



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2026 – 07:06 AM EDT

PDB ID : 8G2D / pdb_00008g2d
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with tylosin, mRNA, deacylated A- and E-site tRNA^{phe}, and deacylated P-site tRNA^{met} at 2.70Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

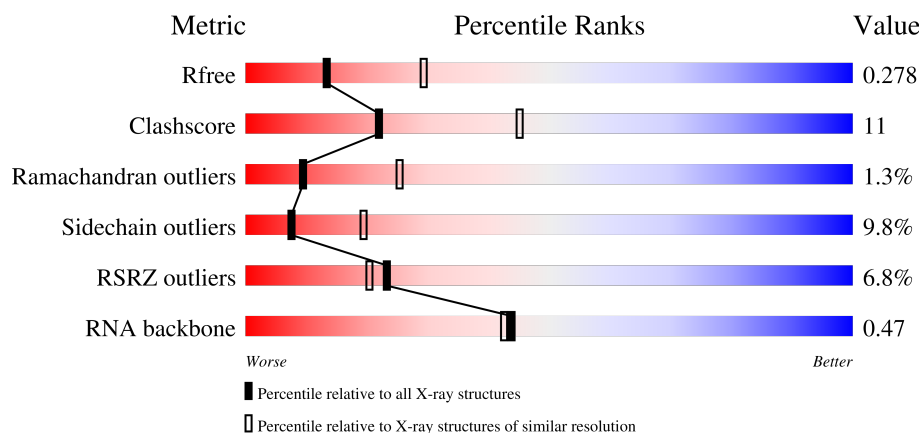
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



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

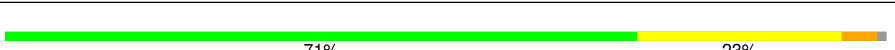
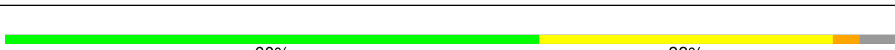
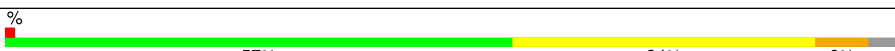
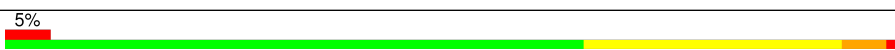
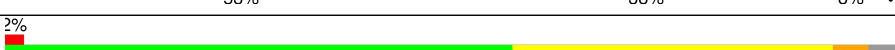
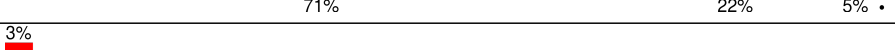
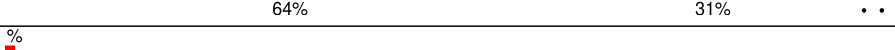
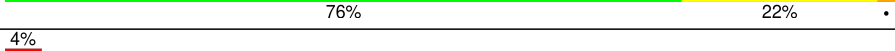
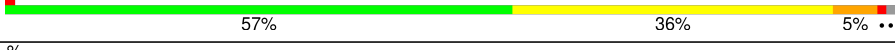
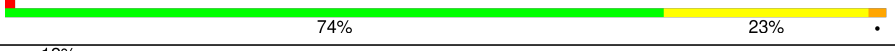
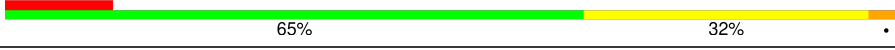
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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

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

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

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

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

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

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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
54	PSU	2y	55	-	-	X	-
59	SF4	1d	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Deacylated tRNA^{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1106	Total	Mg	0	0
			1106	1106		
56	1B	35	Total	Mg	0	0
			35	35		
56	1D	11	Total	Mg	0	0
			11	11		
56	1E	13	Total	Mg	0	0
			13	13		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	5	Total 5	Mg 5	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	5	Total 5	Mg 5	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	6	Total 6	Mg 6	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1U	12	Total 12	Mg 12	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	7	Total 7	Mg 7	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	6	Total 6	Mg 6	0	0
56	15	5	Total 5	Mg 5	0	0
56	16	4	Total 4	Mg 4	0	0
56	17	3	Total 3	Mg 3	0	0
56	18	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	19	1	Total 1	Mg 1	0	0
56	1a	224	Total 224	Mg 224	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1h	1	Total 1	Mg 1	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	7	Total 7	Mg 7	0	0
56	1x	14	Total 14	Mg 14	0	0
56	1y	4	Total 4	Mg 4	0	0
56	2A	877	Total 877	Mg 877	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2E	10	Total 10	Mg 10	0	0

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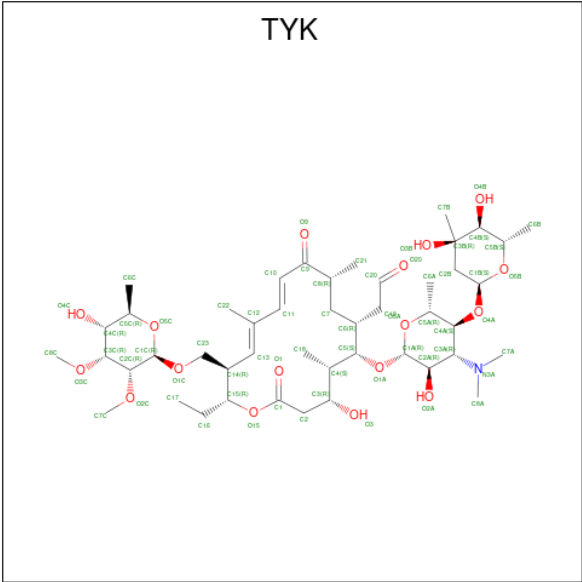
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2F	7	Total 7	Mg 7	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	3	Total 3	Mg 3	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	3	Total 3	Mg 3	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	4	Total 4	Mg 4	0	0
56	25	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	29	1	Total 1	Mg 1	0	0
56	2a	234	Total 234	Mg 234	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0
56	2k	1	Total 1	Mg 1	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2m	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	2	Total 2	Mg 2	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0
56	2w	7	Total 7	Mg 7	0	0
56	2x	4	Total 4	Mg 4	0	0
56	2y	6	Total 6	Mg 6	0	0

- Molecule 57 is TYLOSIN (CCD ID: TYK) (formula: $C_{46}H_{77}NO_{17}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	C	N	O	0	0
			64	46	1	17		
57	2A	1	Total	C	N	O	0	0
			64	46	1	17		

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

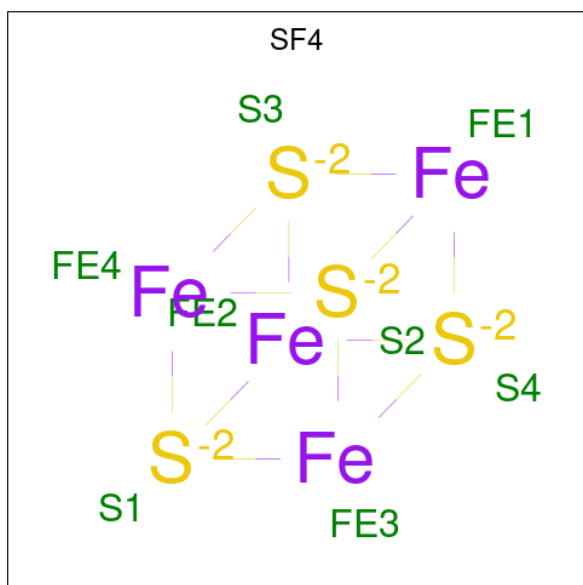
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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 POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1x	1	Total	K	0	0
			1	1		
60	2A	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1864	Total	O	0	0
			1864	1864		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1B	59	Total 59	O 59	0	0
61	1D	24	Total 24	O 24	0	0
61	1E	26	Total 26	O 26	0	0
61	1F	17	Total 17	O 17	0	0
61	1G	5	Total 5	O 5	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	7	Total 7	O 7	0	0
61	1O	9	Total 9	O 9	0	0
61	1P	21	Total 21	O 21	0	0
61	1Q	10	Total 10	O 10	0	0
61	1R	10	Total 10	O 10	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	10	Total 10	O 10	0	0
61	1V	7	Total 7	O 7	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	5	Total 5	O 5	0	0
61	1Y	3	Total 3	O 3	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	11	9	Total 9	O 9	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	14	1	Total 1	O 1	0	0
61	15	5	Total 5	O 5	0	0
61	16	2	Total 2	O 2	0	0
61	17	10	Total 10	O 10	0	0
61	18	13	Total 13	O 13	0	0
61	1a	264	Total 264	O 264	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1i	2	Total 2	O 2	0	0
61	1k	1	Total 1	O 1	0	0
61	1l	4	Total 4	O 4	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	5	Total 5	O 5	0	0
61	1u	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1v	4	Total 4	O 4	0	0
61	1w	13	Total 13	O 13	0	0
61	1x	13	Total 13	O 13	0	0
61	2A	1086	Total 1086	O 1086	0	0
61	2B	21	Total 21	O 21	0	0
61	2D	18	Total 18	O 18	0	0
61	2E	11	Total 11	O 11	0	0
61	2F	13	Total 13	O 13	0	0
61	2I	5	Total 5	O 5	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	9	Total 9	O 9	0	0
61	2Q	3	Total 3	O 3	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	1	Total 1	O 1	0	0
61	2W	1	Total 1	O 1	0	0
61	2X	3	Total 3	O 3	0	0
61	2Y	2	Total 2	O 2	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	5	Total 5	O 5	0	0

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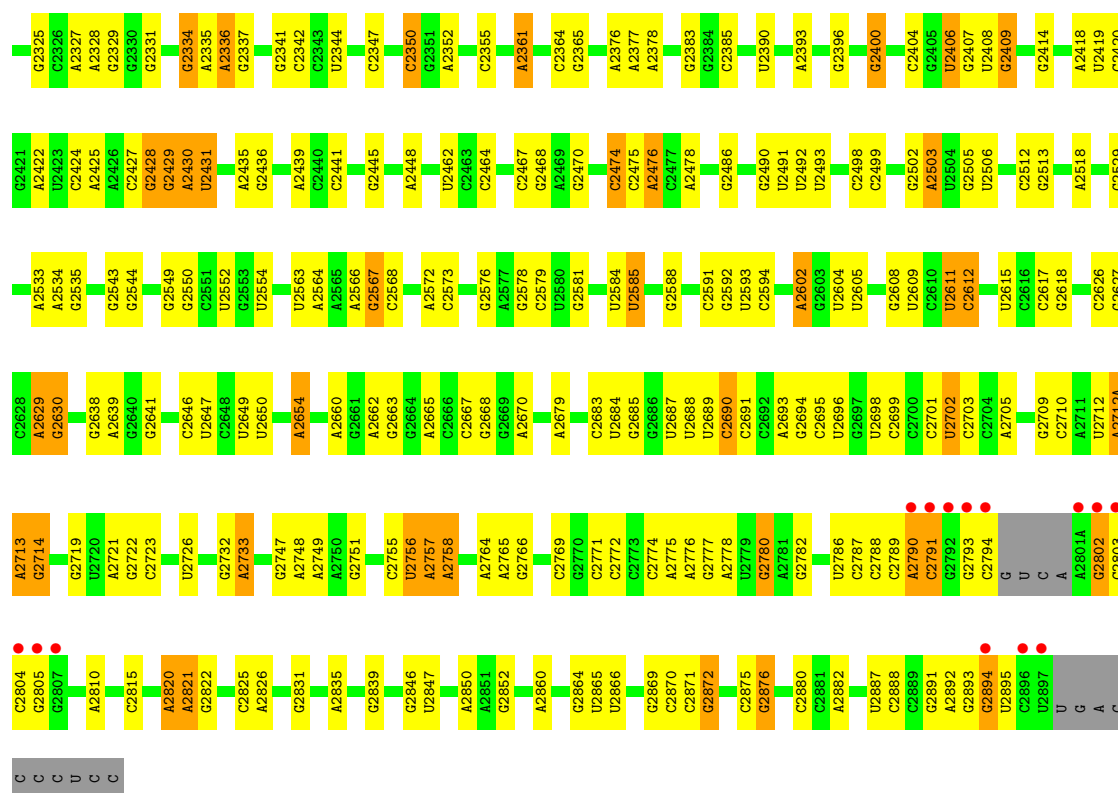
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	21	9	Total 9	O 9	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	3	Total 3	O 3	0	0
61	27	3	Total 3	O 3	0	0
61	28	6	Total 6	O 6	0	0
61	29	1	Total 1	O 1	0	0
61	2a	226	Total 226	O 226	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0
61	2t	4	Total 4	O 4	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	7	Total 7	O 7	0	0
61	2y	16	Total 16	O 16	0	0

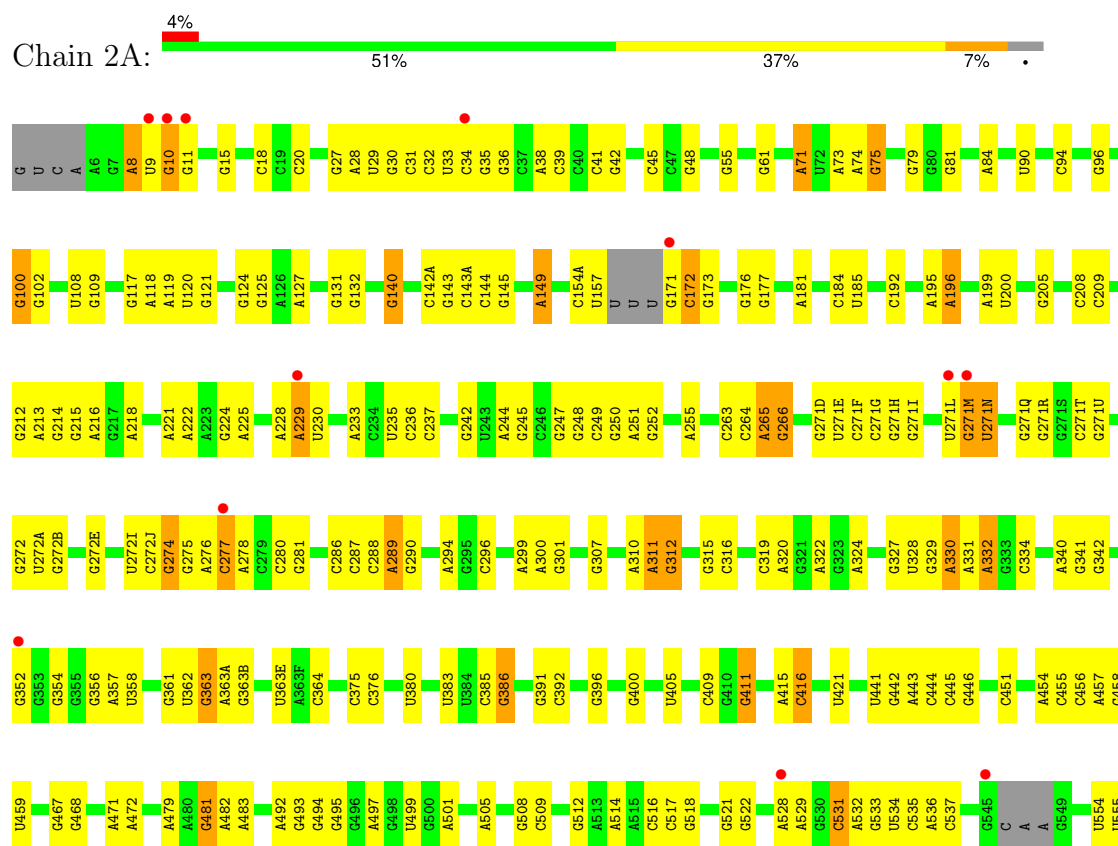
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

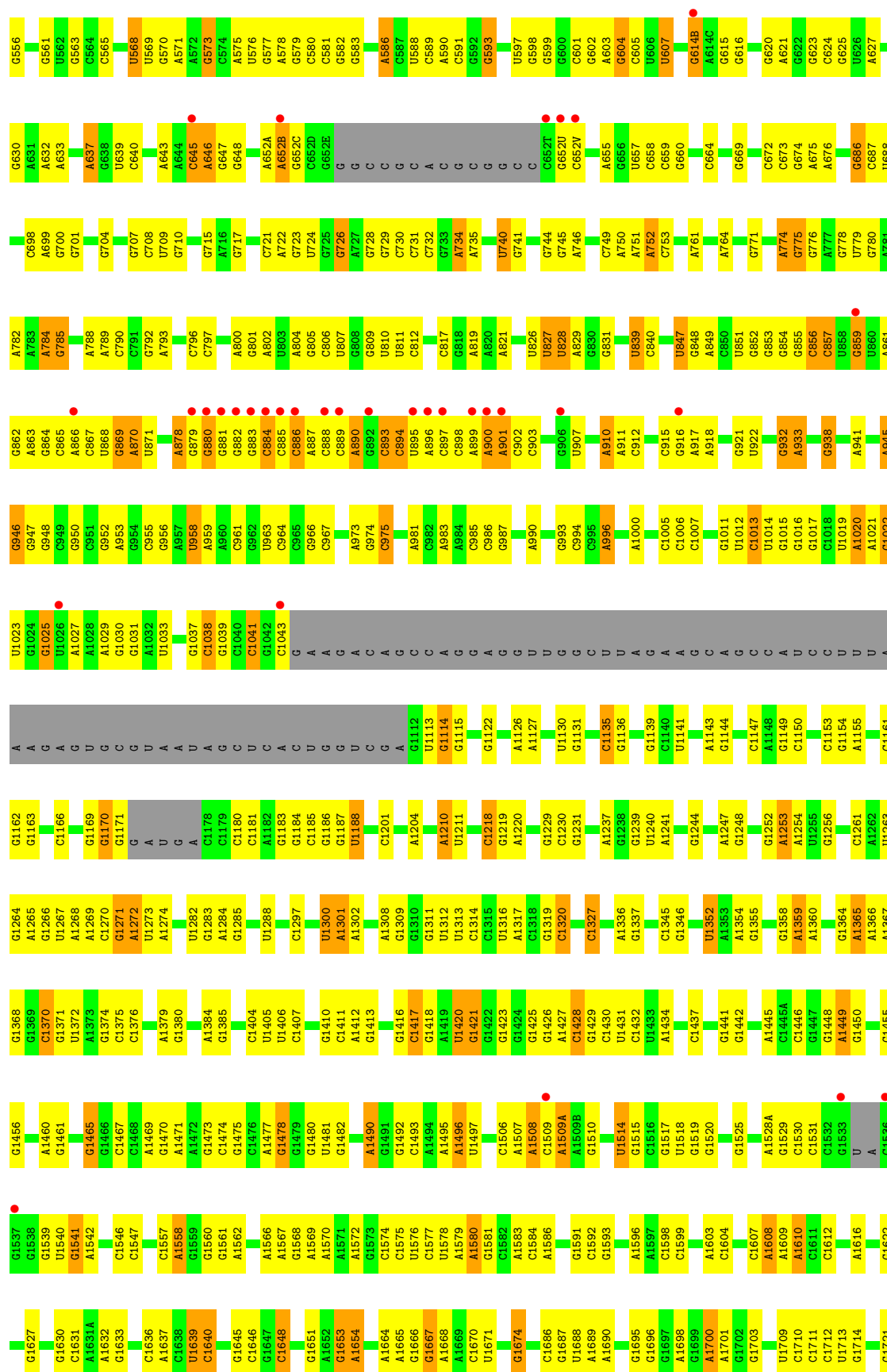
[illegible]

U2233	G2151	C1999	G1785	G1687	C1557	A1489	A1360	C1258	U1165	U1078	C1008
G2234	G2152	C2006	A1786	A1688	A1558	G1450	G1365	G1259	C1166	C1079	A1009
G2235	G2093	G1900	C1790	A1689	A1566	A1452	A1365	G1260	U1167	C1080	A1010
G2236	G2094	G1903	C1791	A1671	A1567	A1453	G1368	G1261	G1170	U1081	C1011
G2237	G2095	G1906	U1794	G1674	A1568	G1455	G1369	G1264	G1171	U1082	C1012
G2238	G2096	G1907	C1795	C1675	A1569	G1456	U1372	A1265	G1173	U1083	C1013
G2239	G2097	G1908	C1796	C1676	A1570	G1461	G1372	G1266	A1174	A1084	U1014
U2243	U2099	G1911	C1797	C1677	A1571	G1466	U1379	U1267	A1175	A1085	A1021
U2244	G2100	U1911	U1798	C1678	A1578	G1467	A1379	A1268	U1176	A1086	G1022
U2245	G2101	U1912	U1799	G1681	A1579	C1468	G1380	A1269	G1177	A1087	G1023
G2251	U2102	C1914	C1800	C1686	A1580	C1469	G1381	G1270	C1178	G1089	G1024
G2252	U2103	U1915	G1801	C1687	A1581	A1469	G1382	A1272	C1179	U1090	G1025
G2253	G2104	A1802	U1688	U1688	C1584	G1482	A1384	U1273	C1180	G1091	U1026
G2254	C2105	A1916	C1687	U1688	C1584	G1482	A1385	U1274	G1183	C1092	A1027
A2268	U2106	U1917	U1688	U1688	C1584	G1482	A1385	A1275	G1184	U1093	A1028
A2269	C2107	A1918	U1688	U1688	C1584	G1482	U1394	A1276	G1185	U1094	A1029
A2270	C2108	A1919	U1688	U1688	C1584	G1482	U1395	A1277	G1186	U1095	A1030
A2271	U2109	C1920	C1684	C1684	C1584	G1482	U1396	A1278	G1187	U1096	U1033
G2272	U2110	G1929	G1812	G1685	C1589	A1485	U1397	U1288	U1188	U1097	G1034
A2273	C2111	G1930	G1813	G1686	C1593	A1486	U1398	C1289	A1189	U1098	U1035
A2274	U2112	A1701	A1814	C1687	G1594	U1503	C1398	C1290	G1190	C1100	G1037
G2275	U2113	G1702	G1815	C1687	G1594	C1504	U1405	U1291	G1191	U1101	C1038
G2276	G2114	G1703	G1816	C1687	G1594	C1505	U1406	G1292	C1196	C1102	G1039
G2277	A2115	A1603	G1817	C1687	A1603	C1506	U1406	C1293	G1196	C1103	C1040
A2278	G2116	C1607	U1825	U1709	C1607	A1507	G1413	U1294	C1201	G1104	C1041
G2279	A2117	G1608	G1826	C1710	A1608	A1508	G1416	C1295	U1205	U1105	A1044
G2280	U2118	C1942	C1827	C1710	A1609	C1509	G1417	G1296	A1204	G1106	A1045
C2283	A2119	U1946	U1828	U1713	A1610	A1509A	G1418	C1297	G1107	U1107	A1046
C2284	G2120	C1947	G1829	G1714	A1611	A1509B	G1419	C1298	U1108	U1108	A1047
C2285	U2121	U1951	U1833	G1721	A1614	U1518	U1420	G1299	A1210	U1109	A1048
A2286	U2122	A1952	C1843	A1722	C1617	G1519	G1421	U1300	U1211	G1110	A1049
A2287	G2123	U1953	C1843	G1739	A1618	G1520	G1422	A1301	G1212	A1111	C1052
A2288	U2124	G1954	G1740	G1740	G1619	G1521	G1423	A1302	A1213	G1112	C1053
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G2290	G2127	U1955	G1742	G1742	A1631A	A1528	G1425	C1315	G1227	G1115	G1055
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• Molecule 1: 23S Ribosomal RNA

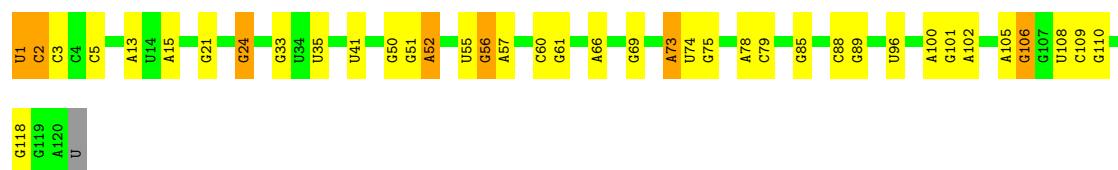




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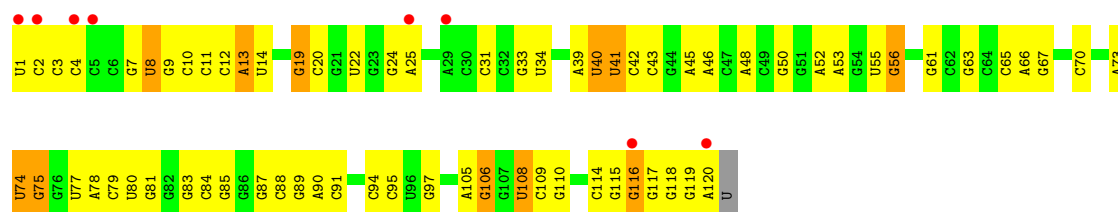
• Molecule 2: 5S Ribosomal RNA

Chain 1B:  67% 26% 6% .



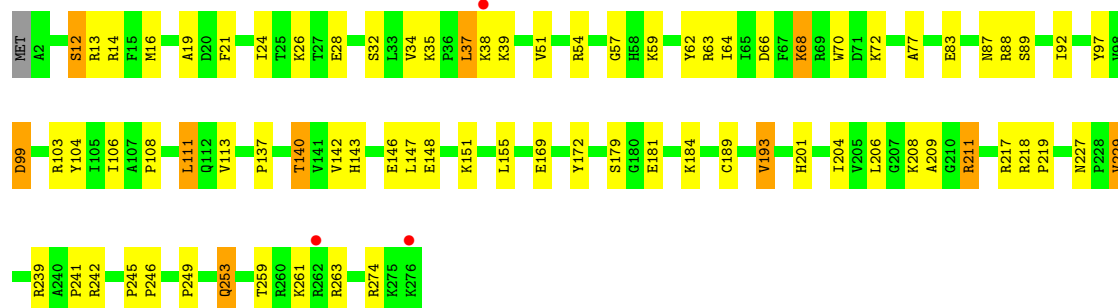
• Molecule 2: 5S Ribosomal RNA

Chain 2B:  7% 41% 49% 9% .



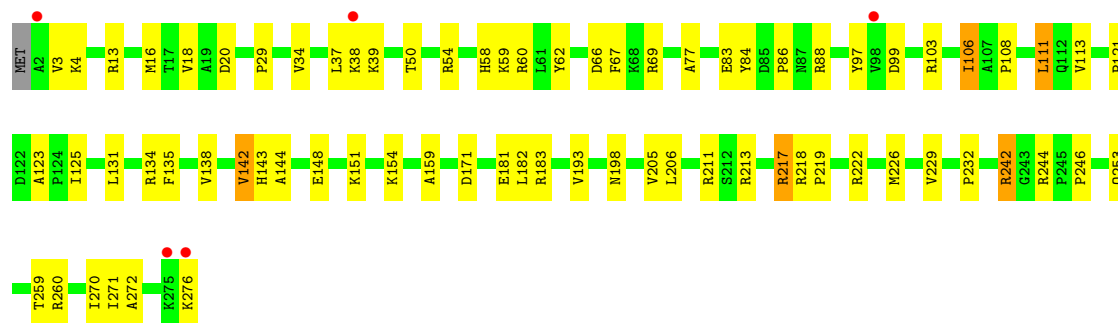
• Molecule 3: 50S ribosomal protein L2

Chain 1D:  71% 25% .



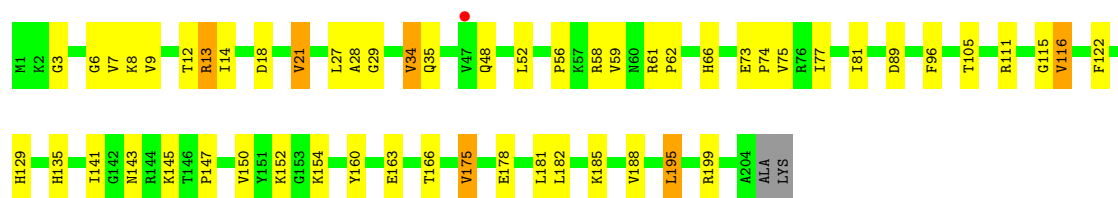
• Molecule 3: 50S ribosomal protein L2

Chain 2D:  2% 73% 25% .



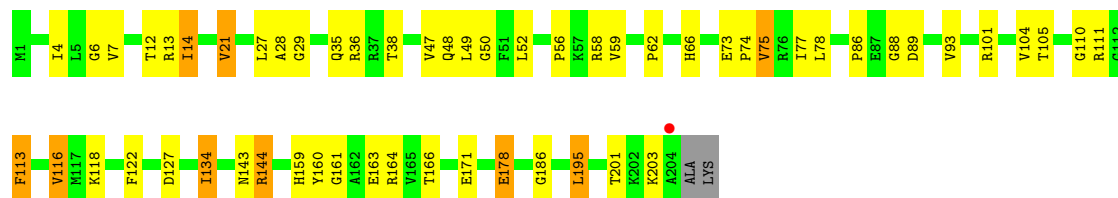
• Molecule 4: 50S ribosomal protein L3

Chain 1E:  72% 24% .



• Molecule 4: 50S ribosomal protein L3

Chain 2E: 71% 23% . .



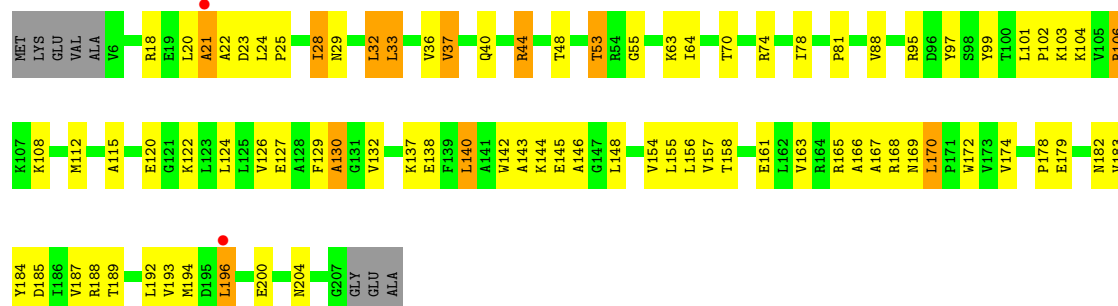
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 60% 33% . .



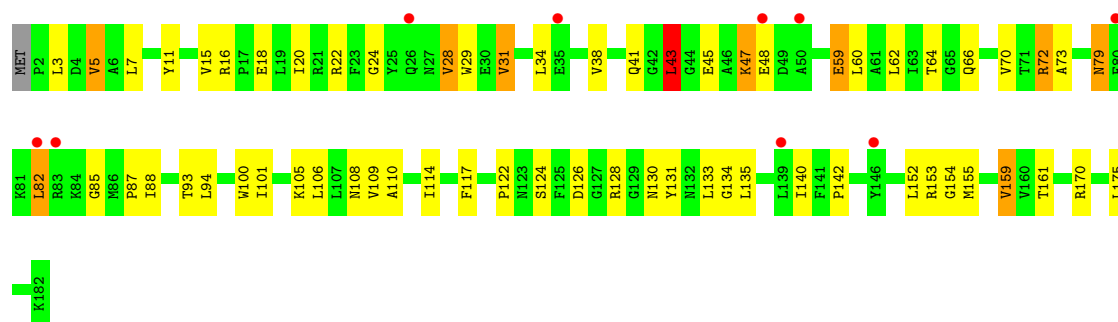
• Molecule 5: 50S ribosomal protein L4

Chain 2F: % 57% 34% 6% .



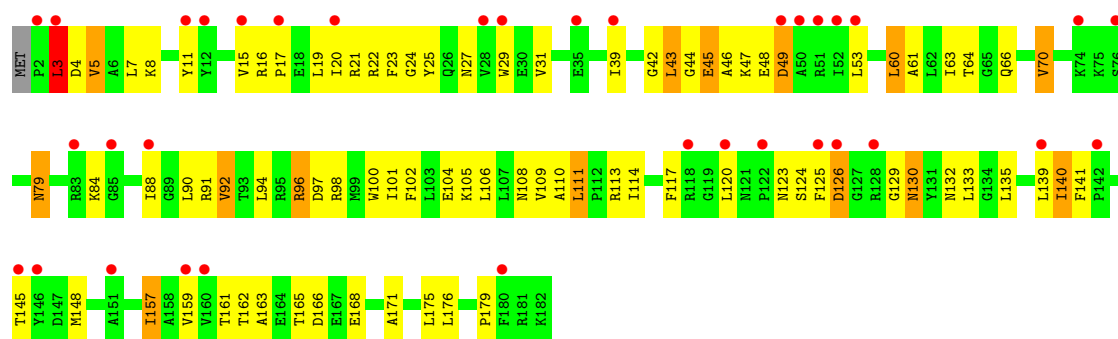
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 5% 65% 29% 5% . .



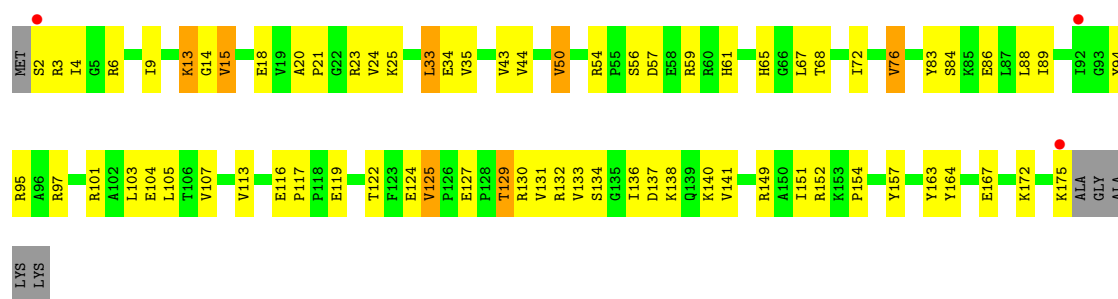
• Molecule 6: 50S ribosomal protein L5

Chain 2G: 19% 53% 38% 8% ..



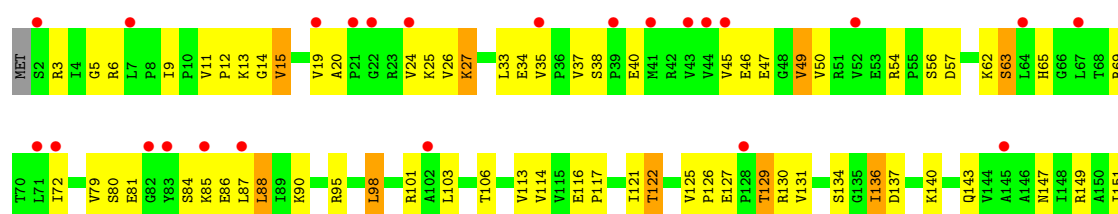
• Molecule 7: 50S ribosomal protein L6

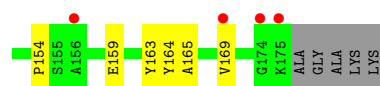
Chain 1H: 2% 57% 36% . .



• Molecule 7: 50S ribosomal protein L6

Chain 2H: 16% 56% 36% 5% .

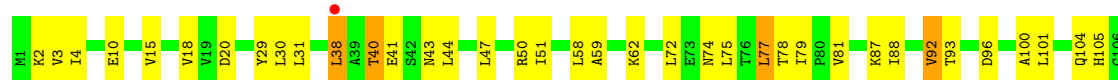




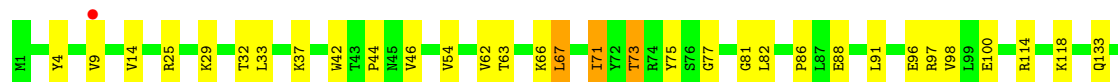
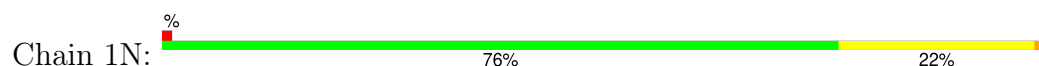
- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

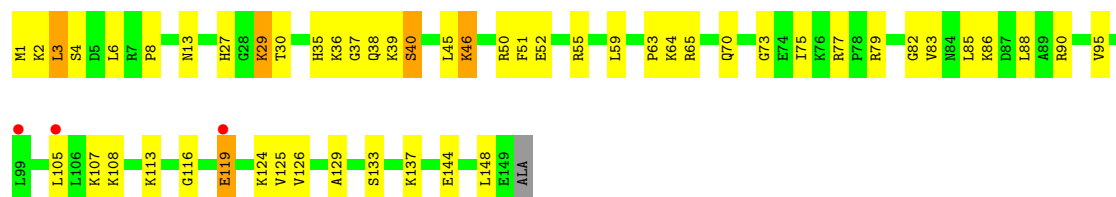




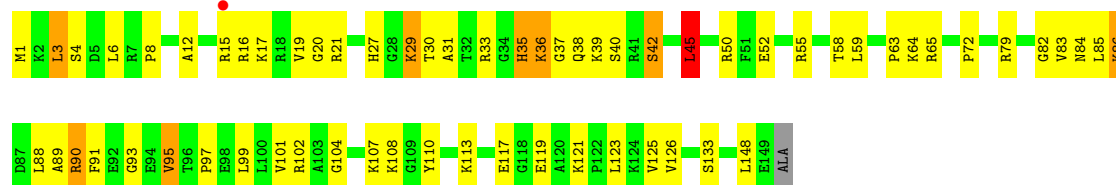
• Molecule 10: 50S ribosomal protein L14



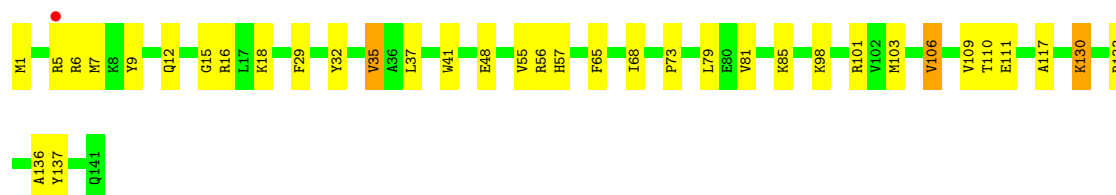
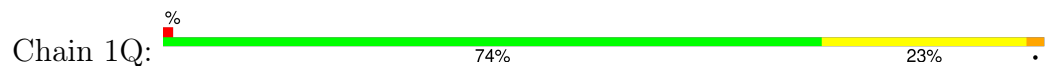
• Molecule 11: 50S ribosomal protein L15



• Molecule 11: 50S ribosomal protein L15

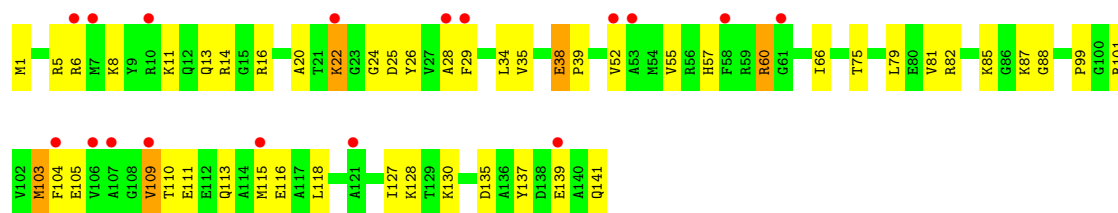


• Molecule 12: 50S ribosomal protein L16



• Molecule 12: 50S ribosomal protein L16





• Molecule 13: 50S ribosomal protein L17

Chain 1R: 73% 25% .



• Molecule 13: 50S ribosomal protein L17

Chain 2R: 70% 25% .



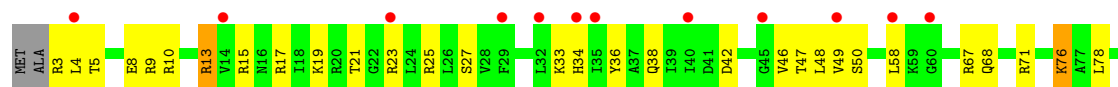
• Molecule 14: 50S ribosomal protein L18

Chain 1S: 72% 23% . .



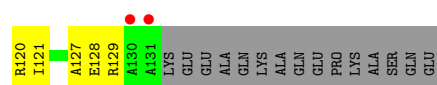
• Molecule 14: 50S ribosomal protein L18

Chain 2S: 12% 61% 33% . .

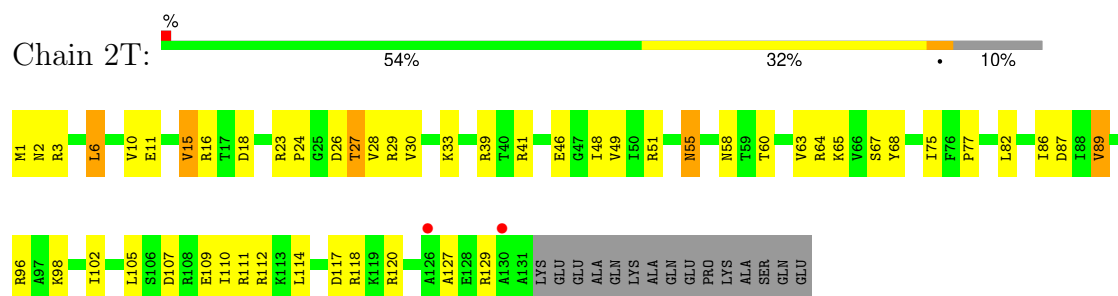


• Molecule 15: 50S ribosomal protein L19

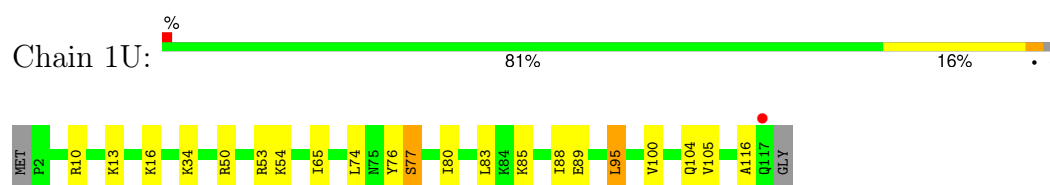
Chain 1T: % 63% 26% 10% .



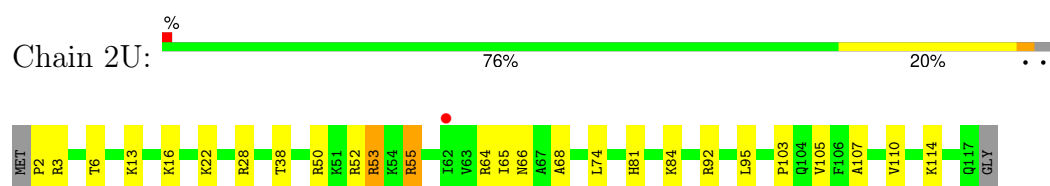
• Molecule 15: 50S ribosomal protein L19



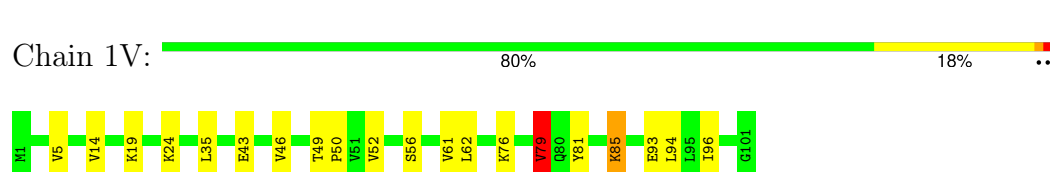
• Molecule 16: 50S ribosomal protein L20



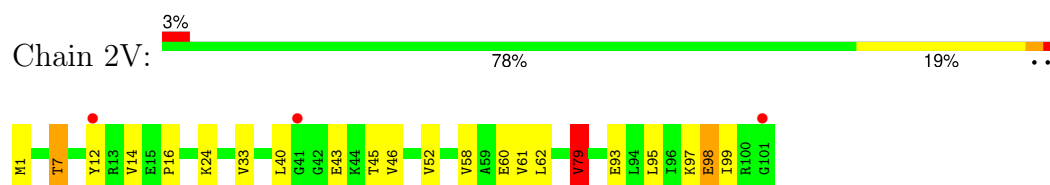
• Molecule 16: 50S ribosomal protein L20



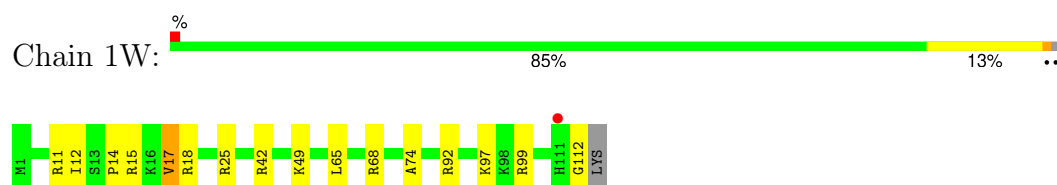
• Molecule 17: 50S ribosomal protein L21



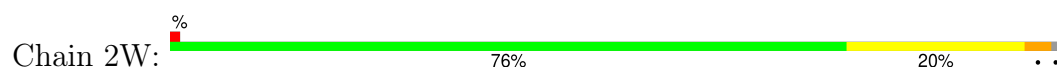
• Molecule 17: 50S ribosomal protein L21

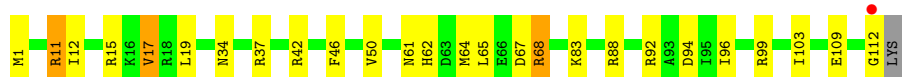


• Molecule 18: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L22





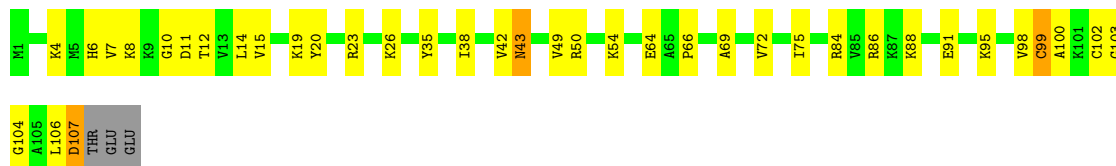
- Molecule 19: 50S ribosomal protein L23



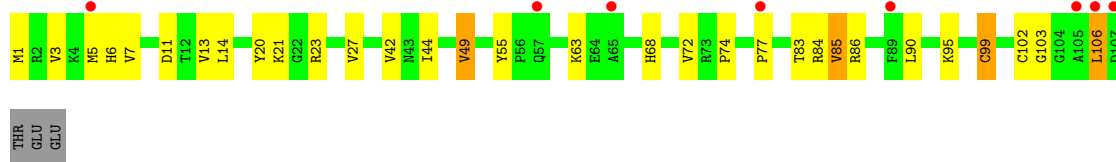
- Molecule 19: 50S ribosomal protein L23



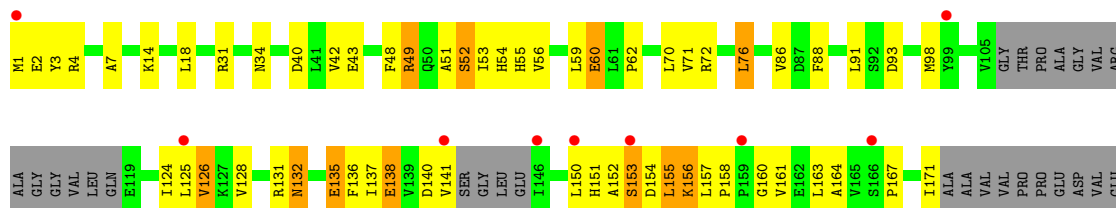
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

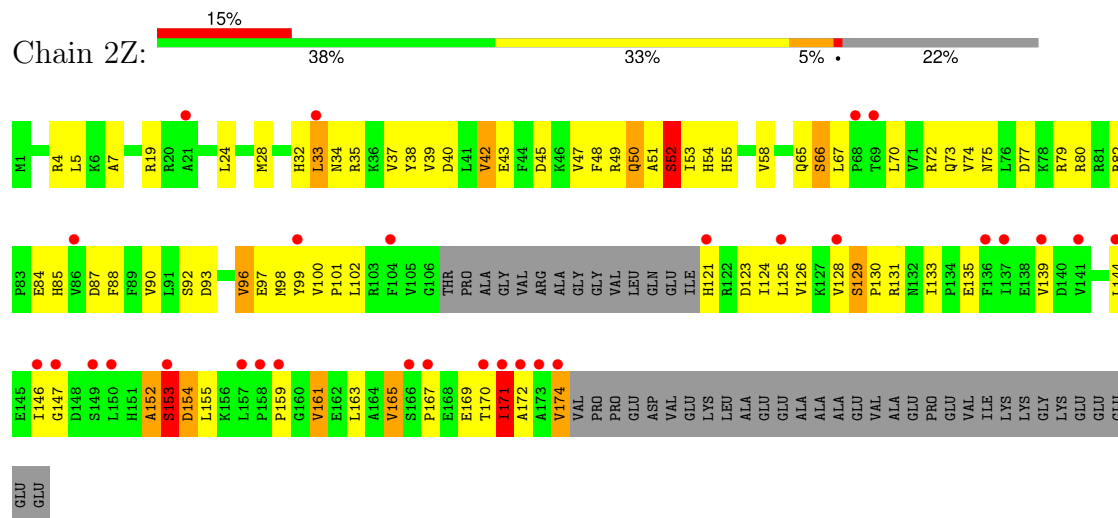


- Molecule 21: 50S ribosomal protein L25

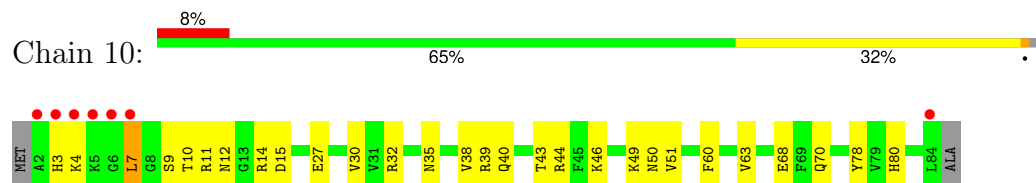


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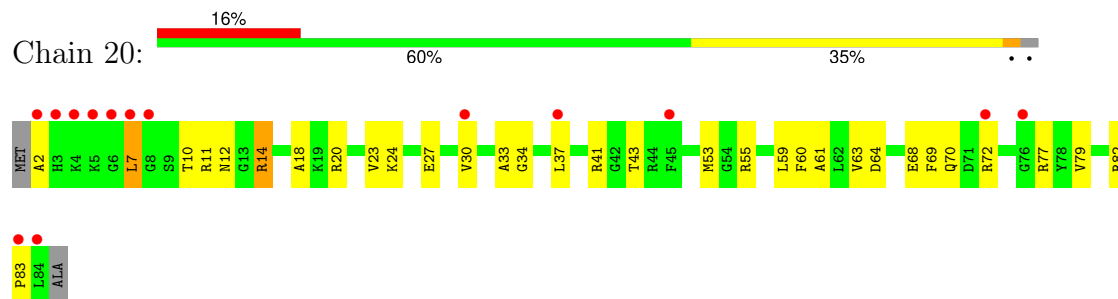
• Molecule 21: 50S ribosomal protein L25



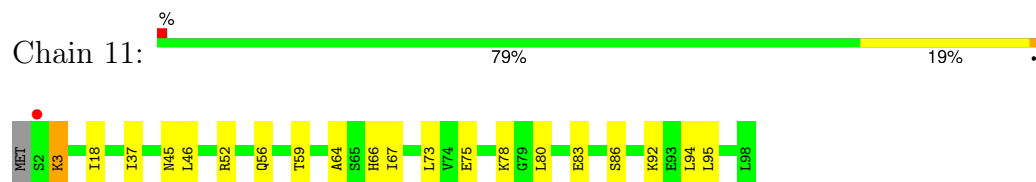
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

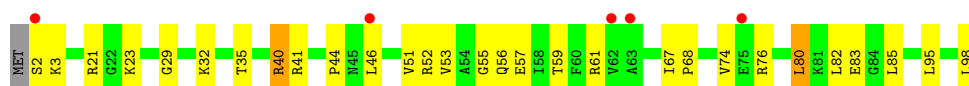


• Molecule 23: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L28

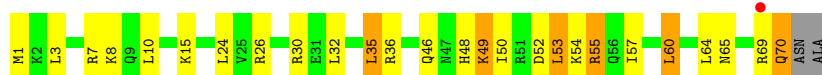




- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



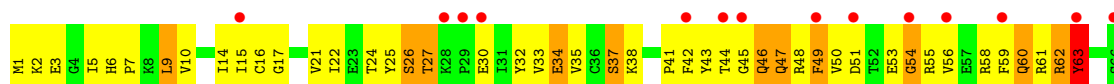
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



• Molecule 27: 50S ribosomal protein L32



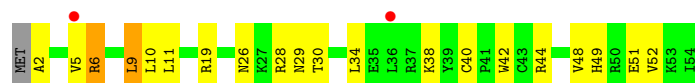
• Molecule 27: 50S ribosomal protein L32



• Molecule 28: 50S ribosomal protein L33



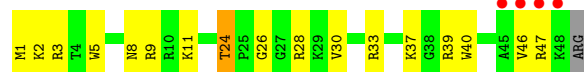
• Molecule 28: 50S ribosomal protein L33



• Molecule 29: 50S ribosomal protein L34



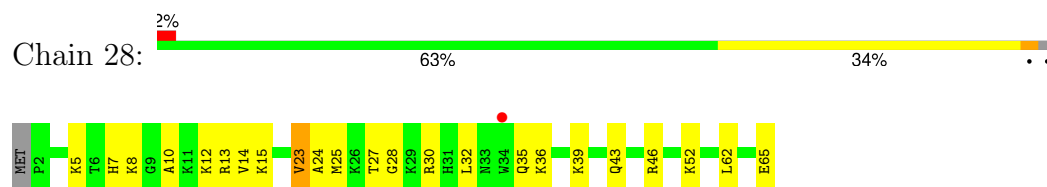
• Molecule 29: 50S ribosomal protein L34



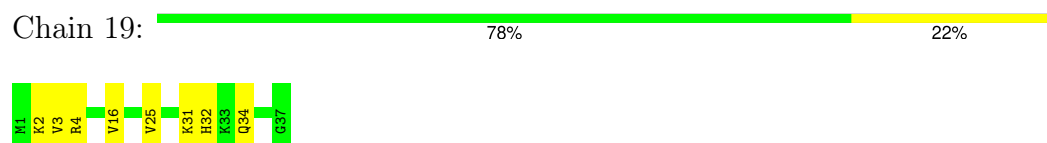
• Molecule 30: 50S ribosomal protein L35



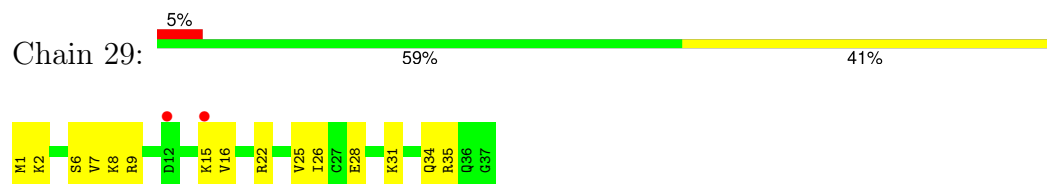
- Molecule 30: 50S ribosomal protein L35



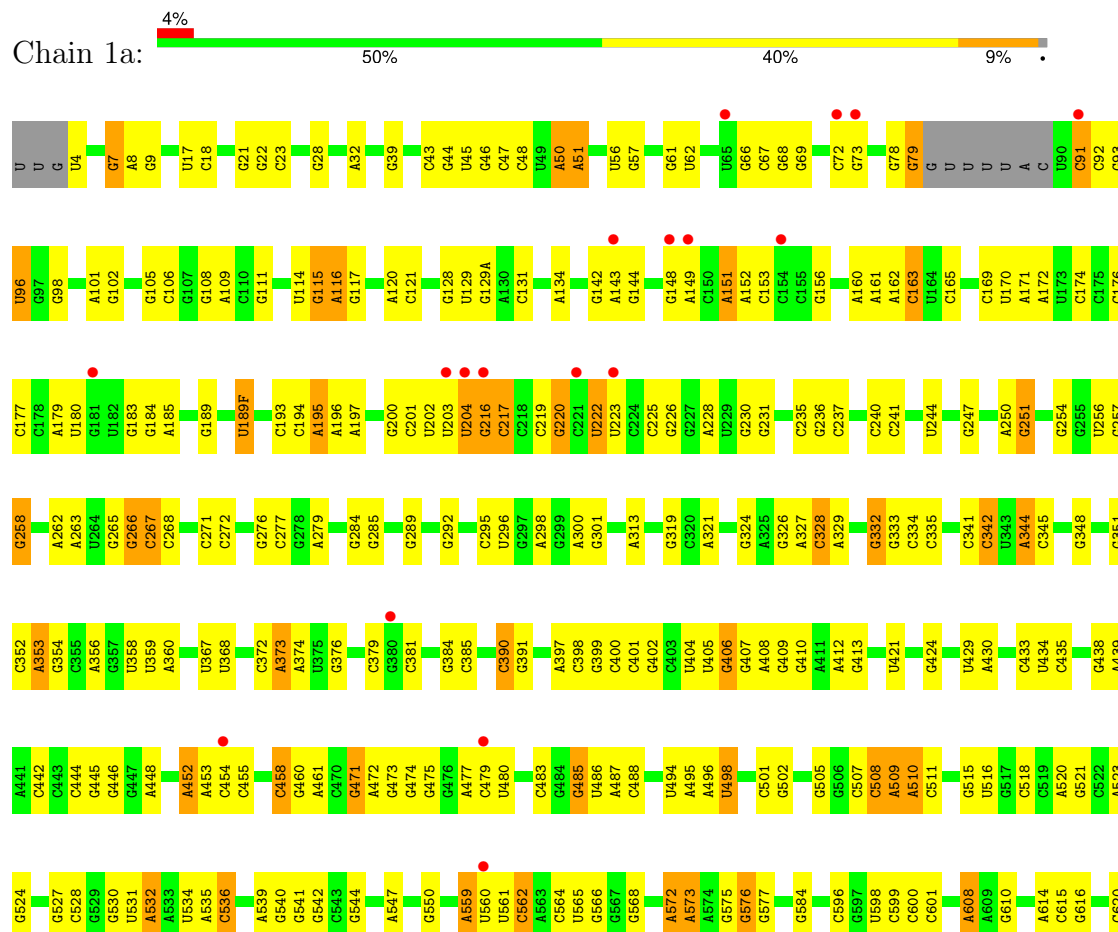
- Molecule 31: 50S ribosomal protein L36

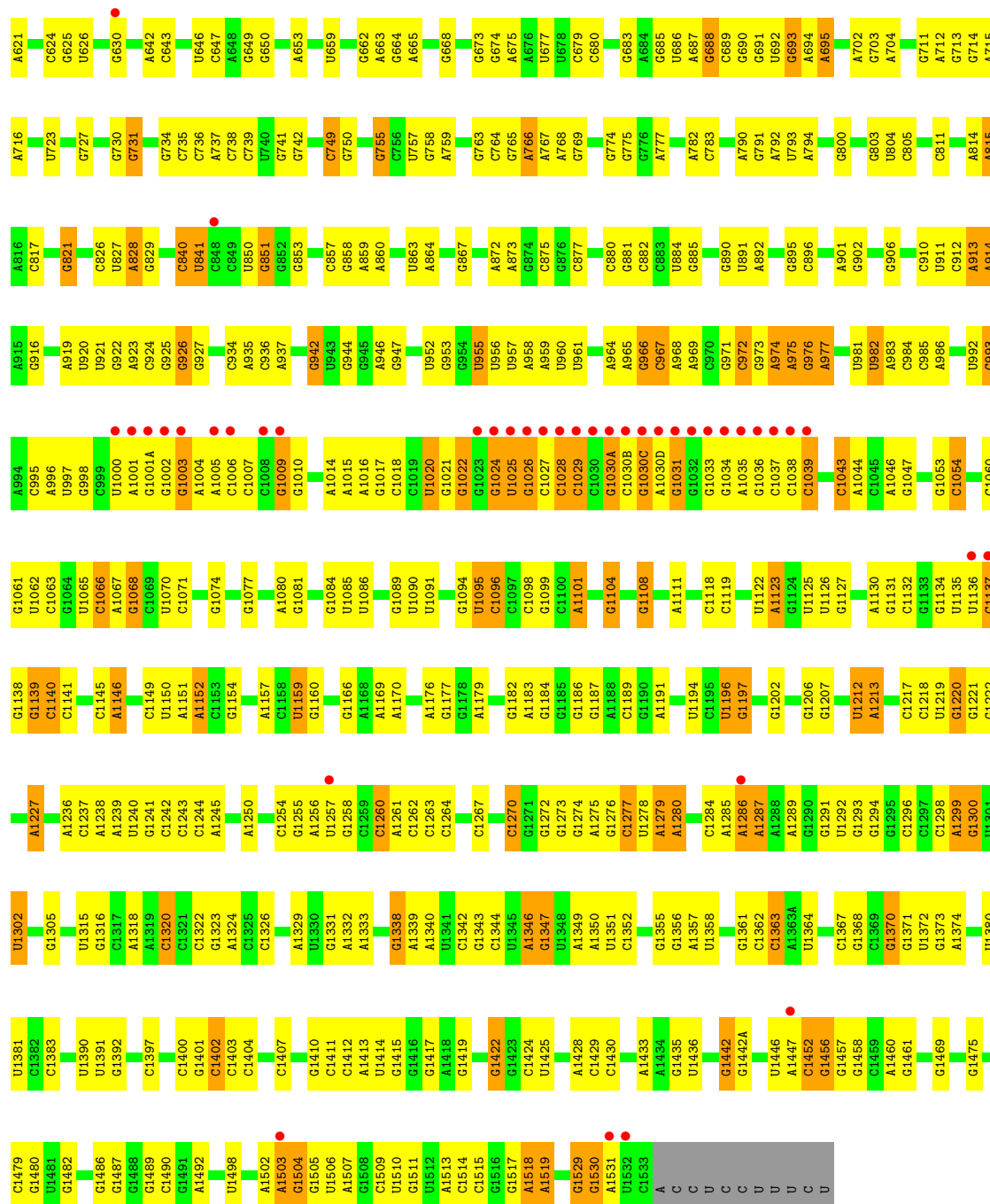


- Molecule 31: 50S ribosomal protein L36

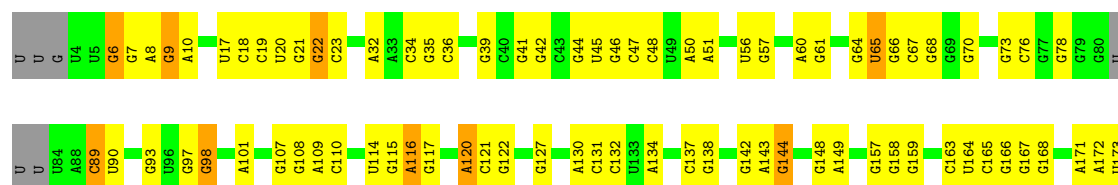


- Molecule 32: 16S Ribosomal RNA

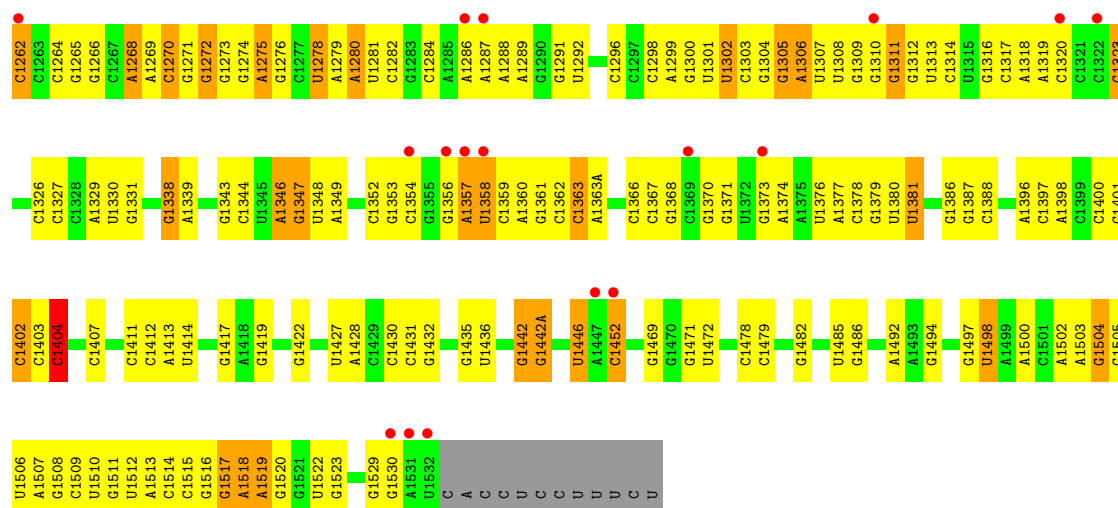




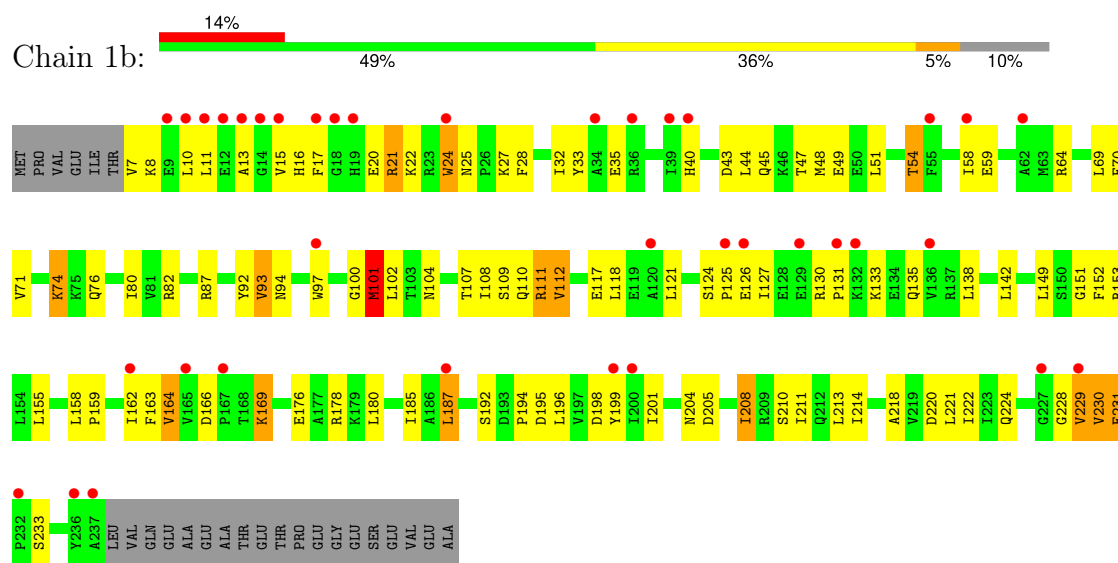
● Molecule 32: 16S Ribosomal RNA



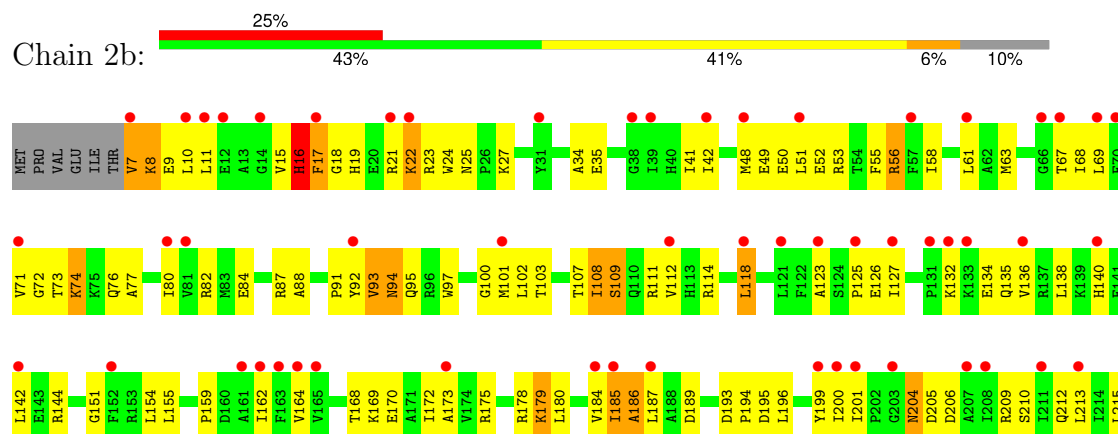
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C1200	C1076	C1019	A958	C875	C783	G713	G617	G544	A453	C175	C268	C176
A1201	G1077	U1020	A959	C876	C784	G714	G618	G545	C457	C177	C269	C178
C1202	U1078	G1021	U960	C877	G785	A716	U619	A647	C458	C179	A279	C180
C1203	G1079	G1022	U961	C878	G786	A717	C620	G548	C459	A180	C280	U181
A1204	A1080	G1023	C880	C879	G787	G718	G621	G549	A461	U182	C281	G181
U1205	G1081	U1024	A964	C881	A790	C719	C624	U552	C470	C182	C282	C183
C1206	U1082	U1025	A965	G882	G791	G720	G625	A553	A471	C184	C283	C185
G1207	U1083	G1026	G966	C885	U792	G721	U626	A554	A472	A186	C284	A187
C1208	U1084	C1027	A967	C886	U793	G722	G627	C554	G473	C188	C285	C189
C1209	U1085	C1028	A968	C887	A794	A723	G628	C555	C474	C190	C286	C191
C1210	U1086	U1029	G969	C888	C806	U724	G629	C556	G475	C192	C287	C193
U1211	U1087	C1030	U970	C889	C807	G725	G630	G557	G481	C194	C288	C195
U1212	G1088	G1030A	G971	A892	A807	C726	C631	G558	A482	U189E	C289	C196
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C1223	U1099	C1038	C984	A913	G821	A737	U652	A572	C506	C207	C300	C207
C1224	C1100	U1039	C985	A914	G822	C738	A653	A573	G507	C208	C301	C208
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C1226	C1102	A1041	A987	A916	G824	G742	G662	G575	A509	C210	C303	C210
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A1229	U1106	G1044	C990	U921	G827	G745	G665	G578	C512	C213	C306	C213
C1230	C1107	U1045	C991	G922	G828	G746	A666	C579	U513	C214	C307	C214
C1231	G1108	A1046	A992	A923	G829	A747	A667	U580	C514	C215	C308	C215
C1232	C1109	G1047	G993	C924	G830	C748	G666	U581	G515	C216	C309	C216
C1233	A1110	U1049	A994	G925	G831	C749	G667	U582	U516	C217	C310	C217
C1234	C1111	G1050	C995	G926	G832	G750	G670	U583	C517	C218	C311	C218
C1235	C1112	C1051	A996	G927	G833	G751	G671	G584	C518	C219	C312	C219
C1236	C1113	U1052	A997	C931	G834	A753	U672	G585	C519	C220	C313	C220
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C1238	C1115	C1054	C999	C933	G836	G755	A674	G587	C521	C222	C315	C222
U1239	C1116	A1055	U1000	A935	G837	C756	A675	G588	C522	C223	C316	C223
U1240	C1117	U1056	A1001	A936	G838	U757	A676	G589	A523	C224	C317	C224
C1241	C1118	G1057	G1001A	A937	G839	G758	U677	G590	C524	C225	C318	C225
C1242	C1119	C1058	G1002	G938	G840	C762	G683	G591	C525	C226	C319	C226
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C1244	U1121	C1060	A1004	C941	G842	C764	G685	U598	C527	C228	C321	C228
C1245	C1122	U1061	A1005	G942	G843	G765	U686	G599	C528	C229	C322	C229
C1246	A1123	G1062	C1006	C943	G844	G766	A687	G600	U531	A250	C323	C230
C1247	U1124	C1063	C1007	A944	G845	A768	G688	G601	A532	C250	C324	C231
C1248	U1125	G1064	U1008	A945	G846	G769	G689	C602	A533	C251	C325	C232
A1251	U1126	U1065	G1009	A946	G847	G770	A695	G603	C536	C252	C326	C233
A1252	G1127	C1066	U863	C947	G848	G771	A696	G604	C537	C253	C327	C234
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C1254	C1129	G1068	A949	A949	G850	G773	A701	G606	C539	C255	C329	C236
C1255	A1130	C1069	U952	U952	G851	G774	A702	G607	C540	C256	C330	C237
A1256	C1131	U1072	G953	G953	G852	A775	G703	A608	G541	C257	C331	C238
U1257	C1132	U1073	G954	U954	G853	G776	G704	A609	G542	C258	C332	C239
C1258	G1133	G1074	U955	U955	G854	G777	G705	G610	C543	C259	C333	C240
C1259	U1134	C1075	U956	U956	G855	G778	G706	G611	C544	C260	C334	C241
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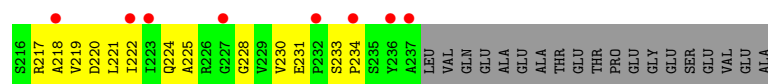


• Molecule 33: 30S ribosomal protein S2

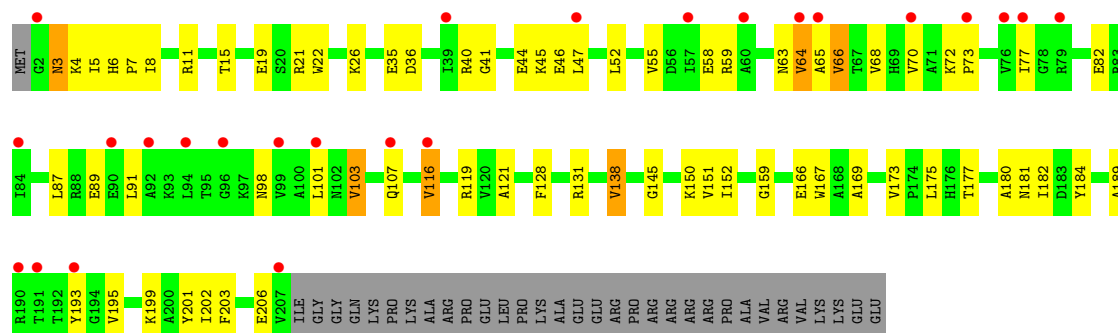


• Molecule 33: 30S ribosomal protein S2

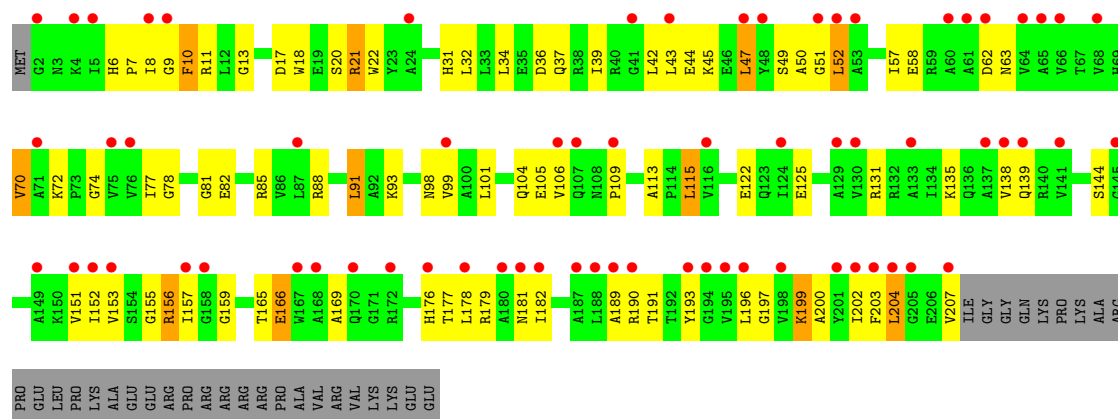




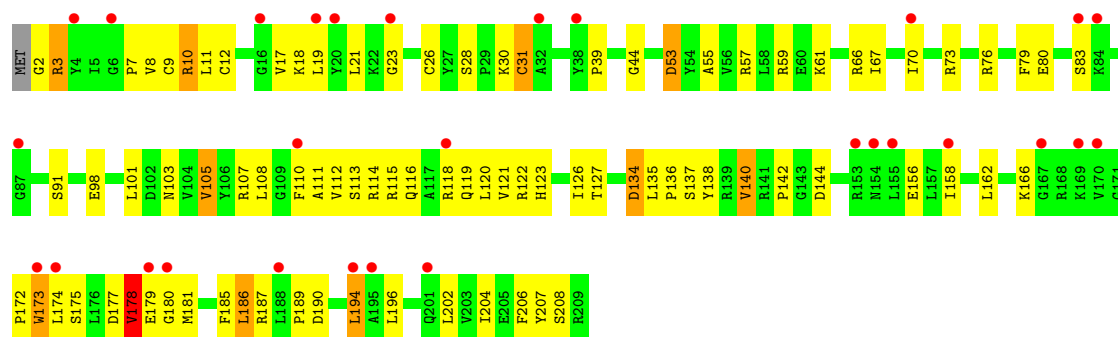
• Molecule 34: 30S ribosomal protein S3



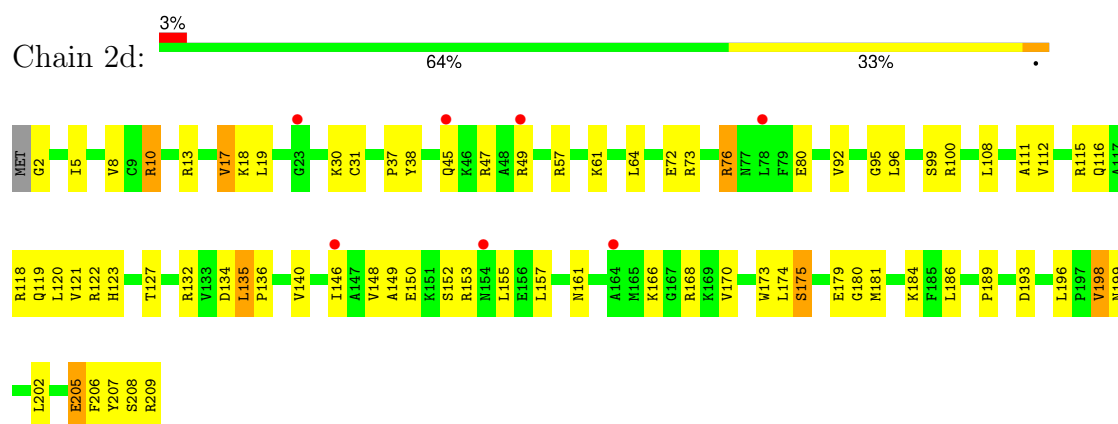
• Molecule 34: 30S ribosomal protein S3



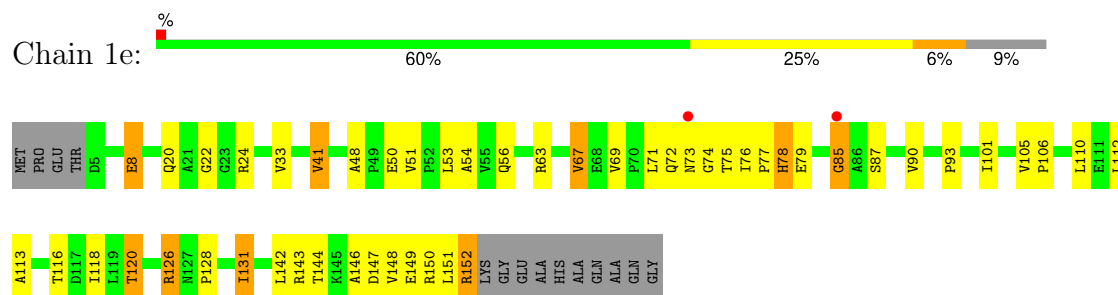
• Molecule 35: 30S ribosomal protein S4



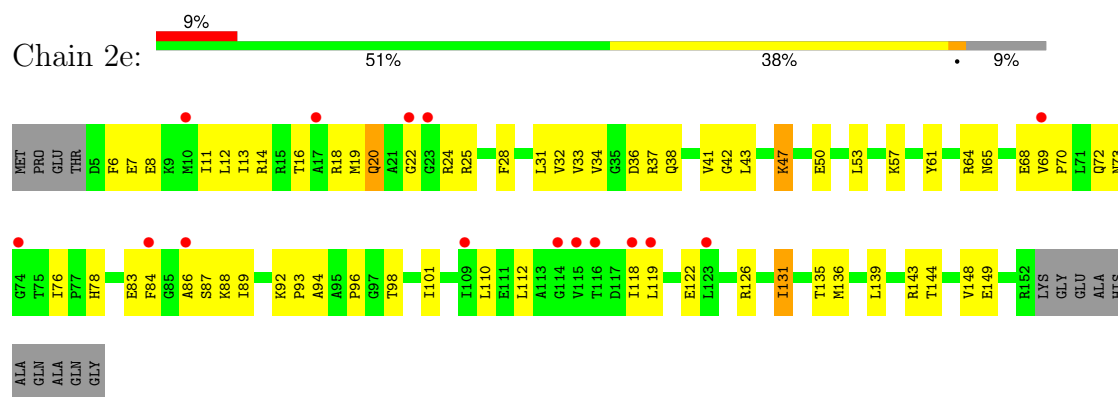
• Molecule 35: 30S ribosomal protein S4



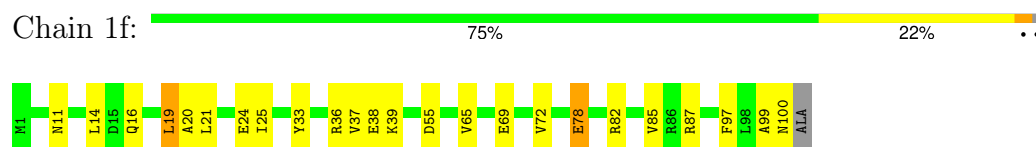
• Molecule 36: 30S ribosomal protein S5



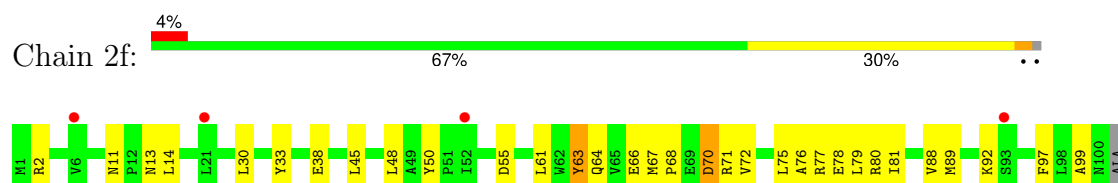
• Molecule 36: 30S ribosomal protein S5



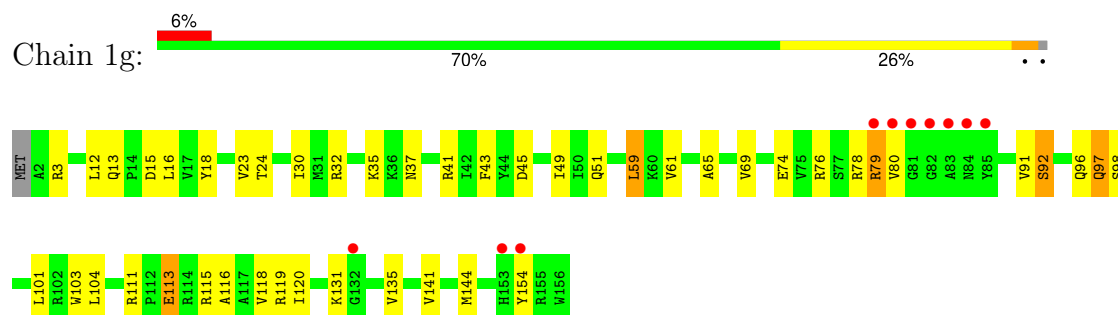
• Molecule 37: 30S ribosomal protein S6



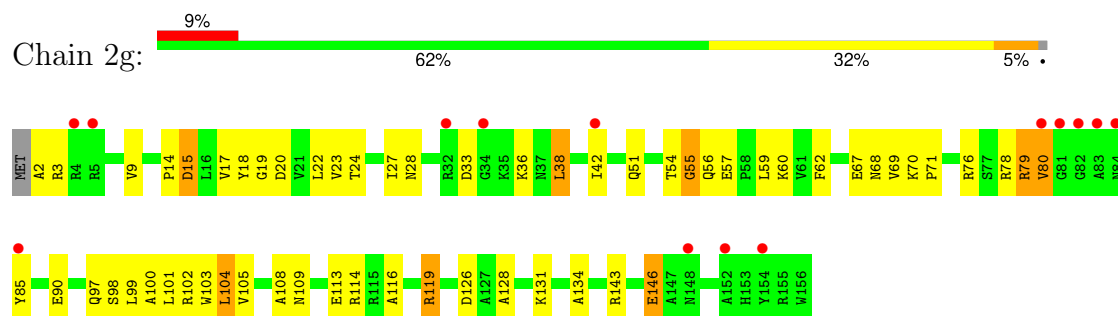
• Molecule 37: 30S ribosomal protein S6



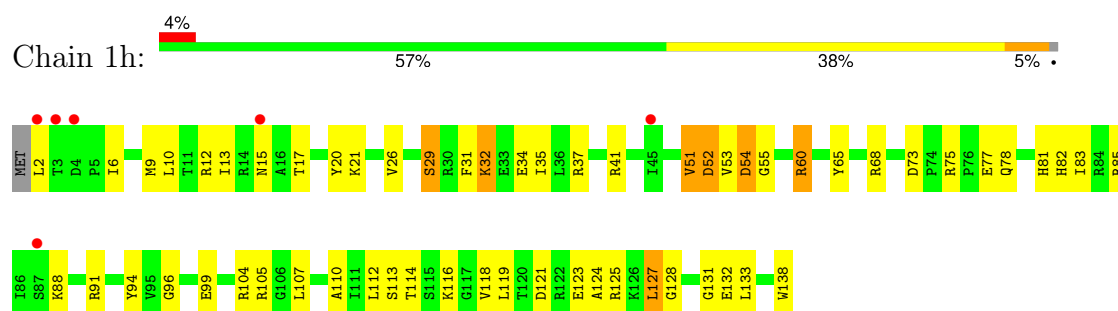
- Molecule 38: 30S ribosomal protein S7



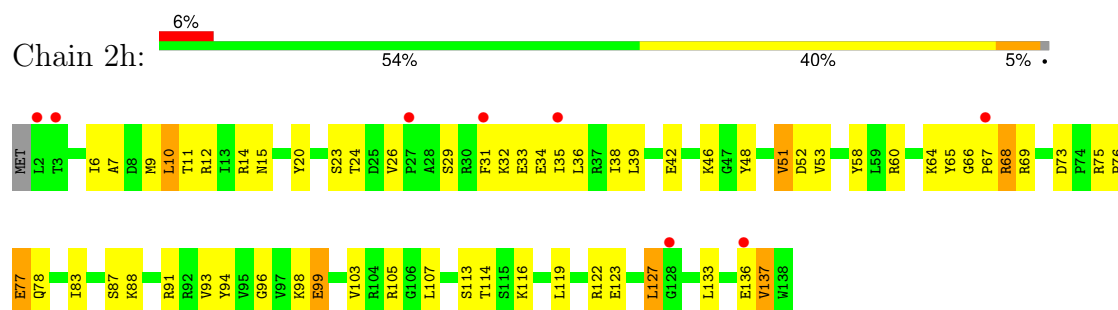
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

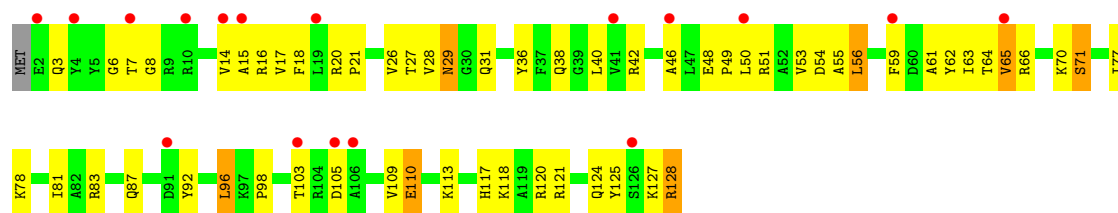


- Molecule 39: 30S ribosomal protein S8

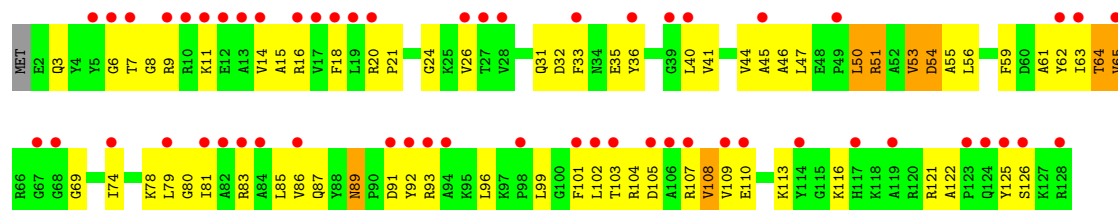
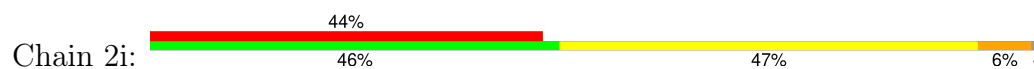


- Molecule 40: 30S ribosomal protein S9





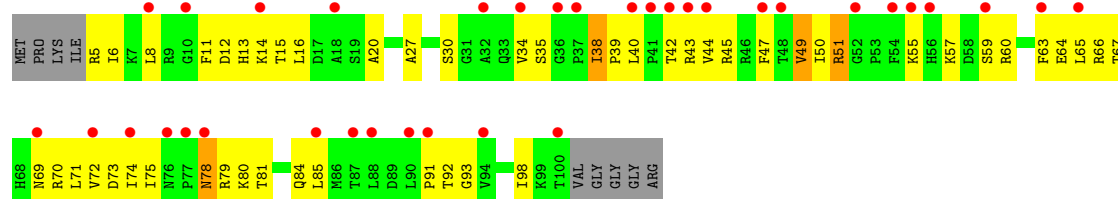
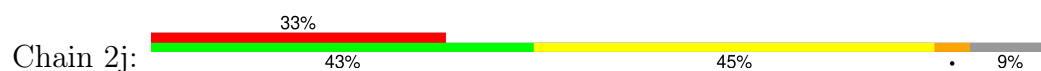
• Molecule 40: 30S ribosomal protein S9



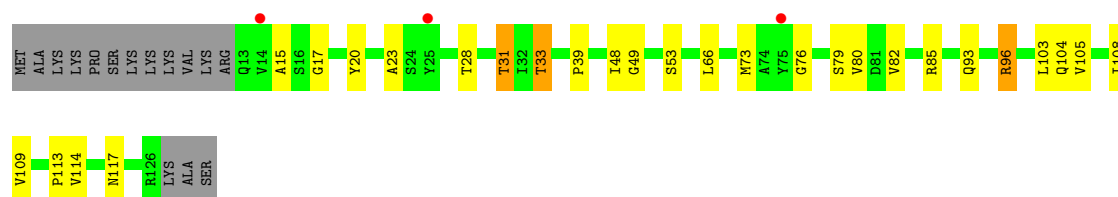
• Molecule 41: 30S ribosomal protein S10



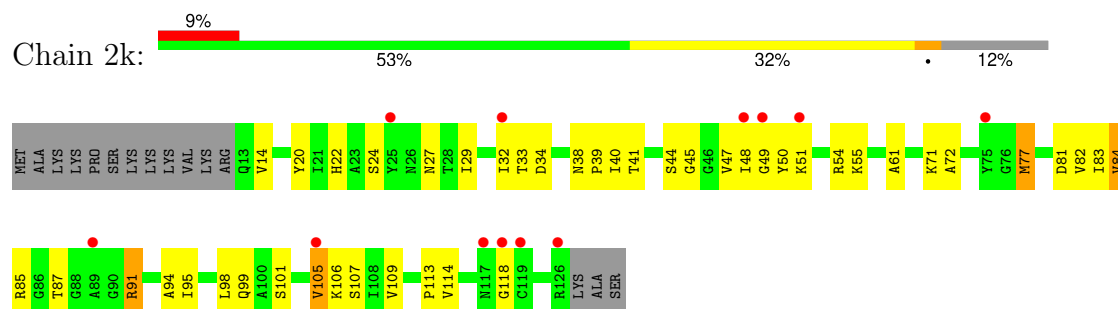
• Molecule 41: 30S ribosomal protein S10



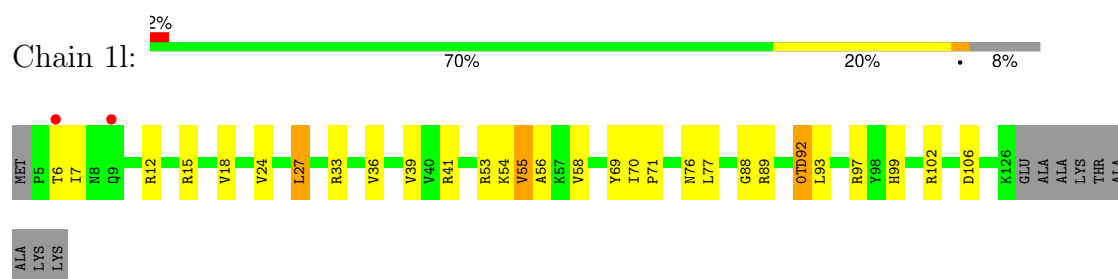
• Molecule 42: 30S ribosomal protein S11



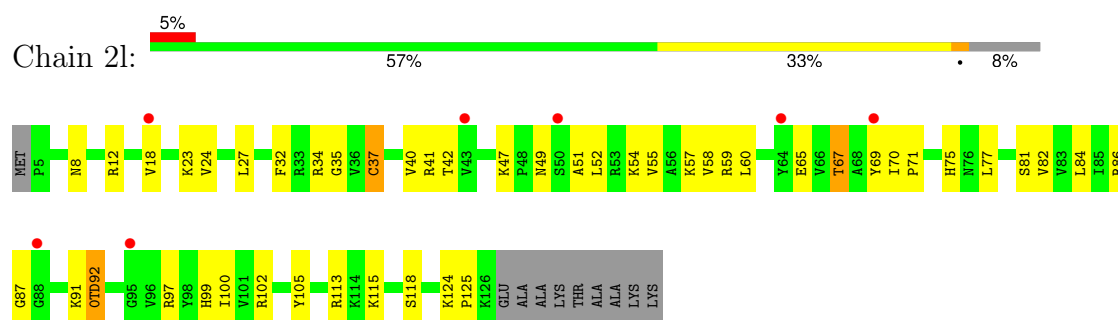
- Molecule 42: 30S ribosomal protein S11



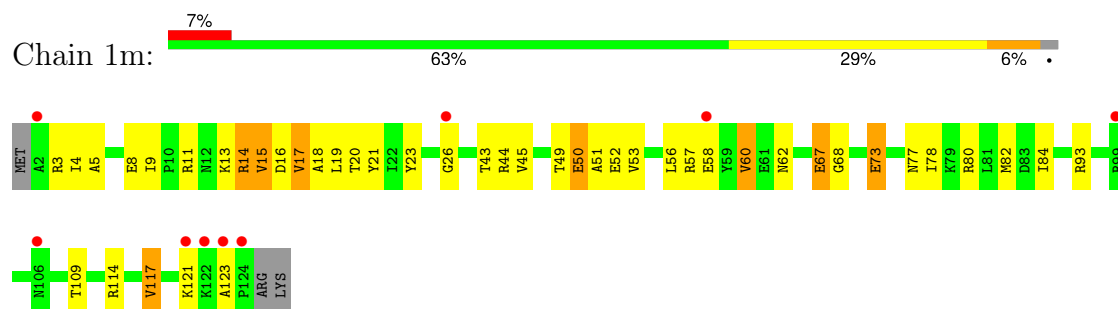
- Molecule 43: 30S ribosomal protein S12



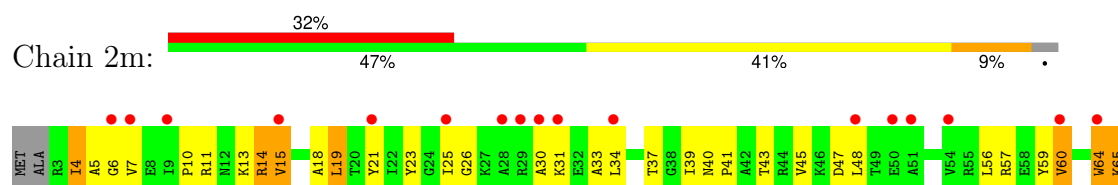
- Molecule 43: 30S ribosomal protein S12

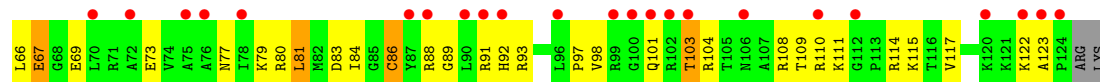


- Molecule 44: 30S ribosomal protein S13

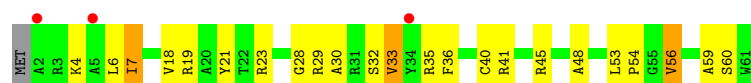


- Molecule 44: 30S ribosomal protein S13

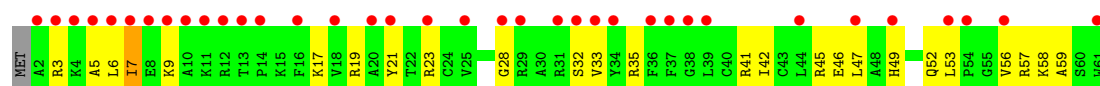




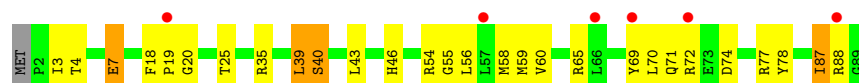
- Molecule 45: 30S ribosomal protein S14 type Z



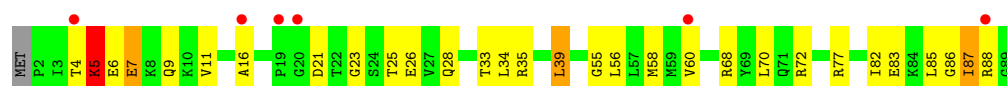
- Molecule 45: 30S ribosomal protein S14 type Z



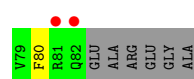
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

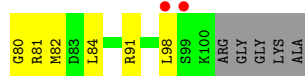


- Molecule 47: 30S ribosomal protein S16

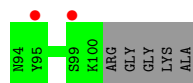
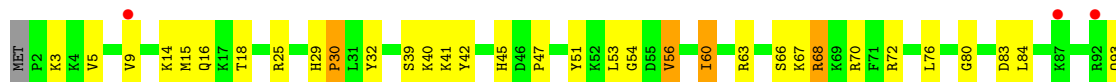




- Molecule 48: 30S ribosomal protein S17



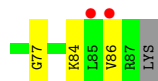
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

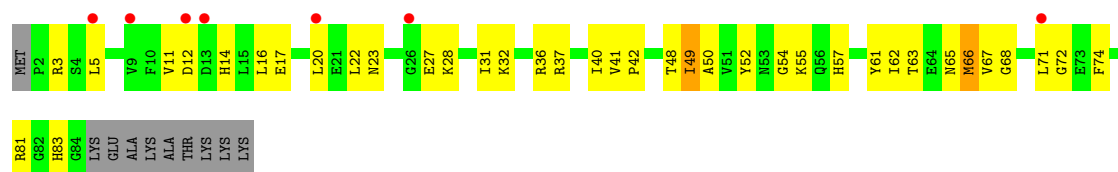


- Molecule 49: 30S ribosomal protein S18

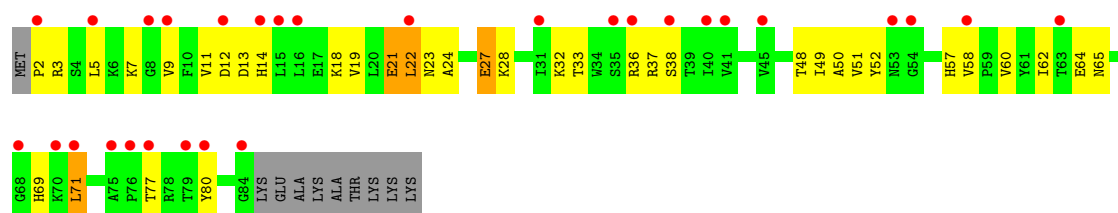


- Molecule 50: 30S ribosomal protein S19

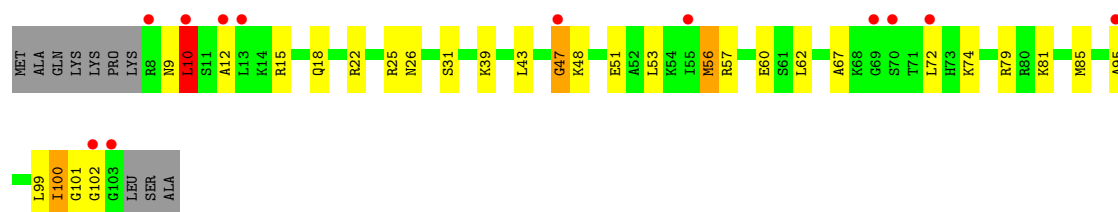




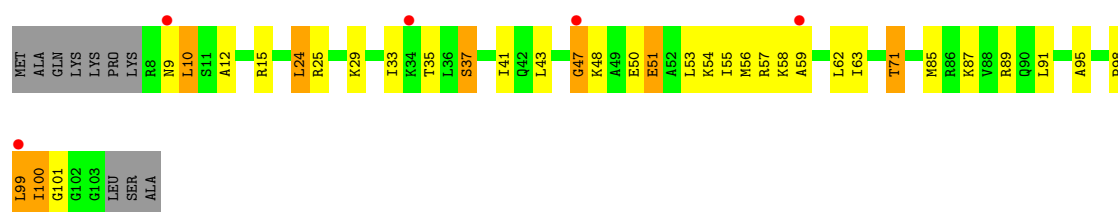
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx

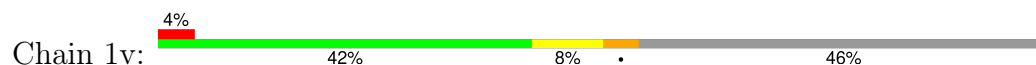


- Molecule 52: 30S ribosomal protein Thx

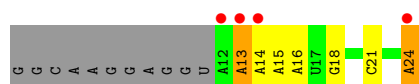
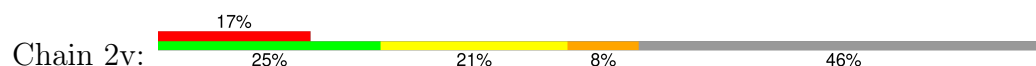




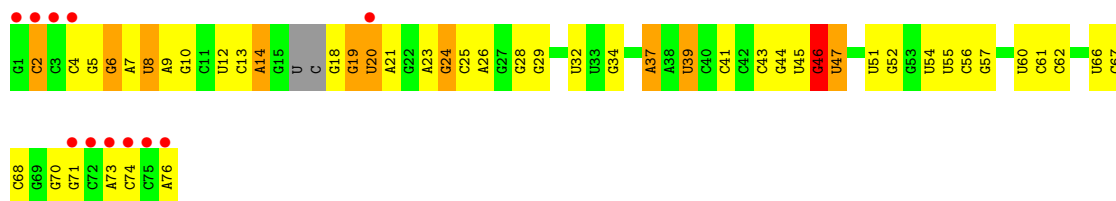
• Molecule 53: MF-mRNA



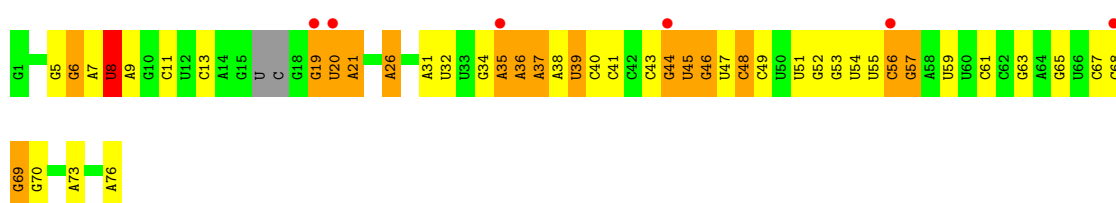
• Molecule 53: MF-mRNA



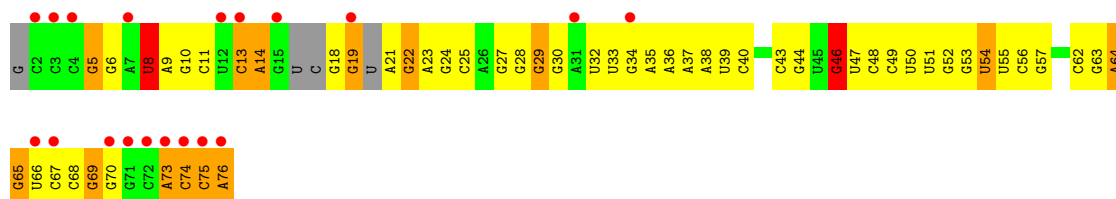
• Molecule 54: A-site and E-site Deacylated tRNAphe



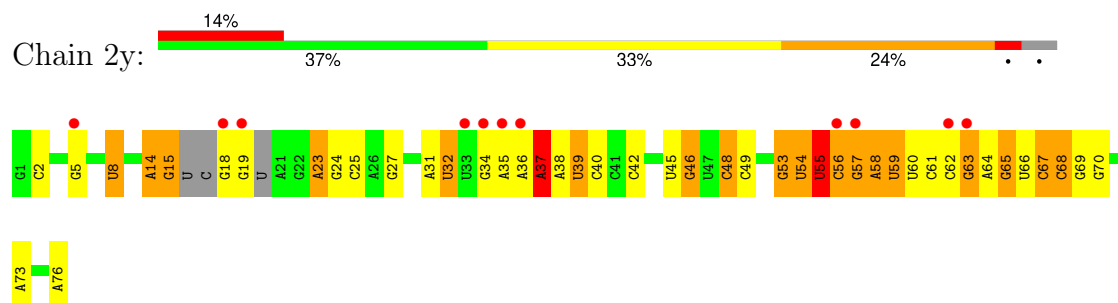
• Molecule 54: A-site and E-site Deacylated tRNAphe



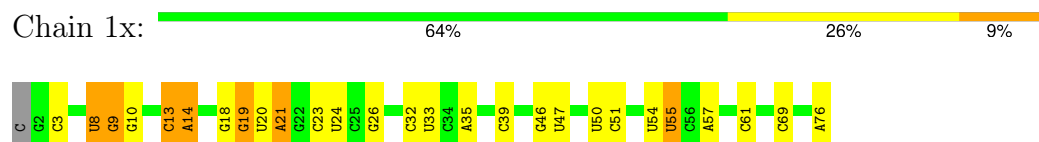
• Molecule 54: A-site and E-site Deacylated tRNAphe



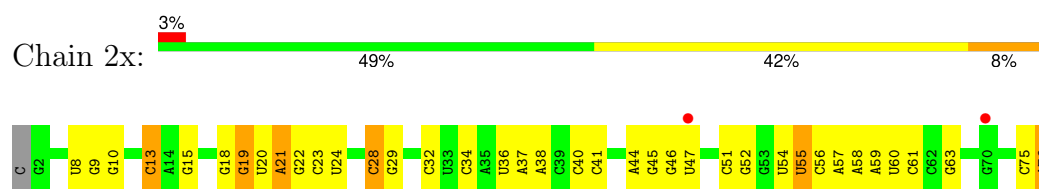
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



- Molecule 55: P-site Deacylated tRNA^{met}



- Molecule 55: P-site Deacylated tRNA^{met}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.36Å 449.77Å 616.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	254.37 – 2.70 254.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (254.37-2.70) 97.1 (254.37-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.224 , 0.277 0.225 , 0.278	Depositor DCC
R_{free} test set	76639 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	299892	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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: M2G, 0TD, G7M, SF4, 2MU, MA6, ZN, K, 4SU, 2MG, 4OC, MG, 5MC, 5MU, PSU, TYK, 2MA, OMC, UR3, OMG, MIA

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	0.28	0/69010	0.46	1/107716 (0.0%)
1	2A	0.22	0/67294	0.40	1/105038 (0.0%)
2	1B	0.23	0/2882	0.40	0/4494
2	2B	0.19	0/2879	0.36	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.28	0/1592	0.50	0/2149
4	2E	0.22	0/1592	0.46	1/2149 (0.0%)
5	1F	0.26	0/1618	0.49	0/2191
5	2F	0.22	0/1614	0.47	2/2186 (0.1%)
6	1G	0.23	0/1448	0.45	0/1957
6	2G	0.20	0/1453	0.46	0/1963
7	1H	0.23	0/1356	0.41	0/1834
7	2H	0.19	0/1356	0.44	0/1834
8	1I	0.21	0/1112	0.44	0/1514
8	2I	0.19	0/1079	0.40	0/1475
9	1N	0.26	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.48	0/1269
10	2O	0.22	0/943	0.47	0/1269
11	1P	0.25	0/1152	0.53	0/1533
11	2P	0.22	0/1152	0.49	0/1533
12	1Q	0.25	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.43	0/1527
13	1R	0.27	0/982	0.49	0/1312
13	2R	0.21	0/982	0.45	0/1312
14	1S	0.27	0/883	0.51	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.26	0/1105	0.54	1/1477 (0.1%)
15	2T	0.21	0/1097	0.43	0/1468
16	1U	0.29	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.42	0/1301
17	1V	0.26	0/782	0.52	0/1049
17	2V	0.19	0/782	0.40	0/1049
18	1W	0.30	0/897	0.49	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.26	0/764	0.54	3/1025 (0.3%)
19	2X	0.21	0/764	0.51	2/1025 (0.2%)
20	1Y	0.25	0/819	0.54	0/1095
20	2Y	0.19	0/819	0.42	0/1095
21	1Z	0.21	0/1267	0.44	0/1717
21	2Z	0.22	0/1299	0.47	0/1763
22	10	0.27	0/662	0.48	0/881
22	20	0.20	0/662	0.43	0/881
23	11	0.26	0/762	0.44	0/1014
23	21	0.23	0/762	0.43	0/1014
24	12	0.26	0/590	0.45	0/781
24	22	0.19	0/590	0.37	0/781
25	13	0.27	0/474	0.48	0/635
25	23	0.20	0/469	0.44	0/630
26	14	0.29	0/565	0.68	1/761 (0.1%)
26	24	0.25	0/545	0.67	1/737 (0.1%)
27	15	0.26	0/469	0.53	0/635
27	25	0.26	0/469	0.49	0/635
28	16	0.27	0/460	0.47	0/613
28	26	0.21	0/456	0.43	0/608
29	17	0.31	0/426	0.52	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.27	0/525	0.47	0/691
30	28	0.22	0/525	0.41	0/691
31	19	0.28	0/310	0.52	0/407
31	29	0.20	0/310	0.45	0/407
32	1a	0.21	0/35795	0.39	0/55864
32	2a	0.20	0/35886	0.38	0/56005
33	1b	0.21	0/1881	0.50	0/2542
33	2b	0.22	0/1860	0.50	0/2518
34	1c	0.19	0/1572	0.43	0/2126
34	2c	0.22	0/1566	0.47	0/2119
35	1d	0.19	0/1685	0.46	0/2262
35	2d	0.21	0/1704	0.44	0/2284
36	1e	0.22	0/1145	0.46	0/1543
36	2e	0.22	0/1149	0.52	0/1548
37	1f	0.21	0/823	0.43	0/1115
37	2f	0.20	0/829	0.43	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.43	0/1679
38	2g	0.19	0/1254	0.42	0/1683
39	1h	0.19	0/1108	0.45	0/1494
39	2h	0.19	0/1108	0.44	0/1494
40	1i	0.20	0/1002	0.51	0/1346
40	2i	0.21	0/997	0.49	0/1343
41	1j	0.20	0/722	0.43	0/982
41	2j	0.22	0/727	0.54	0/988
42	1k	0.19	0/844	0.42	0/1145
42	2k	0.18	0/848	0.41	0/1149
43	1l	0.21	0/937	0.44	0/1260
43	2l	0.19	0/937	0.41	0/1260
44	1m	0.21	0/969	0.48	1/1302 (0.1%)
44	2m	0.21	0/961	0.45	0/1291
45	1n	0.19	0/501	0.46	0/664
45	2n	0.21	0/501	0.47	0/664
46	1o	0.20	0/739	0.38	0/985
46	2o	0.18	0/739	0.38	0/985
47	1p	0.20	0/697	0.47	0/939
47	2p	0.20	0/693	0.46	0/935
48	1q	0.20	0/836	0.43	0/1117
48	2q	0.19	0/836	0.46	0/1117
49	1r	0.22	0/560	0.42	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.24	0/661	0.59	0/893
51	1t	0.20	0/730	0.49	0/965
51	2t	0.21	0/729	0.51	0/965
52	1u	0.19	0/203	0.42	0/266
52	2u	0.22	0/203	0.45	0/266
53	1v	0.19	0/310	0.32	0/480
53	2v	0.21	0/310	0.32	0/480
54	1w	0.29	1/1606 (0.1%)	0.41	0/2497
54	1y	0.28	2/1606 (0.1%)	0.40	0/2497
54	2w	0.30	1/1556 (0.1%)	0.41	0/2418
54	2y	0.29	2/1583 (0.1%)	0.44	0/2459
55	1x	0.27	0/1725	0.42	0/2689
55	2x	0.24	1/1725 (0.1%)	0.36	0/2689
All	All	0.23	7/316686 (0.0%)	0.43	14/474117 (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	1P	0	1
11	2P	0	1
33	2b	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	8	4SU	O3'-P	5.43	1.61	1.56
54	1w	46	G7M	O3'-P	5.34	1.61	1.56
54	2w	46	G7M	O3'-P	5.24	1.61	1.56
55	2x	8	4SU	O3'-P	5.09	1.61	1.56
54	2y	46	G7M	O3'-P	5.07	1.61	1.56

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1T	89	VAL	N-CA-C	-6.52	106.44	112.96
1	1A	1992	G	C2'-C3'-O3'	5.99	118.48	109.50
4	2E	186	GLY	N-CA-C	5.69	118.91	110.60
5	2F	21	ALA	CA-C-N	5.41	131.43	121.70
5	2F	21	ALA	C-N-CA	5.41	131.43	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	Peptide
33	2b	186	ALA	Peptide

5.2 Too-close contacts [i](#)

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	31193	773	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	60322	0	30423	825	0
2	1B	2577	0	1305	28	0
2	2B	2575	0	1303	48	0
3	1D	2136	0	2218	70	0
3	2D	2136	0	2217	61	0
4	1E	1559	0	1618	36	0
4	2E	1559	0	1618	34	0
5	1F	1583	0	1625	47	0
5	2F	1579	0	1619	59	0
6	1G	1423	0	1436	49	0
6	2G	1428	0	1438	59	0
7	1H	1330	0	1407	44	0
7	2H	1330	0	1407	43	0
8	1I	1097	0	1140	27	0
8	2I	1064	0	1082	29	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	25	0
10	2O	933	0	996	28	0
11	1P	1135	0	1212	48	0
11	2P	1135	0	1212	50	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	36	0
13	1R	968	0	1033	25	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	18	0
14	2S	870	0	923	29	0
15	1T	1091	0	1151	25	0
15	2T	1083	0	1136	36	0
16	1U	959	0	1019	19	0
16	2U	959	0	1019	22	0
17	1V	771	0	830	10	1
17	2V	771	0	830	15	0
18	1W	886	0	939	12	0
18	2W	886	0	940	16	0
19	1X	750	0	814	23	0
19	2X	750	0	814	22	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	37	0
21	2Z	1271	0	1273	55	0
22	10	653	0	674	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	25	0
23	11	755	0	826	11	0
23	21	755	0	826	22	0
24	12	588	0	643	11	0
24	22	588	0	643	21	0
25	13	469	0	518	16	0
25	23	464	0	514	18	0
26	14	552	0	533	31	0
26	24	532	0	503	37	0
27	15	455	0	465	12	1
27	25	455	0	465	16	0
28	16	453	0	473	14	0
28	26	449	0	469	15	0
29	17	418	0	467	11	0
29	27	418	0	467	16	0
30	18	517	0	582	27	0
30	28	517	0	582	19	0
31	19	307	0	335	4	0
31	29	307	0	335	8	0
32	1a	32246	0	16294	514	0
32	2a	32327	0	16338	639	1
33	1b	1846	0	1867	74	0
33	2b	1825	0	1828	95	0
34	1c	1548	0	1535	40	0
34	2c	1542	0	1517	61	0
35	1d	1655	0	1672	71	0
35	2d	1674	0	1714	54	0
36	1e	1129	0	1185	31	0
36	2e	1133	0	1191	45	0
37	1f	810	0	804	13	0
37	2f	816	0	808	19	0
38	1g	1231	0	1238	27	0
38	2g	1235	0	1249	37	0
39	1h	1088	0	1126	40	0
39	2h	1088	0	1126	42	0
40	1i	983	0	986	44	0
40	2i	978	0	966	47	0
41	1j	709	0	650	31	0
41	2j	714	0	672	37	0
42	1k	829	0	825	11	0
42	2k	833	0	836	24	0
43	1l	932	0	981	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	36	0
44	1m	958	0	1002	32	0
44	2m	950	0	988	55	0
45	1n	492	0	529	18	0
45	2n	492	0	529	26	0
46	1o	728	0	760	19	0
46	2o	728	0	760	22	0
47	1p	681	0	697	25	0
47	2p	677	0	686	21	0
48	1q	823	0	891	29	0
48	2q	823	0	891	21	0
49	1r	555	0	618	9	0
49	2r	555	0	618	15	0
50	1s	652	0	662	33	0
50	2s	646	0	644	31	0
51	1t	728	0	798	21	0
51	2t	727	0	796	26	0
52	1u	199	0	208	10	0
52	2u	199	0	208	7	0
53	1v	277	0	140	3	0
53	2v	277	0	140	7	0
54	1w	1592	0	818	31	0
54	1y	1585	0	803	18	0
54	2w	1544	0	787	41	0
54	2y	1565	0	794	30	0
55	1x	1625	0	829	15	0
55	2x	1625	0	829	16	0
56	10	7	0	0	0	0
56	11	3	0	0	0	0
56	12	2	0	0	0	0
56	13	6	0	0	0	0
56	15	5	0	0	0	0
56	16	4	0	0	0	0
56	17	3	0	0	0	0
56	18	5	0	0	0	0
56	19	1	0	0	0	0
56	1A	1106	0	0	0	0
56	1B	35	0	0	0	0
56	1D	11	0	0	0	0
56	1E	13	0	0	0	0
56	1F	10	0	0	0	0
56	1G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	6	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1S	3	0	0	0	0
56	1T	3	0	0	0	0
56	1U	12	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	224	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	7	0	0	0	0
56	1x	14	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0
56	23	4	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	4	0	0	0	0
56	29	1	0	0	0	0
56	2A	877	0	0	0	0
56	2B	21	0	0	0	0
56	2D	6	0	0	0	0
56	2E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	3	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	3	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	234	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2m	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	7	0	0	0	0
56	2x	4	0	0	0	0
56	2y	6	0	0	0	0
57	1A	64	0	76	6	0
57	2A	64	0	76	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	5	0
59	2d	8	0	0	0	0
60	1x	1	0	0	0	0
60	2A	1	0	0	0	0
61	10	10	0	0	1	0
61	11	9	0	0	0	0
61	12	4	0	0	1	0
61	13	4	0	0	1	0
61	14	1	0	0	0	0
61	15	5	0	0	0	0
61	16	2	0	0	0	0
61	17	10	0	0	0	0
61	18	13	0	0	1	0
61	1A	1864	0	0	102	0
61	1B	59	0	0	3	0
61	1D	24	0	0	1	0
61	1E	26	0	0	3	0
61	1F	17	0	0	1	0
61	1G	5	0	0	1	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	7	0	0	0	0
61	1O	9	0	0	0	0
61	1P	21	0	0	1	0
61	1Q	10	0	0	0	0
61	1R	10	0	0	1	0
61	1S	5	0	0	0	0
61	1T	7	0	0	0	0
61	1U	10	0	0	0	0
61	1V	7	0	0	0	0
61	1W	8	0	0	2	0
61	1X	5	0	0	1	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	264	0	0	25	0
61	1b	1	0	0	1	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	1	0
61	1i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1k	1	0	0	0	0
6l	1l	4	0	0	0	0
6l	1m	1	0	0	0	0
6l	1o	1	0	0	0	0
6l	1p	1	0	0	0	0
6l	1q	5	0	0	0	0
6l	1u	1	0	0	1	0
6l	1v	4	0	0	0	0
6l	1w	13	0	0	0	0
6l	1x	13	0	0	1	0
6l	20	5	0	0	1	0
6l	21	9	0	0	1	0
6l	22	1	0	0	0	0
6l	23	1	0	0	0	0
6l	25	3	0	0	0	0
6l	27	3	0	0	1	0
6l	28	6	0	0	1	0
6l	29	1	0	0	0	0
6l	2A	1086	0	0	84	0
6l	2B	21	0	0	1	0
6l	2D	18	0	0	1	0
6l	2E	11	0	0	1	0
6l	2F	13	0	0	0	0
6l	2I	5	0	0	1	0
6l	2N	1	0	0	0	0
6l	2O	1	0	0	0	0
6l	2P	9	0	0	0	0
6l	2Q	3	0	0	0	0
6l	2R	3	0	0	0	0
6l	2T	6	0	0	0	0
6l	2U	1	0	0	0	0
6l	2W	1	0	0	0	0
6l	2X	3	0	0	1	0
6l	2Y	2	0	0	0	0
6l	2Z	1	0	0	0	0
6l	2a	226	0	0	28	0
6l	2d	2	0	0	0	0
6l	2e	1	0	0	0	0
6l	2i	1	0	0	0	0
6l	2j	4	0	0	2	0
6l	2l	6	0	0	1	0
6l	2p	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2q	1	0	0	0	0
61	2t	4	0	0	0	0
61	2u	1	0	0	0	0
61	2v	1	0	0	0	0
61	2w	2	0	0	0	0
61	2x	7	0	0	0	0
61	2y	16	0	0	0	0
All	All	299892	0	196834	5098	2

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

The worst 5 of 5098 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.56	1.03
1:1A:1082:U:O4	1:1A:1086:A:N1	1.94	1.00
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.45	0.98
1:1A:2124:G:H1	1:1A:2174:C:H42	1.02	0.97
1:2A:2585:U:H5	54:2w:76:A:HO3'	1.03	0.96

All (2) 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:2136:C:O3'	32:2a:1000:U:O2'[3_654]	2.15	0.05
17:1V:49:THR:OG1	27:15:60:VAL:O[4_545]	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%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	48
4	2E	202/206 (98%)	186 (92%)	13 (6%)	3 (2%)	8	22
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	24	48
5	2F	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	12	32
6	1G	179/182 (98%)	160 (89%)	16 (9%)	3 (2%)	7	19
6	2G	179/182 (98%)	153 (86%)	20 (11%)	6 (3%)	3	7
7	1H	172/180 (96%)	157 (91%)	15 (9%)	0	100	100
7	2H	172/180 (96%)	152 (88%)	18 (10%)	2 (1%)	10	27
8	1I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	18	41
8	2I	144/148 (97%)	120 (83%)	23 (16%)	1 (1%)	18	41
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	37
11	1P	147/150 (98%)	130 (88%)	17 (12%)	0	100	100
11	2P	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	18	41
12	1Q	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	8 (6%)	2 (1%)	9	23
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	100 (93%)	8 (7%)	0	100	100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14	35
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	37
15	2T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	16	37
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	16
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	32
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	5	14
19	2X	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	32
20	2Y	105/110 (96%)	94 (90%)	10 (10%)	1 (1%)	12	32
21	1Z	148/206 (72%)	126 (85%)	17 (12%)	5 (3%)	3	7
21	2Z	156/206 (76%)	124 (80%)	25 (16%)	7 (4%)	2	4
22	10	81/85 (95%)	76 (94%)	4 (5%)	1 (1%)	10	27
22	20	81/85 (95%)	73 (90%)	8 (10%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	29
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	52 (78%)	8 (12%)	7 (10%)	0	0
26	24	67/71 (94%)	43 (64%)	18 (27%)	6 (9%)	0	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	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%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	184 (80%)	38 (17%)	7 (3%)	3	8
33	2b	229/256 (90%)	189 (82%)	32 (14%)	8 (4%)	3	6
34	1c	204/239 (85%)	184 (90%)	16 (8%)	4 (2%)	6	16
34	2c	204/239 (85%)	167 (82%)	31 (15%)	6 (3%)	3	9
35	1d	206/209 (99%)	185 (90%)	19 (9%)	2 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	24	48
36	1e	146/162 (90%)	123 (84%)	20 (14%)	3 (2%)	5	15
36	2e	146/162 (90%)	132 (90%)	12 (8%)	2 (1%)	9	23
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	12	32
38	1g	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	18	41
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	6	16
39	1h	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	8	22
39	2h	135/138 (98%)	118 (87%)	15 (11%)	2 (2%)	8	22
40	1i	125/128 (98%)	105 (84%)	18 (14%)	2 (2%)	7	20
40	2i	125/128 (98%)	104 (83%)	18 (14%)	3 (2%)	4	12
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	2
41	2j	94/105 (90%)	76 (81%)	12 (13%)	6 (6%)	1	1
42	1k	112/129 (87%)	93 (83%)	16 (14%)	3 (3%)	4	10
42	2k	112/129 (87%)	97 (87%)	12 (11%)	3 (3%)	4	10
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	104 (86%)	16 (13%)	1 (1%)	16	37
44	2m	120/126 (95%)	96 (80%)	22 (18%)	2 (2%)	7	19
45	1n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	7	19
45	2n	58/61 (95%)	48 (83%)	10 (17%)	0	100	100
46	1o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10	27
46	2o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10	27
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	5	15
48	2q	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5	15
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	27
50	2s	81/93 (87%)	63 (78%)	16 (20%)	2 (2%)	4	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1	3
51	2t	94/106 (89%)	81 (86%)	9 (10%)	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
All	All	11368/12128 (94%)	10247 (90%)	973 (9%)	148 (1%)	9	25

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
23	11	3	LYS
26	14	58	ARG
26	14	62	ARG
34	1c	66	VAL

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%)	200 (93%)	15 (7%)	14	34
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15	37
4	1E	164/166 (99%)	150 (92%)	14 (8%)	10	25
4	2E	164/166 (99%)	151 (92%)	13 (8%)	11	28
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	14
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	16
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	22
6	2G	143/156 (92%)	122 (85%)	21 (15%)	3	8
7	1H	144/148 (97%)	125 (87%)	19 (13%)	4	10
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	13
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	6
8	2I	105/124 (85%)	91 (87%)	14 (13%)	4	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	30
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10	25
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	48
10	2O	100/100 (100%)	92 (92%)	8 (8%)	11	28
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	17
11	2P	115/116 (99%)	97 (84%)	18 (16%)	2	7
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	27
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	27
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	34
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	42
14	1S	86/88 (98%)	80 (93%)	6 (7%)	14	34
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	10
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	47
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	46
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	64
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	54
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	31
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	23
18	1W	90/92 (98%)	88 (98%)	2 (2%)	45	74
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	36
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	47
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	57
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	13
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	10
21	1Z	135/179 (75%)	119 (88%)	16 (12%)	5	13
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	3	7
22	10	65/67 (97%)	59 (91%)	6 (9%)	8	22
22	20	65/67 (97%)	60 (92%)	5 (8%)	12	30
23	11	80/83 (96%)	71 (89%)	9 (11%)	5	14
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	31
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	22

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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%)	47 (92%)	4 (8%)	11	29
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	28
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	9
26	24	53/63 (84%)	40 (76%)	13 (24%)	1	2
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	19
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	28
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	19
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	12
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	49
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	49
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	32
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	59
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	67
31	29	34/34 (100%)	28 (82%)	6 (18%)	2	5
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4	10
33	2b	187/220 (85%)	163 (87%)	24 (13%)	4	11
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	17
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	10
35	1d	169/181 (93%)	151 (89%)	18 (11%)	6	16
35	2d	173/181 (96%)	156 (90%)	17 (10%)	7	19
36	1e	113/123 (92%)	99 (88%)	14 (12%)	4	11
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	20
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	41
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	33
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	13
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	13
39	1h	114/119 (96%)	101 (89%)	13 (11%)	5	14
39	2h	114/119 (96%)	102 (90%)	12 (10%)	6	17
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4	10
40	2i	89/99 (90%)	74 (83%)	15 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	30
41	2j	69/92 (75%)	65 (94%)	4 (6%)	18	42
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	25
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	20
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	26
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	32
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	13
44	2m	92/101 (91%)	78 (85%)	14 (15%)	3	7
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	12
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	27
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	38
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	30
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	18
47	2p	68/74 (92%)	58 (85%)	10 (15%)	3	8
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	20
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	25
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	48
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	9
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	24
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	17
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13	33
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5	14
52	1u	18/22 (82%)	14 (78%)	4 (22%)	1	3
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	44
All	All	9303/10064 (92%)	8395 (90%)	908 (10%)	7	19

5 of 908 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	2F	32	LEU
49	2r	37	VAL
12	2Q	109	VAL
48	2q	14	LYS
39	2h	52	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
35	2d	116	GLN
36	2e	127	ASN
40	2i	89	ASN
40	1i	31	GLN
40	1i	3	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	472 (16%)	36 (1%)
1	2A	2791/2915 (95%)	518 (18%)	25 (0%)
2	1B	120/121 (99%)	12 (10%)	1 (0%)
2	2B	118/121 (97%)	30 (25%)	0
32	1a	1497/1521 (98%)	270 (18%)	0
32	2a	1501/1521 (98%)	301 (20%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	72/76 (94%)	18 (25%)	0
54	1y	72/76 (94%)	27 (37%)	0
54	2w	69/76 (90%)	22 (31%)	0
54	2y	70/76 (92%)	28 (40%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	17 (22%)	0
All	All	9348/9620 (97%)	1732 (18%)	62 (0%)

5 of 1732 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	27	G
1	1A	34	C

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2181	G
1	2A	1653	G
1	1A	2756	U

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Mol	Chain	Res	Type
1	2A	1530	C
1	2A	2126	A

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

84 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$
1	OMG	2A	2251	1,55	23,26,27	1.21	3 (13%)	32,38,41	1.96	6 (18%)
32	G7M	1a	527	32	23,26,27	1.52	3 (13%)	34,39,42	1.71	5 (14%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.47	0	33,38,41	2.09	8 (24%)
32	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.17	4 (15%)
1	OMG	1A	2251	1,55,56	23,26,27	1.27	3 (13%)	32,38,41	1.92	6 (18%)
1	5MC	2A	1962	1,56	19,22,23	1.61	3 (15%)	26,32,35	1.11	2 (7%)
1	2MA	1A	2503	1,56	22,25,26	1.45	4 (18%)	32,37,40	2.25	9 (28%)
54	MIA	2w	37	54	24,27,32	2.09	6 (25%)	32,39,47	2.28	9 (28%)
32	5MC	1a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.15	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	1.98	9 (27%)
1	5MC	1A	1962	1,56	19,22,23	1.58	3 (15%)	26,32,35	1.14	2 (7%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
1	2MA	2A	2503	1,56	22,25,26	1.45	5 (22%)	32,37,40	2.26	9 (28%)
54	PSU	1y	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.83	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	21,30,33	1.97	4 (19%)
55	4SU	1x	8	55	18,21,22	2.19	5 (27%)	25,30,33	1.58	5 (20%)
54	G7M	2y	46	54	23,26,27	1.61	3 (13%)	34,39,42	1.93	4 (11%)
1	5MU	1A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.06	8 (29%)
1	5MC	1A	1942	1,56	19,22,23	1.50	3 (15%)	26,32,35	1.18	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	2a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.71	3 (11%)
54	G7M	2w	46	54	23,26,27	1.48	3 (13%)	34,39,42	1.63	5 (14%)
54	MIA	2y	37	54	21,24,32	1.58	3 (14%)	30,35,47	2.03	10 (33%)
54	MIA	1y	37	54	21,24,32	1.64	4 (19%)	30,35,47	2.00	7 (23%)
32	5MC	2a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
54	4SU	2w	8	54	18,21,22	1.75	4 (22%)	25,30,33	2.29	5 (20%)
32	5MC	1a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.13	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.13	2 (7%)
55	5MC	2x	32	55	19,22,23	1.70	3 (15%)	26,32,35	1.19	3 (11%)
43	0TD	2l	92	43	8,9,10	4.63	2 (25%)	6,11,13	2.40	3 (50%)
55	5MU	2x	54	55	19,22,23	1.36	5 (26%)	27,32,35	2.02	7 (25%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.87	3 (11%)
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	27,32,35	1.71	6 (22%)
54	PSU	2y	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.90	5 (23%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.14	7 (21%)
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.74	3 (14%)
32	4OC	1a	1402	32	20,23,24	0.78	0	25,32,35	1.00	1 (4%)
54	PSU	1y	32	54	18,21,22	1.39	2 (11%)	21,30,33	1.82	3 (14%)
1	5MU	1A	1939	1,56	19,22,23	1.49	6 (31%)	27,32,35	2.24	6 (22%)
32	PSU	1a	516	32,56	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.91	3 (14%)
1	PSU	1A	1911	1	18,21,22	1.33	2 (11%)	21,30,33	2.13	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.92	1 (4%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.19	9 (27%)
54	PSU	1w	32	56,54	18,21,22	1.34	2 (11%)	21,30,33	1.97	3 (14%)
32	5MC	2a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.32	3 (11%)
54	5MU	2y	54	54	19,22,23	1.51	4 (21%)	27,32,35	2.00	8 (29%)
32	PSU	2a	516	32	18,21,22	1.36	2 (11%)	21,30,33	2.01	5 (23%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.84	6 (18%)
1	2MU	1A	2552	1,56	19,22,24	1.32	3 (15%)	25,31,36	1.85	5 (20%)
54	PSU	1w	39	54	18,21,22	1.34	2 (11%)	21,30,33	1.94	4 (19%)
54	PSU	2w	32	54	18,21,22	1.36	3 (16%)	21,30,33	1.88	3 (14%)
32	5MC	2a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.23	3 (11%)
54	PSU	2w	55	54	18,21,22	1.42	2 (11%)	21,30,33	2.00	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	21,30,33	1.90	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MU	2A	2552	1,56	19,22,24	1.30	2 (10%)	25,31,36	1.80	5 (20%)
55	PSU	1x	55	55,56	18,21,22	1.36	2 (11%)	21,30,33	1.95	4 (19%)
54	4SU	1y	8	56,54	18,21,22	1.72	4 (22%)	25,30,33	2.17	4 (16%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	27,32,35	2.01	7 (25%)
1	5MC	2A	1942	1	19,22,23	1.67	2 (10%)	26,32,35	1.05	2 (7%)
54	MIA	1w	37	54	28,31,32	2.40	7 (25%)	38,44,47	2.61	12 (31%)
43	0TD	1l	92	43	8,9,10	4.51	1 (12%)	6,11,13	7.45	2 (33%)
54	4SU	1w	8	54	18,21,22	1.81	4 (22%)	25,30,33	1.92	6 (24%)
32	4OC	2a	1402	32,56	20,23,24	0.79	0	25,32,35	0.90	1 (4%)
55	5MC	1x	32	55	19,22,23	1.74	3 (15%)	26,32,35	1.19	2 (7%)
54	G7M	1w	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.59	4 (11%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
1	5MU	2A	1939	1,56	19,22,23	1.36	5 (26%)	27,32,35	2.25	6 (22%)
54	PSU	2y	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.90	3 (14%)
54	5MU	1y	54	54	19,22,23	1.50	6 (31%)	27,32,35	2.25	8 (29%)
1	5MU	2A	1915	1	19,22,23	1.47	6 (31%)	27,32,35	2.16	5 (18%)
1	PSU	2A	2605	1	18,21,22	1.31	3 (16%)	21,30,33	2.06	4 (19%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.10	2 (7%)
32	G7M	2a	527	32,56	23,26,27	1.48	4 (17%)	34,39,42	1.78	5 (14%)
32	M2G	2a	966	32	24,27,28	1.26	3 (12%)	33,40,43	1.89	6 (18%)
54	4SU	2y	8	54	18,21,22	1.86	5 (27%)	25,30,33	2.18	5 (20%)
1	PSU	1A	2605	1,56	18,21,22	1.43	4 (22%)	21,30,33	2.04	4 (19%)
54	G7M	1y	46	54	23,26,27	1.51	4 (17%)	34,39,42	1.68	4 (11%)
55	4SU	2x	8	55	18,21,22	2.06	6 (33%)	25,30,33	1.37	3 (12%)
32	MA6	2a	1519	32	23,26,27	0.40	0	33,38,41	2.11	9 (27%)
55	5MU	1x	54	55,56	19,22,23	1.43	5 (26%)	27,32,35	1.92	6 (22%)
1	OMC	2A	1920	1	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.01	10 (30%)

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
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,56	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	1,56	-	1/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	1/7/25/26	0/3/3/3
54	MIA	2w	37	54	-	4/11/29/34	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1962	1,56	-	2/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/7/25/26	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	32	54	-	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	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	4/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	2MU	1A	2552	1,56	-	0/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	3/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	56,54	-	3/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	1/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,56	-	2/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3

The worst 5 of 246 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.58	1.69	1.82
43	1l	92	0TD	CB-SB	-12.34	1.69	1.82
54	1w	37	MIA	C2-S10	-7.20	1.69	1.75
54	1w	37	MIA	C13-C14	7.11	1.53	1.32
54	2w	37	MIA	C2-S10	-6.73	1.70	1.75

The worst 5 of 393 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.77	70.41	102.36
54	1w	37	MIA	C12-C13-C14	-8.35	112.02	127.01
54	2w	37	MIA	C5-C4-N3	-7.83	118.93	127.18
32	1a	1498	UR3	C4-N3-C2	-7.53	118.52	124.58
1	2A	2503	2MA	C5-C4-N3	-7.40	119.39	127.18

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

42 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1519	MA6	2	0
1	1A	2251	OMG	1	0
1	1A	2503	2MA	2	0
32	2a	1518	MA6	4	0
55	2x	55	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2503	2MA	2	0
54	1y	39	PSU	1	0
1	2A	1917	PSU	1	0
55	1x	8	4SU	3	0
1	1A	1915	5MU	1	0
32	2a	1498	UR3	1	0
54	2w	46	G7M	1	0
54	2y	37	MIA	1	0
54	1y	37	MIA	1	0
32	2a	1404	5MC	2	0
54	2w	8	4SU	1	0
32	1a	967	5MC	1	0
43	2l	92	0TD	1	0
54	2w	54	5MU	2	0
54	2y	55	PSU	7	0
32	2a	1207	2MG	1	0
32	1a	1402	4OC	1	0
1	1A	1939	5MU	1	0
54	2y	32	PSU	1	0
1	1A	1911	PSU	1	0
32	1a	966	M2G	1	0
54	1w	39	PSU	1	0
1	2A	2552	2MU	2	0
55	1x	55	PSU	1	0
54	1y	8	4SU	1	0
54	1w	37	MIA	1	0
43	1l	92	0TD	2	0
54	1w	8	4SU	1	0
32	2a	1402	4OC	3	0
54	1w	46	G7M	1	0
1	2A	1939	5MU	1	0
54	2y	39	PSU	1	0
32	2a	967	5MC	1	0
32	2a	966	M2G	1	0
54	2y	8	4SU	1	0
32	2a	1519	MA6	2	0
32	1a	1518	MA6	3	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2807 ligands modelled in this entry, 2803 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
57	TYK	2A	3879	1	67,67,67	1.83	5 (7%)	87,97,97	1.38	13 (14%)
59	SF4	2d	303	35	0,12,12	-	-	-	-	-
57	TYK	1A	4107	1	67,67,67	1.75	8 (11%)	87,97,97	1.26	13 (14%)
59	SF4	1d	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
57	TYK	2A	3879	1	-	4/67/126/126	0/3/4/4
59	SF4	2d	303	35	-	-	0/6/5/5
57	TYK	1A	4107	1	-	2/67/126/126	0/3/4/4
59	SF4	1d	302	35	-	-	0/6/5/5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3879	TYK	C8-C9	-8.87	1.37	1.51
57	1A	4107	TYK	C8-C9	-7.71	1.39	1.51
57	2A	3879	TYK	C14-C13	-7.35	1.37	1.50
57	1A	4107	TYK	C14-C13	-7.15	1.38	1.50
57	2A	3879	TYK	C2-C1	-4.99	1.41	1.50

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3879	TYK	C10-C11-C12	-4.01	120.30	126.23
57	2A	3879	TYK	C23-O1C-C1C	-3.67	105.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3879	TYK	C3B-C2B-C1B	-3.47	108.32	114.77
57	2A	3879	TYK	C18-C4-C3	-3.29	105.84	111.09
57	2A	3879	TYK	C6B-C5B-C4B	-2.74	108.04	112.58

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

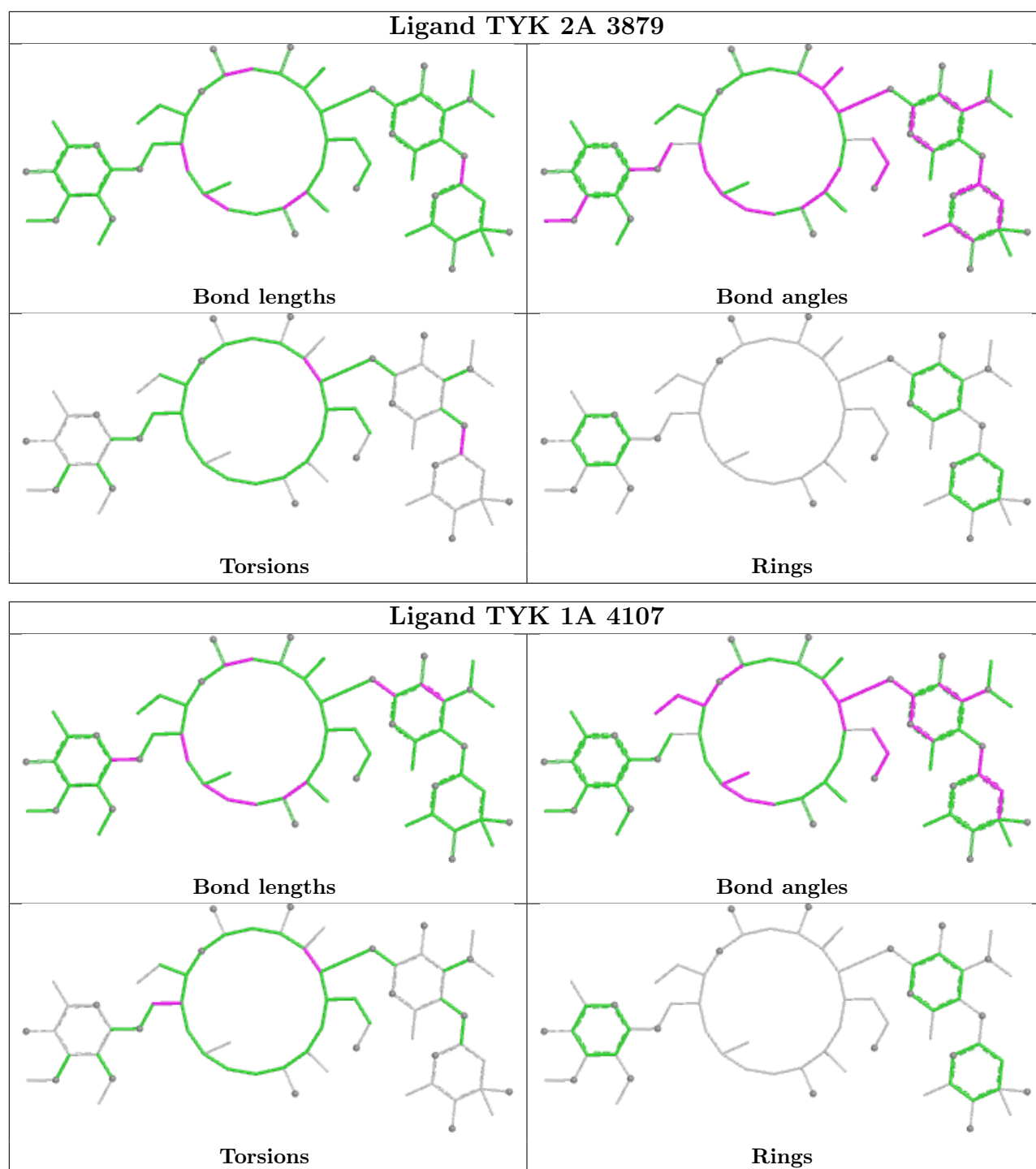
Mol	Chain	Res	Type	Atoms
57	1A	4107	TYK	C15-C14-C23-O1C
57	2A	3879	TYK	C2B-C1B-O4A-C4A
57	2A	3879	TYK	C18-C4-C5-C6
57	1A	4107	TYK	C18-C4-C5-C6
57	2A	3879	TYK	C3-C4-C5-C6

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2A	3879	TYK	4	0
57	1A	4107	TYK	6	0
59	1d	302	SF4	5	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	1A	2860/2915 (98%)	-0.40	125 (4%)	39	35	14, 32, 85, 95	0
1	2A	2789/2915 (95%)	0.18	125 (4%)	38	34	30, 51, 84, 99	0
2	1B	120/121 (99%)	-0.29	0	100	100	27, 46, 59, 76	0
2	2B	120/121 (99%)	1.00	8 (6%)	24	21	55, 71, 78, 84	0
3	1D	275/276 (99%)	-0.15	3 (1%)	78	76	17, 32, 45, 65	0
3	2D	275/276 (99%)	0.34	5 (1%)	67	65	29, 45, 56, 75	0
4	1E	204/206 (99%)	-0.12	1 (0%)	87	86	14, 34, 54, 69	0
4	2E	204/206 (99%)	0.42	1 (0%)	87	86	31, 51, 64, 72	0
5	1F	202/210 (96%)	-0.04	1 (0%)	87	86	15, 37, 59, 77	0
5	2F	202/210 (96%)	0.45	2 (0%)	79	78	29, 59, 70, 77	0
6	1G	181/182 (99%)	0.46	9 (4%)	34	30	39, 53, 66, 78	0
6	2G	181/182 (99%)	1.37	35 (19%)	3	3	61, 70, 75, 86	0
7	1H	174/180 (96%)	0.17	3 (1%)	69	67	35, 46, 58, 68	0
7	2H	174/180 (96%)	1.40	28 (16%)	4	4	58, 73, 81, 88	0
8	1I	146/148 (98%)	0.66	7 (4%)	35	32	38, 64, 74, 78	0
8	2I	146/148 (98%)	0.96	5 (3%)	48	44	46, 62, 71, 77	0
9	1N	140/140 (100%)	-0.04	1 (0%)	84	83	20, 34, 53, 65	0
9	2N	140/140 (100%)	0.61	5 (3%)	46	42	40, 57, 68, 76	0
10	1O	122/122 (100%)	-0.03	0	100	100	24, 36, 50, 53	0
10	2O	122/122 (100%)	0.46	0	100	100	42, 52, 64, 68	0
11	1P	149/150 (99%)	0.11	3 (2%)	65	62	17, 40, 62, 70	0
11	2P	149/150 (99%)	0.65	1 (0%)	84	83	37, 58, 74, 81	0
12	1Q	141/141 (100%)	-0.07	1 (0%)	84	83	24, 38, 52, 68	0
12	2Q	141/141 (100%)	1.03	17 (12%)	8	7	46, 61, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.21	0 100 100	18, 32, 43, 53	0
13	2R	118/118 (100%)	0.22	0 100 100	37, 47, 55, 62	0
14	1S	110/112 (98%)	0.05	0 100 100	34, 46, 55, 63	0
14	2S	110/112 (98%)	1.13	14 (12%) 8 7	55, 65, 74, 79	0
15	1T	131/146 (89%)	0.08	2 (1%) 72 70	25, 39, 60, 65	0
15	2T	131/146 (89%)	0.61	2 (1%) 72 70	45, 54, 67, 74	0
16	1U	116/118 (98%)	-0.31	1 (0%) 81 80	18, 25, 40, 59	0
16	2U	116/118 (98%)	0.57	1 (0%) 81 80	39, 56, 67, 74	0
17	1V	101/101 (100%)	-0.21	0 100 100	18, 34, 51, 65	0
17	2V	101/101 (100%)	0.80	3 (2%) 52 49	39, 62, 69, 83	0
18	1W	112/113 (99%)	-0.27	1 (0%) 81 80	19, 27, 43, 69	0
18	2W	112/113 (99%)	0.23	1 (0%) 81 80	35, 43, 58, 82	0
19	1X	95/96 (98%)	0.06	1 (1%) 78 76	22, 34, 55, 64	0
19	2X	95/96 (98%)	0.71	3 (3%) 50 46	42, 54, 66, 78	0
20	1Y	107/110 (97%)	0.33	0 100 100	31, 44, 58, 70	0
20	2Y	107/110 (97%)	0.89	8 (7%) 20 17	51, 62, 73, 77	0
21	1Z	154/206 (74%)	0.74	9 (5%) 29 25	32, 58, 76, 82	0
21	2Z	160/206 (77%)	1.39	30 (18%) 3 3	63, 72, 79, 86	0
22	10	83/85 (97%)	0.25	7 (8%) 17 14	26, 33, 59, 73	0
22	20	83/85 (97%)	1.28	14 (16%) 4 3	38, 59, 74, 83	0
23	11	97/98 (98%)	0.08	1 (1%) 79 78	23, 38, 62, 68	0
23	21	97/98 (98%)	0.63	5 (5%) 33 29	34, 47, 65, 67	0
24	12	70/72 (97%)	0.11	1 (1%) 73 72	30, 42, 55, 59	0
24	22	70/72 (97%)	0.61	1 (1%) 73 72	50, 60, 67, 73	0
25	13	59/60 (98%)	-0.23	0 100 100	19, 32, 55, 63	0
25	23	59/60 (98%)	0.67	1 (1%) 69 67	48, 59, 69, 74	0
26	14	69/71 (97%)	1.23	14 (20%) 3 2	48, 67, 77, 81	0
26	24	69/71 (97%)	1.58	14 (20%) 3 2	64, 77, 84, 87	0
27	15	59/60 (98%)	-0.14	1 (1%) 69 67	17, 29, 52, 59	0
27	25	59/60 (98%)	0.38	0 100 100	33, 46, 64, 76	0
28	16	53/54 (98%)	-0.26	0 100 100	29, 37, 50, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.64	2 (3%) 44 40	46, 55, 61, 62	0
29	17	48/49 (97%)	-0.27	1 (2%) 63 61	17, 24, 52, 60	0
29	27	48/49 (97%)	0.11	4 (8%) 17 14	29, 36, 58, 68	0
30	18	64/65 (98%)	-0.31	0 100 100	23, 29, 36, 48	0
30	28	64/65 (98%)	0.56	1 (1%) 70 68	42, 50, 55, 59	0
31	19	37/37 (100%)	-0.16	0 100 100	22, 32, 52, 59	0
31	29	37/37 (100%)	0.90	2 (5%) 31 27	54, 61, 68, 72	0
32	1a	1488/1521 (97%)	0.50	58 (3%) 43 39	31, 60, 83, 97	0
32	2a	1491/1521 (98%)	0.84	135 (9%) 15 12	43, 68, 86, 96	0
33	1b	231/256 (90%)	1.31	37 (16%) 5 4	50, 69, 78, 85	0
33	2b	231/256 (90%)	1.52	63 (27%) 1 1	59, 75, 81, 84	0
34	1c	206/239 (86%)	1.05	25 (12%) 8 7	48, 66, 75, 82	0
34	2c	206/239 (86%)	1.65	68 (33%) 1 1	65, 74, 80, 84	0
35	1d	208/209 (99%)	1.13	29 (13%) 6 5	45, 63, 72, 80	0
35	2d	208/209 (99%)	0.84	7 (3%) 48 44	50, 61, 70, 75	0
36	1e	148/162 (91%)	0.60	2 (1%) 73 72	42, 57, 66, 71	0
36	2e	148/162 (91%)	1.10	15 (10%) 12 10	57, 68, 74, 80	0
37	1f	100/101 (99%)	0.63	0 100 100	51, 60, 67, 73	0
37	2f	100/101 (99%)	0.88	4 (4%) 42 38	51, 62, 69, 75	0
38	1g	155/156 (99%)	0.77	10 (6%) 25 22	52, 62, 73, 82	0
38	2g	155/156 (99%)	1.14	14 (9%) 15 13	61, 70, 78, 85	0
39	1h	137/138 (99%)	0.68	6 (4%) 39 35	47, 58, 64, 71	0
39	2h	137/138 (99%)	0.96	8 (5%) 29 25	60, 67, 74, 78	0
40	1i	127/128 (99%)	1.26	17 (13%) 7 6	50, 67, 75, 78	0
40	2i	127/128 (99%)	1.92	56 (44%) 0 0	63, 74, 79, 82	0
41	1j	97/105 (92%)	1.28	10 (10%) 12 10	53, 70, 79, 86	0
41	2j	96/105 (91%)	1.88	35 (36%) 1 0	67, 76, 83, 85	0
42	1k	114/129 (88%)	0.53	3 (2%) 57 54	38, 57, 67, 71	0
42	2k	114/129 (88%)	1.11	12 (10%) 11 9	50, 65, 71, 74	0
43	1l	121/132 (91%)	0.34	2 (1%) 69 67	36, 49, 58, 65	0
43	2l	121/132 (91%)	0.96	7 (5%) 29 25	49, 63, 70, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.92	9 (7%) 21 18	47, 62, 69, 73	0
44	2m	122/126 (96%)	1.71	40 (32%) 1 1	64, 73, 77, 81	0
45	1n	60/61 (98%)	0.99	3 (5%) 34 30	53, 61, 67, 71	0
45	2n	60/61 (98%)	2.37	36 (60%) 0 0	70, 76, 82, 85	0
46	1o	88/89 (98%)	0.79	6 (6%) 23 20	42, 57, 70, 77	0
46	2o	88/89 (98%)	0.91	6 (6%) 23 20	53, 64, 73, 76	0
47	1p	82/88 (93%)	1.50	22 (26%) 1 1	47, 62, 70, 77	0
47	2p	82/88 (93%)	0.88	6 (7%) 21 18	50, 59, 67, 72	0
48	1q	99/105 (94%)	0.80	5 (5%) 33 29	45, 58, 69, 72	0
48	2q	99/105 (94%)	0.98	5 (5%) 33 29	51, 64, 71, 75	0
49	1r	68/88 (77%)	0.61	1 (1%) 72 70	46, 58, 67, 69	0
49	2r	68/88 (77%)	0.97	5 (7%) 20 18	51, 63, 71, 75	0
50	1s	83/93 (89%)	0.94	7 (8%) 17 14	49, 64, 73, 79	0
50	2s	83/93 (89%)	1.75	29 (34%) 1 1	70, 77, 81, 86	0
51	1t	96/106 (90%)	1.09	12 (12%) 8 7	51, 63, 69, 72	0
51	2t	96/106 (90%)	0.93	5 (5%) 33 29	51, 62, 72, 80	0
52	1u	23/27 (85%)	1.05	1 (4%) 40 36	57, 59, 64, 67	0
52	2u	23/27 (85%)	1.81	10 (43%) 0 0	64, 71, 75, 78	0
53	1v	13/24 (54%)	0.72	1 (7%) 19 17	42, 55, 75, 87	0
53	2v	13/24 (54%)	1.68	4 (30%) 1 1	63, 74, 87, 91	0
54	1w	67/76 (88%)	1.27	11 (16%) 4 4	55, 79, 89, 95	0
54	1y	67/76 (88%)	1.09	6 (8%) 15 13	33, 83, 90, 93	0
54	2w	65/76 (85%)	1.62	19 (29%) 1 1	74, 85, 92, 97	0
54	2y	66/76 (86%)	1.35	11 (16%) 4 3	49, 87, 92, 95	0
55	1x	72/77 (93%)	0.29	0 100 100	26, 55, 74, 83	0
55	2x	72/77 (93%)	0.86	2 (2%) 55 51	44, 71, 80, 89	0
All	All	20873/21748 (95%)	0.48	1416 (6%) 23 20	14, 57, 80, 99	0

The worst 5 of 1416 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	2Z	172	ALA	6.3
36	2e	22	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
22	20	7	LEU	5.9
38	2g	84	ASN	5.8
32	2a	1033	G	5.8

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
54	G7M	2w	46	24/25	0.63	0.15	80,90,96,109	0
54	G7M	1w	46	24/25	0.64	0.17	69,79,94,113	0
54	G7M	1y	46	24/25	0.66	0.16	77,87,100,106	0
54	PSU	2y	55	20/21	0.67	0.18	83,90,100,105	0
54	4SU	2w	8	20/21	0.69	0.15	83,90,102,110	0
54	5MU	2y	54	21/22	0.70	0.19	82,87,95,111	0
54	G7M	2y	46	24/25	0.71	0.15	77,86,90,100	0
54	PSU	2w	55	20/21	0.72	0.15	74,85,94,95	0
54	5MU	1y	54	21/22	0.72	0.14	75,79,90,97	0
54	PSU	1y	55	20/21	0.76	0.15	79,86,93,101	0
54	4SU	1y	8	20/21	0.77	0.12	79,86,92,95	0
54	MIA	2y	37	22/30	0.78	0.14	69,78,85,91	0
54	4SU	2y	8	20/21	0.78	0.12	79,87,100,106	0
32	2MG	2a	1207	24/25	0.79	0.17	70,78,84,88	0
54	PSU	2y	32	20/21	0.81	0.13	61,76,85,89	0
54	PSU	1y	32	20/21	0.82	0.13	67,75,82,83	0
54	MIA	1y	37	22/30	0.84	0.14	70,76,80,89	0
54	PSU	2y	39	20/21	0.85	0.12	72,75,93,95	0
54	5MU	2w	54	21/22	0.85	0.13	68,77,83,89	0
54	PSU	1y	39	20/21	0.86	0.12	68,74,83,84	0
43	0TD	2l	92	10/11	0.87	0.15	56,61,65,71	0
55	4SU	2x	8	20/21	0.87	0.12	74,78,83,87	0
54	PSU	1w	55	20/21	0.87	0.12	62,73,80,80	0
55	PSU	2x	55	20/21	0.88	0.11	68,74,78,81	0
54	4SU	1w	8	20/21	0.88	0.10	71,76,84,85	0
1	5MU	2A	1915	21/22	0.89	0.13	62,69,73,75	0
32	M2G	2a	966	25/26	0.90	0.16	61,67,77,80	0
54	PSU	2w	32	20/21	0.90	0.14	68,80,86,87	0
55	5MC	2x	32	21/22	0.90	0.14	64,70,72,79	0
55	5MU	2x	54	21/22	0.90	0.12	67,75,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MIA	2w	37	25/30	0.91	0.14	60,73,79,85	0
55	PSU	1x	55	20/21	0.91	0.10	55,61,66,68	0
32	PSU	2a	516	20/21	0.91	0.11	62,73,80,82	0
32	G7M	2a	527	24/25	0.91	0.12	56,61,66,71	0
43	0TD	1l	92	10/11	0.91	0.12	46,50,51,59	0
32	4OC	2a	1402	22/23	0.92	0.12	48,59,62,71	0
1	PSU	2A	1911	20/21	0.92	0.09	56,59,63,64	0
55	4SU	1x	8	20/21	0.92	0.11	54,60,65,66	0
1	PSU	2A	1917	20/21	0.92	0.10	56,63,69,70	0
55	5MU	1x	54	21/22	0.92	0.11	59,62,66,72	0
54	PSU	2w	39	20/21	0.92	0.13	67,76,80,81	0
32	2MG	1a	1207	24/25	0.92	0.12	59,62,66,70	0
54	5MU	1w	54	21/22	0.92	0.09	60,67,71,74	0
54	PSU	1w	32	20/21	0.92	0.11	60,66,72,75	0
32	5MC	2a	1400	21/22	0.92	0.15	57,65,70,74	0
32	5MC	2a	1404	21/22	0.93	0.11	45,51,54,57	0
32	5MC	2a	967	21/22	0.93	0.12	61,66,74,79	0
32	UR3	2a	1498	21/22	0.94	0.12	41,55,58,63	0
1	5MU	1A	1915	21/22	0.94	0.10	36,48,59,64	0
1	OMC	2A	1920	21/22	0.94	0.10	49,58,62,67	0
32	5MC	2a	1407	21/22	0.94	0.10	42,52,56,57	0
32	MA6	2a	1519	24/25	0.95	0.12	44,59,64,67	0
32	G7M	1a	527	24/25	0.95	0.10	42,46,50,54	0
32	M2G	1a	966	25/26	0.95	0.10	43,48,58,60	0
55	5MC	1x	32	21/22	0.95	0.10	46,48,53,62	0
54	MIA	1w	37	29/30	0.95	0.12	48,56,62,68	0
1	5MC	2A	1942	21/22	0.95	0.10	48,53,57,58	0
1	2MU	2A	2552	21/23	0.95	0.10	31,40,44,50	0
1	PSU	1A	1911	20/21	0.95	0.10	33,44,52,54	0
32	PSU	1a	516	20/21	0.95	0.09	50,55,59,60	0
32	MA6	2a	1518	24/25	0.95	0.10	51,59,64,66	0
1	5MC	1A	1942	21/22	0.96	0.11	32,40,46,48	0
1	5MU	2A	1939	21/22	0.96	0.09	33,36,40,42	0
1	PSU	1A	1917	20/21	0.96	0.09	38,46,54,55	0
1	5MC	2A	1962	21/22	0.96	0.09	33,45,51,56	0
54	PSU	1w	39	20/21	0.96	0.08	37,57,64,66	0
32	5MC	1a	967	21/22	0.96	0.09	45,49,55,56	0
32	5MC	1a	1400	21/22	0.97	0.08	40,44,46,50	0
1	OMG	2A	2251	24/25	0.97	0.09	35,40,44,45	0
32	4OC	1a	1402	22/23	0.97	0.08	33,39,41,45	0
1	PSU	2A	2605	20/21	0.97	0.08	28,37,43,53	0
32	5MC	1a	1407	21/22	0.97	0.08	31,38,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	UR3	1a	1498	21/22	0.97	0.08	30,37,41,44	0
32	MA6	1a	1519	24/25	0.97	0.09	30,37,40,54	0
1	PSU	1A	2605	20/21	0.98	0.06	17,20,31,34	0
32	5MC	1a	1404	21/22	0.98	0.07	32,33,38,41	0
1	5MU	1A	1939	21/22	0.98	0.07	20,28,30,33	0
1	OMC	1A	1920	21/22	0.98	0.07	31,39,46,47	0
32	MA6	1a	1518	24/25	0.98	0.08	27,37,42,42	0
1	5MC	1A	1962	21/22	0.98	0.07	25,30,35,41	0
1	2MA	2A	2503	23/24	0.98	0.07	25,31,35,36	0
1	OMG	1A	2251	24/25	0.98	0.06	17,19,22,29	0
1	2MA	1A	2503	23/24	0.98	0.07	13,17,19,23	0
1	2MU	1A	2552	21/23	0.98	0.07	19,22,28,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4100	1/1	0.21	0.31	76,76,76,76	0
56	MG	2A	3090	1/1	0.58	0.24	60,60,60,60	0
56	MG	2A	3635	1/1	0.59	0.26	76,76,76,76	0
56	MG	1A	3875	1/1	0.65	0.15	68,68,68,68	0
56	MG	2a	3214	1/1	0.67	0.26	64,64,64,64	0
56	MG	2a	3227	1/1	0.67	0.16	66,66,66,66	0
56	MG	2A	3415	1/1	0.68	0.27	67,67,67,67	0
56	MG	2A	3821	1/1	0.68	0.13	58,58,58,58	0
56	MG	2a	3154	1/1	0.70	0.15	60,60,60,60	0
56	MG	1A	3166	1/1	0.71	0.19	59,59,59,59	0
56	MG	2A	3669	1/1	0.71	0.21	79,79,79,79	0
56	MG	2A	3685	1/1	0.71	0.18	58,58,58,58	0
56	MG	2A	3805	1/1	0.71	0.13	75,75,75,75	0
56	MG	2a	3187	1/1	0.72	0.16	61,61,61,61	0
56	MG	2a	3188	1/1	0.72	0.14	65,65,65,65	0
56	MG	1w	104	1/1	0.72	0.22	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3632	1/1	0.72	0.17	68,68,68,68	0
56	MG	2y	104	1/1	0.72	0.13	80,80,80,80	0
56	MG	1y	103	1/1	0.73	0.18	66,66,66,66	0
56	MG	2A	3867	1/1	0.73	0.19	33,33,33,33	0
56	MG	1A	3938	1/1	0.74	0.17	51,51,51,51	0
56	MG	2A	3529	1/1	0.74	0.19	62,62,62,62	0
56	MG	2A	3554	1/1	0.74	0.14	42,42,42,42	0
56	MG	2A	3100	1/1	0.74	0.20	64,64,64,64	0
56	MG	2A	3296	1/1	0.74	0.18	69,69,69,69	0
56	MG	2a	3130	1/1	0.74	0.28	60,60,60,60	0
56	MG	2a	3167	1/1	0.75	0.13	75,75,75,75	0
56	MG	1A	3979	1/1	0.75	0.14	64,64,64,64	0
56	MG	2j	201	1/1	0.75	0.11	69,69,69,69	0
56	MG	2A	3538	1/1	0.75	0.28	61,61,61,61	0
56	MG	2F	307	1/1	0.76	0.17	52,52,52,52	0
56	MG	2A	3766	1/1	0.76	0.10	48,48,48,48	0
56	MG	2A	3661	1/1	0.76	0.20	68,68,68,68	0
56	MG	1A	3520	1/1	0.76	0.14	56,56,56,56	0
56	MG	1x	110	1/1	0.76	0.20	66,66,66,66	0
56	MG	1A	4060	1/1	0.77	0.14	31,31,31,31	0
56	MG	2A	3178	1/1	0.77	0.21	48,48,48,48	0
56	MG	2a	3055	1/1	0.77	0.19	70,70,70,70	0
56	MG	1A	3880	1/1	0.77	0.15	45,45,45,45	0
56	MG	1A	3359	1/1	0.78	0.18	50,50,50,50	0
56	MG	2A	3566	1/1	0.78	0.16	42,42,42,42	0
56	MG	2a	3228	1/1	0.78	0.17	77,77,77,77	0
56	MG	2a	3074	1/1	0.78	0.30	67,67,67,67	0
56	MG	2A	3597	1/1	0.78	0.13	54,54,54,54	0
56	MG	1A	3203	1/1	0.79	0.14	59,59,59,59	0
56	MG	2A	3478	1/1	0.79	0.12	71,71,71,71	0
56	MG	2A	3526	1/1	0.79	0.14	40,40,40,40	0
56	MG	1A	3538	1/1	0.79	0.18	59,59,59,59	0
56	MG	1A	3892	1/1	0.79	0.16	37,37,37,37	0
56	MG	1A	3931	1/1	0.79	0.18	53,53,53,53	0
56	MG	1a	1635	1/1	0.79	0.21	66,66,66,66	0
56	MG	1a	1717	1/1	0.79	0.18	57,57,57,57	0
56	MG	2A	3179	1/1	0.79	0.16	59,59,59,59	0
56	MG	1w	102	1/1	0.79	0.26	68,68,68,68	0
56	MG	1A	3504	1/1	0.80	0.17	47,47,47,47	0
56	MG	2A	3333	1/1	0.80	0.13	62,62,62,62	0
56	MG	2A	3345	1/1	0.80	0.16	64,64,64,64	0
56	MG	2A	3379	1/1	0.80	0.26	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3789	1/1	0.80	0.17	49,49,49,49	0
56	MG	2A	3440	1/1	0.80	0.22	56,56,56,56	0
56	MG	2a	3186	1/1	0.80	0.14	66,66,66,66	0
56	MG	1B	212	1/1	0.80	0.14	62,62,62,62	0
56	MG	1A	3946	1/1	0.80	0.17	38,38,38,38	0
56	MG	2A	3767	1/1	0.80	0.12	40,40,40,40	0
56	MG	1A	3833	1/1	0.80	0.14	58,58,58,58	0
56	MG	2A	3810	1/1	0.80	0.23	77,77,77,77	0
56	MG	1d	301	1/1	0.80	0.31	58,58,58,58	0
56	MG	2l	204	1/1	0.80	0.12	59,59,59,59	0
56	MG	1A	4023	1/1	0.80	0.16	39,39,39,39	0
56	MG	2A	3306	1/1	0.81	0.12	71,71,71,71	0
56	MG	2A	3311	1/1	0.81	0.16	53,53,53,53	0
56	MG	2A	3327	1/1	0.81	0.13	52,52,52,52	0
56	MG	1A	3695	1/1	0.81	0.11	43,43,43,43	0
56	MG	1a	1810	1/1	0.81	0.13	66,66,66,66	0
56	MG	2Q	203	1/1	0.81	0.15	49,49,49,49	0
56	MG	2A	3350	1/1	0.81	0.24	66,66,66,66	0
56	MG	2A	3353	1/1	0.81	0.18	66,66,66,66	0
56	MG	1A	3740	1/1	0.81	0.16	37,37,37,37	0
56	MG	1a	1628	1/1	0.81	0.14	59,59,59,59	0
56	MG	2a	3166	1/1	0.81	0.19	50,50,50,50	0
56	MG	1A	3835	1/1	0.81	0.23	58,58,58,58	0
56	MG	2A	3463	1/1	0.81	0.25	65,65,65,65	0
56	MG	2A	3689	1/1	0.81	0.14	63,63,63,63	0
56	MG	2A	3713	1/1	0.81	0.14	56,56,56,56	0
56	MG	2a	3213	1/1	0.81	0.19	56,56,56,56	0
56	MG	2A	3744	1/1	0.81	0.14	55,55,55,55	0
56	MG	2A	3760	1/1	0.81	0.13	58,58,58,58	0
56	MG	2A	3475	1/1	0.81	0.10	51,51,51,51	0
56	MG	1a	1680	1/1	0.81	0.23	59,59,59,59	0
56	MG	2A	3787	1/1	0.81	0.14	64,64,64,64	0
56	MG	2A	3798	1/1	0.81	0.18	54,54,54,54	0
56	MG	1A	3823	1/1	0.82	0.21	81,81,81,81	0
56	MG	2A	3545	1/1	0.82	0.14	68,68,68,68	0
56	MG	2A	3313	1/1	0.82	0.13	59,59,59,59	0
56	MG	1a	1693	1/1	0.82	0.14	60,60,60,60	0
56	MG	1A	3543	1/1	0.82	0.09	44,44,44,44	0
56	MG	2A	3620	1/1	0.82	0.14	39,39,39,39	0
56	MG	1x	113	1/1	0.82	0.23	51,51,51,51	0
56	MG	2a	3018	1/1	0.82	0.26	66,66,66,66	0
56	MG	2a	3025	1/1	0.82	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1777	1/1	0.82	0.18	64,64,64,64	0
56	MG	1y	104	1/1	0.82	0.24	72,72,72,72	0
56	MG	1a	1781	1/1	0.82	0.14	76,76,76,76	0
56	MG	2A	3684	1/1	0.82	0.17	63,63,63,63	0
56	MG	2A	3414	1/1	0.82	0.23	57,57,57,57	0
56	MG	1a	1788	1/1	0.82	0.35	67,67,67,67	0
56	MG	2a	3185	1/1	0.82	0.16	65,65,65,65	0
56	MG	1a	1803	1/1	0.82	0.17	56,56,56,56	0
56	MG	2A	3737	1/1	0.82	0.12	55,55,55,55	0
56	MG	1a	1805	1/1	0.82	0.16	57,57,57,57	0
56	MG	2A	3753	1/1	0.82	0.13	55,55,55,55	0
56	MG	2A	3261	1/1	0.82	0.23	55,55,55,55	0
56	MG	1A	3764	1/1	0.82	0.18	54,54,54,54	0
56	MG	2A	3304	1/1	0.82	0.24	52,52,52,52	0
56	MG	2A	3773	1/1	0.82	0.22	60,60,60,60	0
56	MG	1A	3473	1/1	0.82	0.19	54,54,54,54	0
56	MG	2v	102	1/1	0.82	0.26	64,64,64,64	0
56	MG	2A	3790	1/1	0.82	0.17	58,58,58,58	0
56	MG	2A	3089	1/1	0.83	0.22	60,60,60,60	0
56	MG	2A	3633	1/1	0.83	0.15	46,46,46,46	0
56	MG	2B	216	1/1	0.83	0.19	58,58,58,58	0
56	MG	1A	3399	1/1	0.83	0.11	62,62,62,62	0
56	MG	2G	201	1/1	0.83	0.28	69,69,69,69	0
56	MG	1A	3799	1/1	0.83	0.12	27,27,27,27	0
56	MG	2A	3663	1/1	0.83	0.11	50,50,50,50	0
56	MG	2A	3403	1/1	0.83	0.22	59,59,59,59	0
56	MG	2A	3125	1/1	0.83	0.13	52,52,52,52	0
56	MG	2a	3069	1/1	0.83	0.22	60,60,60,60	0
56	MG	1a	1641	1/1	0.83	0.20	64,64,64,64	0
56	MG	2a	3096	1/1	0.83	0.15	61,61,61,61	0
56	MG	2a	3115	1/1	0.83	0.15	67,67,67,67	0
56	MG	2a	3119	1/1	0.83	0.26	59,59,59,59	0
56	MG	1a	1656	1/1	0.83	0.30	61,61,61,61	0
56	MG	2A	3457	1/1	0.83	0.16	45,45,45,45	0
56	MG	2A	3720	1/1	0.83	0.14	38,38,38,38	0
56	MG	2A	3201	1/1	0.83	0.20	59,59,59,59	0
56	MG	2A	3742	1/1	0.83	0.14	56,56,56,56	0
56	MG	1A	3550	1/1	0.83	0.12	64,64,64,64	0
56	MG	1A	3920	1/1	0.83	0.13	26,26,26,26	0
56	MG	1a	1713	1/1	0.83	0.17	74,74,74,74	0
56	MG	1A	3756	1/1	0.83	0.16	45,45,45,45	0
56	MG	1a	1763	1/1	0.83	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3217	1/1	0.83	0.18	72,72,72,72	0
56	MG	2a	3221	1/1	0.83	0.26	74,74,74,74	0
56	MG	1A	3673	1/1	0.83	0.16	55,55,55,55	0
56	MG	1X	106	1/1	0.83	0.10	51,51,51,51	0
56	MG	2A	3332	1/1	0.83	0.11	52,52,52,52	0
56	MG	2A	3042	1/1	0.83	0.27	59,59,59,59	0
56	MG	2A	3065	1/1	0.83	0.20	49,49,49,49	0
56	MG	2A	3622	1/1	0.83	0.11	39,39,39,39	0
56	MG	1U	211	1/1	0.84	0.37	52,52,52,52	0
56	MG	2A	3213	1/1	0.84	0.17	61,61,61,61	0
56	MG	2A	3607	1/1	0.84	0.20	53,53,53,53	0
56	MG	2A	3412	1/1	0.84	0.11	57,57,57,57	0
56	MG	1A	3524	1/1	0.84	0.21	55,55,55,55	0
56	MG	2A	3768	1/1	0.84	0.15	60,60,60,60	0
56	MG	1A	3812	1/1	0.84	0.16	36,36,36,36	0
56	MG	1A	4010	1/1	0.84	0.09	11,11,11,11	0
56	MG	1A	3349	1/1	0.84	0.26	55,55,55,55	0
56	MG	2A	3055	1/1	0.84	0.21	60,60,60,60	0
56	MG	2a	3178	1/1	0.84	0.16	69,69,69,69	0
56	MG	2A	3801	1/1	0.84	0.24	66,66,66,66	0
56	MG	1A	4052	1/1	0.84	0.11	38,38,38,38	0
56	MG	1A	3766	1/1	0.84	0.11	57,57,57,57	0
56	MG	1A	3642	1/1	0.84	0.12	33,33,33,33	0
56	MG	2a	3211	1/1	0.84	0.24	68,68,68,68	0
56	MG	2A	3865	1/1	0.84	0.10	46,46,46,46	0
56	MG	1n	102	1/1	0.84	0.16	62,62,62,62	0
56	MG	1A	3842	1/1	0.84	0.15	37,37,37,37	0
56	MG	2A	3708	1/1	0.84	0.19	58,58,58,58	0
56	MG	2a	3222	1/1	0.84	0.14	68,68,68,68	0
56	MG	2a	3226	1/1	0.84	0.20	62,62,62,62	0
56	MG	1B	221	1/1	0.84	0.10	43,43,43,43	0
56	MG	2A	3553	1/1	0.84	0.17	60,60,60,60	0
56	MG	2a	3004	1/1	0.84	0.24	57,57,57,57	0
56	MG	1x	102	1/1	0.84	0.29	57,57,57,57	0
56	MG	2A	3560	1/1	0.84	0.14	51,51,51,51	0
56	MG	2w	104	1/1	0.84	0.40	73,73,73,73	0
56	MG	2y	102	1/1	0.84	0.12	73,73,73,73	0
56	MG	2a	3039	1/1	0.84	0.25	65,65,65,65	0
56	MG	2y	106	1/1	0.84	0.14	81,81,81,81	0
56	MG	2A	3400	1/1	0.85	0.14	68,68,68,68	0
56	MG	2a	3002	1/1	0.85	0.11	63,63,63,63	0
56	MG	1A	3061	1/1	0.85	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3665	1/1	0.85	0.13	56,56,56,56	0
56	MG	1A	3899	1/1	0.85	0.16	43,43,43,43	0
56	MG	2a	3027	1/1	0.85	0.12	61,61,61,61	0
56	MG	2A	3675	1/1	0.85	0.23	61,61,61,61	0
56	MG	1A	3908	1/1	0.85	0.29	41,41,41,41	0
56	MG	1A	3526	1/1	0.85	0.14	47,47,47,47	0
56	MG	2A	3239	1/1	0.85	0.15	54,54,54,54	0
56	MG	2A	3707	1/1	0.85	0.11	67,67,67,67	0
56	MG	1A	3831	1/1	0.85	0.12	41,41,41,41	0
56	MG	2A	3268	1/1	0.85	0.21	77,77,77,77	0
56	MG	2a	3121	1/1	0.85	0.18	66,66,66,66	0
56	MG	2a	3125	1/1	0.85	0.14	50,50,50,50	0
56	MG	2A	3278	1/1	0.85	0.09	55,55,55,55	0
56	MG	2a	3135	1/1	0.85	0.37	67,67,67,67	0
56	MG	2a	3148	1/1	0.85	0.10	56,56,56,56	0
56	MG	1a	1776	1/1	0.85	0.15	57,57,57,57	0
56	MG	2a	3157	1/1	0.85	0.12	57,57,57,57	0
56	MG	2A	3490	1/1	0.85	0.10	49,49,49,49	0
56	MG	1A	3558	1/1	0.85	0.20	41,41,41,41	0
56	MG	2A	3305	1/1	0.85	0.15	53,53,53,53	0
56	MG	1a	1779	1/1	0.85	0.15	65,65,65,65	0
56	MG	1A	3605	1/1	0.85	0.10	42,42,42,42	0
56	MG	1Y	202	1/1	0.85	0.15	58,58,58,58	0
56	MG	1A	3947	1/1	0.85	0.10	34,34,34,34	0
56	MG	2A	3329	1/1	0.85	0.20	56,56,56,56	0
56	MG	1A	3636	1/1	0.85	0.12	23,23,23,23	0
56	MG	2A	3573	1/1	0.85	0.11	31,31,31,31	0
56	MG	2A	3577	1/1	0.85	0.14	67,67,67,67	0
56	MG	1A	3530	1/1	0.85	0.20	52,52,52,52	0
56	MG	1A	3373	1/1	0.85	0.17	54,54,54,54	0
56	MG	1e	201	1/1	0.85	0.08	59,59,59,59	0
56	MG	2A	3621	1/1	0.85	0.13	41,41,41,41	0
56	MG	2A	3136	1/1	0.85	0.14	49,49,49,49	0
56	MG	2a	3233	1/1	0.85	0.21	61,61,61,61	0
56	MG	2A	3367	1/1	0.85	0.12	59,59,59,59	0
56	MG	2A	3878	1/1	0.85	0.11	63,63,63,63	0
56	MG	2B	210	1/1	0.85	0.14	57,57,57,57	0
56	MG	2B	214	1/1	0.85	0.14	73,73,73,73	0
56	MG	2A	3153	1/1	0.85	0.15	60,60,60,60	0
56	MG	2A	3399	1/1	0.85	0.23	54,54,54,54	0
56	MG	2A	3647	1/1	0.85	0.19	49,49,49,49	0
56	MG	2A	3696	1/1	0.86	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3703	1/1	0.86	0.15	52,52,52,52	0
56	MG	1A	3546	1/1	0.86	0.10	37,37,37,37	0
56	MG	1A	3026	1/1	0.86	0.15	45,45,45,45	0
56	MG	16	105	1/1	0.86	0.09	51,51,51,51	0
56	MG	2a	3085	1/1	0.86	0.14	49,49,49,49	0
56	MG	2a	3087	1/1	0.86	0.20	55,55,55,55	0
56	MG	1A	4047	1/1	0.86	0.10	52,52,52,52	0
56	MG	2A	3491	1/1	0.86	0.16	43,43,43,43	0
56	MG	2A	3023	1/1	0.86	0.20	60,60,60,60	0
56	MG	1A	3936	1/1	0.86	0.16	47,47,47,47	0
56	MG	2A	3747	1/1	0.86	0.14	59,59,59,59	0
56	MG	1a	1795	1/1	0.86	0.14	58,58,58,58	0
56	MG	1A	3251	1/1	0.86	0.14	50,50,50,50	0
56	MG	2A	3069	1/1	0.86	0.29	55,55,55,55	0
56	MG	1A	3413	1/1	0.86	0.15	64,64,64,64	0
56	MG	1a	1661	1/1	0.86	0.15	59,59,59,59	0
56	MG	2a	3163	1/1	0.86	0.15	66,66,66,66	0
56	MG	2A	3099	1/1	0.86	0.19	58,58,58,58	0
56	MG	1B	208	1/1	0.86	0.13	56,56,56,56	0
56	MG	2a	3174	1/1	0.86	0.17	58,58,58,58	0
56	MG	2A	3108	1/1	0.86	0.12	68,68,68,68	0
56	MG	2A	3791	1/1	0.86	0.14	66,66,66,66	0
56	MG	2A	3348	1/1	0.86	0.21	61,61,61,61	0
56	MG	1A	3467	1/1	0.86	0.11	63,63,63,63	0
56	MG	1h	201	1/1	0.86	0.08	62,62,62,62	0
56	MG	2a	3197	1/1	0.86	0.19	67,67,67,67	0
56	MG	2a	3203	1/1	0.86	0.20	71,71,71,71	0
56	MG	2A	3807	1/1	0.86	0.13	70,70,70,70	0
56	MG	2A	3362	1/1	0.86	0.24	52,52,52,52	0
56	MG	1l	201	1/1	0.86	0.12	59,59,59,59	0
56	MG	2A	3371	1/1	0.86	0.13	60,60,60,60	0
56	MG	1A	3973	1/1	0.86	0.16	27,27,27,27	0
56	MG	2A	3876	1/1	0.86	0.14	66,66,66,66	0
56	MG	1D	310	1/1	0.86	0.33	49,49,49,49	0
56	MG	2A	3194	1/1	0.86	0.12	49,49,49,49	0
56	MG	1a	1757	1/1	0.86	0.21	66,66,66,66	0
56	MG	2a	3229	1/1	0.86	0.20	66,66,66,66	0
56	MG	1w	106	1/1	0.86	0.15	75,75,75,75	0
56	MG	2A	3221	1/1	0.86	0.18	55,55,55,55	0
56	MG	1A	3912	1/1	0.86	0.11	39,39,39,39	0
56	MG	2A	3243	1/1	0.86	0.15	52,52,52,52	0
56	MG	2A	3448	1/1	0.86	0.17	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2w	106	1/1	0.86	0.10	72,72,72,72	0
56	MG	2A	3246	1/1	0.86	0.15	56,56,56,56	0
56	MG	2A	3461	1/1	0.86	0.19	75,75,75,75	0
56	MG	2A	3690	1/1	0.86	0.15	67,67,67,67	0
56	MG	1S	202	1/1	0.87	0.14	49,49,49,49	0
56	MG	2a	3009	1/1	0.87	0.18	68,68,68,68	0
56	MG	1T	202	1/1	0.87	0.12	46,46,46,46	0
56	MG	1a	1773	1/1	0.87	0.12	58,58,58,58	0
56	MG	1U	210	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3354	1/1	0.87	0.10	60,60,60,60	0
56	MG	2a	3052	1/1	0.87	0.16	54,54,54,54	0
56	MG	2A	3357	1/1	0.87	0.21	65,65,65,65	0
56	MG	1A	3821	1/1	0.87	0.11	42,42,42,42	0
56	MG	2A	3365	1/1	0.87	0.12	56,56,56,56	0
56	MG	1A	3470	1/1	0.87	0.11	62,62,62,62	0
56	MG	1A	4058	1/1	0.87	0.15	49,49,49,49	0
56	MG	2A	3118	1/1	0.87	0.17	66,66,66,66	0
56	MG	1a	1786	1/1	0.87	0.12	74,74,74,74	0
56	MG	2a	3118	1/1	0.87	0.25	61,61,61,61	0
56	MG	10	104	1/1	0.87	0.10	51,51,51,51	0
56	MG	15	105	1/1	0.87	0.11	48,48,48,48	0
56	MG	2a	3124	1/1	0.87	0.10	49,49,49,49	0
56	MG	1A	3898	1/1	0.87	0.09	41,41,41,41	0
56	MG	1a	1604	1/1	0.87	0.10	55,55,55,55	0
56	MG	1a	1806	1/1	0.87	0.10	70,70,70,70	0
56	MG	2a	3146	1/1	0.87	0.12	65,65,65,65	0
56	MG	1a	1609	1/1	0.87	0.16	50,50,50,50	0
56	MG	2A	3209	1/1	0.87	0.08	62,62,62,62	0
56	MG	1A	3089	1/1	0.87	0.09	41,41,41,41	0
56	MG	1a	1629	1/1	0.87	0.17	56,56,56,56	0
56	MG	2a	3165	1/1	0.87	0.25	60,60,60,60	0
56	MG	1a	1634	1/1	0.87	0.17	65,65,65,65	0
56	MG	2A	3470	1/1	0.87	0.10	60,60,60,60	0
56	MG	1A	3426	1/1	0.87	0.14	55,55,55,55	0
56	MG	1l	202	1/1	0.87	0.12	66,66,66,66	0
56	MG	2A	3254	1/1	0.87	0.16	61,61,61,61	0
56	MG	1B	211	1/1	0.87	0.13	57,57,57,57	0
56	MG	1A	3254	1/1	0.87	0.11	53,53,53,53	0
56	MG	2A	3271	1/1	0.87	0.13	55,55,55,55	0
56	MG	1B	214	1/1	0.87	0.09	54,54,54,54	0
56	MG	1a	1667	1/1	0.87	0.20	62,62,62,62	0
56	MG	2A	3549	1/1	0.87	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3298	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3300	1/1	0.87	0.14	53,53,53,53	0
56	MG	2A	3301	1/1	0.87	0.19	58,58,58,58	0
56	MG	1a	1676	1/1	0.87	0.12	45,45,45,45	0
56	MG	1A	3721	1/1	0.87	0.14	29,29,29,29	0
56	MG	2A	3830	1/1	0.87	0.09	66,66,66,66	0
56	MG	1A	3541	1/1	0.87	0.11	60,60,60,60	0
56	MG	1a	1695	1/1	0.87	0.13	47,47,47,47	0
56	MG	2A	3599	1/1	0.87	0.25	63,63,63,63	0
56	MG	2a	3231	1/1	0.87	0.26	58,58,58,58	0
56	MG	1a	1702	1/1	0.87	0.33	57,57,57,57	0
56	MG	2B	205	1/1	0.87	0.15	52,52,52,52	0
56	MG	2A	3613	1/1	0.87	0.17	57,57,57,57	0
56	MG	2A	3614	1/1	0.87	0.18	57,57,57,57	0
56	MG	2w	101	1/1	0.87	0.27	61,61,61,61	0
56	MG	2A	3001	1/1	0.87	0.36	60,60,60,60	0
56	MG	1I	201	1/1	0.87	0.14	63,63,63,63	0
56	MG	2w	107	1/1	0.87	0.20	74,74,74,74	0
56	MG	1O	201	1/1	0.87	0.12	62,62,62,62	0
56	MG	2y	103	1/1	0.87	0.11	56,56,56,56	0
56	MG	2A	3627	1/1	0.87	0.19	59,59,59,59	0
56	MG	2y	105	1/1	0.87	0.12	69,69,69,69	0
56	MG	1a	1726	1/1	0.87	0.14	44,44,44,44	0
56	MG	1w	105	1/1	0.88	0.10	58,58,58,58	0
56	MG	1a	1700	1/1	0.88	0.23	42,42,42,42	0
56	MG	1A	3621	1/1	0.88	0.20	42,42,42,42	0
56	MG	2A	3275	1/1	0.88	0.15	58,58,58,58	0
56	MG	1A	3367	1/1	0.88	0.15	54,54,54,54	0
56	MG	2A	3292	1/1	0.88	0.11	67,67,67,67	0
56	MG	2A	3293	1/1	0.88	0.12	62,62,62,62	0
56	MG	2A	3562	1/1	0.88	0.13	42,42,42,42	0
56	MG	2E	301	1/1	0.88	0.18	50,50,50,50	0
56	MG	2E	308	1/1	0.88	0.11	52,52,52,52	0
56	MG	2F	302	1/1	0.88	0.10	58,58,58,58	0
56	MG	1A	3529	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3567	1/1	0.88	0.13	69,69,69,69	0
56	MG	1A	3656	1/1	0.88	0.12	58,58,58,58	0
56	MG	2W	202	1/1	0.88	0.09	44,44,44,44	0
56	MG	25	104	1/1	0.88	0.12	46,46,46,46	0
56	MG	26	101	1/1	0.88	0.14	52,52,52,52	0
56	MG	1A	3661	1/1	0.88	0.08	21,21,21,21	0
56	MG	1a	1759	1/1	0.88	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3016	1/1	0.88	0.18	60,60,60,60	0
56	MG	2a	3012	1/1	0.88	0.32	62,62,62,62	0
56	MG	2A	3018	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3612	1/1	0.88	0.12	57,57,57,57	0
56	MG	1A	4044	1/1	0.88	0.19	47,47,47,47	0
56	MG	2a	3038	1/1	0.88	0.13	69,69,69,69	0
56	MG	1A	3671	1/1	0.88	0.10	20,20,20,20	0
56	MG	2a	3041	1/1	0.88	0.23	56,56,56,56	0
56	MG	2a	3050	1/1	0.88	0.10	56,56,56,56	0
56	MG	2A	3617	1/1	0.88	0.14	48,48,48,48	0
56	MG	2a	3053	1/1	0.88	0.16	62,62,62,62	0
56	MG	2A	3051	1/1	0.88	0.08	41,41,41,41	0
56	MG	2a	3057	1/1	0.88	0.17	59,59,59,59	0
56	MG	2a	3060	1/1	0.88	0.28	70,70,70,70	0
56	MG	2A	3316	1/1	0.88	0.15	53,53,53,53	0
56	MG	1A	3271	1/1	0.88	0.17	57,57,57,57	0
56	MG	2a	3083	1/1	0.88	0.10	55,55,55,55	0
56	MG	1A	3683	1/1	0.88	0.12	31,31,31,31	0
56	MG	1A	3380	1/1	0.88	0.22	63,63,63,63	0
56	MG	2A	3071	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3076	1/1	0.88	0.08	50,50,50,50	0
56	MG	1A	3715	1/1	0.88	0.12	40,40,40,40	0
56	MG	2A	3660	1/1	0.88	0.15	55,55,55,55	0
56	MG	1A	3480	1/1	0.88	0.12	45,45,45,45	0
56	MG	1a	1630	1/1	0.88	0.25	51,51,51,51	0
56	MG	1a	1794	1/1	0.88	0.16	48,48,48,48	0
56	MG	1A	3730	1/1	0.88	0.11	25,25,25,25	0
56	MG	2A	3360	1/1	0.88	0.12	66,66,66,66	0
56	MG	2a	3140	1/1	0.88	0.10	56,56,56,56	0
56	MG	2a	3141	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3111	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3363	1/1	0.88	0.14	50,50,50,50	0
56	MG	2A	3686	1/1	0.88	0.11	66,66,66,66	0
56	MG	2A	3114	1/1	0.88	0.22	60,60,60,60	0
56	MG	1a	1799	1/1	0.88	0.12	60,60,60,60	0
56	MG	2A	3695	1/1	0.88	0.14	52,52,52,52	0
56	MG	1A	3737	1/1	0.88	0.17	32,32,32,32	0
56	MG	2A	3378	1/1	0.88	0.09	50,50,50,50	0
56	MG	2A	3704	1/1	0.88	0.18	62,62,62,62	0
56	MG	1A	3542	1/1	0.88	0.10	56,56,56,56	0
56	MG	2a	3179	1/1	0.88	0.16	60,60,60,60	0
56	MG	1a	1650	1/1	0.88	0.31	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3154	1/1	0.88	0.12	51,51,51,51	0
56	MG	2A	3164	1/1	0.88	0.12	43,43,43,43	0
56	MG	2A	3725	1/1	0.88	0.10	59,59,59,59	0
56	MG	2A	3173	1/1	0.88	0.17	74,74,74,74	0
56	MG	2A	3740	1/1	0.88	0.10	54,54,54,54	0
56	MG	2A	3175	1/1	0.88	0.10	42,42,42,42	0
56	MG	1A	3489	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3746	1/1	0.88	0.11	43,43,43,43	0
56	MG	2A	3430	1/1	0.88	0.10	44,44,44,44	0
56	MG	2A	3751	1/1	0.88	0.13	54,54,54,54	0
56	MG	2A	3434	1/1	0.88	0.18	49,49,49,49	0
56	MG	2A	3755	1/1	0.88	0.15	39,39,39,39	0
56	MG	2A	3435	1/1	0.88	0.10	56,56,56,56	0
56	MG	2A	3438	1/1	0.88	0.23	53,53,53,53	0
56	MG	1A	3491	1/1	0.88	0.11	48,48,48,48	0
56	MG	1A	3312	1/1	0.88	0.28	64,64,64,64	0
56	MG	1A	3214	1/1	0.88	0.15	61,61,61,61	0
56	MG	2a	3234	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3782	1/1	0.88	0.10	55,55,55,55	0
56	MG	1R	204	1/1	0.88	0.17	49,49,49,49	0
56	MG	2A	3212	1/1	0.88	0.23	60,60,60,60	0
56	MG	1a	1681	1/1	0.88	0.27	66,66,66,66	0
56	MG	1a	1691	1/1	0.88	0.17	55,55,55,55	0
56	MG	1p	101	1/1	0.88	0.10	38,38,38,38	0
56	MG	1w	101	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3232	1/1	0.88	0.14	53,53,53,53	0
56	MG	2A	3503	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3525	1/1	0.88	0.20	47,47,47,47	0
56	MG	1T	201	1/1	0.88	0.15	44,44,44,44	0
56	MG	2A	3863	1/1	0.88	0.10	42,42,42,42	0
56	MG	2A	3853	1/1	0.89	0.12	66,66,66,66	0
56	MG	2A	3497	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3207	1/1	0.89	0.11	54,54,54,54	0
56	MG	1A	3618	1/1	0.89	0.19	49,49,49,49	0
56	MG	1T	203	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3913	1/1	0.89	0.09	18,18,18,18	0
56	MG	1A	3749	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3238	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3189	1/1	0.89	0.07	41,41,41,41	0
56	MG	1A	3935	1/1	0.89	0.09	53,53,53,53	0
56	MG	2B	218	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	3622	1/1	0.89	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2E	303	1/1	0.89	0.06	41,41,41,41	0
56	MG	2A	3251	1/1	0.89	0.13	55,55,55,55	0
56	MG	1A	3383	1/1	0.89	0.09	47,47,47,47	0
56	MG	2A	3563	1/1	0.89	0.15	41,41,41,41	0
56	MG	1A	3640	1/1	0.89	0.09	24,24,24,24	0
56	MG	18	103	1/1	0.89	0.09	48,48,48,48	0
56	MG	2R	201	1/1	0.89	0.16	56,56,56,56	0
56	MG	2V	201	1/1	0.89	0.32	49,49,49,49	0
56	MG	1A	3798	1/1	0.89	0.09	25,25,25,25	0
56	MG	2X	101	1/1	0.89	0.15	60,60,60,60	0
56	MG	1A	3287	1/1	0.89	0.07	39,39,39,39	0
56	MG	1a	1623	1/1	0.89	0.14	50,50,50,50	0
56	MG	1A	3976	1/1	0.89	0.09	34,34,34,34	0
56	MG	1A	3474	1/1	0.89	0.14	56,56,56,56	0
56	MG	1A	3988	1/1	0.89	0.08	18,18,18,18	0
56	MG	2a	3010	1/1	0.89	0.23	67,67,67,67	0
56	MG	1A	4002	1/1	0.89	0.10	58,58,58,58	0
56	MG	1A	3816	1/1	0.89	0.10	77,77,77,77	0
56	MG	2a	3021	1/1	0.89	0.16	58,58,58,58	0
56	MG	1A	4019	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3405	1/1	0.89	0.25	17,17,17,17	0
56	MG	2a	3028	1/1	0.89	0.28	59,59,59,59	0
56	MG	2a	3033	1/1	0.89	0.10	59,59,59,59	0
56	MG	1A	4026	1/1	0.89	0.10	26,26,26,26	0
56	MG	1A	3670	1/1	0.89	0.13	48,48,48,48	0
56	MG	2a	3040	1/1	0.89	0.16	58,58,58,58	0
56	MG	2A	3626	1/1	0.89	0.11	37,37,37,37	0
56	MG	1A	3829	1/1	0.89	0.12	18,18,18,18	0
56	MG	1A	3409	1/1	0.89	0.33	35,35,35,35	0
56	MG	2A	3005	1/1	0.89	0.32	55,55,55,55	0
56	MG	2A	3318	1/1	0.89	0.23	55,55,55,55	0
56	MG	2a	3056	1/1	0.89	0.15	69,69,69,69	0
56	MG	2A	3319	1/1	0.89	0.30	55,55,55,55	0
56	MG	2A	3648	1/1	0.89	0.13	33,33,33,33	0
56	MG	2a	3061	1/1	0.89	0.08	59,59,59,59	0
56	MG	1A	4053	1/1	0.89	0.19	48,48,48,48	0
56	MG	1A	3041	1/1	0.89	0.14	38,38,38,38	0
56	MG	1A	3345	1/1	0.89	0.09	51,51,51,51	0
56	MG	2A	3031	1/1	0.89	0.15	62,62,62,62	0
56	MG	1a	1692	1/1	0.89	0.29	62,62,62,62	0
56	MG	2a	3094	1/1	0.89	0.16	61,61,61,61	0
56	MG	1A	4073	1/1	0.89	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3102	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3518	1/1	0.89	0.16	51,51,51,51	0
56	MG	1A	4102	1/1	0.89	0.09	54,54,54,54	0
56	MG	1A	3843	1/1	0.89	0.10	28,28,28,28	0
56	MG	1a	1705	1/1	0.89	0.25	45,45,45,45	0
56	MG	1A	3869	1/1	0.89	0.11	42,42,42,42	0
56	MG	1a	1715	1/1	0.89	0.10	45,45,45,45	0
56	MG	2a	3128	1/1	0.89	0.29	63,63,63,63	0
56	MG	1A	3710	1/1	0.89	0.16	47,47,47,47	0
56	MG	2A	3702	1/1	0.89	0.12	44,44,44,44	0
56	MG	1a	1725	1/1	0.89	0.12	47,47,47,47	0
56	MG	1A	3713	1/1	0.89	0.10	45,45,45,45	0
56	MG	2A	3104	1/1	0.89	0.16	54,54,54,54	0
56	MG	1a	1733	1/1	0.89	0.24	55,55,55,55	0
56	MG	2A	3712	1/1	0.89	0.23	69,69,69,69	0
56	MG	2A	3109	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3383	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3721	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3390	1/1	0.89	0.22	63,63,63,63	0
56	MG	2A	3726	1/1	0.89	0.07	50,50,50,50	0
56	MG	2a	3170	1/1	0.89	0.14	65,65,65,65	0
56	MG	2A	3729	1/1	0.89	0.15	55,55,55,55	0
56	MG	2A	3736	1/1	0.89	0.13	50,50,50,50	0
56	MG	1a	1755	1/1	0.89	0.23	61,61,61,61	0
56	MG	1B	217	1/1	0.89	0.09	43,43,43,43	0
56	MG	2A	3741	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3883	1/1	0.89	0.08	13,13,13,13	0
56	MG	2A	3743	1/1	0.89	0.12	51,51,51,51	0
56	MG	2A	3408	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3432	1/1	0.89	0.10	52,52,52,52	0
56	MG	2a	3206	1/1	0.89	0.21	58,58,58,58	0
56	MG	2A	3132	1/1	0.89	0.15	71,71,71,71	0
56	MG	1a	1768	1/1	0.89	0.10	61,61,61,61	0
56	MG	2A	3426	1/1	0.89	0.19	35,35,35,35	0
56	MG	2a	3215	1/1	0.89	0.17	61,61,61,61	0
56	MG	1E	308	1/1	0.89	0.09	16,16,16,16	0
56	MG	2A	3757	1/1	0.89	0.09	54,54,54,54	0
56	MG	2A	3759	1/1	0.89	0.10	47,47,47,47	0
56	MG	1G	204	1/1	0.89	0.09	54,54,54,54	0
56	MG	1A	3897	1/1	0.89	0.10	34,34,34,34	0
56	MG	2A	3171	1/1	0.89	0.23	72,72,72,72	0
56	MG	1A	3565	1/1	0.89	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1O	206	1/1	0.89	0.20	57,57,57,57	0
56	MG	2A	3449	1/1	0.89	0.14	65,65,65,65	0
56	MG	2A	3454	1/1	0.89	0.12	45,45,45,45	0
56	MG	1a	1782	1/1	0.89	0.15	55,55,55,55	0
56	MG	1A	3570	1/1	0.89	0.10	54,54,54,54	0
56	MG	2t	201	1/1	0.89	0.17	47,47,47,47	0
56	MG	2A	3793	1/1	0.89	0.09	63,63,63,63	0
56	MG	2A	3185	1/1	0.89	0.20	50,50,50,50	0
56	MG	2A	3189	1/1	0.89	0.10	58,58,58,58	0
56	MG	2A	3190	1/1	0.89	0.19	60,60,60,60	0
56	MG	2A	3193	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3482	1/1	0.89	0.18	56,56,56,56	0
56	MG	2A	3811	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	3906	1/1	0.89	0.15	41,41,41,41	0
56	MG	1A	3448	1/1	0.89	0.11	39,39,39,39	0
56	MG	2A	3831	1/1	0.89	0.14	38,38,38,38	0
58	ZN	24	501	1/1	0.89	0.15	134,134,134,134	0
60	K	2A	3473	1/1	0.89	0.17	75,75,75,75	0
56	MG	1A	3952	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3960	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3968	1/1	0.90	0.08	58,58,58,58	0
56	MG	2A	3629	1/1	0.90	0.23	54,54,54,54	0
56	MG	2A	3630	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	3264	1/1	0.90	0.15	53,53,53,53	0
56	MG	25	102	1/1	0.90	0.14	45,45,45,45	0
56	MG	1A	3229	1/1	0.90	0.09	41,41,41,41	0
56	MG	2A	3351	1/1	0.90	0.09	49,49,49,49	0
56	MG	2A	3352	1/1	0.90	0.08	48,48,48,48	0
56	MG	1A	3553	1/1	0.90	0.24	55,55,55,55	0
56	MG	2a	3008	1/1	0.90	0.18	57,57,57,57	0
56	MG	2A	3650	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3656	1/1	0.90	0.10	39,39,39,39	0
56	MG	1A	3516	1/1	0.90	0.11	37,37,37,37	0
56	MG	2A	3113	1/1	0.90	0.15	50,50,50,50	0
56	MG	1Z	3701	1/1	0.90	0.08	51,51,51,51	0
56	MG	2A	3115	1/1	0.90	0.17	53,53,53,53	0
56	MG	2A	3117	1/1	0.90	0.14	50,50,50,50	0
56	MG	1A	3995	1/1	0.90	0.10	39,39,39,39	0
56	MG	13	104	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3428	1/1	0.90	0.11	38,38,38,38	0
56	MG	1A	4003	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	4007	1/1	0.90	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3381	1/1	0.90	0.18	59,59,59,59	0
56	MG	2a	3042	1/1	0.90	0.25	65,65,65,65	0
56	MG	1A	3050	1/1	0.90	0.16	25,25,25,25	0
56	MG	1a	1797	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3397	1/1	0.90	0.14	58,58,58,58	0
56	MG	1a	1608	1/1	0.90	0.10	42,42,42,42	0
56	MG	1A	3841	1/1	0.90	0.11	42,42,42,42	0
56	MG	1A	3581	1/1	0.90	0.26	64,64,64,64	0
56	MG	1A	3599	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3409	1/1	0.90	0.20	66,66,66,66	0
56	MG	2a	3064	1/1	0.90	0.09	70,70,70,70	0
56	MG	2a	3065	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3853	1/1	0.90	0.09	19,19,19,19	0
56	MG	1a	1821	1/1	0.90	0.27	55,55,55,55	0
56	MG	2a	3076	1/1	0.90	0.20	56,56,56,56	0
56	MG	1a	1824	1/1	0.90	0.18	54,54,54,54	0
56	MG	2A	3723	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3423	1/1	0.90	0.24	42,42,42,42	0
56	MG	1A	3858	1/1	0.90	0.06	27,27,27,27	0
56	MG	1A	3717	1/1	0.90	0.07	39,39,39,39	0
56	MG	2a	3099	1/1	0.90	0.22	58,58,58,58	0
56	MG	1A	3437	1/1	0.90	0.10	50,50,50,50	0
56	MG	2a	3114	1/1	0.90	0.14	65,65,65,65	0
56	MG	1A	3728	1/1	0.90	0.08	20,20,20,20	0
56	MG	2A	3739	1/1	0.90	0.17	62,62,62,62	0
56	MG	1a	1646	1/1	0.90	0.14	53,53,53,53	0
56	MG	2A	3208	1/1	0.90	0.07	32,32,32,32	0
56	MG	1A	3615	1/1	0.90	0.15	33,33,33,33	0
56	MG	1A	3884	1/1	0.90	0.15	47,47,47,47	0
56	MG	2a	3126	1/1	0.90	0.15	62,62,62,62	0
56	MG	1a	1660	1/1	0.90	0.17	63,63,63,63	0
56	MG	2A	3745	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3455	1/1	0.90	0.21	50,50,50,50	0
56	MG	1A	3733	1/1	0.90	0.08	22,22,22,22	0
56	MG	2A	3458	1/1	0.90	0.24	64,64,64,64	0
56	MG	2A	3224	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3226	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	4101	1/1	0.90	0.16	56,56,56,56	0
56	MG	1a	1670	1/1	0.90	0.13	49,49,49,49	0
56	MG	1A	3616	1/1	0.90	0.13	50,50,50,50	0
56	MG	2A	3763	1/1	0.90	0.13	43,43,43,43	0
56	MG	1A	3375	1/1	0.90	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3249	1/1	0.90	0.24	60,60,60,60	0
56	MG	1A	3378	1/1	0.90	0.09	42,42,42,42	0
56	MG	2A	3769	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3253	1/1	0.90	0.09	58,58,58,58	0
56	MG	2A	3780	1/1	0.90	0.09	48,48,48,48	0
56	MG	1a	1683	1/1	0.90	0.19	64,64,64,64	0
56	MG	2A	3504	1/1	0.90	0.30	52,52,52,52	0
56	MG	2A	3505	1/1	0.90	0.11	41,41,41,41	0
56	MG	1x	115	1/1	0.90	0.13	62,62,62,62	0
56	MG	2a	3191	1/1	0.90	0.08	64,64,64,64	0
56	MG	1A	3001	1/1	0.90	0.06	34,34,34,34	0
56	MG	2a	3199	1/1	0.90	0.13	50,50,50,50	0
56	MG	2A	3796	1/1	0.90	0.15	64,64,64,64	0
56	MG	1A	3533	1/1	0.90	0.23	33,33,33,33	0
56	MG	2a	3207	1/1	0.90	0.18	60,60,60,60	0
56	MG	2a	3209	1/1	0.90	0.14	58,58,58,58	0
56	MG	1A	3324	1/1	0.90	0.14	54,54,54,54	0
56	MG	1A	3769	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3291	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3808	1/1	0.90	0.12	58,58,58,58	0
56	MG	1B	230	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3770	1/1	0.90	0.11	47,47,47,47	0
56	MG	2A	3020	1/1	0.90	0.15	55,55,55,55	0
56	MG	2a	3223	1/1	0.90	0.14	58,58,58,58	0
56	MG	2A	3297	1/1	0.90	0.27	68,68,68,68	0
56	MG	1A	3925	1/1	0.90	0.16	54,54,54,54	0
56	MG	2A	3843	1/1	0.90	0.13	41,41,41,41	0
56	MG	2A	3851	1/1	0.90	0.10	55,55,55,55	0
56	MG	2a	3230	1/1	0.90	0.11	60,60,60,60	0
56	MG	1E	310	1/1	0.90	0.11	58,58,58,58	0
56	MG	2A	3041	1/1	0.90	0.16	54,54,54,54	0
56	MG	1A	3341	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3575	1/1	0.90	0.08	40,40,40,40	0
56	MG	2j	202	1/1	0.90	0.07	58,58,58,58	0
56	MG	1A	3172	1/1	0.90	0.14	53,53,53,53	0
56	MG	2A	3586	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3053	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3598	1/1	0.90	0.09	51,51,51,51	0
56	MG	2B	213	1/1	0.90	0.15	55,55,55,55	0
56	MG	2A	3309	1/1	0.90	0.13	49,49,49,49	0
56	MG	1A	3261	1/1	0.90	0.37	46,46,46,46	0
56	MG	2x	103	1/1	0.90	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3810	1/1	0.90	0.08	21,21,21,21	0
56	MG	1a	1732	1/1	0.90	0.23	43,43,43,43	0
56	MG	1A	3667	1/1	0.90	0.08	44,44,44,44	0
56	MG	2E	304	1/1	0.90	0.15	58,58,58,58	0
56	MG	1a	1735	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3084	1/1	0.90	0.19	60,60,60,60	0
56	MG	1A	3669	1/1	0.90	0.09	39,39,39,39	0
56	MG	1A	4040	1/1	0.91	0.07	41,41,41,41	0
56	MG	1A	3410	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	4045	1/1	0.91	0.08	69,69,69,69	0
56	MG	2A	3874	1/1	0.91	0.11	45,45,45,45	0
56	MG	1x	108	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3854	1/1	0.91	0.10	35,35,35,35	0
56	MG	2B	204	1/1	0.91	0.14	71,71,71,71	0
56	MG	2A	3252	1/1	0.91	0.10	55,55,55,55	0
56	MG	1A	3190	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3120	1/1	0.91	0.12	55,55,55,55	0
56	MG	2A	3257	1/1	0.91	0.10	42,42,42,42	0
56	MG	2B	215	1/1	0.91	0.08	52,52,52,52	0
56	MG	2A	3258	1/1	0.91	0.16	62,62,62,62	0
56	MG	1a	1665	1/1	0.91	0.16	55,55,55,55	0
56	MG	2B	221	1/1	0.91	0.12	59,59,59,59	0
56	MG	2A	3267	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3329	1/1	0.91	0.13	52,52,52,52	0
56	MG	1A	3876	1/1	0.91	0.09	53,53,53,53	0
56	MG	2A	3565	1/1	0.91	0.11	33,33,33,33	0
56	MG	2E	309	1/1	0.91	0.10	42,42,42,42	0
56	MG	2A	3273	1/1	0.91	0.07	59,59,59,59	0
56	MG	2F	303	1/1	0.91	0.12	39,39,39,39	0
56	MG	1A	3332	1/1	0.91	0.18	52,52,52,52	0
56	MG	1A	4088	1/1	0.91	0.11	36,36,36,36	0
56	MG	2A	3280	1/1	0.91	0.15	34,34,34,34	0
56	MG	2A	3283	1/1	0.91	0.12	54,54,54,54	0
56	MG	2R	202	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3579	1/1	0.91	0.11	53,53,53,53	0
56	MG	2A	3287	1/1	0.91	0.09	42,42,42,42	0
56	MG	2A	3588	1/1	0.91	0.10	29,29,29,29	0
56	MG	2I	101	1/1	0.91	0.23	44,44,44,44	0
56	MG	2A	3596	1/1	0.91	0.16	53,53,53,53	0
56	MG	2A	3289	1/1	0.91	0.10	41,41,41,41	0
56	MG	1A	3130	1/1	0.91	0.15	44,44,44,44	0
56	MG	1A	3137	1/1	0.91	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3449	1/1	0.91	0.08	42,42,42,42	0
56	MG	2a	3005	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3608	1/1	0.91	0.08	28,28,28,28	0
56	MG	2A	3024	1/1	0.91	0.17	46,46,46,46	0
56	MG	2A	3029	1/1	0.91	0.21	54,54,54,54	0
56	MG	1A	3554	1/1	0.91	0.11	26,26,26,26	0
56	MG	2A	3299	1/1	0.91	0.14	52,52,52,52	0
56	MG	2A	3040	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3152	1/1	0.91	0.25	33,33,33,33	0
56	MG	2A	3302	1/1	0.91	0.09	49,49,49,49	0
56	MG	2A	3624	1/1	0.91	0.16	43,43,43,43	0
56	MG	2a	3031	1/1	0.91	0.19	46,46,46,46	0
56	MG	1A	3562	1/1	0.91	0.08	39,39,39,39	0
56	MG	2a	3034	1/1	0.91	0.25	67,67,67,67	0
56	MG	1A	3468	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	3907	1/1	0.91	0.13	25,25,25,25	0
56	MG	1a	1703	1/1	0.91	0.19	41,41,41,41	0
56	MG	2A	3056	1/1	0.91	0.13	56,56,56,56	0
56	MG	1A	3742	1/1	0.91	0.08	40,40,40,40	0
56	MG	2a	3043	1/1	0.91	0.13	62,62,62,62	0
56	MG	2a	3044	1/1	0.91	0.10	54,54,54,54	0
56	MG	2a	3049	1/1	0.91	0.09	63,63,63,63	0
56	MG	1B	222	1/1	0.91	0.09	41,41,41,41	0
56	MG	1A	3566	1/1	0.91	0.13	50,50,50,50	0
56	MG	1B	231	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3649	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3321	1/1	0.91	0.09	57,57,57,57	0
56	MG	1A	3350	1/1	0.91	0.17	45,45,45,45	0
56	MG	2A	3087	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3571	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3924	1/1	0.91	0.16	55,55,55,55	0
56	MG	2A	3664	1/1	0.91	0.11	67,67,67,67	0
56	MG	2A	3097	1/1	0.91	0.12	50,50,50,50	0
56	MG	2a	3071	1/1	0.91	0.17	45,45,45,45	0
56	MG	2A	3668	1/1	0.91	0.14	59,59,59,59	0
56	MG	1E	311	1/1	0.91	0.22	37,37,37,37	0
56	MG	1F	309	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3680	1/1	0.91	0.08	43,43,43,43	0
56	MG	1a	1739	1/1	0.91	0.34	59,59,59,59	0
56	MG	1A	3237	1/1	0.91	0.18	45,45,45,45	0
56	MG	1A	3930	1/1	0.91	0.09	45,45,45,45	0
56	MG	1N	204	1/1	0.91	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3164	1/1	0.91	0.27	35,35,35,35	0
56	MG	2a	3112	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3933	1/1	0.91	0.20	39,39,39,39	0
56	MG	1P	204	1/1	0.91	0.07	33,33,33,33	0
56	MG	1A	3476	1/1	0.91	0.17	42,42,42,42	0
56	MG	1A	3773	1/1	0.91	0.13	40,40,40,40	0
56	MG	1A	3080	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3706	1/1	0.91	0.07	47,47,47,47	0
56	MG	2A	3368	1/1	0.91	0.08	58,58,58,58	0
56	MG	2A	3369	1/1	0.91	0.11	57,57,57,57	0
56	MG	2a	3127	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3128	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3372	1/1	0.91	0.08	47,47,47,47	0
56	MG	2A	3376	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3942	1/1	0.91	0.18	26,26,26,26	0
56	MG	1A	3791	1/1	0.91	0.10	11,11,11,11	0
56	MG	2A	3141	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3151	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3385	1/1	0.91	0.17	51,51,51,51	0
56	MG	1A	3485	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3948	1/1	0.91	0.17	40,40,40,40	0
56	MG	2A	3155	1/1	0.91	0.11	52,52,52,52	0
56	MG	2A	3163	1/1	0.91	0.18	53,53,53,53	0
56	MG	1A	3487	1/1	0.91	0.15	59,59,59,59	0
56	MG	2A	3406	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3169	1/1	0.91	0.11	61,61,61,61	0
56	MG	2a	3177	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3800	1/1	0.91	0.09	38,38,38,38	0
56	MG	1A	3374	1/1	0.91	0.10	41,41,41,41	0
56	MG	2A	3413	1/1	0.91	0.08	59,59,59,59	0
56	MG	1Z	3702	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3748	1/1	0.91	0.09	57,57,57,57	0
56	MG	2A	3750	1/1	0.91	0.14	56,56,56,56	0
56	MG	1a	1800	1/1	0.91	0.16	38,38,38,38	0
56	MG	2a	3196	1/1	0.91	0.13	68,68,68,68	0
56	MG	1A	3972	1/1	0.91	0.12	31,31,31,31	0
56	MG	2a	3198	1/1	0.91	0.12	53,53,53,53	0
56	MG	2A	3424	1/1	0.91	0.24	36,36,36,36	0
56	MG	2A	3756	1/1	0.91	0.09	53,53,53,53	0
56	MG	1A	3096	1/1	0.91	0.12	49,49,49,49	0
56	MG	2A	3428	1/1	0.91	0.22	49,49,49,49	0
56	MG	2a	3208	1/1	0.91	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3176	1/1	0.91	0.08	33,33,33,33	0
56	MG	16	102	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3765	1/1	0.91	0.12	54,54,54,54	0
56	MG	2A	3192	1/1	0.91	0.11	53,53,53,53	0
56	MG	1A	3511	1/1	0.91	0.12	62,62,62,62	0
56	MG	1A	3265	1/1	0.91	0.11	31,31,31,31	0
56	MG	2a	3218	1/1	0.91	0.08	42,42,42,42	0
56	MG	2a	3219	1/1	0.91	0.14	71,71,71,71	0
56	MG	2A	3441	1/1	0.91	0.14	47,47,47,47	0
56	MG	1A	3269	1/1	0.91	0.15	44,44,44,44	0
56	MG	2A	3203	1/1	0.91	0.16	49,49,49,49	0
56	MG	2a	3225	1/1	0.91	0.12	57,57,57,57	0
56	MG	2A	3205	1/1	0.91	0.10	60,60,60,60	0
56	MG	2A	3784	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3785	1/1	0.91	0.10	64,64,64,64	0
56	MG	1A	3389	1/1	0.91	0.10	38,38,38,38	0
56	MG	1A	3521	1/1	0.91	0.09	50,50,50,50	0
56	MG	1A	3187	1/1	0.91	0.07	53,53,53,53	0
56	MG	1a	1627	1/1	0.91	0.17	36,36,36,36	0
56	MG	2A	3462	1/1	0.91	0.32	51,51,51,51	0
56	MG	1A	3402	1/1	0.91	0.14	42,42,42,42	0
56	MG	2A	3219	1/1	0.91	0.26	57,57,57,57	0
56	MG	2l	202	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3114	1/1	0.91	0.24	35,35,35,35	0
56	MG	2A	3476	1/1	0.91	0.09	52,52,52,52	0
56	MG	1A	3300	1/1	0.91	0.09	37,37,37,37	0
56	MG	1A	3846	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3227	1/1	0.91	0.22	59,59,59,59	0
56	MG	2A	3230	1/1	0.91	0.11	46,46,46,46	0
56	MG	2A	3494	1/1	0.91	0.11	50,50,50,50	0
56	MG	2x	102	1/1	0.91	0.07	52,52,52,52	0
56	MG	2A	3496	1/1	0.91	0.09	61,61,61,61	0
56	MG	2A	3832	1/1	0.91	0.13	30,30,30,30	0
56	MG	2A	3839	1/1	0.91	0.08	51,51,51,51	0
56	MG	1A	4030	1/1	0.91	0.13	36,36,36,36	0
56	MG	2A	3847	1/1	0.91	0.18	48,48,48,48	0
56	MG	2A	3499	1/1	0.91	0.28	54,54,54,54	0
56	MG	2A	3500	1/1	0.91	0.26	49,49,49,49	0
56	MG	2A	3862	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3647	1/1	0.92	0.11	11,11,11,11	0
56	MG	1A	3958	1/1	0.92	0.07	22,22,22,22	0
56	MG	2A	3487	1/1	0.92	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1S	203	1/1	0.92	0.11	70,70,70,70	0
56	MG	2A	3218	1/1	0.92	0.18	45,45,45,45	0
56	MG	1A	3654	1/1	0.92	0.10	35,35,35,35	0
56	MG	1a	1804	1/1	0.92	0.14	47,47,47,47	0
56	MG	2A	3869	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3222	1/1	0.92	0.18	53,53,53,53	0
56	MG	2A	3223	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3877	1/1	0.92	0.07	45,45,45,45	0
56	MG	1A	3306	1/1	0.92	0.14	32,32,32,32	0
56	MG	1A	3307	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3664	1/1	0.92	0.10	54,54,54,54	0
56	MG	2B	206	1/1	0.92	0.13	50,50,50,50	0
56	MG	2B	208	1/1	0.92	0.17	52,52,52,52	0
56	MG	1A	3024	1/1	0.92	0.14	44,44,44,44	0
56	MG	2A	3513	1/1	0.92	0.09	47,47,47,47	0
56	MG	2A	3514	1/1	0.92	0.13	47,47,47,47	0
56	MG	2A	3518	1/1	0.92	0.09	32,32,32,32	0
56	MG	2A	3524	1/1	0.92	0.15	54,54,54,54	0
56	MG	1a	1822	1/1	0.92	0.11	59,59,59,59	0
56	MG	2B	219	1/1	0.92	0.14	49,49,49,49	0
56	MG	2B	220	1/1	0.92	0.22	70,70,70,70	0
56	MG	1X	105	1/1	0.92	0.07	40,40,40,40	0
56	MG	2D	306	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3240	1/1	0.92	0.17	38,38,38,38	0
56	MG	2A	3242	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3542	1/1	0.92	0.13	44,44,44,44	0
56	MG	1A	3196	1/1	0.92	0.16	44,44,44,44	0
56	MG	1A	3981	1/1	0.92	0.09	33,33,33,33	0
56	MG	1f	201	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3326	1/1	0.92	0.12	33,33,33,33	0
56	MG	1A	3991	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3834	1/1	0.92	0.06	43,43,43,43	0
56	MG	1n	101	1/1	0.92	0.22	44,44,44,44	0
56	MG	2A	3256	1/1	0.92	0.14	66,66,66,66	0
56	MG	1A	3997	1/1	0.92	0.14	55,55,55,55	0
56	MG	1A	3999	1/1	0.92	0.07	60,60,60,60	0
56	MG	2A	3260	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	4001	1/1	0.92	0.09	30,30,30,30	0
56	MG	2Z	301	1/1	0.92	0.09	68,68,68,68	0
56	MG	20	102	1/1	0.92	0.13	52,52,52,52	0
56	MG	1A	3545	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3327	1/1	0.92	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4004	1/1	0.92	0.10	74,74,74,74	0
56	MG	1A	3153	1/1	0.92	0.17	31,31,31,31	0
56	MG	1A	4008	1/1	0.92	0.09	67,67,67,67	0
56	MG	2A	3277	1/1	0.92	0.08	40,40,40,40	0
56	MG	1x	104	1/1	0.92	0.11	53,53,53,53	0
56	MG	2a	3006	1/1	0.92	0.11	42,42,42,42	0
56	MG	2a	3007	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3185	1/1	0.92	0.08	45,45,45,45	0
56	MG	2A	3604	1/1	0.92	0.18	50,50,50,50	0
56	MG	1a	1626	1/1	0.92	0.23	53,53,53,53	0
56	MG	2A	3284	1/1	0.92	0.19	56,56,56,56	0
56	MG	2A	3610	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	4014	1/1	0.92	0.09	34,34,34,34	0
56	MG	2a	3024	1/1	0.92	0.09	38,38,38,38	0
56	MG	2A	3288	1/1	0.92	0.10	40,40,40,40	0
56	MG	2a	3026	1/1	0.92	0.09	50,50,50,50	0
56	MG	1A	4015	1/1	0.92	0.09	29,29,29,29	0
56	MG	1A	3340	1/1	0.92	0.07	46,46,46,46	0
56	MG	1A	3218	1/1	0.92	0.07	36,36,36,36	0
56	MG	1a	1632	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3226	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3007	1/1	0.92	0.13	43,43,43,43	0
56	MG	1A	4028	1/1	0.92	0.07	66,66,66,66	0
56	MG	1a	1637	1/1	0.92	0.13	43,43,43,43	0
56	MG	1A	3054	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3022	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3860	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	4042	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	3505	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3638	1/1	0.92	0.08	30,30,30,30	0
56	MG	2A	3642	1/1	0.92	0.18	39,39,39,39	0
56	MG	2A	3643	1/1	0.92	0.19	47,47,47,47	0
56	MG	2A	3645	1/1	0.92	0.09	43,43,43,43	0
56	MG	1A	3722	1/1	0.92	0.12	16,16,16,16	0
56	MG	2A	3039	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3425	1/1	0.92	0.07	36,36,36,36	0
56	MG	1A	3512	1/1	0.92	0.16	54,54,54,54	0
56	MG	2A	3651	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3655	1/1	0.92	0.11	44,44,44,44	0
56	MG	1a	1666	1/1	0.92	0.09	50,50,50,50	0
56	MG	2a	3070	1/1	0.92	0.14	49,49,49,49	0
56	MG	2A	3047	1/1	0.92	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3279	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3052	1/1	0.92	0.15	66,66,66,66	0
56	MG	2a	3080	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3325	1/1	0.92	0.13	49,49,49,49	0
56	MG	1A	3734	1/1	0.92	0.10	17,17,17,17	0
56	MG	2A	3667	1/1	0.92	0.12	42,42,42,42	0
56	MG	2a	3088	1/1	0.92	0.16	53,53,53,53	0
56	MG	2a	3093	1/1	0.92	0.12	72,72,72,72	0
56	MG	1a	1671	1/1	0.92	0.18	56,56,56,56	0
56	MG	1A	3886	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	4064	1/1	0.92	0.14	28,28,28,28	0
56	MG	2A	3343	1/1	0.92	0.10	55,55,55,55	0
56	MG	2a	3108	1/1	0.92	0.19	63,63,63,63	0
56	MG	2a	3109	1/1	0.92	0.09	48,48,48,48	0
56	MG	2a	3110	1/1	0.92	0.14	65,65,65,65	0
56	MG	1A	4066	1/1	0.92	0.09	24,24,24,24	0
56	MG	2A	3346	1/1	0.92	0.06	54,54,54,54	0
56	MG	1A	3597	1/1	0.92	0.19	30,30,30,30	0
56	MG	2a	3117	1/1	0.92	0.20	73,73,73,73	0
56	MG	2A	3349	1/1	0.92	0.23	64,64,64,64	0
56	MG	1A	4076	1/1	0.92	0.14	63,63,63,63	0
56	MG	2A	3694	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3598	1/1	0.92	0.23	33,33,33,33	0
56	MG	2A	3086	1/1	0.92	0.07	40,40,40,40	0
56	MG	2A	3698	1/1	0.92	0.07	37,37,37,37	0
56	MG	1A	3351	1/1	0.92	0.09	39,39,39,39	0
56	MG	1A	3743	1/1	0.92	0.09	37,37,37,37	0
56	MG	1a	1696	1/1	0.92	0.21	61,61,61,61	0
56	MG	2a	3133	1/1	0.92	0.16	45,45,45,45	0
56	MG	2A	3093	1/1	0.92	0.08	41,41,41,41	0
56	MG	2a	3138	1/1	0.92	0.12	64,64,64,64	0
56	MG	1A	3900	1/1	0.92	0.12	28,28,28,28	0
56	MG	1A	4105	1/1	0.92	0.17	50,50,50,50	0
56	MG	2a	3143	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3711	1/1	0.92	0.10	24,24,24,24	0
56	MG	2a	3147	1/1	0.92	0.16	64,64,64,64	0
56	MG	2A	3364	1/1	0.92	0.13	56,56,56,56	0
56	MG	2a	3153	1/1	0.92	0.10	73,73,73,73	0
56	MG	1B	207	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3715	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3719	1/1	0.92	0.10	29,29,29,29	0
56	MG	2A	3366	1/1	0.92	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3101	1/1	0.92	0.15	49,49,49,49	0
56	MG	1a	1704	1/1	0.92	0.18	53,53,53,53	0
56	MG	2a	3169	1/1	0.92	0.08	55,55,55,55	0
56	MG	1A	3903	1/1	0.92	0.10	29,29,29,29	0
56	MG	1a	1709	1/1	0.92	0.17	43,43,43,43	0
56	MG	1a	1710	1/1	0.92	0.34	61,61,61,61	0
56	MG	2A	3112	1/1	0.92	0.18	57,57,57,57	0
56	MG	1a	1711	1/1	0.92	0.15	48,48,48,48	0
56	MG	2a	3180	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3745	1/1	0.92	0.20	50,50,50,50	0
56	MG	1A	3747	1/1	0.92	0.13	55,55,55,55	0
56	MG	1a	1716	1/1	0.92	0.11	49,49,49,49	0
56	MG	1B	213	1/1	0.92	0.17	50,50,50,50	0
56	MG	2A	3386	1/1	0.92	0.12	46,46,46,46	0
56	MG	2A	3389	1/1	0.92	0.26	53,53,53,53	0
56	MG	1A	3430	1/1	0.92	0.14	48,48,48,48	0
56	MG	1A	3614	1/1	0.92	0.08	34,34,34,34	0
56	MG	1a	1730	1/1	0.92	0.14	46,46,46,46	0
56	MG	1B	220	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	3280	1/1	0.92	0.13	43,43,43,43	0
56	MG	2A	3404	1/1	0.92	0.13	65,65,65,65	0
56	MG	2A	3145	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3522	1/1	0.92	0.13	31,31,31,31	0
56	MG	1A	3365	1/1	0.92	0.12	50,50,50,50	0
56	MG	1a	1752	1/1	0.92	0.10	41,41,41,41	0
56	MG	2A	3758	1/1	0.92	0.07	35,35,35,35	0
56	MG	1a	1753	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3159	1/1	0.92	0.08	58,58,58,58	0
56	MG	1A	3620	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3418	1/1	0.92	0.13	43,43,43,43	0
56	MG	1B	233	1/1	0.92	0.10	63,63,63,63	0
56	MG	1D	301	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3929	1/1	0.92	0.10	41,41,41,41	0
56	MG	1a	1767	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3770	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3525	1/1	0.92	0.09	42,42,42,42	0
56	MG	2A	3779	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3431	1/1	0.92	0.14	54,54,54,54	0
56	MG	1a	1770	1/1	0.92	0.19	46,46,46,46	0
56	MG	1A	3780	1/1	0.92	0.08	39,39,39,39	0
56	MG	2A	3180	1/1	0.92	0.18	58,58,58,58	0
56	MG	1a	1774	1/1	0.92	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2d	302	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3783	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3188	1/1	0.92	0.24	67,67,67,67	0
56	MG	2A	3191	1/1	0.92	0.17	55,55,55,55	0
56	MG	2A	3450	1/1	0.92	0.18	51,51,51,51	0
56	MG	2r	101	1/1	0.92	0.10	56,56,56,56	0
56	MG	2r	102	1/1	0.92	0.11	54,54,54,54	0
56	MG	1G	203	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3800	1/1	0.92	0.11	37,37,37,37	0
56	MG	1A	3088	1/1	0.92	0.22	37,37,37,37	0
56	MG	2w	103	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3792	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3200	1/1	0.92	0.28	63,63,63,63	0
56	MG	1A	3794	1/1	0.92	0.13	18,18,18,18	0
56	MG	1A	3639	1/1	0.92	0.09	50,50,50,50	0
56	MG	2A	3204	1/1	0.92	0.16	54,54,54,54	0
56	MG	2x	104	1/1	0.92	0.14	48,48,48,48	0
56	MG	2A	3464	1/1	0.92	0.15	46,46,46,46	0
56	MG	2A	3823	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3466	1/1	0.92	0.11	40,40,40,40	0
56	MG	1A	3455	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3472	1/1	0.92	0.07	45,45,45,45	0
56	MG	1A	3532	1/1	0.92	0.14	37,37,37,37	0
56	MG	1a	1796	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	4024	1/1	0.93	0.12	20,20,20,20	0
56	MG	2A	3852	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3489	1/1	0.93	0.07	56,56,56,56	0
56	MG	2A	3854	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3861	1/1	0.93	0.10	51,51,51,51	0
56	MG	1a	1605	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3606	1/1	0.93	0.13	32,32,32,32	0
56	MG	2A	3492	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3613	1/1	0.93	0.23	56,56,56,56	0
56	MG	2A	3495	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3871	1/1	0.93	0.07	52,52,52,52	0
56	MG	1a	1611	1/1	0.93	0.07	57,57,57,57	0
56	MG	1a	1613	1/1	0.93	0.12	48,48,48,48	0
56	MG	1w	103	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3889	1/1	0.93	0.13	44,44,44,44	0
56	MG	1a	1624	1/1	0.93	0.22	47,47,47,47	0
56	MG	2A	3250	1/1	0.93	0.16	56,56,56,56	0
56	MG	1a	1625	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
56	MG	2A	3506	1/1	0.93	0.14	53,53,53,53	0
56	MG	2B	209	1/1	0.93	0.19	53,53,53,53	0
56	MG	2A	3509	1/1	0.93	0.19	58,58,58,58	0
56	MG	2A	3510	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3103	1/1	0.93	0.11	56,56,56,56	0
56	MG	1A	3234	1/1	0.93	0.21	26,26,26,26	0
56	MG	2A	3515	1/1	0.93	0.15	35,35,35,35	0
56	MG	2A	3517	1/1	0.93	0.14	55,55,55,55	0
56	MG	1x	105	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3192	1/1	0.93	0.09	35,35,35,35	0
56	MG	1x	109	1/1	0.93	0.18	65,65,65,65	0
56	MG	2D	301	1/1	0.93	0.12	41,41,41,41	0
56	MG	1A	3754	1/1	0.93	0.10	45,45,45,45	0
56	MG	2A	3259	1/1	0.93	0.18	49,49,49,49	0
56	MG	2E	302	1/1	0.93	0.13	52,52,52,52	0
56	MG	2A	3532	1/1	0.93	0.15	32,32,32,32	0
56	MG	2A	3536	1/1	0.93	0.06	38,38,38,38	0
56	MG	1A	3246	1/1	0.93	0.09	26,26,26,26	0
56	MG	2A	3539	1/1	0.93	0.08	31,31,31,31	0
56	MG	1A	3901	1/1	0.93	0.07	33,33,33,33	0
56	MG	2A	3264	1/1	0.93	0.17	46,46,46,46	0
56	MG	2A	3265	1/1	0.93	0.12	43,43,43,43	0
56	MG	2A	3266	1/1	0.93	0.07	42,42,42,42	0
56	MG	2P	201	1/1	0.93	0.25	46,46,46,46	0
56	MG	2P	202	1/1	0.93	0.06	52,52,52,52	0
56	MG	2Q	202	1/1	0.93	0.08	44,44,44,44	0
56	MG	1y	101	1/1	0.93	0.18	41,41,41,41	0
56	MG	1A	3757	1/1	0.93	0.05	47,47,47,47	0
56	MG	1A	4057	1/1	0.93	0.16	40,40,40,40	0
56	MG	2T	201	1/1	0.93	0.11	49,49,49,49	0
56	MG	1A	3759	1/1	0.93	0.10	45,45,45,45	0
56	MG	2A	3274	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	4059	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3438	1/1	0.93	0.13	44,44,44,44	0
56	MG	20	101	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3569	1/1	0.93	0.08	31,31,31,31	0
56	MG	2A	3012	1/1	0.93	0.07	34,34,34,34	0
56	MG	23	101	1/1	0.93	0.16	54,54,54,54	0
56	MG	25	101	1/1	0.93	0.25	53,53,53,53	0
56	MG	2A	3279	1/1	0.93	0.07	48,48,48,48	0
56	MG	1A	3440	1/1	0.93	0.19	51,51,51,51	0
56	MG	2A	3282	1/1	0.93	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	28	102	1/1	0.93	0.18	47,47,47,47	0
56	MG	28	104	1/1	0.93	0.17	53,53,53,53	0
56	MG	2A	3580	1/1	0.93	0.09	37,37,37,37	0
56	MG	2A	3584	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3444	1/1	0.93	0.12	36,36,36,36	0
56	MG	1a	1659	1/1	0.93	0.21	58,58,58,58	0
56	MG	2A	3589	1/1	0.93	0.12	54,54,54,54	0
56	MG	2A	3591	1/1	0.93	0.08	33,33,33,33	0
56	MG	2A	3595	1/1	0.93	0.22	58,58,58,58	0
56	MG	2A	3285	1/1	0.93	0.10	45,45,45,45	0
56	MG	1A	4072	1/1	0.93	0.06	18,18,18,18	0
56	MG	1A	3623	1/1	0.93	0.24	37,37,37,37	0
56	MG	2a	3019	1/1	0.93	0.12	59,59,59,59	0
56	MG	1a	1662	1/1	0.93	0.10	54,54,54,54	0
56	MG	2a	3023	1/1	0.93	0.28	65,65,65,65	0
56	MG	1a	1663	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3624	1/1	0.93	0.17	54,54,54,54	0
56	MG	2A	3036	1/1	0.93	0.12	43,43,43,43	0
56	MG	2A	3294	1/1	0.93	0.06	50,50,50,50	0
56	MG	1A	3922	1/1	0.93	0.07	22,22,22,22	0
56	MG	2a	3030	1/1	0.93	0.06	46,46,46,46	0
56	MG	1A	4089	1/1	0.93	0.10	20,20,20,20	0
56	MG	1A	4095	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	4097	1/1	0.93	0.08	49,49,49,49	0
56	MG	2a	3037	1/1	0.93	0.17	46,46,46,46	0
56	MG	1a	1672	1/1	0.93	0.20	48,48,48,48	0
56	MG	1A	3923	1/1	0.93	0.11	22,22,22,22	0
56	MG	1A	3778	1/1	0.93	0.21	52,52,52,52	0
56	MG	1A	3625	1/1	0.93	0.16	39,39,39,39	0
56	MG	1A	3631	1/1	0.93	0.16	49,49,49,49	0
56	MG	1B	202	1/1	0.93	0.18	38,38,38,38	0
56	MG	2A	3060	1/1	0.93	0.20	53,53,53,53	0
56	MG	2a	3048	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3063	1/1	0.93	0.20	57,57,57,57	0
56	MG	1A	3087	1/1	0.93	0.16	21,21,21,21	0
56	MG	2A	3315	1/1	0.93	0.27	57,57,57,57	0
56	MG	1A	3314	1/1	0.93	0.24	40,40,40,40	0
56	MG	2a	3054	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3070	1/1	0.93	0.08	46,46,46,46	0
56	MG	1B	210	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3073	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3324	1/1	0.93	0.10	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3454	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3323	1/1	0.93	0.15	36,36,36,36	0
56	MG	1A	3252	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3330	1/1	0.93	0.16	60,60,60,60	0
56	MG	1A	3184	1/1	0.93	0.10	29,29,29,29	0
56	MG	1A	3940	1/1	0.93	0.15	46,46,46,46	0
56	MG	2A	3341	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3657	1/1	0.93	0.09	51,51,51,51	0
56	MG	2a	3078	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3342	1/1	0.93	0.13	56,56,56,56	0
56	MG	2a	3081	1/1	0.93	0.18	60,60,60,60	0
56	MG	1A	3381	1/1	0.93	0.13	50,50,50,50	0
56	MG	2a	3084	1/1	0.93	0.23	62,62,62,62	0
56	MG	2A	3091	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3945	1/1	0.93	0.08	15,15,15,15	0
56	MG	2A	3347	1/1	0.93	0.13	54,54,54,54	0
56	MG	2a	3092	1/1	0.93	0.21	51,51,51,51	0
56	MG	2A	3666	1/1	0.93	0.10	58,58,58,58	0
56	MG	2A	3096	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3803	1/1	0.93	0.08	18,18,18,18	0
56	MG	2a	3098	1/1	0.93	0.14	67,67,67,67	0
56	MG	1B	224	1/1	0.93	0.07	46,46,46,46	0
56	MG	2a	3100	1/1	0.93	0.11	58,58,58,58	0
56	MG	1B	226	1/1	0.93	0.08	36,36,36,36	0
56	MG	2a	3104	1/1	0.93	0.15	62,62,62,62	0
56	MG	2a	3105	1/1	0.93	0.18	53,53,53,53	0
56	MG	1B	228	1/1	0.93	0.07	59,59,59,59	0
56	MG	2A	3103	1/1	0.93	0.17	50,50,50,50	0
56	MG	1A	3804	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3356	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3687	1/1	0.93	0.07	61,61,61,61	0
56	MG	2A	3688	1/1	0.93	0.09	36,36,36,36	0
56	MG	1A	3208	1/1	0.93	0.07	42,42,42,42	0
56	MG	1B	232	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3692	1/1	0.93	0.14	43,43,43,43	0
56	MG	2A	3693	1/1	0.93	0.17	57,57,57,57	0
56	MG	2a	3123	1/1	0.93	0.27	59,59,59,59	0
56	MG	2A	3361	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3950	1/1	0.93	0.11	34,34,34,34	0
56	MG	1A	3951	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3095	1/1	0.93	0.19	44,44,44,44	0
56	MG	2A	3700	1/1	0.93	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3154	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3959	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3337	1/1	0.93	0.07	35,35,35,35	0
56	MG	2A	3705	1/1	0.93	0.12	47,47,47,47	0
56	MG	1a	1740	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3121	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3481	1/1	0.93	0.10	27,27,27,27	0
56	MG	2a	3144	1/1	0.93	0.15	76,76,76,76	0
56	MG	1A	3825	1/1	0.93	0.14	46,46,46,46	0
56	MG	2A	3131	1/1	0.93	0.07	46,46,46,46	0
56	MG	1A	3220	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3224	1/1	0.93	0.10	40,40,40,40	0
56	MG	1a	1758	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3121	1/1	0.93	0.08	30,30,30,30	0
56	MG	2A	3150	1/1	0.93	0.16	52,52,52,52	0
56	MG	1a	1761	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3387	1/1	0.93	0.06	48,48,48,48	0
56	MG	2A	3152	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3728	1/1	0.93	0.11	39,39,39,39	0
56	MG	1a	1762	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3391	1/1	0.93	0.10	47,47,47,47	0
56	MG	2a	3176	1/1	0.93	0.16	40,40,40,40	0
56	MG	2A	3393	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3738	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3694	1/1	0.93	0.10	17,17,17,17	0
56	MG	2A	3398	1/1	0.93	0.15	60,60,60,60	0
56	MG	1a	1765	1/1	0.93	0.19	52,52,52,52	0
56	MG	1A	3985	1/1	0.93	0.07	40,40,40,40	0
56	MG	2A	3162	1/1	0.93	0.11	60,60,60,60	0
56	MG	1A	3347	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3989	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3407	1/1	0.93	0.09	62,62,62,62	0
56	MG	2A	3166	1/1	0.93	0.18	51,51,51,51	0
56	MG	1R	205	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3569	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3503	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3417	1/1	0.93	0.09	45,45,45,45	0
56	MG	1A	3998	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3416	1/1	0.93	0.09	50,50,50,50	0
56	MG	1a	1780	1/1	0.93	0.08	51,51,51,51	0
56	MG	2A	3419	1/1	0.93	0.21	41,41,41,41	0
56	MG	2A	3421	1/1	0.93	0.18	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3573	1/1	0.93	0.14	33,33,33,33	0
56	MG	2A	3762	1/1	0.93	0.22	60,60,60,60	0
56	MG	1U	205	1/1	0.93	0.22	38,38,38,38	0
56	MG	2A	3187	1/1	0.93	0.18	49,49,49,49	0
56	MG	1a	1783	1/1	0.93	0.11	49,49,49,49	0
56	MG	1A	3577	1/1	0.93	0.41	35,35,35,35	0
56	MG	1A	3421	1/1	0.93	0.09	39,39,39,39	0
56	MG	1a	1790	1/1	0.93	0.18	77,77,77,77	0
56	MG	2a	3224	1/1	0.93	0.23	62,62,62,62	0
56	MG	1W	202	1/1	0.93	0.12	34,34,34,34	0
56	MG	2A	3772	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3437	1/1	0.93	0.23	46,46,46,46	0
56	MG	1W	205	1/1	0.93	0.12	28,28,28,28	0
56	MG	1A	3590	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3729	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3202	1/1	0.93	0.10	39,39,39,39	0
56	MG	1A	4005	1/1	0.93	0.13	68,68,68,68	0
56	MG	1A	3422	1/1	0.93	0.12	42,42,42,42	0
56	MG	2A	3453	1/1	0.93	0.23	43,43,43,43	0
56	MG	1A	3873	1/1	0.93	0.13	39,39,39,39	0
56	MG	2A	3206	1/1	0.93	0.10	45,45,45,45	0
56	MG	2l	201	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3424	1/1	0.93	0.09	34,34,34,34	0
56	MG	10	106	1/1	0.93	0.07	40,40,40,40	0
56	MG	10	107	1/1	0.93	0.16	63,63,63,63	0
56	MG	12	101	1/1	0.93	0.09	44,44,44,44	0
56	MG	1A	4011	1/1	0.93	0.07	21,21,21,21	0
56	MG	2v	101	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3217	1/1	0.93	0.12	51,51,51,51	0
56	MG	15	102	1/1	0.93	0.18	32,32,32,32	0
56	MG	2w	102	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3809	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3468	1/1	0.93	0.10	36,36,36,36	0
56	MG	1A	3058	1/1	0.93	0.12	36,36,36,36	0
56	MG	1A	3877	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	3601	1/1	0.93	0.07	34,34,34,34	0
56	MG	2A	3824	1/1	0.93	0.10	34,34,34,34	0
56	MG	2A	3826	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3285	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3477	1/1	0.93	0.16	48,48,48,48	0
56	MG	1a	1601	1/1	0.93	0.18	60,60,60,60	0
56	MG	2A	3479	1/1	0.93	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3842	1/1	0.93	0.12	60,60,60,60	0
58	ZN	14	501	1/1	0.93	0.14	110,110,110,110	0
56	MG	1a	1602	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3486	1/1	0.93	0.17	41,41,41,41	0
56	MG	1U	207	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	3797	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3229	1/1	0.94	0.07	31,31,31,31	0
56	MG	1A	3982	1/1	0.94	0.07	37,37,37,37	0
56	MG	2A	3233	1/1	0.94	0.27	43,43,43,43	0
56	MG	2A	3875	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3508	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3165	1/1	0.94	0.13	34,34,34,34	0
56	MG	1A	3986	1/1	0.94	0.06	32,32,32,32	0
56	MG	2B	202	1/1	0.94	0.07	53,53,53,53	0
56	MG	2B	203	1/1	0.94	0.15	63,63,63,63	0
56	MG	1a	1811	1/1	0.94	0.10	56,56,56,56	0
56	MG	1a	1812	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3083	1/1	0.94	0.24	28,28,28,28	0
56	MG	1A	3407	1/1	0.94	0.07	37,37,37,37	0
56	MG	2A	3248	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3519	1/1	0.94	0.15	57,57,57,57	0
56	MG	2B	211	1/1	0.94	0.16	52,52,52,52	0
56	MG	1Z	3700	1/1	0.94	0.13	57,57,57,57	0
56	MG	1A	3309	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3805	1/1	0.94	0.09	12,12,12,12	0
56	MG	1A	3626	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3628	1/1	0.94	0.08	32,32,32,32	0
56	MG	1A	4000	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3814	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3540	1/1	0.94	0.13	48,48,48,48	0
56	MG	1A	3815	1/1	0.94	0.09	23,23,23,23	0
56	MG	2D	302	1/1	0.94	0.16	42,42,42,42	0
56	MG	2A	3544	1/1	0.94	0.15	53,53,53,53	0
56	MG	13	105	1/1	0.94	0.11	19,19,19,19	0
56	MG	2A	3547	1/1	0.94	0.09	43,43,43,43	0
56	MG	1t	201	1/1	0.94	0.26	50,50,50,50	0
56	MG	2A	3552	1/1	0.94	0.11	38,38,38,38	0
56	MG	1v	101	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3262	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3227	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3561	1/1	0.94	0.11	32,32,32,32	0
56	MG	2F	304	1/1	0.94	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3168	1/1	0.94	0.13	23,23,23,23	0
56	MG	1A	3523	1/1	0.94	0.11	30,30,30,30	0
56	MG	1A	3317	1/1	0.94	0.16	33,33,33,33	0
56	MG	1A	3641	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3830	1/1	0.94	0.08	10,10,10,10	0
56	MG	1w	107	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3319	1/1	0.94	0.20	46,46,46,46	0
56	MG	1a	1603	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3231	1/1	0.94	0.09	37,37,37,37	0
56	MG	2U	201	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3651	1/1	0.94	0.09	29,29,29,29	0
56	MG	1a	1606	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3527	1/1	0.94	0.08	44,44,44,44	0
56	MG	1x	112	1/1	0.94	0.18	50,50,50,50	0
56	MG	2A	3587	1/1	0.94	0.16	70,70,70,70	0
56	MG	1A	4022	1/1	0.94	0.10	45,45,45,45	0
56	MG	20	103	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3022	1/1	0.94	0.13	36,36,36,36	0
56	MG	1A	3002	1/1	0.94	0.11	52,52,52,52	0
56	MG	23	102	1/1	0.94	0.10	59,59,59,59	0
56	MG	23	104	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3592	1/1	0.94	0.16	44,44,44,44	0
56	MG	1a	1621	1/1	0.94	0.16	50,50,50,50	0
56	MG	1a	1622	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3123	1/1	0.94	0.16	32,32,32,32	0
56	MG	27	101	1/1	0.94	0.25	44,44,44,44	0
56	MG	1A	3844	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3244	1/1	0.94	0.10	44,44,44,44	0
56	MG	2a	3001	1/1	0.94	0.18	60,60,60,60	0
56	MG	2A	3009	1/1	0.94	0.11	44,44,44,44	0
56	MG	2a	3003	1/1	0.94	0.07	62,62,62,62	0
56	MG	2A	3606	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3010	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3295	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	4031	1/1	0.94	0.10	27,27,27,27	0
56	MG	2A	3611	1/1	0.94	0.14	53,53,53,53	0
56	MG	2A	3013	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	4033	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	4039	1/1	0.94	0.08	65,65,65,65	0
56	MG	2a	3013	1/1	0.94	0.20	62,62,62,62	0
56	MG	2a	3014	1/1	0.94	0.13	48,48,48,48	0
56	MG	2a	3017	1/1	0.94	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3429	1/1	0.94	0.12	29,29,29,29	0
56	MG	2A	3619	1/1	0.94	0.08	58,58,58,58	0
56	MG	2a	3020	1/1	0.94	0.10	71,71,71,71	0
56	MG	1A	3127	1/1	0.94	0.19	35,35,35,35	0
56	MG	1A	4043	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3249	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3026	1/1	0.94	0.27	43,43,43,43	0
56	MG	1A	3436	1/1	0.94	0.06	38,38,38,38	0
56	MG	2A	3308	1/1	0.94	0.09	60,60,60,60	0
56	MG	2A	3628	1/1	0.94	0.08	54,54,54,54	0
56	MG	2A	3030	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3310	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	4046	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3032	1/1	0.94	0.09	45,45,45,45	0
56	MG	2a	3036	1/1	0.94	0.18	44,44,44,44	0
56	MG	2A	3035	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3636	1/1	0.94	0.10	28,28,28,28	0
56	MG	1a	1640	1/1	0.94	0.11	32,32,32,32	0
56	MG	2A	3641	1/1	0.94	0.07	33,33,33,33	0
56	MG	2A	3038	1/1	0.94	0.09	29,29,29,29	0
56	MG	1A	3861	1/1	0.94	0.12	27,27,27,27	0
56	MG	1a	1644	1/1	0.94	0.16	61,61,61,61	0
56	MG	2A	3646	1/1	0.94	0.11	35,35,35,35	0
56	MG	2A	3322	1/1	0.94	0.22	57,57,57,57	0
56	MG	2A	3323	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	4050	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3865	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3326	1/1	0.94	0.15	51,51,51,51	0
56	MG	2A	3043	1/1	0.94	0.06	45,45,45,45	0
56	MG	2A	3045	1/1	0.94	0.23	65,65,65,65	0
56	MG	1A	3677	1/1	0.94	0.08	28,28,28,28	0
56	MG	2A	3658	1/1	0.94	0.19	61,61,61,61	0
56	MG	2a	3058	1/1	0.94	0.05	56,56,56,56	0
56	MG	2A	3659	1/1	0.94	0.22	46,46,46,46	0
56	MG	2A	3331	1/1	0.94	0.31	63,63,63,63	0
56	MG	2a	3063	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3870	1/1	0.94	0.09	61,61,61,61	0
56	MG	1A	3678	1/1	0.94	0.07	27,27,27,27	0
56	MG	2a	3067	1/1	0.94	0.09	63,63,63,63	0
56	MG	1A	3128	1/1	0.94	0.25	36,36,36,36	0
56	MG	1A	3688	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	4061	1/1	0.94	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3073	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3344	1/1	0.94	0.06	37,37,37,37	0
56	MG	2A	3059	1/1	0.94	0.14	41,41,41,41	0
56	MG	1a	1664	1/1	0.94	0.07	45,45,45,45	0
56	MG	2a	3079	1/1	0.94	0.21	52,52,52,52	0
56	MG	2A	3670	1/1	0.94	0.07	51,51,51,51	0
56	MG	2A	3061	1/1	0.94	0.07	52,52,52,52	0
56	MG	2A	3062	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3682	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3690	1/1	0.94	0.09	24,24,24,24	0
56	MG	2a	3086	1/1	0.94	0.12	44,44,44,44	0
56	MG	1A	3879	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	4071	1/1	0.94	0.08	38,38,38,38	0
56	MG	1a	1669	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3692	1/1	0.94	0.07	28,28,28,28	0
56	MG	1A	3006	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3549	1/1	0.94	0.18	31,31,31,31	0
56	MG	2A	3078	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3081	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3083	1/1	0.94	0.11	44,44,44,44	0
56	MG	2a	3101	1/1	0.94	0.16	55,55,55,55	0
56	MG	1a	1674	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	4077	1/1	0.94	0.06	35,35,35,35	0
56	MG	1a	1677	1/1	0.94	0.16	47,47,47,47	0
56	MG	2a	3106	1/1	0.94	0.18	48,48,48,48	0
56	MG	1a	1678	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	4080	1/1	0.94	0.16	59,59,59,59	0
56	MG	1A	3885	1/1	0.94	0.16	47,47,47,47	0
56	MG	2a	3111	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3696	1/1	0.94	0.07	28,28,28,28	0
56	MG	2A	3095	1/1	0.94	0.11	50,50,50,50	0
56	MG	1a	1684	1/1	0.94	0.10	47,47,47,47	0
56	MG	1a	1689	1/1	0.94	0.17	48,48,48,48	0
56	MG	2A	3374	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	4094	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3887	1/1	0.94	0.09	26,26,26,26	0
56	MG	1A	3699	1/1	0.94	0.07	26,26,26,26	0
56	MG	1A	3702	1/1	0.94	0.08	28,28,28,28	0
56	MG	1A	3706	1/1	0.94	0.10	12,12,12,12	0
56	MG	2A	3384	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3133	1/1	0.94	0.14	31,31,31,31	0
56	MG	1A	3442	1/1	0.94	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4106	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3257	1/1	0.94	0.09	31,31,31,31	0
56	MG	1B	203	1/1	0.94	0.20	52,52,52,52	0
56	MG	1a	1708	1/1	0.94	0.24	48,48,48,48	0
56	MG	2a	3139	1/1	0.94	0.15	71,71,71,71	0
56	MG	2A	3731	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3733	1/1	0.94	0.08	35,35,35,35	0
56	MG	2A	3735	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3556	1/1	0.94	0.17	52,52,52,52	0
56	MG	2A	3395	1/1	0.94	0.10	46,46,46,46	0
56	MG	1A	3348	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3561	1/1	0.94	0.21	38,38,38,38	0
56	MG	1a	1712	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3123	1/1	0.94	0.21	59,59,59,59	0
56	MG	2A	3401	1/1	0.94	0.09	55,55,55,55	0
56	MG	2a	3158	1/1	0.94	0.09	68,68,68,68	0
56	MG	1A	3725	1/1	0.94	0.08	19,19,19,19	0
56	MG	2a	3164	1/1	0.94	0.10	65,65,65,65	0
56	MG	2A	3126	1/1	0.94	0.08	61,61,61,61	0
56	MG	2A	3127	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3040	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3563	1/1	0.94	0.17	53,53,53,53	0
56	MG	1A	3262	1/1	0.94	0.15	31,31,31,31	0
56	MG	1a	1721	1/1	0.94	0.22	59,59,59,59	0
56	MG	1a	1722	1/1	0.94	0.32	54,54,54,54	0
56	MG	1A	3146	1/1	0.94	0.09	39,39,39,39	0
56	MG	1A	3148	1/1	0.94	0.10	19,19,19,19	0
56	MG	1A	3268	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3201	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3369	1/1	0.94	0.08	52,52,52,52	0
56	MG	1a	1734	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3926	1/1	0.94	0.13	27,27,27,27	0
56	MG	1a	1737	1/1	0.94	0.19	55,55,55,55	0
56	MG	2a	3190	1/1	0.94	0.20	63,63,63,63	0
56	MG	2A	3425	1/1	0.94	0.12	43,43,43,43	0
56	MG	2a	3194	1/1	0.94	0.09	58,58,58,58	0
56	MG	2A	3160	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3576	1/1	0.94	0.14	28,28,28,28	0
56	MG	1A	3202	1/1	0.94	0.05	28,28,28,28	0
56	MG	1a	1742	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3432	1/1	0.94	0.25	45,45,45,45	0
56	MG	1A	3580	1/1	0.94	0.19	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3771	1/1	0.94	0.09	28,28,28,28	0
56	MG	1A	3068	1/1	0.94	0.11	43,43,43,43	0
56	MG	1A	3585	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3777	1/1	0.94	0.11	64,64,64,64	0
56	MG	2a	3212	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3172	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3479	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3781	1/1	0.94	0.10	70,70,70,70	0
56	MG	2a	3216	1/1	0.94	0.14	58,58,58,58	0
56	MG	1D	308	1/1	0.94	0.06	35,35,35,35	0
56	MG	2A	3176	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3596	1/1	0.94	0.08	37,37,37,37	0
56	MG	1E	304	1/1	0.94	0.11	26,26,26,26	0
56	MG	2A	3789	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3451	1/1	0.94	0.10	37,37,37,37	0
56	MG	1E	307	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3101	1/1	0.94	0.05	58,58,58,58	0
56	MG	1A	3376	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3007	1/1	0.94	0.06	30,30,30,30	0
56	MG	1E	312	1/1	0.94	0.13	45,45,45,45	0
56	MG	1a	1769	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3160	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3602	1/1	0.94	0.08	30,30,30,30	0
56	MG	1A	3288	1/1	0.94	0.05	30,30,30,30	0
56	MG	2A	3197	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3776	1/1	0.94	0.08	42,42,42,42	0
56	MG	1N	201	1/1	0.94	0.23	43,43,43,43	0
56	MG	2A	3813	1/1	0.94	0.08	67,67,67,67	0
56	MG	2k	201	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3815	1/1	0.94	0.10	41,41,41,41	0
56	MG	2A	3818	1/1	0.94	0.06	45,45,45,45	0
56	MG	1A	3292	1/1	0.94	0.13	26,26,26,26	0
56	MG	2q	202	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3498	1/1	0.94	0.13	41,41,41,41	0
56	MG	1O	205	1/1	0.94	0.09	47,47,47,47	0
56	MG	2A	3825	1/1	0.94	0.11	43,43,43,43	0
56	MG	1A	3953	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3956	1/1	0.94	0.10	66,66,66,66	0
56	MG	1a	1785	1/1	0.94	0.08	63,63,63,63	0
56	MG	1Q	206	1/1	0.94	0.16	36,36,36,36	0
56	MG	2A	3833	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3781	1/1	0.94	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3499	1/1	0.94	0.08	47,47,47,47	0
56	MG	1a	1792	1/1	0.94	0.15	36,36,36,36	0
56	MG	2A	3845	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3846	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3786	1/1	0.94	0.13	25,25,25,25	0
56	MG	2y	101	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3850	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	3788	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3386	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3105	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	3395	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3301	1/1	0.94	0.21	48,48,48,48	0
56	MG	1a	1802	1/1	0.94	0.08	52,52,52,52	0
56	MG	2A	3225	1/1	0.94	0.43	44,44,44,44	0
56	MG	1a	1823	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3256	1/1	0.95	0.15	40,40,40,40	0
56	MG	2A	3241	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3527	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3994	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3414	1/1	0.95	0.16	44,44,44,44	0
56	MG	2A	3244	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3537	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3245	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3627	1/1	0.95	0.16	29,29,29,29	0
56	MG	2B	212	1/1	0.95	0.10	52,52,52,52	0
56	MG	1f	202	1/1	0.95	0.19	58,58,58,58	0
56	MG	1A	3513	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3416	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3633	1/1	0.95	0.07	23,23,23,23	0
56	MG	2B	217	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3546	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3635	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3140	1/1	0.95	0.09	28,28,28,28	0
56	MG	1A	3420	1/1	0.95	0.06	34,34,34,34	0
56	MG	1A	3144	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	3338	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3817	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3819	1/1	0.95	0.06	52,52,52,52	0
56	MG	1A	3042	1/1	0.95	0.12	22,22,22,22	0
56	MG	1A	3644	1/1	0.95	0.07	30,30,30,30	0
56	MG	2A	3564	1/1	0.95	0.10	46,46,46,46	0
56	MG	18	104	1/1	0.95	0.12	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	18	105	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	4013	1/1	0.95	0.07	17,17,17,17	0
56	MG	1A	3200	1/1	0.95	0.14	26,26,26,26	0
56	MG	1A	3104	1/1	0.95	0.08	33,33,33,33	0
56	MG	1A	3653	1/1	0.95	0.05	23,23,23,23	0
56	MG	2A	3270	1/1	0.95	0.10	44,44,44,44	0
56	MG	2N	201	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	4020	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3272	1/1	0.95	0.07	54,54,54,54	0
56	MG	2P	203	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3427	1/1	0.95	0.06	37,37,37,37	0
56	MG	1a	1607	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3150	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3034	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	4025	1/1	0.95	0.15	29,29,29,29	0
56	MG	2T	202	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3270	1/1	0.95	0.16	48,48,48,48	0
56	MG	1a	1615	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3431	1/1	0.95	0.13	33,33,33,33	0
56	MG	2W	203	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	4029	1/1	0.95	0.06	55,55,55,55	0
56	MG	2X	102	1/1	0.95	0.13	44,44,44,44	0
56	MG	2A	3004	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3082	1/1	0.95	0.16	23,23,23,23	0
56	MG	1A	3435	1/1	0.95	0.16	43,43,43,43	0
56	MG	2A	3008	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	4032	1/1	0.95	0.06	22,22,22,22	0
56	MG	2A	3290	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3272	1/1	0.95	0.21	54,54,54,54	0
56	MG	1A	4036	1/1	0.95	0.05	28,28,28,28	0
56	MG	1A	3672	1/1	0.95	0.09	10,10,10,10	0
56	MG	1A	3851	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3539	1/1	0.95	0.06	42,42,42,42	0
56	MG	1a	1631	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3352	1/1	0.95	0.14	32,32,32,32	0
56	MG	2A	3618	1/1	0.95	0.11	58,58,58,58	0
56	MG	1A	3856	1/1	0.95	0.11	31,31,31,31	0
56	MG	1A	3117	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3859	1/1	0.95	0.09	38,38,38,38	0
56	MG	1a	1639	1/1	0.95	0.20	52,52,52,52	0
56	MG	2A	3623	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3679	1/1	0.95	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3625	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	4049	1/1	0.95	0.05	33,33,33,33	0
56	MG	1a	1643	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3033	1/1	0.95	0.16	39,39,39,39	0
56	MG	1A	3051	1/1	0.95	0.10	25,25,25,25	0
56	MG	1A	3862	1/1	0.95	0.16	57,57,57,57	0
56	MG	2A	3631	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3686	1/1	0.95	0.08	48,48,48,48	0
56	MG	2a	3016	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3867	1/1	0.95	0.08	32,32,32,32	0
56	MG	2A	3634	1/1	0.95	0.06	26,26,26,26	0
56	MG	1a	1657	1/1	0.95	0.09	45,45,45,45	0
56	MG	1a	1658	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3053	1/1	0.95	0.07	44,44,44,44	0
56	MG	2a	3022	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3640	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3443	1/1	0.95	0.07	32,32,32,32	0
56	MG	2A	3044	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3871	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	3872	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3050	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3036	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3445	1/1	0.95	0.08	40,40,40,40	0
56	MG	2a	3032	1/1	0.95	0.18	51,51,51,51	0
56	MG	1A	4069	1/1	0.95	0.09	32,32,32,32	0
56	MG	1A	3446	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3328	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3652	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3654	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3447	1/1	0.95	0.08	39,39,39,39	0
56	MG	2A	3058	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3698	1/1	0.95	0.08	18,18,18,18	0
56	MG	1A	4075	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3371	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3336	1/1	0.95	0.07	38,38,38,38	0
56	MG	2a	3047	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3225	1/1	0.95	0.09	32,32,32,32	0
56	MG	1A	4078	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	4079	1/1	0.95	0.16	35,35,35,35	0
56	MG	1A	3705	1/1	0.95	0.05	15,15,15,15	0
56	MG	1A	4083	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3560	1/1	0.95	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3450	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3074	1/1	0.95	0.09	43,43,43,43	0
56	MG	1a	1682	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	4093	1/1	0.95	0.17	42,42,42,42	0
56	MG	2a	3059	1/1	0.95	0.24	46,46,46,46	0
56	MG	2A	3679	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3079	1/1	0.95	0.15	51,51,51,51	0
56	MG	2a	3062	1/1	0.95	0.15	64,64,64,64	0
56	MG	1A	3452	1/1	0.95	0.08	34,34,34,34	0
56	MG	2A	3683	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3082	1/1	0.95	0.14	45,45,45,45	0
56	MG	1a	1686	1/1	0.95	0.12	31,31,31,31	0
56	MG	1A	3124	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	3125	1/1	0.95	0.10	23,23,23,23	0
56	MG	1A	3895	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3088	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3461	1/1	0.95	0.15	35,35,35,35	0
56	MG	2a	3075	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	3568	1/1	0.95	0.12	52,52,52,52	0
56	MG	2a	3077	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	4103	1/1	0.95	0.17	47,47,47,47	0
56	MG	1a	1698	1/1	0.95	0.06	53,53,53,53	0
56	MG	1A	3462	1/1	0.95	0.13	34,34,34,34	0
56	MG	1a	1701	1/1	0.95	0.22	45,45,45,45	0
56	MG	2a	3082	1/1	0.95	0.16	50,50,50,50	0
56	MG	2A	3697	1/1	0.95	0.18	56,56,56,56	0
56	MG	1A	3465	1/1	0.95	0.10	56,56,56,56	0
56	MG	2A	3699	1/1	0.95	0.06	54,54,54,54	0
56	MG	1B	201	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3171	1/1	0.95	0.13	19,19,19,19	0
56	MG	1A	3902	1/1	0.95	0.11	30,30,30,30	0
56	MG	2a	3089	1/1	0.95	0.19	53,53,53,53	0
56	MG	2a	3090	1/1	0.95	0.12	59,59,59,59	0
56	MG	2a	3091	1/1	0.95	0.15	47,47,47,47	0
56	MG	2A	3102	1/1	0.95	0.09	37,37,37,37	0
56	MG	2A	3375	1/1	0.95	0.14	49,49,49,49	0
56	MG	1B	206	1/1	0.95	0.12	36,36,36,36	0
56	MG	2a	3095	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3018	1/1	0.95	0.08	32,32,32,32	0
56	MG	2a	3097	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3904	1/1	0.95	0.17	25,25,25,25	0
56	MG	2A	3710	1/1	0.95	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3731	1/1	0.95	0.07	31,31,31,31	0
56	MG	2A	3110	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3574	1/1	0.95	0.09	42,42,42,42	0
56	MG	2a	3103	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3469	1/1	0.95	0.15	33,33,33,33	0
56	MG	1A	3910	1/1	0.95	0.06	23,23,23,23	0
56	MG	1A	3735	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	3175	1/1	0.95	0.16	42,42,42,42	0
56	MG	2A	3116	1/1	0.95	0.06	48,48,48,48	0
56	MG	1a	1720	1/1	0.95	0.18	50,50,50,50	0
56	MG	2A	3392	1/1	0.95	0.10	43,43,43,43	0
56	MG	1B	218	1/1	0.95	0.08	36,36,36,36	0
56	MG	2a	3113	1/1	0.95	0.13	58,58,58,58	0
56	MG	2A	3394	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3915	1/1	0.95	0.12	21,21,21,21	0
56	MG	2A	3732	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3738	1/1	0.95	0.07	28,28,28,28	0
56	MG	1A	3472	1/1	0.95	0.08	43,43,43,43	0
56	MG	2a	3120	1/1	0.95	0.28	67,67,67,67	0
56	MG	1a	1727	1/1	0.95	0.09	37,37,37,37	0
56	MG	1a	1729	1/1	0.95	0.21	46,46,46,46	0
56	MG	1B	223	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3741	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3023	1/1	0.95	0.05	21,21,21,21	0
56	MG	2A	3133	1/1	0.95	0.06	35,35,35,35	0
56	MG	2A	3135	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3583	1/1	0.95	0.21	40,40,40,40	0
56	MG	2a	3132	1/1	0.95	0.18	58,58,58,58	0
56	MG	2A	3137	1/1	0.95	0.11	36,36,36,36	0
56	MG	2a	3134	1/1	0.95	0.21	49,49,49,49	0
56	MG	2A	3411	1/1	0.95	0.05	41,41,41,41	0
56	MG	1B	229	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3183	1/1	0.95	0.05	25,25,25,25	0
56	MG	2A	3146	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3148	1/1	0.95	0.19	37,37,37,37	0
56	MG	1a	1738	1/1	0.95	0.26	47,47,47,47	0
56	MG	2A	3752	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3241	1/1	0.95	0.13	62,62,62,62	0
56	MG	2A	3754	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3591	1/1	0.95	0.19	38,38,38,38	0
56	MG	2A	3420	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3752	1/1	0.95	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1744	1/1	0.95	0.10	52,52,52,52	0
56	MG	1a	1748	1/1	0.95	0.09	34,34,34,34	0
56	MG	2a	3162	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3388	1/1	0.95	0.18	46,46,46,46	0
56	MG	2A	3761	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3755	1/1	0.95	0.10	40,40,40,40	0
56	MG	1a	1754	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3315	1/1	0.95	0.09	35,35,35,35	0
56	MG	1D	311	1/1	0.95	0.16	29,29,29,29	0
56	MG	2A	3165	1/1	0.95	0.20	46,46,46,46	0
56	MG	2a	3171	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3433	1/1	0.95	0.24	49,49,49,49	0
56	MG	1E	301	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3062	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3484	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3761	1/1	0.95	0.06	30,30,30,30	0
56	MG	1A	3396	1/1	0.95	0.10	48,48,48,48	0
56	MG	2a	3184	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3776	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3398	1/1	0.95	0.16	37,37,37,37	0
56	MG	2A	3444	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3446	1/1	0.95	0.18	40,40,40,40	0
56	MG	2a	3189	1/1	0.95	0.10	49,49,49,49	0
56	MG	1a	1766	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3768	1/1	0.95	0.18	44,44,44,44	0
56	MG	2a	3192	1/1	0.95	0.24	55,55,55,55	0
56	MG	2A	3783	1/1	0.95	0.07	53,53,53,53	0
56	MG	1F	306	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3488	1/1	0.95	0.06	52,52,52,52	0
56	MG	1G	202	1/1	0.95	0.06	46,46,46,46	0
56	MG	2A	3186	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3132	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3456	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3771	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3607	1/1	0.95	0.07	31,31,31,31	0
56	MG	2A	3460	1/1	0.95	0.11	50,50,50,50	0
56	MG	2a	3210	1/1	0.95	0.20	54,54,54,54	0
56	MG	1A	3774	1/1	0.95	0.11	12,12,12,12	0
56	MG	1N	202	1/1	0.95	0.06	46,46,46,46	0
56	MG	2A	3802	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3803	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3804	1/1	0.95	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3955	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3775	1/1	0.95	0.13	26,26,26,26	0
56	MG	2A	3196	1/1	0.95	0.08	48,48,48,48	0
56	MG	1O	203	1/1	0.95	0.14	43,43,43,43	0
56	MG	2a	3220	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3198	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3608	1/1	0.95	0.06	42,42,42,42	0
56	MG	1a	1784	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3777	1/1	0.95	0.07	12,12,12,12	0
56	MG	2A	3816	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3610	1/1	0.95	0.14	34,34,34,34	0
56	MG	2A	3819	1/1	0.95	0.09	61,61,61,61	0
56	MG	1Q	204	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3964	1/1	0.95	0.10	45,45,45,45	0
56	MG	1a	1791	1/1	0.95	0.12	61,61,61,61	0
56	MG	2A	3485	1/1	0.95	0.10	56,56,56,56	0
56	MG	1R	203	1/1	0.95	0.25	42,42,42,42	0
56	MG	1a	1793	1/1	0.95	0.12	50,50,50,50	0
56	MG	2d	301	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	3967	1/1	0.95	0.07	29,29,29,29	0
56	MG	2e	201	1/1	0.95	0.08	52,52,52,52	0
56	MG	2g	201	1/1	0.95	0.16	64,64,64,64	0
56	MG	1A	3490	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3401	1/1	0.95	0.09	42,42,42,42	0
56	MG	2A	3215	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3216	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3493	1/1	0.95	0.20	52,52,52,52	0
56	MG	2l	203	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3186	1/1	0.95	0.08	41,41,41,41	0
56	MG	2m	201	1/1	0.95	0.21	61,61,61,61	0
56	MG	1A	3787	1/1	0.95	0.05	42,42,42,42	0
56	MG	2A	3220	1/1	0.95	0.13	49,49,49,49	0
56	MG	2A	3849	1/1	0.95	0.13	61,61,61,61	0
56	MG	1A	3980	1/1	0.95	0.06	59,59,59,59	0
56	MG	2A	3502	1/1	0.95	0.20	45,45,45,45	0
56	MG	1U	204	1/1	0.95	0.05	26,26,26,26	0
56	MG	1A	3100	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3500	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3856	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3858	1/1	0.95	0.06	55,55,55,55	0
56	MG	2A	3860	1/1	0.95	0.13	28,28,28,28	0
56	MG	1A	3067	1/1	0.95	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1809	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3138	1/1	0.95	0.11	23,23,23,23	0
56	MG	1A	3328	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3509	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3868	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3232	1/1	0.95	0.14	37,37,37,37	0
56	MG	1W	207	1/1	0.95	0.08	18,18,18,18	0
56	MG	2A	3873	1/1	0.95	0.15	59,59,59,59	0
56	MG	2A	3516	1/1	0.95	0.17	48,48,48,48	0
56	MG	2A	3237	1/1	0.95	0.26	55,55,55,55	0
56	MG	1A	3990	1/1	0.95	0.06	38,38,38,38	0
56	MG	2A	3522	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3584	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3267	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3368	1/1	0.96	0.06	58,58,58,58	0
56	MG	2A	3157	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3939	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3198	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3594	1/1	0.96	0.15	23,23,23,23	0
56	MG	2A	3859	1/1	0.96	0.08	51,51,51,51	0
56	MG	2A	3469	1/1	0.96	0.11	42,42,42,42	0
56	MG	1D	305	1/1	0.96	0.13	33,33,33,33	0
56	MG	2A	3471	1/1	0.96	0.08	47,47,47,47	0
56	MG	1D	306	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3595	1/1	0.96	0.25	33,33,33,33	0
56	MG	2A	3866	1/1	0.96	0.07	44,44,44,44	0
56	MG	1A	3471	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3167	1/1	0.96	0.13	34,34,34,34	0
56	MG	2A	3168	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3370	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3170	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3483	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3484	1/1	0.96	0.11	42,42,42,42	0
56	MG	1a	1741	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3767	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3949	1/1	0.96	0.07	44,44,44,44	0
56	MG	2B	201	1/1	0.96	0.15	52,52,52,52	0
56	MG	1A	3199	1/1	0.96	0.26	29,29,29,29	0
56	MG	1a	1749	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3112	1/1	0.96	0.12	23,23,23,23	0
56	MG	1E	309	1/1	0.96	0.14	19,19,19,19	0
56	MG	1A	3113	1/1	0.96	0.14	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3182	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3477	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3954	1/1	0.96	0.11	41,41,41,41	0
56	MG	1F	303	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3005	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3501	1/1	0.96	0.14	53,53,53,53	0
56	MG	1F	308	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3273	1/1	0.96	0.06	28,28,28,28	0
56	MG	1F	310	1/1	0.96	0.11	31,31,31,31	0
56	MG	1a	1764	1/1	0.96	0.12	33,33,33,33	0
56	MG	1G	201	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3957	1/1	0.96	0.07	30,30,30,30	0
56	MG	1A	3274	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3379	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3511	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3609	1/1	0.96	0.11	31,31,31,31	0
56	MG	2D	305	1/1	0.96	0.24	40,40,40,40	0
56	MG	1A	3115	1/1	0.96	0.06	31,31,31,31	0
56	MG	1a	1772	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3611	1/1	0.96	0.19	40,40,40,40	0
56	MG	1A	3204	1/1	0.96	0.11	35,35,35,35	0
56	MG	1a	1775	1/1	0.96	0.07	41,41,41,41	0
56	MG	2E	307	1/1	0.96	0.07	26,26,26,26	0
56	MG	1N	205	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3970	1/1	0.96	0.05	44,44,44,44	0
56	MG	1a	1778	1/1	0.96	0.22	54,54,54,54	0
56	MG	1A	3205	1/1	0.96	0.12	18,18,18,18	0
56	MG	2A	3211	1/1	0.96	0.10	51,51,51,51	0
56	MG	2F	306	1/1	0.96	0.11	47,47,47,47	0
56	MG	2A	3528	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3084	1/1	0.96	0.10	22,22,22,22	0
56	MG	2A	3531	1/1	0.96	0.06	54,54,54,54	0
56	MG	2O	201	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3974	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3535	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3214	1/1	0.96	0.10	43,43,43,43	0
56	MG	1P	203	1/1	0.96	0.25	29,29,29,29	0
56	MG	1A	3387	1/1	0.96	0.12	47,47,47,47	0
56	MG	1Q	203	1/1	0.96	0.04	33,33,33,33	0
56	MG	1A	3617	1/1	0.96	0.21	40,40,40,40	0
56	MG	2A	3541	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3213	1/1	0.96	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3543	1/1	0.96	0.10	39,39,39,39	0
56	MG	1a	1787	1/1	0.96	0.09	70,70,70,70	0
56	MG	1R	202	1/1	0.96	0.18	38,38,38,38	0
56	MG	1a	1789	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3290	1/1	0.96	0.20	25,25,25,25	0
56	MG	1A	3494	1/1	0.96	0.08	38,38,38,38	0
56	MG	2Y	201	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3983	1/1	0.96	0.12	39,39,39,39	0
56	MG	1S	201	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3984	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3556	1/1	0.96	0.12	28,28,28,28	0
56	MG	2A	3228	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3495	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3795	1/1	0.96	0.09	37,37,37,37	0
56	MG	23	103	1/1	0.96	0.14	53,53,53,53	0
56	MG	2A	3231	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3796	1/1	0.96	0.06	19,19,19,19	0
56	MG	1A	3497	1/1	0.96	0.21	38,38,38,38	0
56	MG	25	103	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3236	1/1	0.96	0.07	35,35,35,35	0
56	MG	1U	203	1/1	0.96	0.10	23,23,23,23	0
56	MG	2A	3568	1/1	0.96	0.07	51,51,51,51	0
56	MG	28	101	1/1	0.96	0.14	59,59,59,59	0
56	MG	1A	3392	1/1	0.96	0.05	35,35,35,35	0
56	MG	28	103	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3571	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3393	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3574	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3291	1/1	0.96	0.10	40,40,40,40	0
56	MG	1U	208	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3501	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3156	1/1	0.96	0.19	35,35,35,35	0
56	MG	1V	204	1/1	0.96	0.08	39,39,39,39	0
56	MG	2A	3585	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3299	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	3809	1/1	0.96	0.08	32,32,32,32	0
56	MG	2a	3011	1/1	0.96	0.06	49,49,49,49	0
56	MG	1a	1813	1/1	0.96	0.08	52,52,52,52	0
56	MG	1a	1814	1/1	0.96	0.14	51,51,51,51	0
56	MG	2A	3590	1/1	0.96	0.13	40,40,40,40	0
56	MG	1a	1815	1/1	0.96	0.06	48,48,48,48	0
56	MG	1a	1816	1/1	0.96	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1817	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3118	1/1	0.96	0.19	22,22,22,22	0
56	MG	1X	104	1/1	0.96	0.19	34,34,34,34	0
56	MG	2A	3255	1/1	0.96	0.12	60,60,60,60	0
56	MG	1A	3506	1/1	0.96	0.13	33,33,33,33	0
56	MG	2A	3603	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3813	1/1	0.96	0.07	35,35,35,35	0
56	MG	1b	301	1/1	0.96	0.05	70,70,70,70	0
56	MG	1Y	201	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3508	1/1	0.96	0.06	42,42,42,42	0
56	MG	1e	202	1/1	0.96	0.10	51,51,51,51	0
56	MG	2a	3029	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3400	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3162	1/1	0.96	0.13	25,25,25,25	0
56	MG	1A	3302	1/1	0.96	0.08	44,44,44,44	0
56	MG	10	102	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3222	1/1	0.96	0.11	28,28,28,28	0
56	MG	2a	3035	1/1	0.96	0.11	38,38,38,38	0
56	MG	10	105	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3269	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	4009	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3086	1/1	0.96	0.11	22,22,22,22	0
56	MG	11	101	1/1	0.96	0.20	29,29,29,29	0
56	MG	11	102	1/1	0.96	0.06	47,47,47,47	0
56	MG	11	103	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3822	1/1	0.96	0.09	20,20,20,20	0
56	MG	2A	3276	1/1	0.96	0.22	50,50,50,50	0
56	MG	2a	3046	1/1	0.96	0.20	55,55,55,55	0
56	MG	12	102	1/1	0.96	0.12	39,39,39,39	0
56	MG	13	103	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3646	1/1	0.96	0.05	31,31,31,31	0
56	MG	1A	3063	1/1	0.96	0.12	46,46,46,46	0
56	MG	2a	3051	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3281	1/1	0.96	0.06	36,36,36,36	0
56	MG	13	106	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3064	1/1	0.96	0.05	29,29,29,29	0
56	MG	1A	4016	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	4018	1/1	0.96	0.09	53,53,53,53	0
56	MG	1x	106	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	3412	1/1	0.96	0.18	38,38,38,38	0
56	MG	18	102	1/1	0.96	0.16	38,38,38,38	0
56	MG	1A	3066	1/1	0.96	0.11	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1x	111	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	4021	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3091	1/1	0.96	0.11	32,32,32,32	0
56	MG	1x	114	1/1	0.96	0.13	60,60,60,60	0
56	MG	19	101	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3230	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3663	1/1	0.96	0.05	16,16,16,16	0
56	MG	1A	3836	1/1	0.96	0.08	19,19,19,19	0
56	MG	1A	3838	1/1	0.96	0.08	43,43,43,43	0
56	MG	2a	3072	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3002	1/1	0.96	0.27	45,45,45,45	0
56	MG	1A	3839	1/1	0.96	0.05	17,17,17,17	0
56	MG	1A	3318	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3303	1/1	0.96	0.13	46,46,46,46	0
56	MG	2A	3006	1/1	0.96	0.20	50,50,50,50	0
56	MG	1A	3419	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3668	1/1	0.96	0.05	36,36,36,36	0
56	MG	1A	3094	1/1	0.96	0.06	18,18,18,18	0
56	MG	1A	3173	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3662	1/1	0.96	0.10	43,43,43,43	0
56	MG	2A	3011	1/1	0.96	0.08	48,48,48,48	0
56	MG	1a	1612	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3312	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3849	1/1	0.96	0.05	40,40,40,40	0
56	MG	2A	3014	1/1	0.96	0.12	49,49,49,49	0
56	MG	1a	1614	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3317	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3528	1/1	0.96	0.19	41,41,41,41	0
56	MG	2A	3671	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3673	1/1	0.96	0.08	48,48,48,48	0
56	MG	2A	3674	1/1	0.96	0.10	34,34,34,34	0
56	MG	1a	1616	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3676	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3677	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3320	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3021	1/1	0.96	0.06	37,37,37,37	0
56	MG	1a	1620	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3852	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	4041	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3025	1/1	0.96	0.20	44,44,44,44	0
56	MG	1A	3027	1/1	0.96	0.10	65,65,65,65	0
56	MG	2A	3028	1/1	0.96	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3325	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3674	1/1	0.96	0.10	52,52,52,52	0
56	MG	2a	3107	1/1	0.96	0.06	61,61,61,61	0
56	MG	1A	3531	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3236	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3129	1/1	0.96	0.24	32,32,32,32	0
56	MG	1A	3680	1/1	0.96	0.08	37,37,37,37	0
56	MG	2A	3334	1/1	0.96	0.07	53,53,53,53	0
56	MG	2A	3335	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3681	1/1	0.96	0.07	41,41,41,41	0
56	MG	2A	3338	1/1	0.96	0.12	46,46,46,46	0
56	MG	2a	3116	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3037	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3864	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3535	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3537	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3239	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3689	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3178	1/1	0.96	0.34	28,28,28,28	0
56	MG	1A	3330	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	4062	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3709	1/1	0.96	0.08	59,59,59,59	0
56	MG	2A	3046	1/1	0.96	0.10	49,49,49,49	0
56	MG	2a	3129	1/1	0.96	0.22	46,46,46,46	0
56	MG	1A	4063	1/1	0.96	0.05	34,34,34,34	0
56	MG	2a	3131	1/1	0.96	0.25	58,58,58,58	0
56	MG	2A	3048	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3049	1/1	0.96	0.07	20,20,20,20	0
56	MG	2A	3714	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3057	1/1	0.96	0.12	19,19,19,19	0
56	MG	2a	3136	1/1	0.96	0.07	60,60,60,60	0
56	MG	2A	3716	1/1	0.96	0.07	37,37,37,37	0
56	MG	2A	3718	1/1	0.96	0.10	43,43,43,43	0
56	MG	1a	1645	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	4065	1/1	0.96	0.09	22,22,22,22	0
56	MG	2A	3358	1/1	0.96	0.21	42,42,42,42	0
56	MG	1a	1649	1/1	0.96	0.14	49,49,49,49	0
56	MG	1A	3874	1/1	0.96	0.06	32,32,32,32	0
56	MG	1a	1651	1/1	0.96	0.13	49,49,49,49	0
56	MG	2A	3057	1/1	0.96	0.13	38,38,38,38	0
56	MG	2a	3150	1/1	0.96	0.11	38,38,38,38	0
56	MG	2a	3152	1/1	0.96	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1655	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	4067	1/1	0.96	0.25	45,45,45,45	0
56	MG	2a	3156	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3335	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3070	1/1	0.96	0.06	12,12,12,12	0
56	MG	2a	3161	1/1	0.96	0.12	60,60,60,60	0
56	MG	1A	3433	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3878	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3064	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3071	1/1	0.96	0.07	18,18,18,18	0
56	MG	2A	3373	1/1	0.96	0.07	41,41,41,41	0
56	MG	2A	3066	1/1	0.96	0.20	47,47,47,47	0
56	MG	2a	3168	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3339	1/1	0.96	0.09	31,31,31,31	0
56	MG	1A	3551	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3377	1/1	0.96	0.17	57,57,57,57	0
56	MG	2a	3173	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3552	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3708	1/1	0.96	0.06	15,15,15,15	0
56	MG	1A	3102	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3382	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3079	1/1	0.96	0.10	26,26,26,26	0
56	MG	1A	4084	1/1	0.96	0.07	44,44,44,44	0
56	MG	2a	3181	1/1	0.96	0.22	52,52,52,52	0
56	MG	2a	3182	1/1	0.96	0.16	47,47,47,47	0
56	MG	1A	4087	1/1	0.96	0.08	28,28,28,28	0
56	MG	2A	3080	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3888	1/1	0.96	0.10	23,23,23,23	0
56	MG	2A	3388	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3342	1/1	0.96	0.22	49,49,49,49	0
56	MG	1A	3344	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3720	1/1	0.96	0.06	33,33,33,33	0
56	MG	2A	3085	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3896	1/1	0.96	0.05	33,33,33,33	0
56	MG	2a	3193	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	4096	1/1	0.96	0.08	46,46,46,46	0
56	MG	2a	3195	1/1	0.96	0.07	62,62,62,62	0
56	MG	1a	1679	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3559	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	4098	1/1	0.96	0.07	29,29,29,29	0
56	MG	2A	3764	1/1	0.96	0.06	48,48,48,48	0
56	MG	2a	3201	1/1	0.96	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	3202	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3253	1/1	0.96	0.07	43,43,43,43	0
56	MG	2a	3205	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3723	1/1	0.96	0.08	21,21,21,21	0
56	MG	1A	3139	1/1	0.96	0.26	25,25,25,25	0
56	MG	2A	3402	1/1	0.96	0.10	38,38,38,38	0
56	MG	1a	1685	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3727	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3405	1/1	0.96	0.10	48,48,48,48	0
56	MG	1a	1687	1/1	0.96	0.11	32,32,32,32	0
56	MG	1a	1688	1/1	0.96	0.15	53,53,53,53	0
56	MG	1A	4104	1/1	0.96	0.05	46,46,46,46	0
56	MG	1a	1690	1/1	0.96	0.09	58,58,58,58	0
56	MG	2A	3410	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3010	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3142	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3052	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1694	1/1	0.96	0.13	43,43,43,43	0
56	MG	1A	3193	1/1	0.96	0.14	29,29,29,29	0
56	MG	1A	3263	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3786	1/1	0.96	0.17	56,56,56,56	0
56	MG	1a	1697	1/1	0.96	0.11	36,36,36,36	0
56	MG	1B	204	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3355	1/1	0.96	0.09	49,49,49,49	0
56	MG	1A	3356	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3422	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3794	1/1	0.96	0.04	46,46,46,46	0
56	MG	1A	3358	1/1	0.96	0.04	45,45,45,45	0
56	MG	2A	3797	1/1	0.96	0.05	52,52,52,52	0
56	MG	1B	209	1/1	0.96	0.13	31,31,31,31	0
56	MG	2A	3799	1/1	0.96	0.13	68,68,68,68	0
56	MG	1A	3194	1/1	0.96	0.15	27,27,27,27	0
56	MG	1A	3457	1/1	0.96	0.11	39,39,39,39	0
56	MG	2A	3427	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3917	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3429	1/1	0.96	0.17	30,30,30,30	0
56	MG	1A	3361	1/1	0.96	0.21	26,26,26,26	0
56	MG	1A	3363	1/1	0.96	0.11	23,23,23,23	0
56	MG	1B	215	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3578	1/1	0.96	0.17	31,31,31,31	0
56	MG	2A	3129	1/1	0.96	0.11	46,46,46,46	0
56	MG	2A	3130	1/1	0.96	0.09	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3436	1/1	0.96	0.13	47,47,47,47	0
56	MG	2q	201	1/1	0.96	0.08	58,58,58,58	0
56	MG	2A	3814	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3744	1/1	0.96	0.05	32,32,32,32	0
56	MG	1a	1714	1/1	0.96	0.27	52,52,52,52	0
56	MG	1B	219	1/1	0.96	0.07	31,31,31,31	0
56	MG	2A	3134	1/1	0.96	0.14	41,41,41,41	0
56	MG	2A	3442	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3579	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3445	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3746	1/1	0.96	0.07	13,13,13,13	0
56	MG	1a	1718	1/1	0.96	0.13	56,56,56,56	0
56	MG	2w	105	1/1	0.96	0.13	67,67,67,67	0
56	MG	1a	1719	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3142	1/1	0.96	0.16	38,38,38,38	0
56	MG	2x	101	1/1	0.96	0.15	66,66,66,66	0
56	MG	1A	3463	1/1	0.96	0.25	43,43,43,43	0
56	MG	2A	3452	1/1	0.96	0.09	32,32,32,32	0
56	MG	2A	3834	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3109	1/1	0.96	0.19	28,28,28,28	0
56	MG	2A	3841	1/1	0.96	0.09	65,65,65,65	0
56	MG	1A	3751	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3149	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3844	1/1	0.96	0.10	47,47,47,47	0
56	MG	1a	1723	1/1	0.96	0.28	44,44,44,44	0
57	TYK	2A	3879	64/64	0.96	0.09	26,33,41,50	0
56	MG	1A	3366	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3934	1/1	0.96	0.22	22,22,22,22	0
56	MG	2A	3459	1/1	0.96	0.24	43,43,43,43	0
56	MG	1A	3693	1/1	0.97	0.05	18,18,18,18	0
56	MG	2A	3578	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	4074	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3141	1/1	0.97	0.11	30,30,30,30	0
56	MG	1A	3074	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3108	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3075	1/1	0.97	0.05	22,22,22,22	0
56	MG	2E	310	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3195	1/1	0.97	0.19	27,27,27,27	0
56	MG	1A	3881	1/1	0.97	0.07	50,50,50,50	0
56	MG	1a	1638	1/1	0.97	0.22	38,38,38,38	0
56	MG	2F	305	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3019	1/1	0.97	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4082	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3439	1/1	0.97	0.06	39,39,39,39	0
56	MG	2A	3593	1/1	0.97	0.12	34,34,34,34	0
56	MG	2A	3594	1/1	0.97	0.12	39,39,39,39	0
56	MG	1A	3343	1/1	0.97	0.09	35,35,35,35	0
56	MG	1a	1642	1/1	0.97	0.16	42,42,42,42	0
56	MG	1A	4086	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3441	1/1	0.97	0.13	39,39,39,39	0
56	MG	1A	3557	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3602	1/1	0.97	0.06	41,41,41,41	0
56	MG	2A	3027	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3709	1/1	0.97	0.05	24,24,24,24	0
56	MG	1a	1647	1/1	0.97	0.08	40,40,40,40	0
56	MG	2T	203	1/1	0.97	0.12	39,39,39,39	0
56	MG	1a	1648	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	4091	1/1	0.97	0.10	37,37,37,37	0
56	MG	2V	202	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3609	1/1	0.97	0.14	56,56,56,56	0
56	MG	1A	4092	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3111	1/1	0.97	0.04	21,21,21,21	0
56	MG	1a	1653	1/1	0.97	0.11	45,45,45,45	0
56	MG	2A	3307	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3711	1/1	0.97	0.09	45,45,45,45	0
56	MG	1A	3891	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3258	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3894	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3346	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	4099	1/1	0.97	0.08	35,35,35,35	0
56	MG	2A	3314	1/1	0.97	0.04	53,53,53,53	0
56	MG	1A	3260	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3197	1/1	0.97	0.23	29,29,29,29	0
56	MG	1A	3078	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3564	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3030	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	3724	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3032	1/1	0.97	0.19	20,20,20,20	0
56	MG	1a	1668	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3567	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3019	1/1	0.97	0.21	43,43,43,43	0
56	MG	1A	3354	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3453	1/1	0.97	0.16	35,35,35,35	0
56	MG	29	101	1/1	0.97	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1673	1/1	0.97	0.04	34,34,34,34	0
56	MG	1A	3266	1/1	0.97	0.04	31,31,31,31	0
56	MG	2A	3637	1/1	0.97	0.13	53,53,53,53	0
56	MG	1a	1675	1/1	0.97	0.07	56,56,56,56	0
56	MG	2A	3639	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3572	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3035	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3357	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3458	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3916	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3459	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3919	1/1	0.97	0.09	17,17,17,17	0
56	MG	1A	3739	1/1	0.97	0.07	34,34,34,34	0
56	MG	2A	3340	1/1	0.97	0.06	56,56,56,56	0
56	MG	2a	3015	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3460	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3067	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3157	1/1	0.97	0.10	33,33,33,33	0
56	MG	2A	3653	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	3159	1/1	0.97	0.06	28,28,28,28	0
56	MG	1A	3360	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3582	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3927	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3464	1/1	0.97	0.19	27,27,27,27	0
56	MG	2A	3077	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3020	1/1	0.97	0.04	30,30,30,30	0
56	MG	1A	3466	1/1	0.97	0.10	25,25,25,25	0
56	MG	1B	225	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3932	1/1	0.97	0.07	34,34,34,34	0
56	MG	1B	227	1/1	0.97	0.04	39,39,39,39	0
56	MG	1A	3748	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3588	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3750	1/1	0.97	0.12	34,34,34,34	0
56	MG	2A	3359	1/1	0.97	0.05	38,38,38,38	0
56	MG	1a	1699	1/1	0.97	0.16	35,35,35,35	0
56	MG	1A	3362	1/1	0.97	0.16	34,34,34,34	0
56	MG	1A	3085	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3593	1/1	0.97	0.09	32,32,32,32	0
56	MG	1B	234	1/1	0.97	0.05	33,33,33,33	0
56	MG	1A	3209	1/1	0.97	0.08	19,19,19,19	0
56	MG	1D	303	1/1	0.97	0.09	10,10,10,10	0
56	MG	2A	3094	1/1	0.97	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3678	1/1	0.97	0.13	50,50,50,50	0
56	MG	1a	1706	1/1	0.97	0.26	48,48,48,48	0
56	MG	2a	3045	1/1	0.97	0.05	46,46,46,46	0
56	MG	1D	304	1/1	0.97	0.05	28,28,28,28	0
56	MG	2A	3681	1/1	0.97	0.13	46,46,46,46	0
56	MG	2A	3370	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3210	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3211	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3758	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3277	1/1	0.97	0.05	28,28,28,28	0
56	MG	1A	3278	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3059	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3765	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3105	1/1	0.97	0.06	48,48,48,48	0
56	MG	2A	3691	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3106	1/1	0.97	0.05	39,39,39,39	0
56	MG	2A	3107	1/1	0.97	0.05	33,33,33,33	0
56	MG	1E	305	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3600	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3122	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3372	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3604	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3281	1/1	0.97	0.09	49,49,49,49	0
56	MG	2a	3066	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3282	1/1	0.97	0.12	36,36,36,36	0
56	MG	2A	3701	1/1	0.97	0.05	54,54,54,54	0
56	MG	1F	302	1/1	0.97	0.09	33,33,33,33	0
56	MG	1a	1724	1/1	0.97	0.14	31,31,31,31	0
56	MG	1A	3772	1/1	0.97	0.08	32,32,32,32	0
56	MG	1F	304	1/1	0.97	0.15	25,25,25,25	0
56	MG	2A	3120	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3283	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3122	1/1	0.97	0.10	51,51,51,51	0
56	MG	1a	1728	1/1	0.97	0.13	35,35,35,35	0
56	MG	2A	3124	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3483	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	3284	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3215	1/1	0.97	0.07	30,30,30,30	0
56	MG	1A	3966	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3216	1/1	0.97	0.11	36,36,36,36	0
56	MG	1A	3003	1/1	0.97	0.04	22,22,22,22	0
56	MG	1a	1736	1/1	0.97	0.25	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3779	1/1	0.97	0.04	47,47,47,47	0
56	MG	1A	3219	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3167	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3722	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3782	1/1	0.97	0.08	33,33,33,33	0
56	MG	1N	203	1/1	0.97	0.13	45,45,45,45	0
56	MG	1A	3975	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3139	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3385	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3730	1/1	0.97	0.07	35,35,35,35	0
56	MG	1a	1747	1/1	0.97	0.09	58,58,58,58	0
56	MG	2A	3144	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3978	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3734	1/1	0.97	0.05	38,38,38,38	0
56	MG	1O	202	1/1	0.97	0.14	49,49,49,49	0
56	MG	1a	1750	1/1	0.97	0.11	25,25,25,25	0
56	MG	1a	1751	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3011	1/1	0.97	0.09	31,31,31,31	0
56	MG	1O	204	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3294	1/1	0.97	0.23	27,27,27,27	0
56	MG	1A	3298	1/1	0.97	0.07	38,38,38,38	0
56	MG	1P	202	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3169	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3790	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3390	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3391	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3015	1/1	0.97	0.21	32,32,32,32	0
56	MG	1A	3987	1/1	0.97	0.05	34,34,34,34	0
56	MG	1A	3126	1/1	0.97	0.23	28,28,28,28	0
56	MG	1A	3502	1/1	0.97	0.05	26,26,26,26	0
56	MG	1A	3043	1/1	0.97	0.16	27,27,27,27	0
56	MG	1R	206	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3303	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3092	1/1	0.97	0.12	28,28,28,28	0
56	MG	1a	1771	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3632	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3996	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3801	1/1	0.97	0.13	23,23,23,23	0
56	MG	2A	3174	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3802	1/1	0.97	0.07	20,20,20,20	0
56	MG	1U	201	1/1	0.97	0.07	26,26,26,26	0
56	MG	2A	3447	1/1	0.97	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3065	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3634	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3308	1/1	0.97	0.05	36,36,36,36	0
56	MG	2A	3181	1/1	0.97	0.04	36,36,36,36	0
56	MG	1A	3806	1/1	0.97	0.09	20,20,20,20	0
56	MG	2A	3183	1/1	0.97	0.15	48,48,48,48	0
56	MG	2A	3184	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3808	1/1	0.97	0.08	51,51,51,51	0
56	MG	1A	3046	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3638	1/1	0.97	0.07	17,17,17,17	0
56	MG	2A	3775	1/1	0.97	0.18	55,55,55,55	0
56	MG	1U	212	1/1	0.97	0.07	36,36,36,36	0
56	MG	2a	3142	1/1	0.97	0.08	50,50,50,50	0
56	MG	1V	201	1/1	0.97	0.34	25,25,25,25	0
56	MG	1A	4006	1/1	0.97	0.04	43,43,43,43	0
56	MG	1V	206	1/1	0.97	0.07	39,39,39,39	0
56	MG	1W	201	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3510	1/1	0.97	0.10	33,33,33,33	0
56	MG	2a	3149	1/1	0.97	0.09	42,42,42,42	0
56	MG	1W	203	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3465	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3311	1/1	0.97	0.17	33,33,33,33	0
56	MG	1W	206	1/1	0.97	0.07	34,34,34,34	0
56	MG	2a	3155	1/1	0.97	0.09	67,67,67,67	0
56	MG	2A	3199	1/1	0.97	0.11	45,45,45,45	0
56	MG	2A	3788	1/1	0.97	0.05	33,33,33,33	0
56	MG	1A	3403	1/1	0.97	0.27	44,44,44,44	0
56	MG	2a	3159	1/1	0.97	0.10	39,39,39,39	0
56	MG	1X	101	1/1	0.97	0.23	25,25,25,25	0
56	MG	1X	102	1/1	0.97	0.13	28,28,28,28	0
56	MG	2A	3792	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3180	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3643	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3795	1/1	0.97	0.12	42,42,42,42	0
56	MG	1a	1798	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3514	1/1	0.97	0.10	22,22,22,22	0
56	MG	1A	3645	1/1	0.97	0.08	12,12,12,12	0
56	MG	2A	3480	1/1	0.97	0.17	28,28,28,28	0
56	MG	2A	3481	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	3515	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3313	1/1	0.97	0.17	22,22,22,22	0
56	MG	2a	3175	1/1	0.97	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3210	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	4017	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3649	1/1	0.97	0.12	27,27,27,27	0
56	MG	2A	3806	1/1	0.97	0.14	64,64,64,64	0
56	MG	10	101	1/1	0.97	0.15	43,43,43,43	0
56	MG	2A	3488	1/1	0.97	0.09	40,40,40,40	0
56	MG	1a	1807	1/1	0.97	0.09	36,36,36,36	0
56	MG	2a	3183	1/1	0.97	0.08	40,40,40,40	0
56	MG	1A	3408	1/1	0.97	0.30	32,32,32,32	0
56	MG	10	103	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3812	1/1	0.97	0.07	63,63,63,63	0
56	MG	1A	3826	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3652	1/1	0.97	0.04	20,20,20,20	0
56	MG	1A	3233	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	3182	1/1	0.97	0.10	17,17,17,17	0
56	MG	2A	3817	1/1	0.97	0.07	53,53,53,53	0
56	MG	1A	3655	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3498	1/1	0.97	0.11	38,38,38,38	0
56	MG	2A	3820	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3411	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3316	1/1	0.97	0.09	23,23,23,23	0
56	MG	1a	1819	1/1	0.97	0.17	43,43,43,43	0
56	MG	1a	1820	1/1	0.97	0.13	27,27,27,27	0
56	MG	1A	3662	1/1	0.97	0.08	24,24,24,24	0
56	MG	2a	3200	1/1	0.97	0.09	63,63,63,63	0
56	MG	2A	3827	1/1	0.97	0.08	35,35,35,35	0
56	MG	2A	3828	1/1	0.97	0.05	32,32,32,32	0
56	MG	2A	3829	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3837	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3235	1/1	0.97	0.16	25,25,25,25	0
56	MG	1A	3048	1/1	0.97	0.07	22,22,22,22	0
56	MG	2A	3507	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3665	1/1	0.97	0.12	23,23,23,23	0
56	MG	2A	3837	1/1	0.97	0.08	50,50,50,50	0
56	MG	1b	302	1/1	0.97	0.12	58,58,58,58	0
56	MG	1A	3666	1/1	0.97	0.08	13,13,13,13	0
56	MG	15	101	1/1	0.97	0.18	29,29,29,29	0
56	MG	2A	3234	1/1	0.97	0.11	35,35,35,35	0
56	MG	2A	3235	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	4034	1/1	0.97	0.07	19,19,19,19	0
56	MG	15	104	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3415	1/1	0.97	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	16	101	1/1	0.97	0.06	37,37,37,37	0
56	MG	2A	3520	1/1	0.97	0.10	21,21,21,21	0
56	MG	1A	4037	1/1	0.97	0.04	32,32,32,32	0
56	MG	16	103	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3049	1/1	0.97	0.11	35,35,35,35	0
56	MG	18	101	1/1	0.97	0.08	33,33,33,33	0
56	MG	2A	3855	1/1	0.97	0.07	64,64,64,64	0
56	MG	1A	3320	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3848	1/1	0.97	0.04	17,17,17,17	0
56	MG	1A	3322	1/1	0.97	0.05	36,36,36,36	0
56	MG	2A	3530	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3247	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3850	1/1	0.97	0.28	29,29,29,29	0
56	MG	2A	3534	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3864	1/1	0.97	0.10	32,32,32,32	0
56	MG	1A	3238	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3136	1/1	0.97	0.04	29,29,29,29	0
56	MG	1A	3240	1/1	0.97	0.17	35,35,35,35	0
56	MG	2f	201	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3423	1/1	0.97	0.17	39,39,39,39	0
56	MG	1A	3855	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3870	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3676	1/1	0.97	0.07	19,19,19,19	0
56	MG	1A	3069	1/1	0.97	0.09	28,28,28,28	0
56	MG	1x	103	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3534	1/1	0.97	0.11	29,29,29,29	0
56	MG	1A	4056	1/1	0.97	0.04	36,36,36,36	0
56	MG	1A	3242	1/1	0.97	0.24	24,24,24,24	0
56	MG	1x	107	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3017	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3548	1/1	0.97	0.07	56,56,56,56	0
56	MG	1A	3245	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3551	1/1	0.97	0.06	39,39,39,39	0
56	MG	2A	3263	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3682	1/1	0.97	0.04	20,20,20,20	0
56	MG	2B	207	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3008	1/1	0.97	0.07	19,19,19,19	0
56	MG	1A	3866	1/1	0.97	0.05	32,32,32,32	0
56	MG	2A	3557	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3684	1/1	0.97	0.07	35,35,35,35	0
56	MG	1a	1617	1/1	0.97	0.06	36,36,36,36	0
56	MG	1a	1618	1/1	0.97	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1619	1/1	0.97	0.07	40,40,40,40	0
56	MG	1y	102	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3868	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3540	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3687	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3247	1/1	0.97	0.21	31,31,31,31	0
56	MG	2A	3003	1/1	0.97	0.18	47,47,47,47	0
56	MG	1A	4068	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3334	1/1	0.97	0.17	22,22,22,22	0
56	MG	1A	3072	1/1	0.97	0.21	27,27,27,27	0
57	TYK	1A	4107	64/64	0.97	0.08	13,21,29,34	0
56	MG	2D	303	1/1	0.97	0.22	41,41,41,41	0
56	MG	2D	304	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3250	1/1	0.97	0.07	48,48,48,48	0
60	K	1x	101	1/1	0.97	0.07	62,62,62,62	0
56	MG	2A	3576	1/1	0.97	0.09	43,43,43,43	0
56	MG	1X	103	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3321	1/1	0.98	0.03	25,25,25,25	0
56	MG	1A	3038	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3601	1/1	0.98	0.03	29,29,29,29	0
56	MG	1A	3110	1/1	0.98	0.14	24,24,24,24	0
56	MG	1X	107	1/1	0.98	0.12	32,32,32,32	0
56	MG	2A	3396	1/1	0.98	0.04	38,38,38,38	0
56	MG	2A	3605	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3824	1/1	0.98	0.04	34,34,34,34	0
56	MG	1A	4090	1/1	0.98	0.04	31,31,31,31	0
56	MG	1Y	203	1/1	0.98	0.17	39,39,39,39	0
56	MG	2a	3068	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3028	1/1	0.98	0.16	25,25,25,25	0
56	MG	1A	3217	1/1	0.98	0.17	26,26,26,26	0
56	MG	2A	3034	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3828	1/1	0.98	0.07	15,15,15,15	0
56	MG	1A	3612	1/1	0.98	0.28	38,38,38,38	0
56	MG	1A	3716	1/1	0.98	0.04	20,20,20,20	0
56	MG	2A	3615	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3456	1/1	0.98	0.05	44,44,44,44	0
56	MG	1a	1731	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3832	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3718	1/1	0.98	0.04	18,18,18,18	0
56	MG	1A	3719	1/1	0.98	0.04	17,17,17,17	0
56	MG	1A	3961	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3962	1/1	0.98	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3174	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3965	1/1	0.98	0.09	17,17,17,17	0
56	MG	1A	3029	1/1	0.98	0.08	28,28,28,28	0
56	MG	1A	3056	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3835	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3417	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3838	1/1	0.98	0.15	32,32,32,32	0
56	MG	13	101	1/1	0.98	0.06	25,25,25,25	0
56	MG	2A	3840	1/1	0.98	0.04	37,37,37,37	0
56	MG	13	102	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3177	1/1	0.98	0.10	34,34,34,34	0
56	MG	1a	1745	1/1	0.98	0.09	35,35,35,35	0
56	MG	1a	1746	1/1	0.98	0.07	39,39,39,39	0
56	MG	2A	3054	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3223	1/1	0.98	0.04	36,36,36,36	0
56	MG	1A	3971	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3840	1/1	0.98	0.18	17,17,17,17	0
56	MG	1A	3536	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3726	1/1	0.98	0.04	25,25,25,25	0
56	MG	15	103	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	3394	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3016	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	3333	1/1	0.98	0.06	24,24,24,24	0
56	MG	2A	3644	1/1	0.98	0.14	52,52,52,52	0
56	MG	1A	3847	1/1	0.98	0.10	49,49,49,49	0
56	MG	1A	3179	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3013	1/1	0.98	0.13	23,23,23,23	0
56	MG	17	101	1/1	0.98	0.07	25,25,25,25	0
56	MG	2A	3068	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3275	1/1	0.98	0.05	28,28,28,28	0
56	MG	2A	3439	1/1	0.98	0.21	45,45,45,45	0
56	MG	1A	3143	1/1	0.98	0.09	17,17,17,17	0
56	MG	1A	3544	1/1	0.98	0.12	41,41,41,41	0
56	MG	2A	3072	1/1	0.98	0.06	41,41,41,41	0
56	MG	1B	216	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3736	1/1	0.98	0.06	18,18,18,18	0
56	MG	2A	3075	1/1	0.98	0.12	33,33,33,33	0
56	MG	1A	3629	1/1	0.98	0.10	38,38,38,38	0
56	MG	2A	3872	1/1	0.98	0.10	30,30,30,30	0
56	MG	2a	3122	1/1	0.98	0.12	53,53,53,53	0
56	MG	1A	3228	1/1	0.98	0.11	37,37,37,37	0
56	MG	1A	3073	1/1	0.98	0.05	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3857	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3547	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3404	1/1	0.98	0.24	24,24,24,24	0
56	MG	1A	3992	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3993	1/1	0.98	0.06	19,19,19,19	0
56	MG	1A	3145	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3406	1/1	0.98	0.11	17,17,17,17	0
56	MG	1A	3093	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3475	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3147	1/1	0.98	0.19	28,28,28,28	0
56	MG	1A	3555	1/1	0.98	0.14	32,32,32,32	0
56	MG	2A	3672	1/1	0.98	0.04	28,28,28,28	0
56	MG	2a	3137	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3044	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3149	1/1	0.98	0.06	28,28,28,28	0
56	MG	2A	3092	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3060	1/1	0.98	0.08	25,25,25,25	0
56	MG	1B	235	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3286	1/1	0.98	0.11	33,33,33,33	0
56	MG	2A	3467	1/1	0.98	0.13	56,56,56,56	0
56	MG	2a	3145	1/1	0.98	0.04	45,45,45,45	0
56	MG	1D	302	1/1	0.98	0.12	23,23,23,23	0
56	MG	1A	3482	1/1	0.98	0.15	24,24,24,24	0
56	MG	2A	3098	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3151	1/1	0.98	0.15	20,20,20,20	0
56	MG	1A	3648	1/1	0.98	0.10	30,30,30,30	0
56	MG	2a	3151	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	3191	1/1	0.98	0.12	28,28,28,28	0
56	MG	1A	3650	1/1	0.98	0.12	54,54,54,54	0
56	MG	2A	3286	1/1	0.98	0.10	46,46,46,46	0
56	MG	1D	309	1/1	0.98	0.25	22,22,22,22	0
56	MG	1A	3289	1/1	0.98	0.07	19,19,19,19	0
56	MG	1A	3486	1/1	0.98	0.10	38,38,38,38	0
56	MG	1A	3077	1/1	0.98	0.12	37,37,37,37	0
56	MG	1E	303	1/1	0.98	0.07	31,31,31,31	0
56	MG	2a	3160	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	4012	1/1	0.98	0.10	26,26,26,26	0
56	MG	1A	3763	1/1	0.98	0.04	21,21,21,21	0
56	MG	1a	1633	1/1	0.98	0.08	19,19,19,19	0
56	MG	2E	306	1/1	0.98	0.10	40,40,40,40	0
56	MG	1E	306	1/1	0.98	0.07	20,20,20,20	0
56	MG	1A	3097	1/1	0.98	0.10	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1636	1/1	0.98	0.17	45,45,45,45	0
56	MG	1A	3418	1/1	0.98	0.04	44,44,44,44	0
56	MG	2F	301	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3882	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3353	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3657	1/1	0.98	0.06	23,23,23,23	0
56	MG	2A	3493	1/1	0.98	0.05	25,25,25,25	0
56	MG	1a	1808	1/1	0.98	0.05	40,40,40,40	0
56	MG	2A	3119	1/1	0.98	0.08	31,31,31,31	0
56	MG	1A	3659	1/1	0.98	0.03	15,15,15,15	0
56	MG	1E	313	1/1	0.98	0.05	23,23,23,23	0
56	MG	1F	301	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	3660	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3099	1/1	0.98	0.09	19,19,19,19	0
56	MG	1A	3293	1/1	0.98	0.22	29,29,29,29	0
56	MG	2Q	201	1/1	0.98	0.05	45,45,45,45	0
56	MG	1F	305	1/1	0.98	0.11	22,22,22,22	0
56	MG	1A	3155	1/1	0.98	0.04	23,23,23,23	0
56	MG	1F	307	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3297	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3045	1/1	0.98	0.06	22,22,22,22	0
56	MG	1a	1652	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3033	1/1	0.98	0.17	18,18,18,18	0
56	MG	1a	1654	1/1	0.98	0.10	47,47,47,47	0
56	MG	1A	3575	1/1	0.98	0.07	17,17,17,17	0
56	MG	1A	3158	1/1	0.98	0.10	25,25,25,25	0
56	MG	2W	201	1/1	0.98	0.27	40,40,40,40	0
56	MG	1A	3025	1/1	0.98	0.07	32,32,32,32	0
56	MG	2A	3724	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3081	1/1	0.98	0.12	30,30,30,30	0
56	MG	2A	3138	1/1	0.98	0.21	38,38,38,38	0
56	MG	2A	3727	1/1	0.98	0.05	58,58,58,58	0
56	MG	1A	3248	1/1	0.98	0.10	19,19,19,19	0
56	MG	1A	3364	1/1	0.98	0.24	28,28,28,28	0
56	MG	1A	3304	1/1	0.98	0.12	12,12,12,12	0
56	MG	2A	3519	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	4035	1/1	0.98	0.03	27,27,27,27	0
56	MG	2A	3521	1/1	0.98	0.07	57,57,57,57	0
56	MG	1A	3305	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3784	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	4038	1/1	0.98	0.08	30,30,30,30	0
56	MG	1A	3785	1/1	0.98	0.05	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3905	1/1	0.98	0.16	24,24,24,24	0
56	MG	1A	3675	1/1	0.98	0.12	19,19,19,19	0
56	MG	1A	3161	1/1	0.98	0.08	28,28,28,28	0
56	MG	1A	3507	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3909	1/1	0.98	0.04	42,42,42,42	0
56	MG	1A	3434	1/1	0.98	0.21	30,30,30,30	0
56	MG	2A	3337	1/1	0.98	0.09	52,52,52,52	0
56	MG	2A	3156	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3339	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3911	1/1	0.98	0.06	31,31,31,31	0
56	MG	1P	205	1/1	0.98	0.13	34,34,34,34	0
56	MG	2A	3749	1/1	0.98	0.09	47,47,47,47	0
56	MG	1Q	201	1/1	0.98	0.06	22,22,22,22	0
56	MG	2A	3161	1/1	0.98	0.15	32,32,32,32	0
56	MG	1Q	202	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3586	1/1	0.98	0.12	26,26,26,26	0
56	MG	1A	3587	1/1	0.98	0.04	18,18,18,18	0
56	MG	1Q	205	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3914	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3021	1/1	0.98	0.04	15,15,15,15	0
56	MG	1A	3589	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	3163	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	3918	1/1	0.98	0.04	39,39,39,39	0
56	MG	2A	3550	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3009	1/1	0.98	0.06	23,23,23,23	0
56	MG	1A	3685	1/1	0.98	0.04	48,48,48,48	0
56	MG	2A	3355	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3921	1/1	0.98	0.07	17,17,17,17	0
56	MG	1A	3592	1/1	0.98	0.07	21,21,21,21	0
56	MG	1A	3131	1/1	0.98	0.04	20,20,20,20	0
56	MG	2A	3558	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3206	1/1	0.98	0.06	24,24,24,24	0
56	MG	2A	3177	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3255	1/1	0.98	0.12	23,23,23,23	0
56	MG	1A	3207	1/1	0.98	0.08	26,26,26,26	0
56	MG	1U	202	1/1	0.98	0.22	31,31,31,31	0
56	MG	2A	3774	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	3691	1/1	0.98	0.04	19,19,19,19	0
56	MG	1A	3928	1/1	0.98	0.04	23,23,23,23	0
56	MG	1A	3106	1/1	0.98	0.04	28,28,28,28	0
56	MG	1U	206	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3517	1/1	0.98	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3037	1/1	0.98	0.12	18,18,18,18	0
56	MG	2A	3572	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3377	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3188	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3259	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3134	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3811	1/1	0.98	0.04	21,21,21,21	0
56	MG	1V	202	1/1	0.98	0.13	25,25,25,25	0
56	MG	1A	3603	1/1	0.98	0.07	37,37,37,37	0
56	MG	1V	205	1/1	0.98	0.06	30,30,30,30	0
56	MG	2A	3581	1/1	0.98	0.07	41,41,41,41	0
56	MG	2A	3195	1/1	0.98	0.05	41,41,41,41	0
56	MG	1a	1707	1/1	0.98	0.20	50,50,50,50	0
56	MG	2A	3380	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3701	1/1	0.98	0.07	17,17,17,17	0
56	MG	1A	3135	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3704	1/1	0.98	0.05	18,18,18,18	0
56	MG	2A	3017	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	3170	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	4081	1/1	0.98	0.07	21,21,21,21	0
56	MG	1A	3382	1/1	0.98	0.21	38,38,38,38	0
58	ZN	2Y	202	1/1	0.98	0.04	83,83,83,83	0
56	MG	1A	3818	1/1	0.98	0.04	26,26,26,26	0
58	ZN	25	105	1/1	0.98	0.05	74,74,74,74	0
58	ZN	2n	501	1/1	0.98	0.04	86,86,86,86	0
56	MG	1A	3707	1/1	0.98	0.06	20,20,20,20	0
56	MG	1A	4085	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3107	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3619	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3969	1/1	0.99	0.05	28,28,28,28	0
56	MG	1E	302	1/1	0.99	0.06	28,28,28,28	0
56	MG	1A	4027	1/1	0.99	0.03	21,21,21,21	0
56	MG	1U	209	1/1	0.99	0.06	23,23,23,23	0
56	MG	1A	3031	1/1	0.99	0.18	22,22,22,22	0
56	MG	1A	3863	1/1	0.99	0.07	35,35,35,35	0
56	MG	1a	1610	1/1	0.99	0.06	17,17,17,17	0
56	MG	1k	201	1/1	0.99	0.12	36,36,36,36	0
56	MG	2A	3555	1/1	0.99	0.07	41,41,41,41	0
56	MG	1a	1756	1/1	0.99	0.10	28,28,28,28	0
56	MG	1A	3098	1/1	0.99	0.05	29,29,29,29	0
56	MG	1m	3001	1/1	0.99	0.04	53,53,53,53	0
56	MG	2A	3559	1/1	0.99	0.07	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3397	1/1	0.99	0.08	18,18,18,18	0
56	MG	1A	3004	1/1	0.99	0.06	19,19,19,19	0
56	MG	1a	1760	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3090	1/1	0.99	0.08	29,29,29,29	0
56	MG	2A	3857	1/1	0.99	0.03	28,28,28,28	0
56	MG	1A	3658	1/1	0.99	0.06	33,33,33,33	0
56	MG	2A	3474	1/1	0.99	0.13	20,20,20,20	0
56	MG	1A	3977	1/1	0.99	0.03	30,30,30,30	0
56	MG	1A	3820	1/1	0.99	0.03	24,24,24,24	0
56	MG	1A	3732	1/1	0.99	0.07	17,17,17,17	0
56	MG	1A	3047	1/1	0.99	0.04	30,30,30,30	0
56	MG	2A	3570	1/1	0.99	0.09	51,51,51,51	0
56	MG	2a	3204	1/1	0.99	0.05	65,65,65,65	0
56	MG	2A	3140	1/1	0.99	0.12	39,39,39,39	0
56	MG	1W	204	1/1	0.99	0.04	22,22,22,22	0
56	MG	1A	3451	1/1	0.99	0.09	26,26,26,26	0
56	MG	2A	3143	1/1	0.99	0.11	37,37,37,37	0
56	MG	1A	3478	1/1	0.99	0.03	31,31,31,31	0
56	MG	1A	3221	1/1	0.99	0.06	33,33,33,33	0
56	MG	1A	3697	1/1	0.99	0.04	29,29,29,29	0
56	MG	2A	3147	1/1	0.99	0.14	40,40,40,40	0
56	MG	1A	3827	1/1	0.99	0.04	17,17,17,17	0
56	MG	1A	3331	1/1	0.99	0.07	40,40,40,40	0
56	MG	1A	3630	1/1	0.99	0.11	12,12,12,12	0
56	MG	2A	3582	1/1	0.99	0.10	30,30,30,30	0
56	MG	2A	3583	1/1	0.99	0.09	35,35,35,35	0
56	MG	1A	3700	1/1	0.99	0.08	12,12,12,12	0
56	MG	2A	3778	1/1	0.99	0.09	38,38,38,38	0
56	MG	1A	3310	1/1	0.99	0.07	28,28,28,28	0
56	MG	1B	205	1/1	0.99	0.04	37,37,37,37	0
56	MG	1A	4048	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3014	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3703	1/1	0.99	0.04	18,18,18,18	0
56	MG	1A	4051	1/1	0.99	0.08	35,35,35,35	0
56	MG	2A	3158	1/1	0.99	0.09	30,30,30,30	0
56	MG	1A	3076	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3055	1/1	0.99	0.07	27,27,27,27	0
56	MG	1A	4054	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3336	1/1	0.99	0.03	21,21,21,21	0
56	MG	1A	3181	1/1	0.99	0.06	30,30,30,30	0
56	MG	2a	3232	1/1	0.99	0.07	48,48,48,48	0
56	MG	1A	3637	1/1	0.99	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3384	1/1	0.99	0.11	31,31,31,31	0
56	MG	1A	3941	1/1	0.99	0.04	29,29,29,29	0
56	MG	2A	3600	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3793	1/1	0.99	0.06	28,28,28,28	0
56	MG	1A	3943	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3944	1/1	0.99	0.02	22,22,22,22	0
56	MG	1P	201	1/1	0.99	0.14	26,26,26,26	0
56	MG	1A	3890	1/1	0.99	0.16	26,26,26,26	0
56	MG	1A	3276	1/1	0.99	0.10	26,26,26,26	0
56	MG	2A	3512	1/1	0.99	0.07	44,44,44,44	0
56	MG	1A	3295	1/1	0.99	0.11	33,33,33,33	0
56	MG	1A	3893	1/1	0.99	0.03	27,27,27,27	0
56	MG	1A	3712	1/1	0.99	0.03	18,18,18,18	0
56	MG	1A	3753	1/1	0.99	0.06	13,13,13,13	0
56	MG	1A	4070	1/1	0.99	0.09	23,23,23,23	0
56	MG	1a	1801	1/1	0.99	0.03	46,46,46,46	0
56	MG	2A	3015	1/1	0.99	0.08	34,34,34,34	0
56	MG	2E	305	1/1	0.99	0.07	27,27,27,27	0
56	MG	1A	3845	1/1	0.99	0.10	48,48,48,48	0
56	MG	2A	3616	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3548	1/1	0.99	0.11	30,30,30,30	0
56	MG	1A	3714	1/1	0.99	0.07	17,17,17,17	0
56	MG	2A	3523	1/1	0.99	0.06	31,31,31,31	0
56	MG	1R	201	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3296	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3116	1/1	0.99	0.07	33,33,33,33	0
56	MG	1A	3492	1/1	0.99	0.11	40,40,40,40	0
56	MG	1A	3243	1/1	0.99	0.11	18,18,18,18	0
56	MG	1A	3760	1/1	0.99	0.04	31,31,31,31	0
56	MG	1A	3012	1/1	0.99	0.03	21,21,21,21	0
56	MG	1A	3762	1/1	0.99	0.04	17,17,17,17	0
56	MG	2A	3822	1/1	0.99	0.03	26,26,26,26	0
56	MG	2A	3443	1/1	0.99	0.11	43,43,43,43	0
56	MG	2A	3533	1/1	0.99	0.04	44,44,44,44	0
56	MG	17	102	1/1	0.99	0.07	23,23,23,23	0
56	MG	17	103	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3807	1/1	0.99	0.04	22,22,22,22	0
56	MG	1A	3212	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3963	1/1	0.99	0.04	14,14,14,14	0
56	MG	1a	1818	1/1	0.99	0.02	46,46,46,46	0
58	ZN	1Y	204	1/1	0.99	0.03	67,67,67,67	0
56	MG	1A	3496	1/1	0.99	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	1n	103	1/1	0.99	0.03	58,58,58,58	0
56	MG	1a	1743	1/1	0.99	0.07	38,38,38,38	0
56	MG	2a	3172	1/1	0.99	0.09	41,41,41,41	0
56	MG	1D	307	1/1	0.99	0.14	37,37,37,37	0
58	ZN	26	102	1/1	0.99	0.04	57,57,57,57	0
58	ZN	29	102	1/1	0.99	0.03	64,64,64,64	0
56	MG	1A	3039	1/1	0.99	0.14	29,29,29,29	0
59	SF4	1d	302	8/8	0.99	0.04	51,55,66,66	0
59	SF4	2d	303	8/8	0.99	0.04	53,64,70,73	0
56	MG	1A	3119	1/1	0.99	0.11	27,27,27,27	0
56	MG	2A	3836	1/1	0.99	0.07	27,27,27,27	0
56	MG	1A	3937	1/1	1.00	0.07	27,27,27,27	0
56	MG	2A	3717	1/1	1.00	0.02	27,27,27,27	0
58	ZN	15	106	1/1	1.00	0.02	52,52,52,52	0
58	ZN	16	104	1/1	1.00	0.02	28,28,28,28	0
58	ZN	19	102	1/1	1.00	0.03	39,39,39,39	0
56	MG	1V	203	1/1	1.00	0.11	27,27,27,27	0
56	MG	1A	4055	1/1	1.00	0.02	16,16,16,16	0
56	MG	2A	3848	1/1	1.00	0.05	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.