	1/1	0.94	0.32	43,43,43,43	0
57	MG	2A	3525	1/1	0.94	0.07	63,63,63,63	0
57	MG	1a	1636	1/1	0.94	0.18	49,49,49,49	0
57	MG	1A	3756	1/1	0.94	0.08	29,29,29,29	0
57	MG	2A	3237	1/1	0.94	0.17	44,44,44,44	0
57	MG	2A	3530	1/1	0.94	0.08	55,55,55,55	0
57	MG	1A	3141	1/1	0.94	0.10	32,32,32,32	0
57	MG	2a	1697	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3142	1/1	0.94	0.28	31,31,31,31	0
57	MG	2A	3009	1/1	0.94	0.13	57,57,57,57	0
57	MG	2A	3011	1/1	0.94	0.13	43,43,43,43	0
57	MG	1a	1641	1/1	0.94	0.10	44,44,44,44	0
57	MG	2A	3016	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3017	1/1	0.94	0.07	55,55,55,55	0
57	MG	2A	3253	1/1	0.94	0.07	46,46,46,46	0
57	MG	2a	1709	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3469	1/1	0.94	0.11	32,32,32,32	0
57	MG	1a	1644	1/1	0.94	0.17	49,49,49,49	0
57	MG	2A	3023	1/1	0.94	0.13	52,52,52,52	0
57	MG	2A	3259	1/1	0.94	0.08	46,46,46,46	0
57	MG	1A	3145	1/1	0.94	0.14	27,27,27,27	0
57	MG	2A	3551	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3620	1/1	0.94	0.06	19,19,19,19	0
57	MG	1A	3149	1/1	0.94	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3472	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3151	1/1	0.94	0.05	32,32,32,32	0
57	MG	2a	1725	1/1	0.94	0.14	46,46,46,46	0
57	MG	1A	3475	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3772	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3244	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3038	1/1	0.94	0.16	36,36,36,36	0
57	MG	1a	1655	1/1	0.94	0.31	60,60,60,60	0
57	MG	1A	3070	1/1	0.94	0.08	33,33,33,33	0
57	MG	2a	1733	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3777	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3154	1/1	0.94	0.16	40,40,40,40	0
57	MG	1A	3044	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3045	1/1	0.94	0.08	58,58,58,58	0
57	MG	2A	3573	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3574	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3576	1/1	0.94	0.16	60,60,60,60	0
57	MG	2a	1743	1/1	0.94	0.22	59,59,59,59	0
57	MG	1A	3257	1/1	0.94	0.08	34,34,34,34	0
57	MG	2a	1746	1/1	0.94	0.12	62,62,62,62	0
57	MG	2A	3047	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3258	1/1	0.94	0.20	37,37,37,37	0
57	MG	2a	1750	1/1	0.94	0.10	60,60,60,60	0
57	MG	2a	1751	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3582	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3004	1/1	0.94	0.09	31,31,31,31	0
57	MG	2A	3293	1/1	0.94	0.15	54,54,54,54	0
57	MG	2a	1755	1/1	0.94	0.21	57,57,57,57	0
57	MG	2A	3050	1/1	0.94	0.20	59,59,59,59	0
57	MG	1a	1666	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3788	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3299	1/1	0.94	0.06	57,57,57,57	0
57	MG	1A	3640	1/1	0.94	0.12	34,34,34,34	0
57	MG	2A	3054	1/1	0.94	0.21	57,57,57,57	0
57	MG	2A	3592	1/1	0.94	0.14	53,53,53,53	0
57	MG	1A	3372	1/1	0.94	0.13	62,62,62,62	0
57	MG	2a	1765	1/1	0.94	0.14	72,72,72,72	0
57	MG	2A	3056	1/1	0.94	0.12	64,64,64,64	0
57	MG	2A	3057	1/1	0.94	0.17	36,36,36,36	0
57	MG	2A	3599	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3792	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3046	1/1	0.94	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3063	1/1	0.94	0.05	24,24,24,24	0
57	MG	1A	3512	1/1	0.94	0.06	21,21,21,21	0
57	MG	2A	3604	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3264	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3607	1/1	0.94	0.10	61,61,61,61	0
57	MG	1a	1677	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3177	1/1	0.94	0.30	43,43,43,43	0
57	MG	1A	3271	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3073	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3328	1/1	0.94	0.09	59,59,59,59	0
57	MG	2w	402	1/1	0.94	0.14	62,62,62,62	0
57	MG	2A	3614	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3332	1/1	0.94	0.11	50,50,50,50	0
57	MG	2x	103	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	3112	1/1	0.94	0.19	42,42,42,42	0
57	MG	1A	3520	1/1	0.94	0.09	32,32,32,32	0
57	MG	2A	3619	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3438	1/1	0.95	0.10	37,37,37,37	0
57	MG	2B	203	1/1	0.95	0.21	65,65,65,65	0
57	MG	2A	3427	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3179	1/1	0.95	0.14	36,36,36,36	0
57	MG	1A	3005	1/1	0.95	0.10	48,48,48,48	0
57	MG	2B	207	1/1	0.95	0.13	54,54,54,54	0
57	MG	1x	102	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3799	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3340	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3436	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3803	1/1	0.95	0.08	35,35,35,35	0
57	MG	2A	3187	1/1	0.95	0.31	58,58,58,58	0
57	MG	1A	3033	1/1	0.95	0.08	24,24,24,24	0
57	MG	1A	3805	1/1	0.95	0.10	24,24,24,24	0
57	MG	1A	3444	1/1	0.95	0.06	23,23,23,23	0
57	MG	1A	3445	1/1	0.95	0.07	22,22,22,22	0
57	MG	2E	301	1/1	0.95	0.12	46,46,46,46	0
57	MG	2E	303	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3557	1/1	0.95	0.07	17,17,17,17	0
57	MG	1A	3558	1/1	0.95	0.09	33,33,33,33	0
57	MG	1A	3561	1/1	0.95	0.05	62,62,62,62	0
57	MG	1A	3568	1/1	0.95	0.06	22,22,22,22	0
57	MG	1a	1662	1/1	0.95	0.14	61,61,61,61	0
57	MG	2A	3015	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3680	1/1	0.95	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	207	1/1	0.95	0.10	33,33,33,33	0
57	MG	2A	3203	1/1	0.95	0.23	53,53,53,53	0
57	MG	1A	3342	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3579	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3465	1/1	0.95	0.15	67,67,67,67	0
57	MG	1A	3686	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3208	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3072	1/1	0.95	0.28	47,47,47,47	0
57	MG	1A	3266	1/1	0.95	0.18	31,31,31,31	0
57	MG	1A	3205	1/1	0.95	0.09	32,32,32,32	0
57	MG	25	101	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3206	1/1	0.95	0.13	27,27,27,27	0
57	MG	28	103	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3028	1/1	0.95	0.15	38,38,38,38	0
57	MG	2A	3215	1/1	0.95	0.20	41,41,41,41	0
57	MG	1B	220	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3691	1/1	0.95	0.09	48,48,48,48	0
57	MG	1A	3693	1/1	0.95	0.08	42,42,42,42	0
57	MG	1A	3272	1/1	0.95	0.14	25,25,25,25	0
57	MG	1A	3697	1/1	0.95	0.23	35,35,35,35	0
57	MG	2a	1609	1/1	0.95	0.22	68,68,68,68	0
57	MG	1A	3273	1/1	0.95	0.12	28,28,28,28	0
57	MG	2A	3226	1/1	0.95	0.25	43,43,43,43	0
57	MG	1F	304	1/1	0.95	0.18	27,27,27,27	0
57	MG	2A	3483	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3155	1/1	0.95	0.10	23,23,23,23	0
57	MG	2A	3038	1/1	0.95	0.14	46,46,46,46	0
57	MG	1G	201	1/1	0.95	0.11	54,54,54,54	0
57	MG	2A	3488	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3073	1/1	0.95	0.29	46,46,46,46	0
57	MG	2A	3042	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3214	1/1	0.95	0.20	52,52,52,52	0
57	MG	2A	3492	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3704	1/1	0.95	0.14	21,21,21,21	0
57	MG	1A	3463	1/1	0.95	0.09	19,19,19,19	0
57	MG	2A	3496	1/1	0.95	0.19	29,29,29,29	0
57	MG	2a	1628	1/1	0.95	0.19	39,39,39,39	0
57	MG	1O	201	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	3216	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3365	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3060	1/1	0.95	0.09	37,37,37,37	0
57	MG	1P	203	1/1	0.95	0.25	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3280	1/1	0.95	0.11	33,33,33,33	0
57	MG	2A	3254	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3597	1/1	0.95	0.10	28,28,28,28	0
57	MG	2a	1638	1/1	0.95	0.14	73,73,73,73	0
57	MG	1a	1705	1/1	0.95	0.10	51,51,51,51	0
57	MG	1Q	203	1/1	0.95	0.12	34,34,34,34	0
57	MG	1Q	204	1/1	0.95	0.11	41,41,41,41	0
57	MG	1a	1709	1/1	0.95	0.21	46,46,46,46	0
57	MG	1A	3598	1/1	0.95	0.06	45,45,45,45	0
57	MG	1T	201	1/1	0.95	0.08	37,37,37,37	0
57	MG	2A	3062	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3516	1/1	0.95	0.15	45,45,45,45	0
57	MG	2A	3517	1/1	0.95	0.21	55,55,55,55	0
57	MG	2A	3063	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3220	1/1	0.95	0.23	46,46,46,46	0
57	MG	1a	1716	1/1	0.95	0.16	60,60,60,60	0
57	MG	2A	3270	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3272	1/1	0.95	0.08	40,40,40,40	0
57	MG	2a	1654	1/1	0.95	0.30	57,57,57,57	0
57	MG	1A	3601	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3275	1/1	0.95	0.11	48,48,48,48	0
57	MG	1U	204	1/1	0.95	0.12	28,28,28,28	0
57	MG	1A	3721	1/1	0.95	0.07	25,25,25,25	0
57	MG	1A	3722	1/1	0.95	0.09	36,36,36,36	0
57	MG	1X	101	1/1	0.95	0.08	41,41,41,41	0
57	MG	2A	3280	1/1	0.95	0.14	52,52,52,52	0
57	MG	1a	1723	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3171	1/1	0.95	0.12	37,37,37,37	0
57	MG	1Z	302	1/1	0.95	0.13	40,40,40,40	0
57	MG	10	101	1/1	0.95	0.16	27,27,27,27	0
57	MG	2A	3080	1/1	0.95	0.11	52,52,52,52	0
57	MG	1a	1728	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3022	1/1	0.95	0.05	26,26,26,26	0
57	MG	2a	1670	1/1	0.95	0.20	61,61,61,61	0
57	MG	10	103	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3082	1/1	0.95	0.20	28,28,28,28	0
57	MG	1A	3285	1/1	0.95	0.17	45,45,45,45	0
57	MG	2A	3297	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3226	1/1	0.95	0.10	34,34,34,34	0
57	MG	2A	3089	1/1	0.95	0.13	43,43,43,43	0
57	MG	2A	3300	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3609	1/1	0.95	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3304	1/1	0.95	0.09	34,34,34,34	0
57	MG	2a	1682	1/1	0.95	0.13	66,66,66,66	0
57	MG	1A	3479	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3480	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3309	1/1	0.95	0.08	39,39,39,39	0
57	MG	2A	3562	1/1	0.95	0.14	31,31,31,31	0
57	MG	2A	3310	1/1	0.95	0.06	48,48,48,48	0
57	MG	1a	1739	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3483	1/1	0.95	0.12	42,42,42,42	0
57	MG	2a	1692	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3135	1/1	0.95	0.08	29,29,29,29	0
57	MG	2A	3101	1/1	0.95	0.08	46,46,46,46	0
57	MG	2a	1695	1/1	0.95	0.08	48,48,48,48	0
57	MG	2a	1696	1/1	0.95	0.17	54,54,54,54	0
57	MG	2A	3103	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3179	1/1	0.95	0.14	43,43,43,43	0
57	MG	2a	1699	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3387	1/1	0.95	0.07	63,63,63,63	0
57	MG	1a	1745	1/1	0.95	0.16	54,54,54,54	0
57	MG	1A	3742	1/1	0.95	0.10	38,38,38,38	0
57	MG	2a	1705	1/1	0.95	0.11	55,55,55,55	0
57	MG	2A	3325	1/1	0.95	0.15	42,42,42,42	0
57	MG	1A	3136	1/1	0.95	0.10	32,32,32,32	0
57	MG	1A	3296	1/1	0.95	0.20	40,40,40,40	0
57	MG	1a	1749	1/1	0.95	0.06	40,40,40,40	0
57	MG	1a	1602	1/1	0.95	0.22	56,56,56,56	0
57	MG	2a	1712	1/1	0.95	0.11	57,57,57,57	0
57	MG	1a	1751	1/1	0.95	0.12	68,68,68,68	0
57	MG	1A	3299	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3084	1/1	0.95	0.23	50,50,50,50	0
57	MG	1A	3498	1/1	0.95	0.11	42,42,42,42	0
57	MG	1a	1755	1/1	0.95	0.15	54,54,54,54	0
57	MG	2a	1718	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3124	1/1	0.95	0.20	39,39,39,39	0
57	MG	2A	3342	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3125	1/1	0.95	0.11	40,40,40,40	0
57	MG	1A	3184	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3594	1/1	0.95	0.06	74,74,74,74	0
57	MG	1A	3308	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3507	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3350	1/1	0.95	0.07	33,33,33,33	0
57	MG	2A	3351	1/1	0.95	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3630	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3400	1/1	0.95	0.05	18,18,18,18	0
57	MG	2a	1732	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3511	1/1	0.95	0.09	38,38,38,38	0
57	MG	2A	3132	1/1	0.95	0.13	28,28,28,28	0
57	MG	1A	3759	1/1	0.95	0.08	26,26,26,26	0
57	MG	2A	3360	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3139	1/1	0.95	0.14	23,23,23,23	0
57	MG	2a	1739	1/1	0.95	0.12	67,67,67,67	0
57	MG	2A	3364	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3245	1/1	0.95	0.04	20,20,20,20	0
57	MG	1A	3037	1/1	0.95	0.17	28,28,28,28	0
57	MG	1A	3109	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3139	1/1	0.95	0.26	56,56,56,56	0
57	MG	1A	3639	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3375	1/1	0.95	0.16	44,44,44,44	0
57	MG	2A	3378	1/1	0.95	0.05	51,51,51,51	0
57	MG	1A	3769	1/1	0.95	0.24	46,46,46,46	0
57	MG	1A	3322	1/1	0.95	0.09	41,41,41,41	0
57	MG	1A	3023	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3408	1/1	0.95	0.07	34,34,34,34	0
57	MG	2A	3145	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3386	1/1	0.95	0.15	60,60,60,60	0
57	MG	2A	3146	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3065	1/1	0.95	0.21	25,25,25,25	0
57	MG	1A	3416	1/1	0.95	0.07	15,15,15,15	0
57	MG	2A	3391	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3150	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3394	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3532	1/1	0.95	0.14	22,22,22,22	0
57	MG	1A	3420	1/1	0.95	0.08	24,24,24,24	0
57	MG	1A	3146	1/1	0.95	0.24	40,40,40,40	0
57	MG	2A	3154	1/1	0.95	0.08	36,36,36,36	0
57	MG	2A	3637	1/1	0.95	0.11	38,38,38,38	0
57	MG	1A	3113	1/1	0.95	0.13	35,35,35,35	0
57	MG	2A	3402	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3330	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3782	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3334	1/1	0.95	0.08	33,33,33,33	0
57	MG	1A	3659	1/1	0.95	0.07	30,30,30,30	0
57	MG	1a	1786	1/1	0.95	0.16	44,44,44,44	0
57	MG	2A	3650	1/1	0.95	0.07	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3787	1/1	0.95	0.06	20,20,20,20	0
57	MG	1A	3040	1/1	0.95	0.12	36,36,36,36	0
57	MG	1d	301	1/1	0.95	0.23	37,37,37,37	0
57	MG	1f	201	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3170	1/1	0.95	0.14	49,49,49,49	0
57	MG	1m	3001	1/1	0.95	0.10	64,64,64,64	0
57	MG	1a	1643	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3663	1/1	0.95	0.04	29,29,29,29	0
57	MG	1A	3260	1/1	0.95	0.27	49,49,49,49	0
57	MG	2A	3175	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3665	1/1	0.95	0.07	54,54,54,54	0
57	MG	1A	3666	1/1	0.95	0.08	37,37,37,37	0
57	MG	2A	3408	1/1	0.96	0.05	48,48,48,48	0
57	MG	1A	3161	1/1	0.96	0.11	32,32,32,32	0
57	MG	1A	3486	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3162	1/1	0.96	0.08	25,25,25,25	0
57	MG	1a	1619	1/1	0.96	0.05	65,65,65,65	0
57	MG	1a	1785	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3489	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3415	1/1	0.96	0.09	29,29,29,29	0
57	MG	1a	1621	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3417	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3760	1/1	0.96	0.07	18,18,18,18	0
57	MG	1A	3170	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3382	1/1	0.96	0.14	39,39,39,39	0
57	MG	1k	201	1/1	0.96	0.11	53,53,53,53	0
57	MG	1A	3385	1/1	0.96	0.08	34,34,34,34	0
57	MG	1A	3627	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	3766	1/1	0.96	0.18	43,43,43,43	0
57	MG	1A	3223	1/1	0.96	0.17	30,30,30,30	0
57	MG	1a	1629	1/1	0.96	0.17	41,41,41,41	0
57	MG	1A	3768	1/1	0.96	0.14	15,15,15,15	0
57	MG	1a	1631	1/1	0.96	0.11	53,53,53,53	0
57	MG	2A	3432	1/1	0.96	0.09	44,44,44,44	0
57	MG	2D	303	1/1	0.96	0.09	35,35,35,35	0
57	MG	1w	403	1/1	0.96	0.11	31,31,31,31	0
57	MG	2D	305	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3098	1/1	0.96	0.19	35,35,35,35	0
57	MG	1A	3497	1/1	0.96	0.12	43,43,43,43	0
57	MG	2A	3437	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3225	1/1	0.96	0.07	32,32,32,32	0
57	MG	1x	104	1/1	0.96	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1x	106	1/1	0.96	0.04	40,40,40,40	0
57	MG	2F	302	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3126	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3174	1/1	0.96	0.17	29,29,29,29	0
57	MG	2F	306	1/1	0.96	0.10	44,44,44,44	0
57	MG	2N	201	1/1	0.96	0.05	41,41,41,41	0
57	MG	2A	3444	1/1	0.96	0.13	50,50,50,50	0
57	MG	2A	3445	1/1	0.96	0.05	60,60,60,60	0
57	MG	2Q	202	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3446	1/1	0.96	0.09	34,34,34,34	0
57	MG	2A	3447	1/1	0.96	0.11	41,41,41,41	0
57	MG	1A	3774	1/1	0.96	0.22	28,28,28,28	0
57	MG	2A	3449	1/1	0.96	0.17	49,49,49,49	0
57	MG	1A	3055	1/1	0.96	0.16	14,14,14,14	0
57	MG	1a	1640	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3300	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3396	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3398	1/1	0.96	0.09	49,49,49,49	0
57	MG	2A	3008	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3779	1/1	0.96	0.08	41,41,41,41	0
57	MG	20	102	1/1	0.96	0.08	53,53,53,53	0
57	MG	2A	3010	1/1	0.96	0.06	45,45,45,45	0
57	MG	2A	3460	1/1	0.96	0.17	65,65,65,65	0
57	MG	23	102	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3513	1/1	0.96	0.12	28,28,28,28	0
57	MG	2A	3012	1/1	0.96	0.07	46,46,46,46	0
57	MG	28	102	1/1	0.96	0.07	67,67,67,67	0
57	MG	1A	3130	1/1	0.96	0.32	22,22,22,22	0
57	MG	1A	3643	1/1	0.96	0.06	33,33,33,33	0
57	MG	2a	1601	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3178	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3304	1/1	0.96	0.30	32,32,32,32	0
57	MG	2A	3217	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3234	1/1	0.96	0.23	32,32,32,32	0
57	MG	1A	3519	1/1	0.96	0.19	35,35,35,35	0
57	MG	2A	3022	1/1	0.96	0.04	24,24,24,24	0
57	MG	1A	3309	1/1	0.96	0.08	32,32,32,32	0
57	MG	1A	3235	1/1	0.96	0.08	38,38,38,38	0
57	MG	1a	1654	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3475	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3405	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3652	1/1	0.96	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3655	1/1	0.96	0.15	49,49,49,49	0
57	MG	1A	3797	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3312	1/1	0.96	0.06	39,39,39,39	0
57	MG	2a	1619	1/1	0.96	0.06	55,55,55,55	0
57	MG	2A	3235	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3525	1/1	0.96	0.04	36,36,36,36	0
57	MG	1A	3660	1/1	0.96	0.05	24,24,24,24	0
57	MG	2A	3238	1/1	0.96	0.05	44,44,44,44	0
57	MG	1A	3313	1/1	0.96	0.06	18,18,18,18	0
57	MG	1a	1663	1/1	0.96	0.08	50,50,50,50	0
57	MG	1A	3662	1/1	0.96	0.06	36,36,36,36	0
57	MG	2A	3242	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	3014	1/1	0.96	0.07	24,24,24,24	0
57	MG	1A	3534	1/1	0.96	0.10	32,32,32,32	0
57	MG	2A	3246	1/1	0.96	0.12	50,50,50,50	0
57	MG	2A	3247	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3494	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3238	1/1	0.96	0.36	35,35,35,35	0
57	MG	1A	3412	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3413	1/1	0.96	0.08	23,23,23,23	0
57	MG	2A	3044	1/1	0.96	0.17	41,41,41,41	0
57	MG	1A	3316	1/1	0.96	0.08	42,42,42,42	0
57	MG	1B	204	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3417	1/1	0.96	0.06	26,26,26,26	0
57	MG	1a	1674	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3418	1/1	0.96	0.06	24,24,24,24	0
57	MG	1a	1676	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3239	1/1	0.96	0.05	34,34,34,34	0
57	MG	1B	208	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3673	1/1	0.96	0.08	27,27,27,27	0
57	MG	1A	3422	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3549	1/1	0.96	0.13	15,15,15,15	0
57	MG	2A	3269	1/1	0.96	0.04	30,30,30,30	0
57	MG	1a	1684	1/1	0.96	0.18	42,42,42,42	0
57	MG	2A	3271	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3676	1/1	0.96	0.13	43,43,43,43	0
57	MG	2a	1655	1/1	0.96	0.27	52,52,52,52	0
57	MG	2A	3273	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3319	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3024	1/1	0.96	0.05	23,23,23,23	0
57	MG	2A	3522	1/1	0.96	0.08	63,63,63,63	0
57	MG	1B	218	1/1	0.96	0.04	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3027	1/1	0.96	0.18	28,28,28,28	0
57	MG	1A	3246	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3064	1/1	0.96	0.11	54,54,54,54	0
57	MG	2A	3527	1/1	0.96	0.06	62,62,62,62	0
57	MG	1D	301	1/1	0.96	0.26	43,43,43,43	0
57	MG	1A	3327	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3282	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3283	1/1	0.96	0.10	44,44,44,44	0
57	MG	1E	301	1/1	0.96	0.24	28,28,28,28	0
57	MG	2A	3070	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	3434	1/1	0.96	0.06	26,26,26,26	0
57	MG	2a	1672	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3685	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3560	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3289	1/1	0.96	0.10	38,38,38,38	0
57	MG	1A	3015	1/1	0.96	0.10	34,34,34,34	0
57	MG	1F	301	1/1	0.96	0.17	24,24,24,24	0
57	MG	2a	1678	1/1	0.96	0.08	70,70,70,70	0
57	MG	1F	302	1/1	0.96	0.25	34,34,34,34	0
57	MG	2A	3077	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3545	1/1	0.96	0.10	90,90,90,90	0
57	MG	1A	3562	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3547	1/1	0.96	0.05	51,51,51,51	0
57	MG	1F	306	1/1	0.96	0.05	42,42,42,42	0
57	MG	2A	3550	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	3564	1/1	0.96	0.06	22,22,22,22	0
57	MG	1A	3565	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3301	1/1	0.96	0.08	39,39,39,39	0
57	MG	1G	203	1/1	0.96	0.13	41,41,41,41	0
57	MG	1a	1713	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3009	1/1	0.96	0.05	21,21,21,21	0
57	MG	2A	3306	1/1	0.96	0.14	62,62,62,62	0
57	MG	1A	3692	1/1	0.96	0.12	18,18,18,18	0
57	MG	2A	3560	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3561	1/1	0.96	0.16	29,29,29,29	0
57	MG	1A	3569	1/1	0.96	0.05	68,68,68,68	0
57	MG	2A	3563	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3087	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3039	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	3696	1/1	0.96	0.12	40,40,40,40	0
57	MG	2a	1704	1/1	0.96	0.14	57,57,57,57	0
57	MG	2A	3567	1/1	0.96	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3572	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3573	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3575	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3251	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3702	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3051	1/1	0.96	0.12	23,23,23,23	0
57	MG	1a	1727	1/1	0.96	0.15	35,35,35,35	0
57	MG	1A	3443	1/1	0.96	0.08	23,23,23,23	0
57	MG	1A	3255	1/1	0.96	0.06	25,25,25,25	0
57	MG	1A	3256	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3708	1/1	0.96	0.11	31,31,31,31	0
57	MG	1A	3584	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3087	1/1	0.96	0.05	20,20,20,20	0
57	MG	2a	1721	1/1	0.96	0.12	47,47,47,47	0
57	MG	2A	3111	1/1	0.96	0.06	47,47,47,47	0
57	MG	2A	3586	1/1	0.96	0.14	48,48,48,48	0
57	MG	2A	3336	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3586	1/1	0.96	0.05	56,56,56,56	0
57	MG	2A	3338	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3113	1/1	0.96	0.13	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.12	28,28,28,28	0
57	MG	1a	1736	1/1	0.96	0.05	55,55,55,55	0
57	MG	2A	3117	1/1	0.96	0.19	35,35,35,35	0
57	MG	1a	1737	1/1	0.96	0.08	48,48,48,48	0
57	MG	1V	202	1/1	0.96	0.14	26,26,26,26	0
57	MG	2A	3596	1/1	0.96	0.06	65,65,65,65	0
57	MG	1A	3713	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3714	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3448	1/1	0.96	0.09	17,17,17,17	0
57	MG	1A	3088	1/1	0.96	0.07	62,62,62,62	0
57	MG	1A	3143	1/1	0.96	0.10	29,29,29,29	0
57	MG	1A	3006	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3115	1/1	0.96	0.16	21,21,21,21	0
57	MG	2A	3605	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3116	1/1	0.96	0.07	30,30,30,30	0
57	MG	10	104	1/1	0.96	0.06	53,53,53,53	0
57	MG	2a	1745	1/1	0.96	0.14	63,63,63,63	0
57	MG	10	105	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3609	1/1	0.96	0.09	40,40,40,40	0
57	MG	11	102	1/1	0.96	0.38	42,42,42,42	0
57	MG	2a	1749	1/1	0.96	0.13	63,63,63,63	0
57	MG	1A	3353	1/1	0.96	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
57	MG	2A	3365	1/1	0.96	0.11	45,45,45,45	0
57	MG	1l	104	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3150	1/1	0.96	0.19	46,46,46,46	0
57	MG	1A	3725	1/1	0.96	0.08	32,32,32,32	0
57	MG	2A	3616	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3357	1/1	0.96	0.07	20,20,20,20	0
57	MG	2a	1757	1/1	0.96	0.04	52,52,52,52	0
57	MG	1A	3069	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3199	1/1	0.96	0.14	40,40,40,40	0
57	MG	2A	3376	1/1	0.96	0.15	45,45,45,45	0
57	MG	1A	3202	1/1	0.96	0.40	31,31,31,31	0
57	MG	1A	3600	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3118	1/1	0.96	0.18	45,45,45,45	0
57	MG	17	103	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3737	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3054	1/1	0.96	0.16	40,40,40,40	0
57	MG	1A	3207	1/1	0.96	0.09	17,17,17,17	0
57	MG	1a	1766	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3630	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3149	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3120	1/1	0.96	0.15	41,41,41,41	0
57	MG	2a	1772	1/1	0.96	0.10	59,59,59,59	0
57	MG	2d	301	1/1	0.96	0.19	45,45,45,45	0
57	MG	1a	1768	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3121	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3369	1/1	0.96	0.06	12,12,12,12	0
57	MG	1A	3743	1/1	0.96	0.11	22,22,22,22	0
57	MG	1A	3608	1/1	0.96	0.13	57,57,57,57	0
57	MG	2k	202	1/1	0.96	0.06	72,72,72,72	0
57	MG	1a	1606	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3213	1/1	0.96	0.11	29,29,29,29	0
57	MG	2A	3400	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3071	1/1	0.96	0.19	48,48,48,48	0
57	MG	2w	401	1/1	0.96	0.06	38,38,38,38	0
57	MG	2A	3643	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3644	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3157	1/1	0.96	0.04	37,37,37,37	0
57	MG	1A	3478	1/1	0.96	0.08	65,65,65,65	0
57	MG	1A	3373	1/1	0.96	0.12	22,22,22,22	0
57	MG	1A	3217	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	3096	1/1	0.96	0.16	29,29,29,29	0
57	MG	2x	109	1/1	0.96	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3499	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3163	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3165	1/1	0.97	0.07	29,29,29,29	0
57	MG	1A	3318	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3625	1/1	0.97	0.15	30,30,30,30	0
57	MG	2A	3265	1/1	0.97	0.08	45,45,45,45	0
57	MG	1A	3166	1/1	0.97	0.05	15,15,15,15	0
57	MG	1A	3509	1/1	0.97	0.11	56,56,56,56	0
57	MG	2A	3268	1/1	0.97	0.07	60,60,60,60	0
57	MG	1A	3320	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3208	1/1	0.97	0.04	29,29,29,29	0
57	MG	13	101	1/1	0.97	0.12	28,28,28,28	0
57	MG	2A	3487	1/1	0.97	0.18	48,48,48,48	0
57	MG	1A	3631	1/1	0.97	0.09	34,34,34,34	0
57	MG	2A	3088	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3323	1/1	0.97	0.04	39,39,39,39	0
57	MG	1A	3755	1/1	0.97	0.08	21,21,21,21	0
57	MG	2A	3091	1/1	0.97	0.11	26,26,26,26	0
57	MG	1A	3137	1/1	0.97	0.09	27,27,27,27	0
57	MG	1A	3053	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3094	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	3409	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3326	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3097	1/1	0.97	0.10	54,54,54,54	0
57	MG	1A	3172	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3100	1/1	0.97	0.10	36,36,36,36	0
57	MG	17	106	1/1	0.97	0.18	45,45,45,45	0
57	MG	2A	3102	1/1	0.97	0.07	48,48,48,48	0
57	MG	17	107	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3008	1/1	0.97	0.13	22,22,22,22	0
57	MG	1A	3414	1/1	0.97	0.07	18,18,18,18	0
57	MG	2A	3506	1/1	0.97	0.07	48,48,48,48	0
57	MG	2a	1607	1/1	0.97	0.23	46,46,46,46	0
57	MG	2A	3507	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3291	1/1	0.97	0.06	47,47,47,47	0
57	MG	19	101	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3265	1/1	0.97	0.13	19,19,19,19	0
57	MG	1A	3079	1/1	0.97	0.13	33,33,33,33	0
57	MG	1A	3331	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3526	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3515	1/1	0.97	0.14	59,59,59,59	0
57	MG	1A	3530	1/1	0.97	0.14	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1617	1/1	0.97	0.18	40,40,40,40	0
57	MG	1A	3332	1/1	0.97	0.14	10,10,10,10	0
57	MG	2A	3114	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3080	1/1	0.97	0.11	11,11,11,11	0
57	MG	1A	3268	1/1	0.97	0.09	29,29,29,29	0
57	MG	2A	3521	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3649	1/1	0.97	0.07	40,40,40,40	0
57	MG	1a	1610	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3536	1/1	0.97	0.20	47,47,47,47	0
57	MG	1A	3269	1/1	0.97	0.23	40,40,40,40	0
57	MG	2a	1627	1/1	0.97	0.26	55,55,55,55	0
57	MG	2A	3308	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3428	1/1	0.97	0.09	24,24,24,24	0
57	MG	2A	3122	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3312	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3123	1/1	0.97	0.06	41,41,41,41	0
57	MG	2a	1633	1/1	0.97	0.21	61,61,61,61	0
57	MG	1A	3653	1/1	0.97	0.13	36,36,36,36	0
57	MG	1A	3654	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3429	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3656	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3657	1/1	0.97	0.03	30,30,30,30	0
57	MG	1A	3540	1/1	0.97	0.05	19,19,19,19	0
57	MG	1A	3218	1/1	0.97	0.19	40,40,40,40	0
57	MG	1A	3338	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3784	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3176	1/1	0.97	0.30	27,27,27,27	0
57	MG	1A	3081	1/1	0.97	0.30	34,34,34,34	0
57	MG	1A	3002	1/1	0.97	0.09	46,46,46,46	0
57	MG	2A	3329	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3330	1/1	0.97	0.08	49,49,49,49	0
57	MG	2A	3331	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3547	1/1	0.97	0.07	22,22,22,22	0
57	MG	1A	3790	1/1	0.97	0.05	14,14,14,14	0
57	MG	2a	1651	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3343	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3144	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3793	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3551	1/1	0.97	0.14	29,29,29,29	0
57	MG	1A	3180	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3348	1/1	0.97	0.05	22,22,22,22	0
57	MG	1A	3554	1/1	0.97	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3349	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3672	1/1	0.97	0.08	35,35,35,35	0
57	MG	2A	3344	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3345	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3067	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3352	1/1	0.97	0.06	13,13,13,13	0
57	MG	1A	3104	1/1	0.97	0.08	21,21,21,21	0
57	MG	2A	3349	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3183	1/1	0.97	0.16	38,38,38,38	0
57	MG	1A	3147	1/1	0.97	0.26	36,36,36,36	0
57	MG	1A	3563	1/1	0.97	0.06	16,16,16,16	0
57	MG	1A	3450	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3355	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3451	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3357	1/1	0.97	0.17	50,50,50,50	0
57	MG	2A	3577	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3156	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3681	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3158	1/1	0.97	0.12	33,33,33,33	0
57	MG	2A	3581	1/1	0.97	0.08	41,41,41,41	0
57	MG	2A	3361	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3566	1/1	0.97	0.07	38,38,38,38	0
57	MG	1x	101	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3567	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3684	1/1	0.97	0.06	14,14,14,14	0
57	MG	1A	3228	1/1	0.97	0.17	36,36,36,36	0
57	MG	1A	3453	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3057	1/1	0.97	0.11	26,26,26,26	0
57	MG	2A	3166	1/1	0.97	0.08	35,35,35,35	0
57	MG	2A	3167	1/1	0.97	0.17	41,41,41,41	0
57	MG	2a	1690	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3125	1/1	0.97	0.04	19,19,19,19	0
57	MG	2A	3377	1/1	0.97	0.09	46,46,46,46	0
57	MG	2A	3169	1/1	0.97	0.24	44,44,44,44	0
57	MG	1A	3018	1/1	0.97	0.04	20,20,20,20	0
57	MG	1B	213	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3597	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3127	1/1	0.97	0.03	24,24,24,24	0
57	MG	2A	3004	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3578	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3385	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3043	1/1	0.97	0.28	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1702	1/1	0.97	0.12	65,65,65,65	0
57	MG	1A	3029	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	3460	1/1	0.97	0.08	26,26,26,26	0
57	MG	1A	3366	1/1	0.97	0.10	38,38,38,38	0
57	MG	1D	302	1/1	0.97	0.04	19,19,19,19	0
57	MG	2A	3180	1/1	0.97	0.16	56,56,56,56	0
57	MG	1D	303	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3290	1/1	0.97	0.10	20,20,20,20	0
57	MG	2a	1710	1/1	0.97	0.11	42,42,42,42	0
57	MG	1D	306	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3014	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3398	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3464	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3465	1/1	0.97	0.09	47,47,47,47	0
57	MG	2A	3188	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3292	1/1	0.97	0.10	25,25,25,25	0
57	MG	2A	3403	1/1	0.97	0.09	49,49,49,49	0
57	MG	2a	1719	1/1	0.97	0.09	70,70,70,70	0
57	MG	2A	3018	1/1	0.97	0.17	38,38,38,38	0
57	MG	1E	305	1/1	0.97	0.07	46,46,46,46	0
57	MG	2A	3020	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3131	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3295	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3062	1/1	0.97	0.08	31,31,31,31	0
57	MG	1A	3297	1/1	0.97	0.12	30,30,30,30	0
57	MG	2A	3625	1/1	0.97	0.13	65,65,65,65	0
57	MG	1F	303	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3298	1/1	0.97	0.09	33,33,33,33	0
57	MG	1a	1678	1/1	0.97	0.04	47,47,47,47	0
57	MG	1F	305	1/1	0.97	0.17	34,34,34,34	0
57	MG	2A	3202	1/1	0.97	0.24	56,56,56,56	0
57	MG	1A	3240	1/1	0.97	0.10	16,16,16,16	0
57	MG	2A	3204	1/1	0.97	0.10	69,69,69,69	0
57	MG	1F	307	1/1	0.97	0.09	32,32,32,32	0
57	MG	1a	1682	1/1	0.97	0.04	39,39,39,39	0
57	MG	2a	1737	1/1	0.97	0.24	59,59,59,59	0
57	MG	1A	3473	1/1	0.97	0.08	52,52,52,52	0
57	MG	1A	3010	1/1	0.97	0.05	24,24,24,24	0
57	MG	1G	202	1/1	0.97	0.11	35,35,35,35	0
57	MG	1A	3711	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3301	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3158	1/1	0.97	0.14	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3197	1/1	0.97	0.07	33,33,33,33	0
57	MG	2A	3642	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3383	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3134	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3481	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3718	1/1	0.97	0.06	42,42,42,42	0
57	MG	1a	1695	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3482	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3305	1/1	0.97	0.05	23,23,23,23	0
57	MG	2A	3224	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3484	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3605	1/1	0.97	0.04	25,25,25,25	0
57	MG	1Q	202	1/1	0.97	0.10	31,31,31,31	0
57	MG	2A	3228	1/1	0.97	0.33	54,54,54,54	0
57	MG	1A	3306	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3307	1/1	0.97	0.12	40,40,40,40	0
57	MG	2A	3231	1/1	0.97	0.11	54,54,54,54	0
57	MG	1A	3389	1/1	0.97	0.08	21,21,21,21	0
57	MG	2A	3663	1/1	0.97	0.17	45,45,45,45	0
57	MG	2A	3664	1/1	0.97	0.06	37,37,37,37	0
57	MG	1R	201	1/1	0.97	0.12	31,31,31,31	0
57	MG	1R	202	1/1	0.97	0.28	40,40,40,40	0
57	MG	1A	3091	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3392	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3200	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3732	1/1	0.97	0.30	29,29,29,29	0
57	MG	2A	3061	1/1	0.97	0.10	47,47,47,47	0
57	MG	1U	205	1/1	0.97	0.19	30,30,30,30	0
57	MG	1A	3075	1/1	0.97	0.06	40,40,40,40	0
57	MG	1a	1719	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3734	1/1	0.97	0.16	26,26,26,26	0
57	MG	1A	3735	1/1	0.97	0.13	42,42,42,42	0
57	MG	1W	201	1/1	0.97	0.23	41,41,41,41	0
57	MG	2D	302	1/1	0.97	0.14	32,32,32,32	0
57	MG	2A	3068	1/1	0.97	0.10	40,40,40,40	0
57	MG	2A	3249	1/1	0.97	0.19	39,39,39,39	0
57	MG	1A	3252	1/1	0.97	0.13	22,22,22,22	0
57	MG	2A	3251	1/1	0.97	0.06	40,40,40,40	0
57	MG	1W	203	1/1	0.97	0.17	27,27,27,27	0
57	MG	1W	204	1/1	0.97	0.06	40,40,40,40	0
57	MG	2A	3255	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3495	1/1	0.97	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2E	302	1/1	0.97	0.16	44,44,44,44	0
57	MG	1A	3203	1/1	0.97	0.17	26,26,26,26	0
57	MG	2E	304	1/1	0.97	0.09	33,33,33,33	0
57	MG	2x	104	1/1	0.97	0.13	61,61,61,61	0
57	MG	2E	305	1/1	0.97	0.08	46,46,46,46	0
57	MG	2F	301	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3254	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3204	1/1	0.97	0.12	22,22,22,22	0
58	ZN	1n	102	1/1	0.97	0.04	97,97,97,97	0
58	ZN	2n	501	1/1	0.97	0.06	86,86,86,86	0
57	MG	2A	3223	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3110	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3160	1/1	0.98	0.04	37,37,37,37	0
57	MG	1a	1715	1/1	0.98	0.17	58,58,58,58	0
57	MG	1A	3462	1/1	0.98	0.06	8,8,8,8	0
57	MG	1A	3528	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3529	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3353	1/1	0.98	0.06	55,55,55,55	0
57	MG	1A	3074	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3531	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3351	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3270	1/1	0.98	0.08	26,26,26,26	0
57	MG	2A	3234	1/1	0.98	0.10	55,55,55,55	0
57	MG	1A	3237	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3762	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3535	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3128	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3311	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3611	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3210	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3646	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3614	1/1	0.98	0.17	53,53,53,53	0
57	MG	2A	3243	1/1	0.98	0.09	48,48,48,48	0
57	MG	2A	3649	1/1	0.98	0.03	35,35,35,35	0
57	MG	1A	3185	1/1	0.98	0.03	20,20,20,20	0
57	MG	2A	3373	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3241	1/1	0.98	0.06	32,32,32,32	0
57	MG	2A	3653	1/1	0.98	0.06	33,33,33,33	0
57	MG	2A	3510	1/1	0.98	0.09	39,39,39,39	0
57	MG	1A	3276	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3133	1/1	0.98	0.08	48,48,48,48	0
57	MG	1a	1635	1/1	0.98	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3242	1/1	0.98	0.03	21,21,21,21	0
57	MG	1A	3363	1/1	0.98	0.06	12,12,12,12	0
57	MG	2A	3660	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3243	1/1	0.98	0.11	31,31,31,31	0
57	MG	2a	1686	1/1	0.98	0.19	48,48,48,48	0
57	MG	2A	3252	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3382	1/1	0.98	0.10	67,67,67,67	0
57	MG	2A	3030	1/1	0.98	0.17	41,41,41,41	0
57	MG	1A	3476	1/1	0.98	0.06	15,15,15,15	0
57	MG	1A	3694	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3186	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3548	1/1	0.98	0.07	28,28,28,28	0
57	MG	2A	3388	1/1	0.98	0.05	66,66,66,66	0
57	MG	1a	1742	1/1	0.98	0.12	69,69,69,69	0
57	MG	1A	3097	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	3698	1/1	0.98	0.09	25,25,25,25	0
57	MG	2A	3392	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3367	1/1	0.98	0.04	35,35,35,35	0
57	MG	1A	3421	1/1	0.98	0.10	18,18,18,18	0
57	MG	1A	3164	1/1	0.98	0.12	37,37,37,37	0
57	MG	2A	3041	1/1	0.98	0.21	32,32,32,32	0
57	MG	1U	202	1/1	0.98	0.14	34,34,34,34	0
57	MG	2A	3534	1/1	0.98	0.17	43,43,43,43	0
57	MG	1A	3628	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3321	1/1	0.98	0.05	15,15,15,15	0
57	MG	1A	3786	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3215	1/1	0.98	0.16	28,28,28,28	0
57	MG	1V	201	1/1	0.98	0.25	21,21,21,21	0
57	MG	2A	3541	1/1	0.98	0.07	57,57,57,57	0
57	MG	1A	3705	1/1	0.98	0.05	35,35,35,35	0
57	MG	1V	203	1/1	0.98	0.36	26,26,26,26	0
57	MG	1A	3427	1/1	0.98	0.06	31,31,31,31	0
57	MG	1V	205	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3632	1/1	0.98	0.05	51,51,51,51	0
57	MG	1A	3556	1/1	0.98	0.07	16,16,16,16	0
57	MG	1A	3058	1/1	0.98	0.03	17,17,17,17	0
57	MG	2A	3549	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3249	1/1	0.98	0.13	25,25,25,25	0
57	MG	2F	305	1/1	0.98	0.17	47,47,47,47	0
57	MG	1A	3559	1/1	0.98	0.06	14,14,14,14	0
57	MG	1X	103	1/1	0.98	0.07	24,24,24,24	0
57	MG	1a	1664	1/1	0.98	0.04	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1765	1/1	0.98	0.05	58,58,58,58	0
57	MG	1A	3430	1/1	0.98	0.03	27,27,27,27	0
57	MG	1A	3099	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3167	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3376	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3800	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	3168	1/1	0.98	0.08	48,48,48,48	0
57	MG	1A	3493	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3290	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3148	1/1	0.98	0.18	31,31,31,31	0
57	MG	2X	103	1/1	0.98	0.06	51,51,51,51	0
57	MG	2A	3425	1/1	0.98	0.05	37,37,37,37	0
57	MG	2A	3069	1/1	0.98	0.12	53,53,53,53	0
57	MG	1A	3719	1/1	0.98	0.13	43,43,43,43	0
57	MG	2A	3294	1/1	0.98	0.09	45,45,45,45	0
57	MG	2A	3429	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3436	1/1	0.98	0.06	44,44,44,44	0
57	MG	2A	3571	1/1	0.98	0.12	46,46,46,46	0
57	MG	1A	3042	1/1	0.98	0.18	33,33,33,33	0
57	MG	1A	3291	1/1	0.98	0.06	23,23,23,23	0
57	MG	2A	3181	1/1	0.98	0.23	50,50,50,50	0
57	MG	2A	3575	1/1	0.98	0.05	59,59,59,59	0
57	MG	1A	3381	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3435	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3025	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3500	1/1	0.98	0.05	18,18,18,18	0
57	MG	2A	3302	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3439	1/1	0.98	0.05	58,58,58,58	0
57	MG	1A	3502	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3576	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3729	1/1	0.98	0.09	35,35,35,35	0
57	MG	1A	3026	1/1	0.98	0.04	15,15,15,15	0
57	MG	17	101	1/1	0.98	0.09	32,32,32,32	0
57	MG	2A	3190	1/1	0.98	0.09	56,56,56,56	0
57	MG	17	102	1/1	0.98	0.15	34,34,34,34	0
57	MG	1A	3294	1/1	0.98	0.15	41,41,41,41	0
57	MG	2A	3311	1/1	0.98	0.09	30,30,30,30	0
57	MG	1A	3505	1/1	0.98	0.04	39,39,39,39	0
57	MG	2A	3313	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3506	1/1	0.98	0.09	40,40,40,40	0
57	MG	2A	3315	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3013	1/1	0.98	0.08	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3454	1/1	0.98	0.10	37,37,37,37	0
57	MG	1a	1690	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3318	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3034	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3092	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3106	1/1	0.98	0.12	42,42,42,42	0
57	MG	1B	217	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3462	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3339	1/1	0.98	0.05	23,23,23,23	0
57	MG	1a	1696	1/1	0.98	0.15	54,54,54,54	0
57	MG	1a	1697	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3391	1/1	0.98	0.14	46,46,46,46	0
57	MG	1a	1700	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3201	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3098	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3262	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	3093	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3517	1/1	0.98	0.07	41,41,41,41	0
57	MG	1x	105	1/1	0.98	0.06	60,60,60,60	0
57	MG	1A	3035	1/1	0.98	0.17	32,32,32,32	0
57	MG	2A	3213	1/1	0.98	0.15	52,52,52,52	0
57	MG	1A	3231	1/1	0.98	0.19	23,23,23,23	0
57	MG	1A	3747	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3397	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3107	1/1	0.98	0.07	44,44,44,44	0
57	MG	1a	1710	1/1	0.98	0.06	29,29,29,29	0
57	MG	2x	107	1/1	0.98	0.05	76,76,76,76	0
57	MG	1A	3345	1/1	0.98	0.04	18,18,18,18	0
57	MG	2A	3003	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3041	1/1	0.98	0.10	19,19,19,19	0
58	ZN	2Y	202	1/1	0.98	0.04	89,89,89,89	0
58	ZN	24	501	1/1	0.98	0.09	125,125,125,125	0
57	MG	2A	3222	1/1	0.98	0.04	37,37,37,37	0
59	SF4	2d	302	8/8	0.98	0.04	55,65,83,89	0
57	MG	1B	216	1/1	0.99	0.04	34,34,34,34	0
57	MG	1x	108	1/1	0.99	0.03	42,42,42,42	0
57	MG	1A	3384	1/1	0.99	0.03	16,16,16,16	0
57	MG	2A	3539	1/1	0.99	0.06	44,44,44,44	0
57	MG	1A	3114	1/1	0.99	0.22	45,45,45,45	0
57	MG	1A	3487	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3356	1/1	0.99	0.07	20,20,20,20	0
57	MG	1A	3169	1/1	0.99	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3333	1/1	0.99	0.05	38,38,38,38	0
57	MG	1A	3541	1/1	0.99	0.09	23,23,23,23	0
57	MG	1A	3333	1/1	0.99	0.03	23,23,23,23	0
57	MG	17	104	1/1	0.99	0.10	24,24,24,24	0
57	MG	1D	304	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3570	1/1	0.99	0.05	37,37,37,37	0
57	MG	1A	3795	1/1	0.99	0.04	37,37,37,37	0
57	MG	1A	3446	1/1	0.99	0.08	19,19,19,19	0
57	MG	1A	3728	1/1	0.99	0.03	50,50,50,50	0
57	MG	1A	3012	1/1	0.99	0.03	22,22,22,22	0
57	MG	1E	304	1/1	0.99	0.07	16,16,16,16	0
57	MG	1A	3425	1/1	0.99	0.02	26,26,26,26	0
57	MG	1A	3574	1/1	0.99	0.09	34,34,34,34	0
57	MG	1A	3801	1/1	0.99	0.09	27,27,27,27	0
57	MG	2A	3558	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3426	1/1	0.99	0.04	21,21,21,21	0
57	MG	1A	3374	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3577	1/1	0.99	0.04	44,44,44,44	0
57	MG	1A	3521	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	3047	1/1	0.99	0.11	27,27,27,27	0
57	MG	1A	3347	1/1	0.99	0.05	37,37,37,37	0
57	MG	1X	102	1/1	0.99	0.03	31,31,31,31	0
57	MG	1A	3056	1/1	0.99	0.09	19,19,19,19	0
57	MG	2A	3459	1/1	0.99	0.03	34,34,34,34	0
57	MG	1a	1699	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3410	1/1	0.99	0.07	40,40,40,40	0
57	MG	1A	3078	1/1	0.99	0.06	32,32,32,32	0
57	MG	1a	1615	1/1	0.99	0.03	45,45,45,45	0
57	MG	1A	3527	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3501	1/1	0.99	0.03	10,10,10,10	0
57	MG	1A	3233	1/1	0.99	0.36	30,30,30,30	0
57	MG	1A	3209	1/1	0.99	0.11	25,25,25,25	0
57	MG	1A	3745	1/1	0.99	0.06	30,30,30,30	0
57	MG	1a	1708	1/1	0.99	0.04	29,29,29,29	0
57	MG	11	101	1/1	0.99	0.18	39,39,39,39	0
57	MG	2A	3367	1/1	0.99	0.04	53,53,53,53	0
57	MG	1A	3588	1/1	0.99	0.03	15,15,15,15	0
57	MG	1A	3289	1/1	0.99	0.07	14,14,14,14	0
57	MG	2A	3421	1/1	0.99	0.11	48,48,48,48	0
57	MG	1A	3748	1/1	0.99	0.05	19,19,19,19	0
57	MG	2A	3371	1/1	0.99	0.04	34,34,34,34	0
57	MG	2A	3372	1/1	0.99	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	1Y	501	1/1	0.99	0.03	56,56,56,56	0
58	ZN	14	501	1/1	0.99	0.08	107,107,107,107	0
58	ZN	15	105	1/1	0.99	0.02	38,38,38,38	0
58	ZN	16	102	1/1	0.99	0.03	42,42,42,42	0
57	MG	1A	3415	1/1	0.99	0.08	14,14,14,14	0
57	MG	1A	3437	1/1	0.99	0.03	14,14,14,14	0
57	MG	1A	3083	1/1	0.99	0.03	12,12,12,12	0
58	ZN	25	102	1/1	0.99	0.05	52,52,52,52	0
58	ZN	26	501	1/1	0.99	0.02	55,55,55,55	0
58	ZN	29	102	1/1	0.99	0.04	69,69,69,69	0
57	MG	1A	3354	1/1	0.99	0.07	13,13,13,13	0
59	SF4	1d	302	8/8	0.99	0.04	61,72,77,81	0
57	MG	2A	3043	1/1	0.99	0.04	39,39,39,39	0
57	MG	2A	3363	1/1	1.00	0.10	35,35,35,35	0
57	MG	1A	3440	1/1	1.00	0.07	17,17,17,17	0
58	ZN	19	102	1/1	1.00	0.02	39,39,39,39	0
57	MG	1A	3419	1/1	1.00	0.01	21,21,21,21	0
57	MG	1A	3612	1/1	1.00	0.01	18,18,18,18	0
57	MG	1A	3510	1/1	1.00	0.03	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.