



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 04:45 PM UTC

PDB ID : 9DFD / pdb_00009dfd
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with lasso peptide lariocidin B, mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.60Å resolution
Authors : Aleksandrova, E.V.; Travin, D.Y.; Jangra, M.; Kaur, M.; Darwish, L.; Koteva, K.; Klepacki, D.; Wang, W.; Tiffany, M.; Sokaribo, A.; Coombes, B.K.; Vazquez-Laslop, N.; Wright, G.D.; Mankin, A.S.; Polikanov, Y.S.
Deposited on : 2024-08-29
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

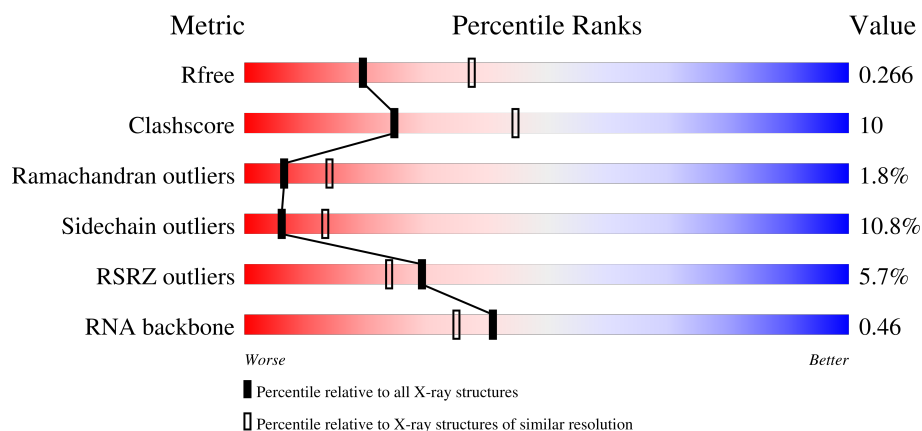
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)




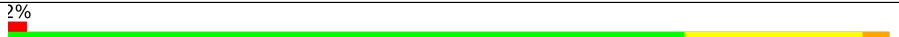
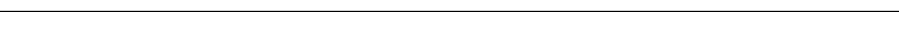
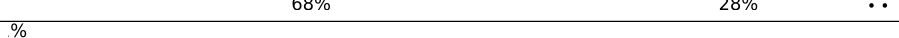
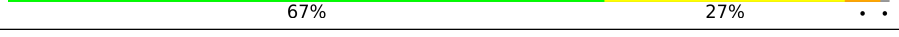




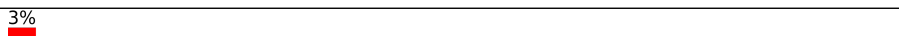

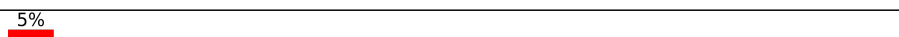





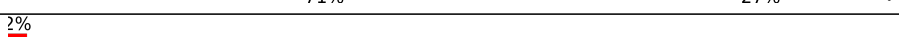





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>6%</div> <div>63% 29% 7%</div> </div>
1	2A	2915	<div> <div>6%</div> <div>57% 31% 7%</div> </div>

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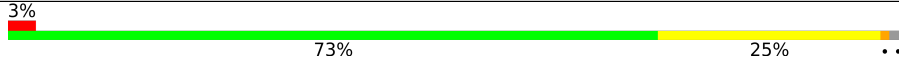
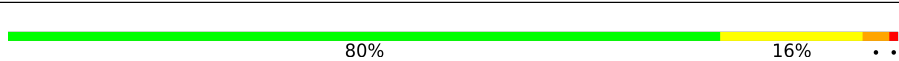
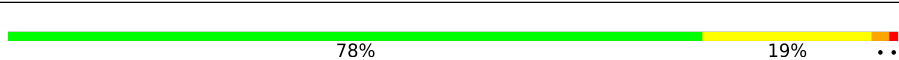
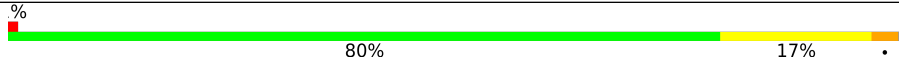
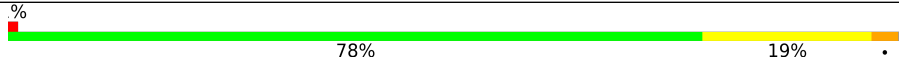
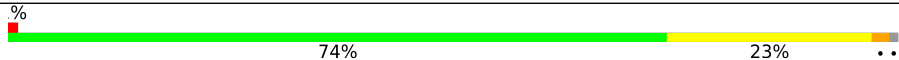
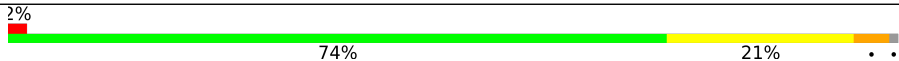
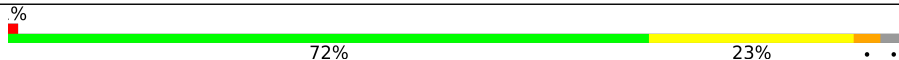

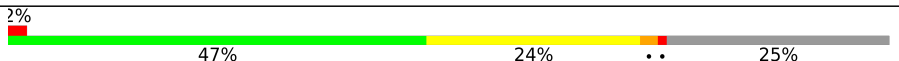
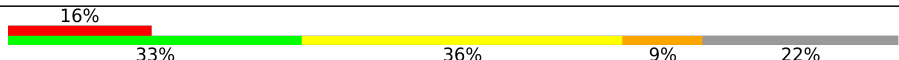
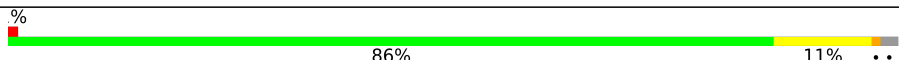
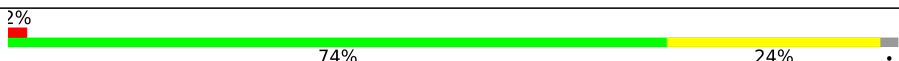
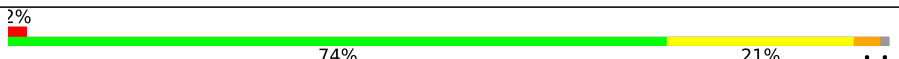
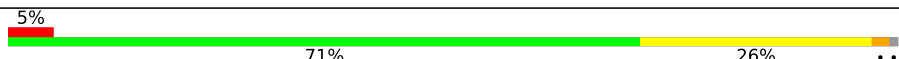

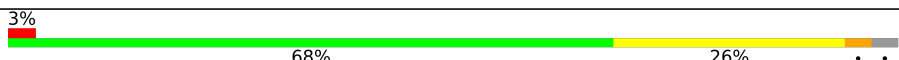
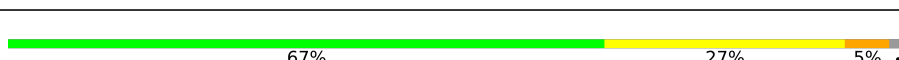
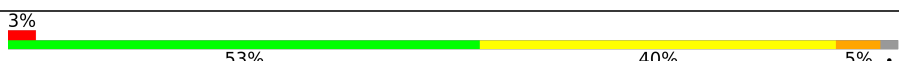
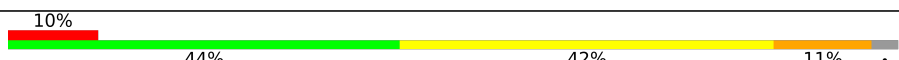
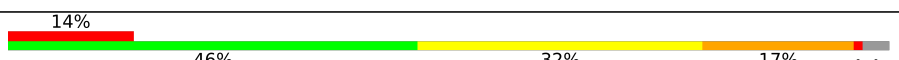
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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


























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

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

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

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Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	
57	1z	17	
57	2z	17	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	29	101	-	-	-	X
61	SF4	1d	302	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	125	Total	C	N	O	S	0	0	0
			979	604	204	169	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MET-PHE-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 Aminoacylated Phe-tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	75	Total	C	N	O	P	S	0	0	0
			1623	731	289	526	75	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNA^{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 57 is a protein called Lasso peptide lariocidin B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	1z	17	Total	C	N	O	0	0	0
			127	79	28	20			
57	2z	17	Total	C	N	O	0	0	0
			127	79	28	20			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1105	Total	Mg	0	0
			1105	1105		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	12	Total 12	Mg 12	0	0
58	1E	14	Total 14	Mg 14	0	0
58	1F	13	Total 13	Mg 13	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	7	Total 7	Mg 7	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	4	Total 4	Mg 4	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	4	Total 4	Mg 4	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	3	Total 3	Mg 3	0	0
58	1U	11	Total 11	Mg 11	0	0
58	1V	7	Total 7	Mg 7	0	0
58	1W	8	Total 8	Mg 8	0	0
58	1X	6	Total 6	Mg 6	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	3	Total 3	Mg 3	0	0
58	10	9	Total 9	Mg 9	0	0
58	11	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	12	2	Total 2	Mg 2	0	0
58	13	3	Total 3	Mg 3	0	0
58	15	9	Total 9	Mg 9	0	0
58	16	2	Total 2	Mg 2	0	0
58	17	3	Total 3	Mg 3	0	0
58	18	5	Total 5	Mg 5	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	218	Total 218	Mg 218	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1h	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	1	Total 1	Mg 1	0	0
58	1p	1	Total 1	Mg 1	0	0
58	1s	1	Total 1	Mg 1	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1v	2	Total 2	Mg 2	0	0
58	1w	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1x	13	Total 13	Mg 13	0	0
58	1y	1	Total 1	Mg 1	0	0
58	2A	883	Total 883	Mg 883	0	0
58	2B	19	Total 19	Mg 19	0	0
58	2D	7	Total 7	Mg 7	0	0
58	2E	11	Total 11	Mg 11	0	0
58	2F	9	Total 9	Mg 9	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	1	Total 1	Mg 1	0	0
58	2Q	3	Total 3	Mg 3	0	0
58	2R	3	Total 3	Mg 3	0	0
58	2S	1	Total 1	Mg 1	0	0
58	2T	3	Total 3	Mg 3	0	0
58	2U	2	Total 2	Mg 2	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	2	Total 2	Mg 2	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	21	1	Total 1	Mg 1	0	0
58	23	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	25	4	Total 4	Mg 4	0	0
58	26	1	Total 1	Mg 1	0	0
58	27	3	Total 3	Mg 3	0	0
58	28	4	Total 4	Mg 4	0	0
58	29	1	Total 1	Mg 1	0	0
58	2a	242	Total 242	Mg 242	0	0
58	2d	1	Total 1	Mg 1	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2i	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2l	5	Total 5	Mg 5	0	0
58	2p	1	Total 1	Mg 1	0	0
58	2q	2	Total 2	Mg 2	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	1	Total 1	Mg 1	0	0
58	2v	3	Total 3	Mg 3	0	0
58	2w	12	Total 12	Mg 12	0	0
58	2x	5	Total 5	Mg 5	0	0
58	2y	6	Total 6	Mg 6	0	0

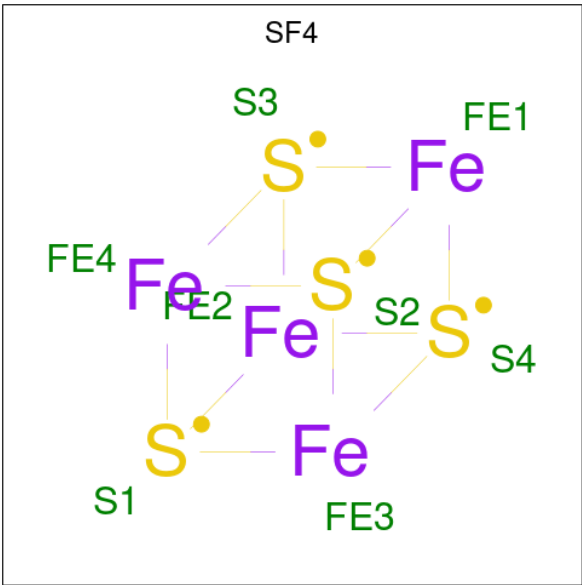
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

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

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	2019	Total	O	0	0
			2019	2019		
62	1B	63	Total	O	0	0
			63	63		
62	1D	24	Total	O	0	0
			24	24		
62	1E	24	Total	O	0	0
			24	24		
62	1F	15	Total	O	0	0
			15	15		
62	1G	2	Total	O	0	0
			2	2		
62	1H	2	Total	O	0	0
			2	2		
62	1I	1	Total	O	0	0
			1	1		
62	1N	5	Total	O	0	0
			5	5		
62	1O	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	19	Total 19	O 19	0	0
62	1Q	8	Total 8	O 8	0	0
62	1R	12	Total 12	O 12	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	9	Total 9	O 9	0	0
62	1U	15	Total 15	O 15	0	0
62	1V	8	Total 8	O 8	0	0
62	1W	9	Total 9	O 9	0	0
62	1X	4	Total 4	O 4	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	13	Total 13	O 13	0	0
62	11	11	Total 11	O 11	0	0
62	12	4	Total 4	O 4	0	0
62	13	5	Total 5	O 5	0	0
62	14	1	Total 1	O 1	0	0
62	15	5	Total 5	O 5	0	0
62	16	4	Total 4	O 4	0	0
62	17	7	Total 7	O 7	0	0
62	18	9	Total 9	O 9	0	0
62	1a	388	Total 388	O 388	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1b	1	Total 1	O 1	0	0
62	1f	1	Total 1	O 1	0	0
62	1l	8	Total 8	O 8	0	0
62	1m	2	Total 2	O 2	0	0
62	1n	1	Total 1	O 1	0	0
62	1o	1	Total 1	O 1	0	0
62	1p	1	Total 1	O 1	0	0
62	1q	2	Total 2	O 2	0	0
62	1u	1	Total 1	O 1	0	0
62	1v	6	Total 6	O 6	0	0
62	1w	20	Total 20	O 20	0	0
62	1x	15	Total 15	O 15	0	0
62	1y	2	Total 2	O 2	0	0
62	1z	1	Total 1	O 1	0	0
62	2A	1153	Total 1153	O 1153	0	0
62	2B	23	Total 23	O 23	0	0
62	2D	24	Total 24	O 24	0	0
62	2E	14	Total 14	O 14	0	0
62	2F	13	Total 13	O 13	0	0
62	2I	2	Total 2	O 2	0	0
62	2N	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2O	3	Total 3	O 3	0	0
62	2P	14	Total 14	O 14	0	0
62	2Q	3	Total 3	O 3	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	4	Total 4	O 4	0	0
62	2U	2	Total 2	O 2	0	0
62	2W	2	Total 2	O 2	0	0
62	2X	2	Total 2	O 2	0	0
62	2Y	1	Total 1	O 1	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	3	Total 3	O 3	0	0
62	21	13	Total 13	O 13	0	0
62	23	1	Total 1	O 1	0	0
62	25	1	Total 1	O 1	0	0
62	27	5	Total 5	O 5	0	0
62	28	4	Total 4	O 4	0	0
62	29	1	Total 1	O 1	0	0
62	2a	283	Total 283	O 283	0	0
62	2c	2	Total 2	O 2	0	0
62	2d	2	Total 2	O 2	0	0
62	2e	1	Total 1	O 1	0	0

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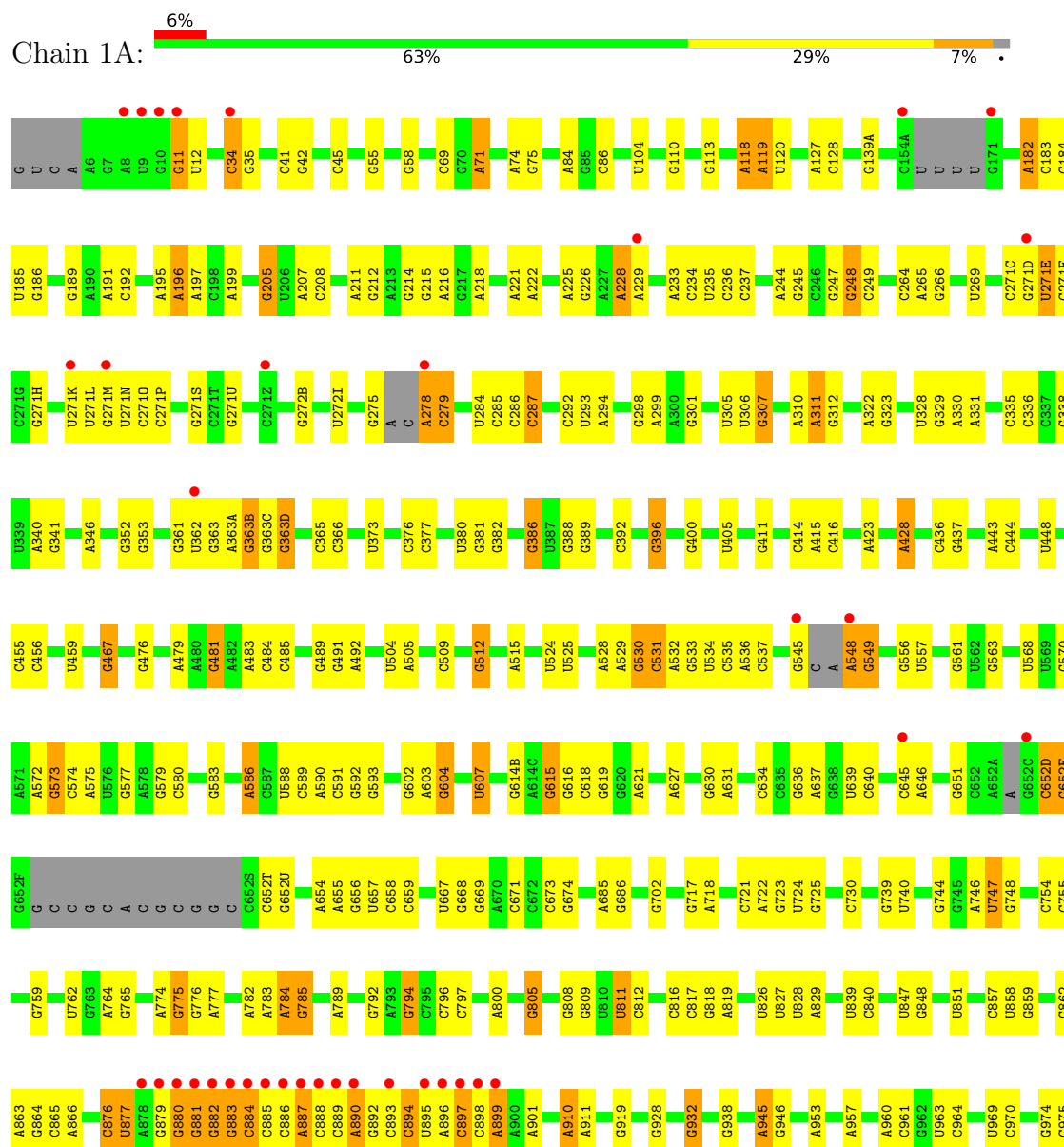
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2j	3	Total 3	O 3	0	0
62	2l	6	Total 6	O 6	0	0
62	2p	1	Total 1	O 1	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	1	Total 1	O 1	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	10	Total 10	O 10	0	0
62	2x	6	Total 6	O 6	0	0
62	2y	9	Total 9	O 9	0	0

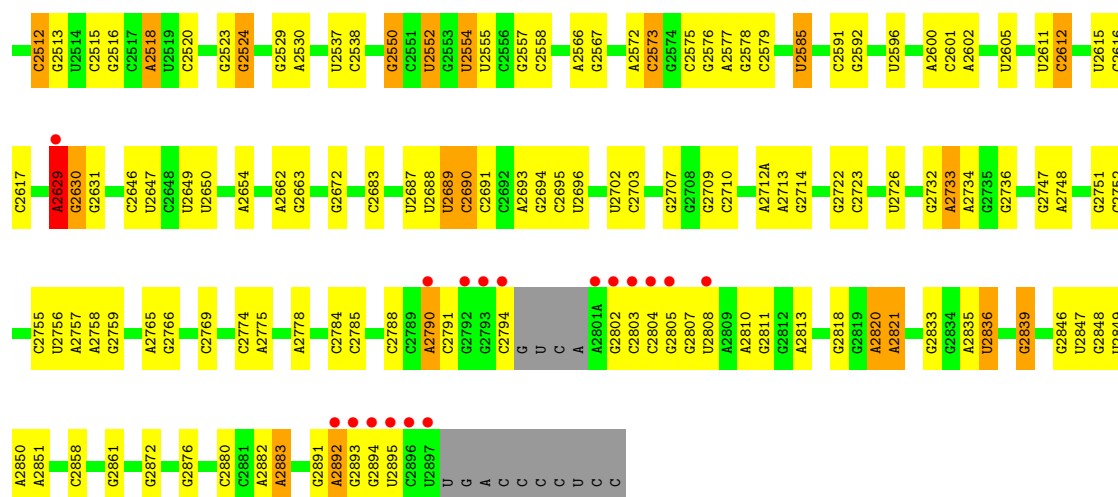
3 Residue-property plots [i](#)

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

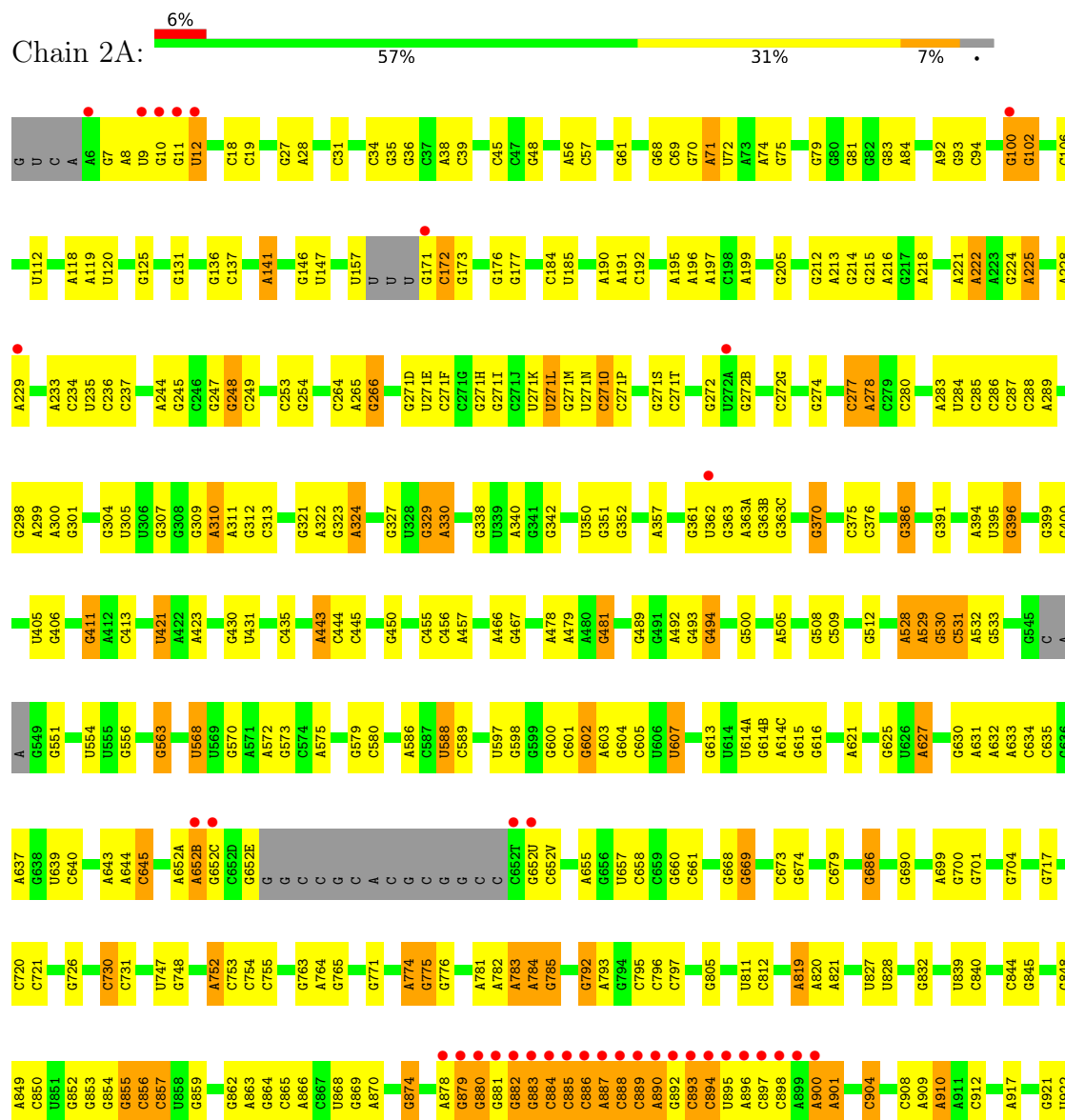
• Molecule 1: 23S Ribosomal RNA



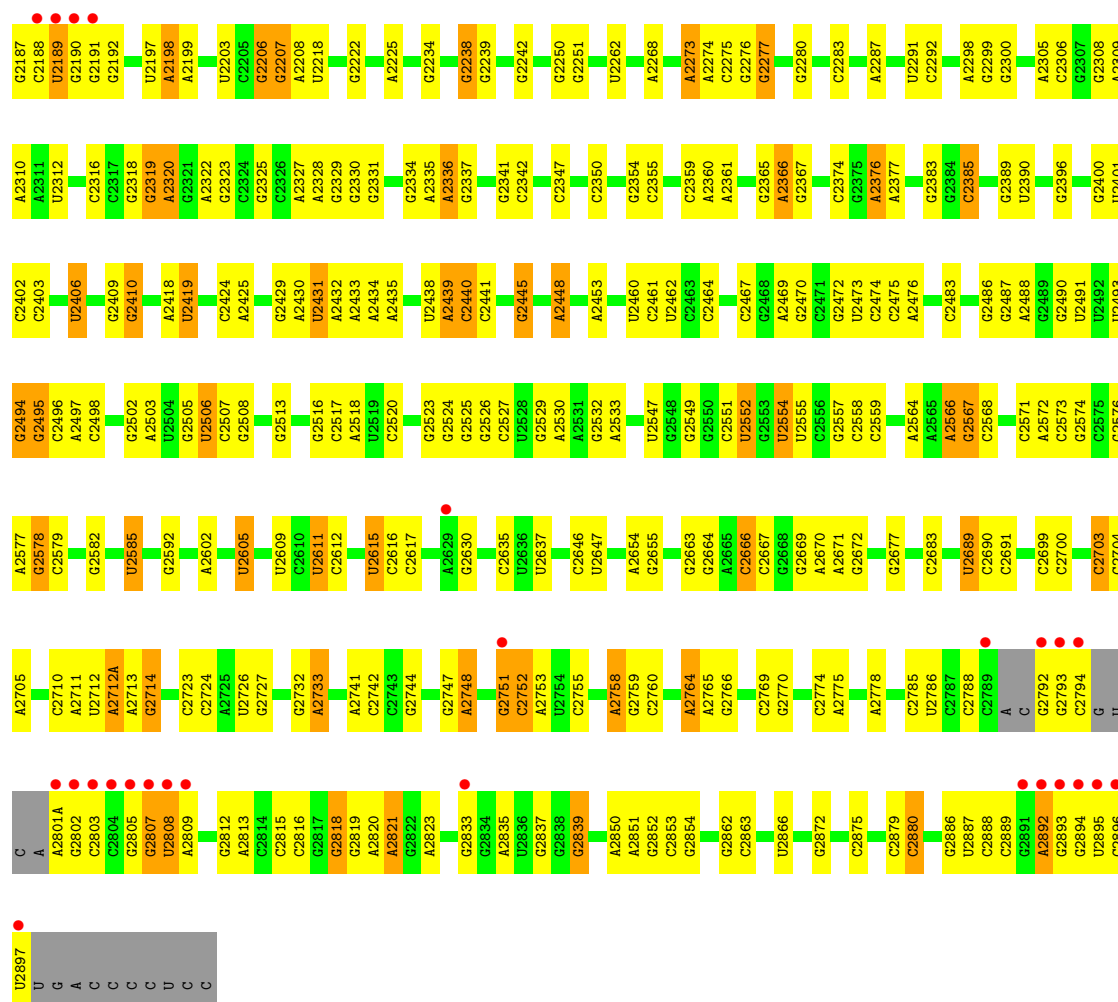


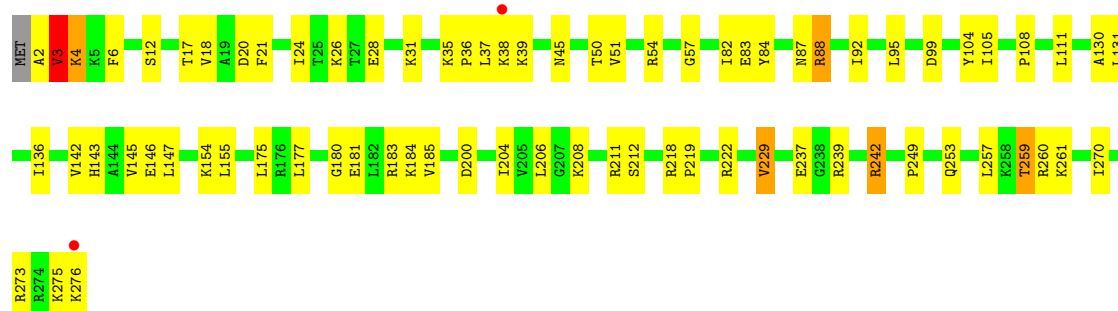


• Molecule 1: 23S Ribosomal RNA

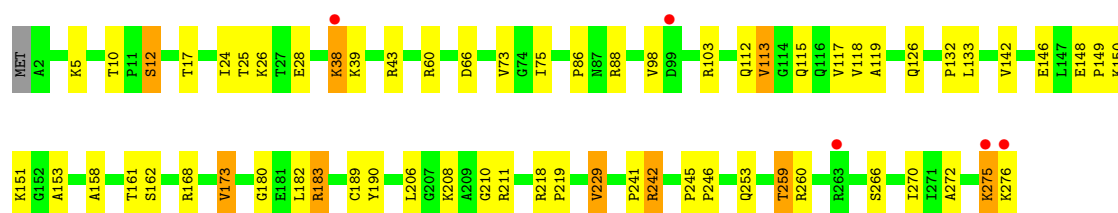
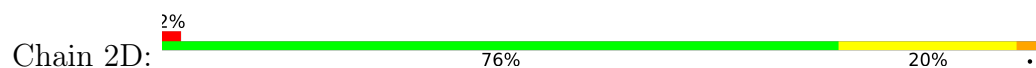




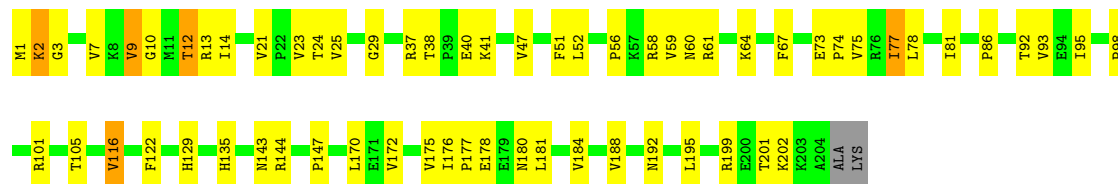




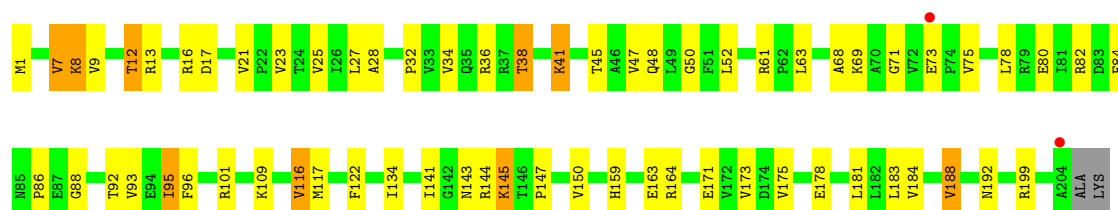
• Molecule 3: 50S ribosomal protein L2



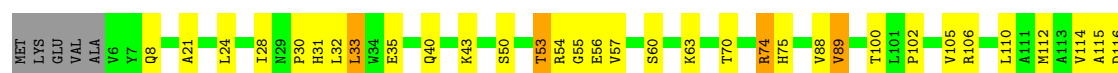
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

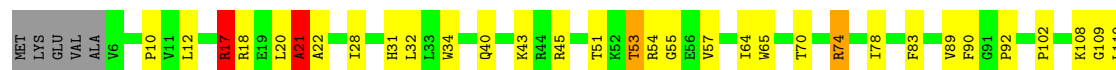


• Molecule 5: 50S ribosomal protein L4

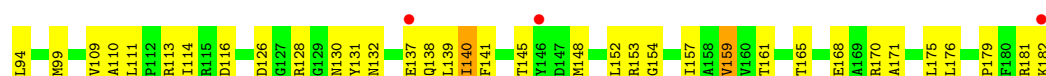
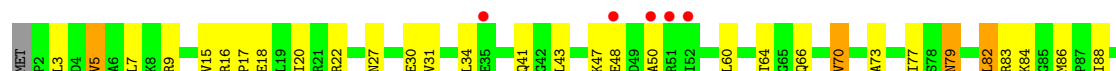




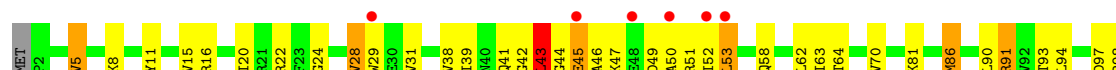
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5



• Molecule 6: 50S ribosomal protein L5

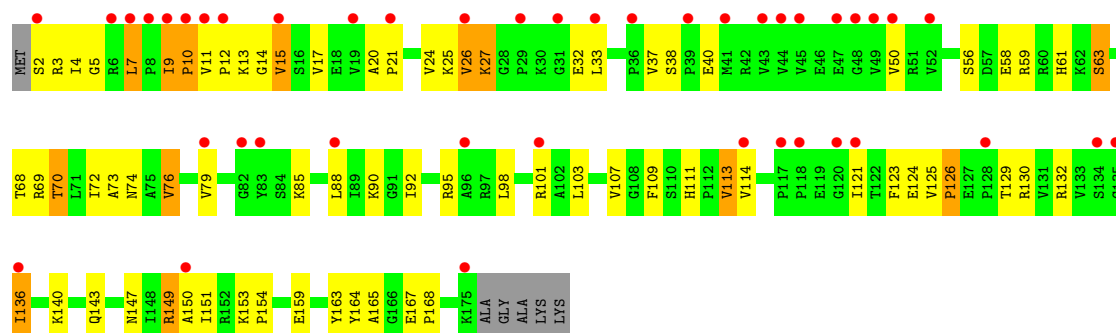


• Molecule 7: 50S ribosomal protein L6

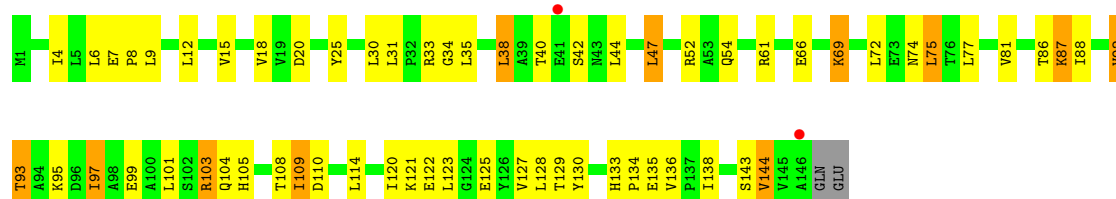




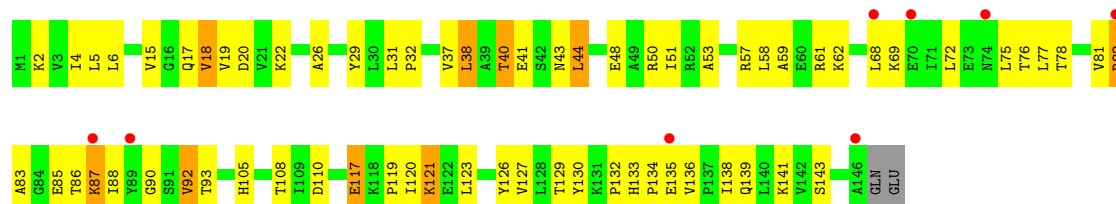
• Molecule 7: 50S ribosomal protein L6



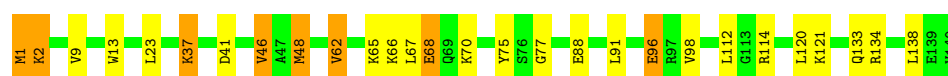
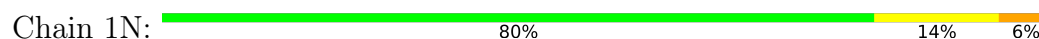
• Molecule 8: 50S ribosomal protein L9



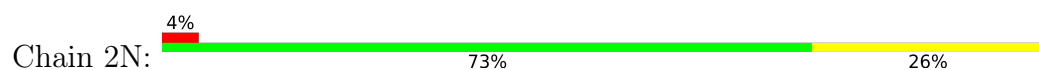
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

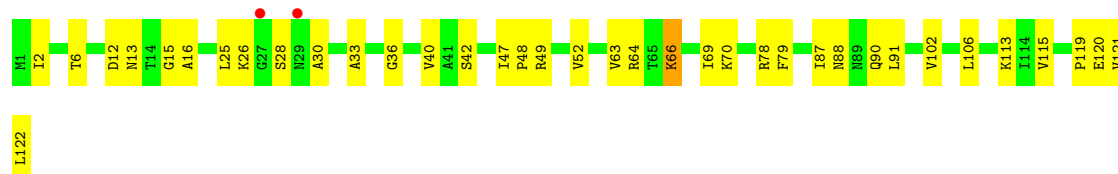




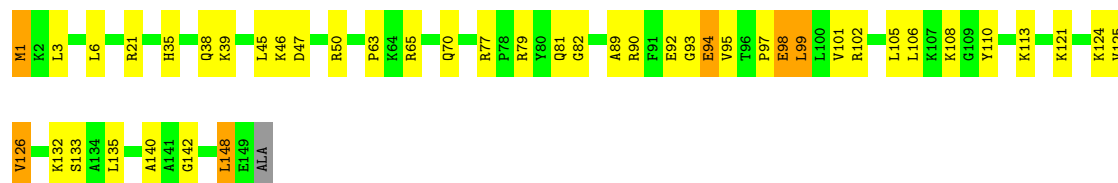
- Molecule 10: 50S ribosomal protein L14



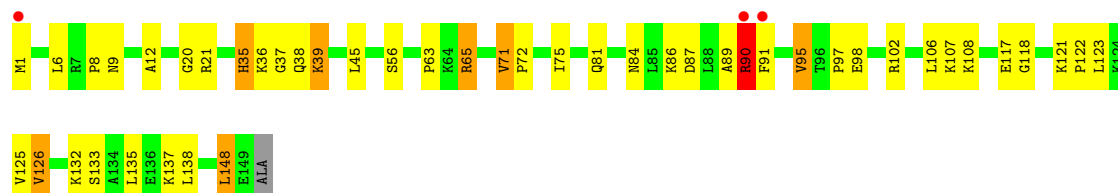
- Molecule 10: 50S ribosomal protein L14



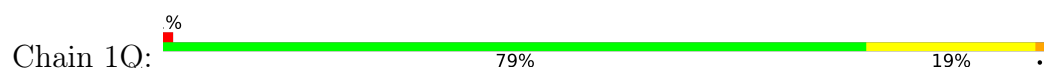
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15

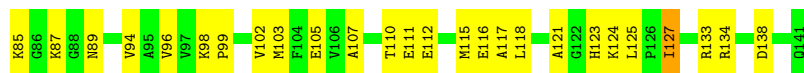
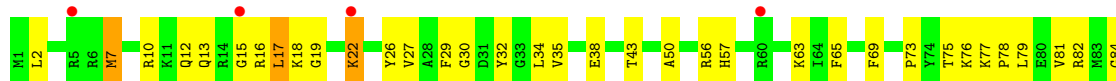


- Molecule 12: 50S ribosomal protein L16

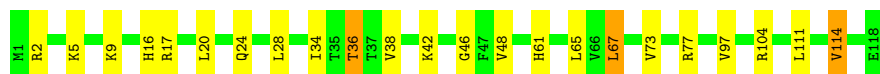
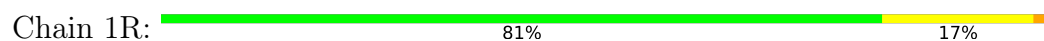




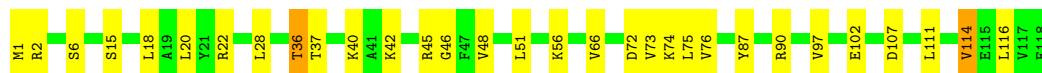
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17



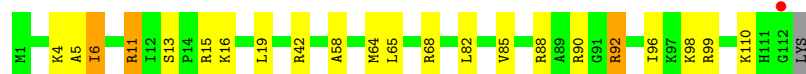
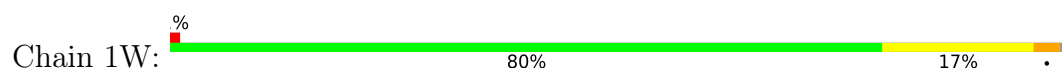
- Molecule 14: 50S ribosomal protein L18



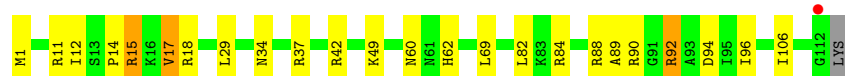
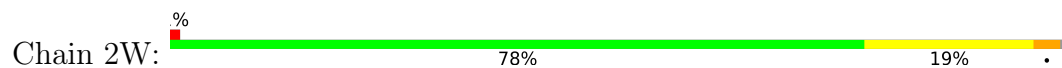
- Molecule 14: 50S ribosomal protein L18



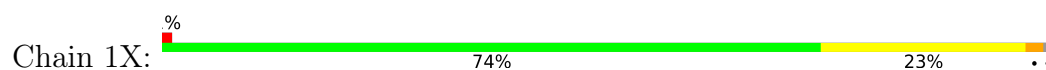
- Molecule 15: 50S ribosomal protein L19



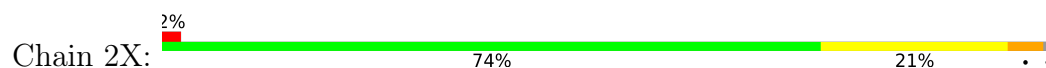
- Molecule 18: 50S ribosomal protein L22



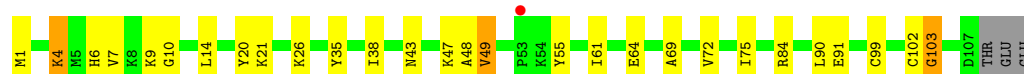
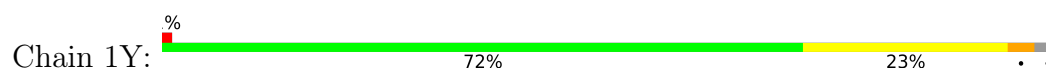
- Molecule 19: 50S ribosomal protein L23



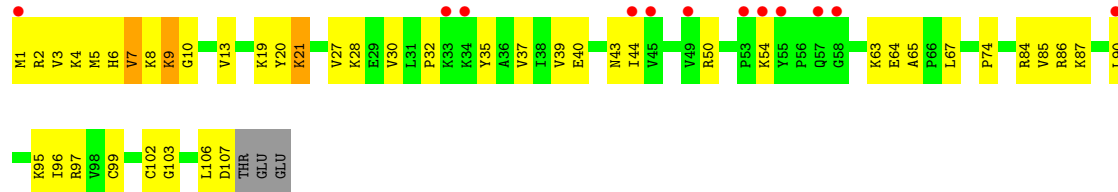
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



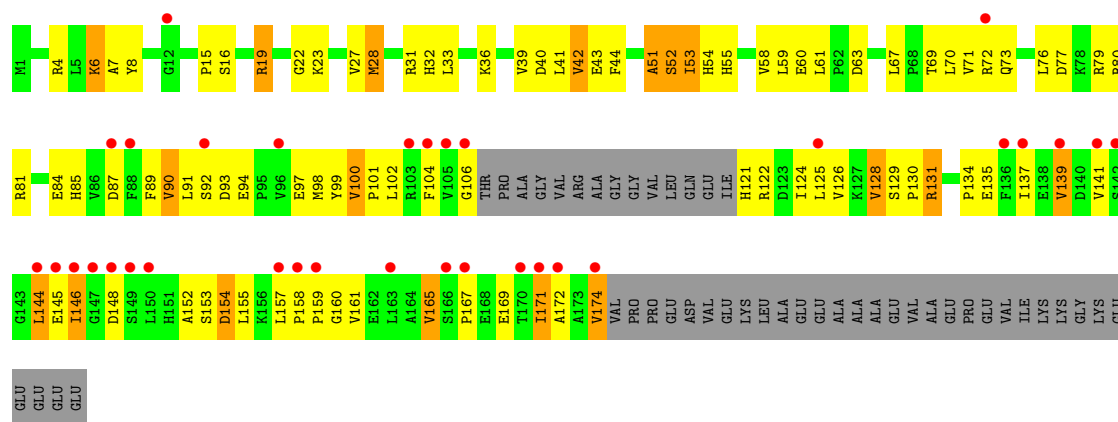
- Molecule 20: 50S ribosomal protein L24



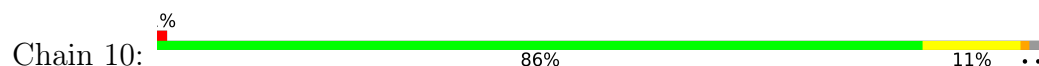
- Molecule 21: 50S ribosomal protein L25



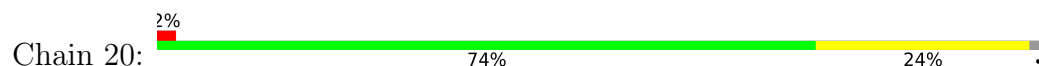
- Molecule 21: 50S ribosomal protein L25



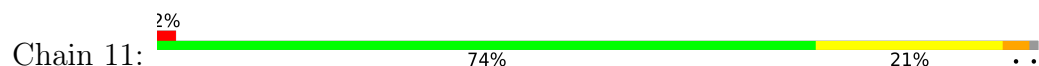
- Molecule 22: 50S ribosomal protein L27



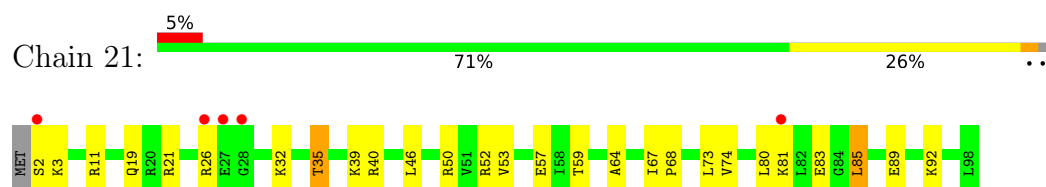
- Molecule 22: 50S ribosomal protein L27



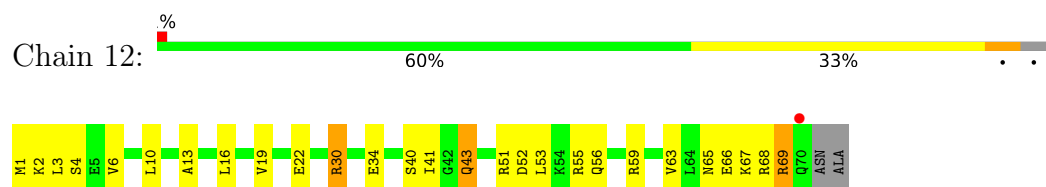
- Molecule 23: 50S ribosomal protein L28



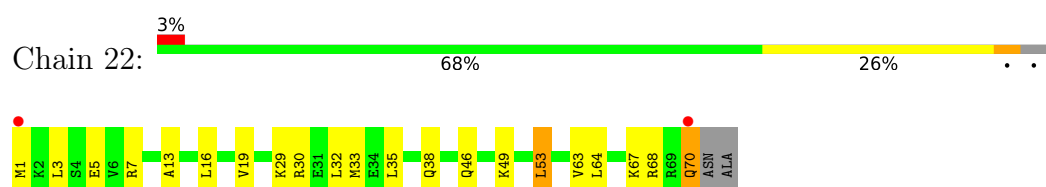
- Molecule 23: 50S ribosomal protein L28



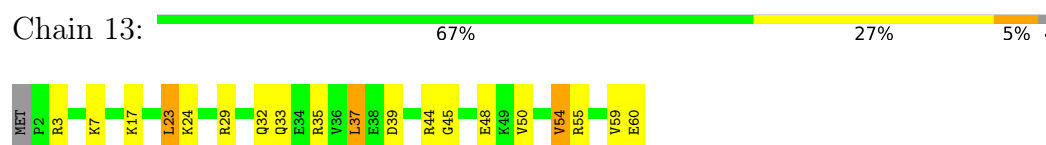
- Molecule 24: 50S ribosomal protein L29



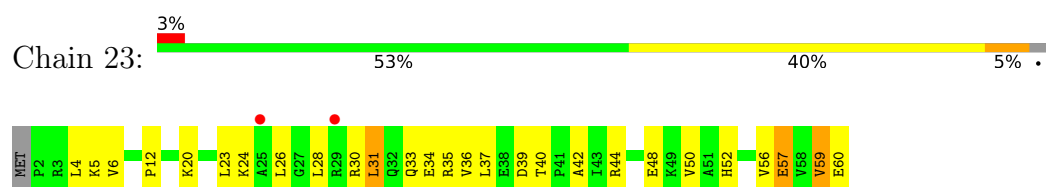
- Molecule 24: 50S ribosomal protein L29



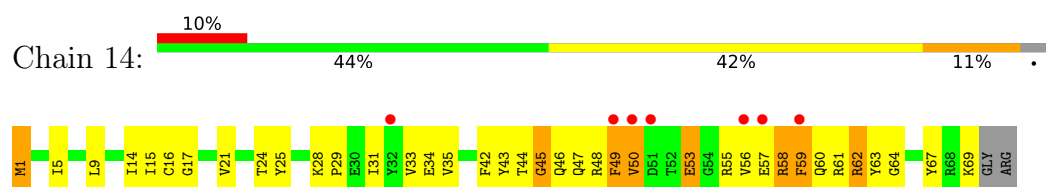
- Molecule 25: 50S ribosomal protein L30



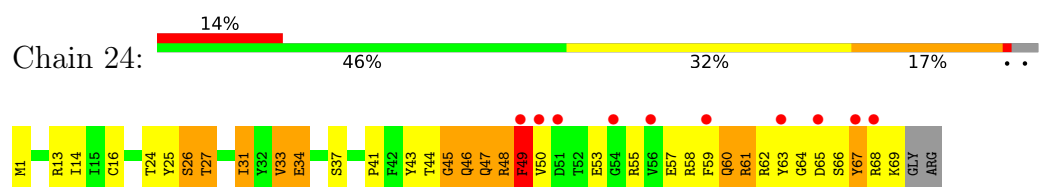
- Molecule 25: 50S ribosomal protein L30




- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31




- Molecule 27: 50S ribosomal protein L32

Chain 15:  75% 22% ..



- Molecule 27: 50S ribosomal protein L32

Chain 25:  82% 17% .



- Molecule 28: 50S ribosomal protein L33

Chain 16:  69% 28% ..




- Molecule 28: 50S ribosomal protein L33

Chain 26:  2% 65% 26% 7% .



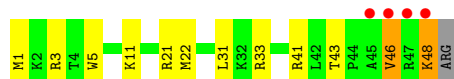
- Molecule 29: 50S ribosomal protein L34

Chain 17:  4% 76% 18% ..



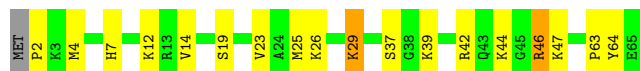
- Molecule 29: 50S ribosomal protein L34

Chain 27:  8% 73% 20% ..

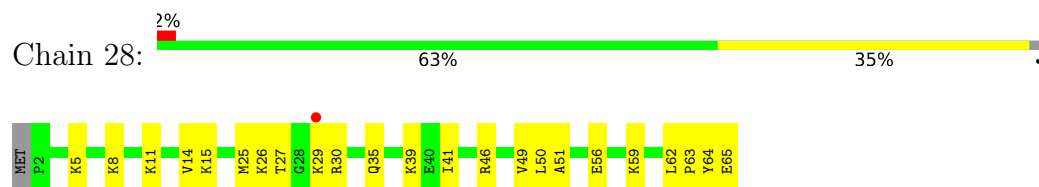


- Molecule 30: 50S ribosomal protein L35

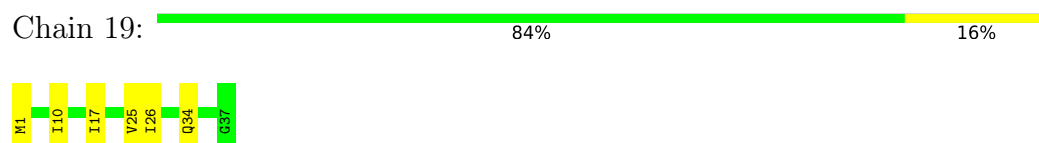
Chain 18:  71% 25% ..



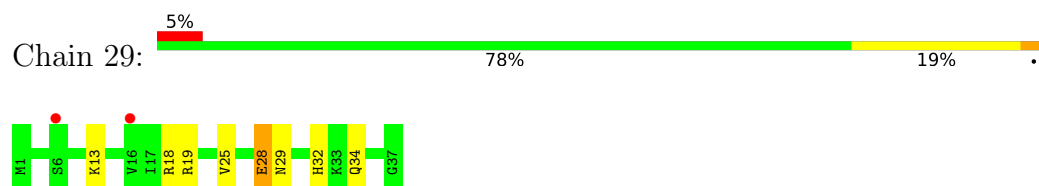
- Molecule 30: 50S ribosomal protein L35



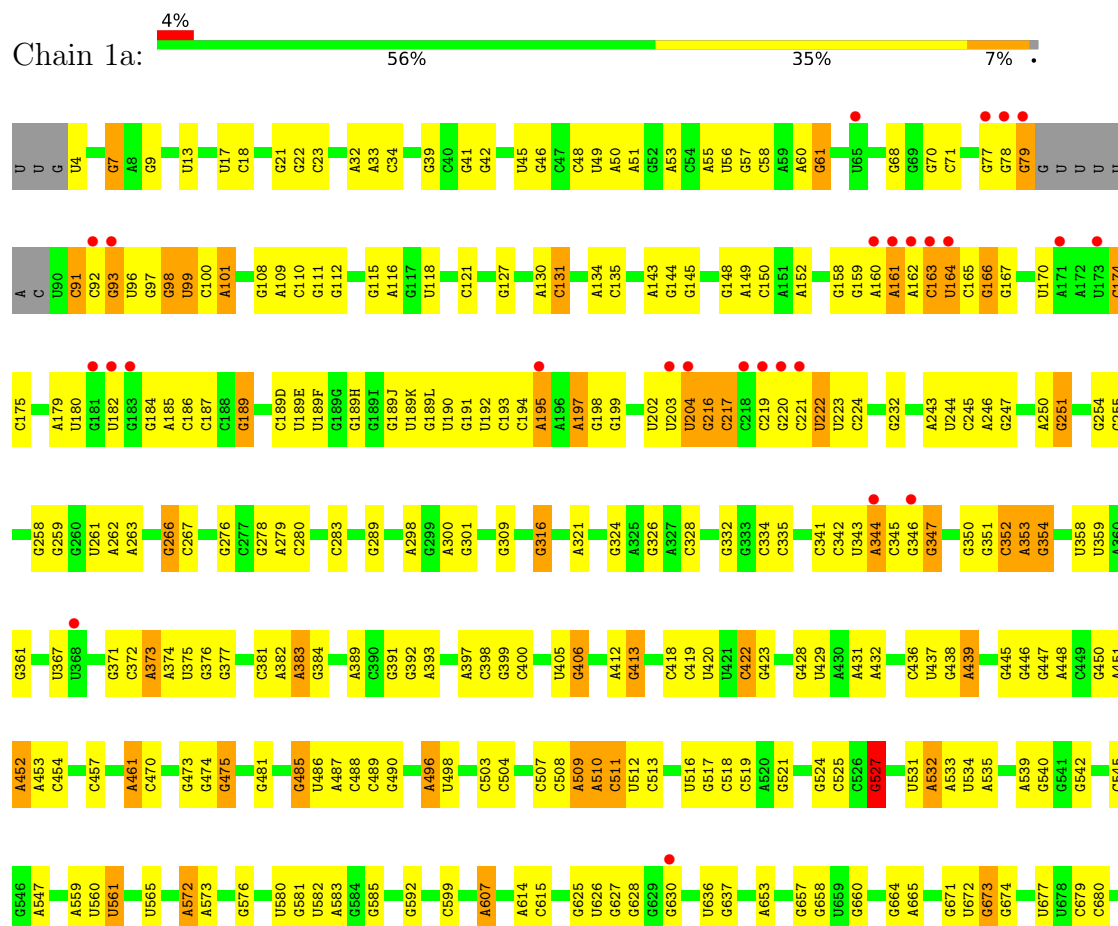
- Molecule 31: 50S ribosomal protein L36

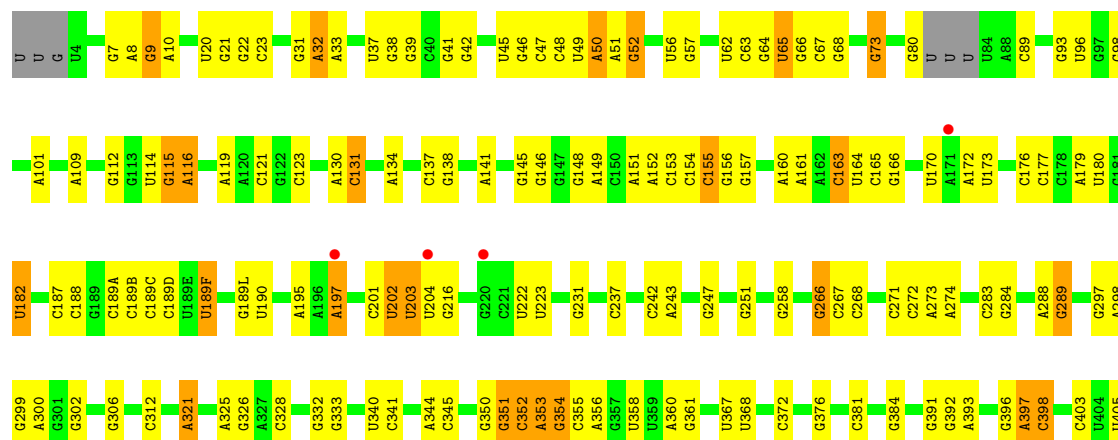
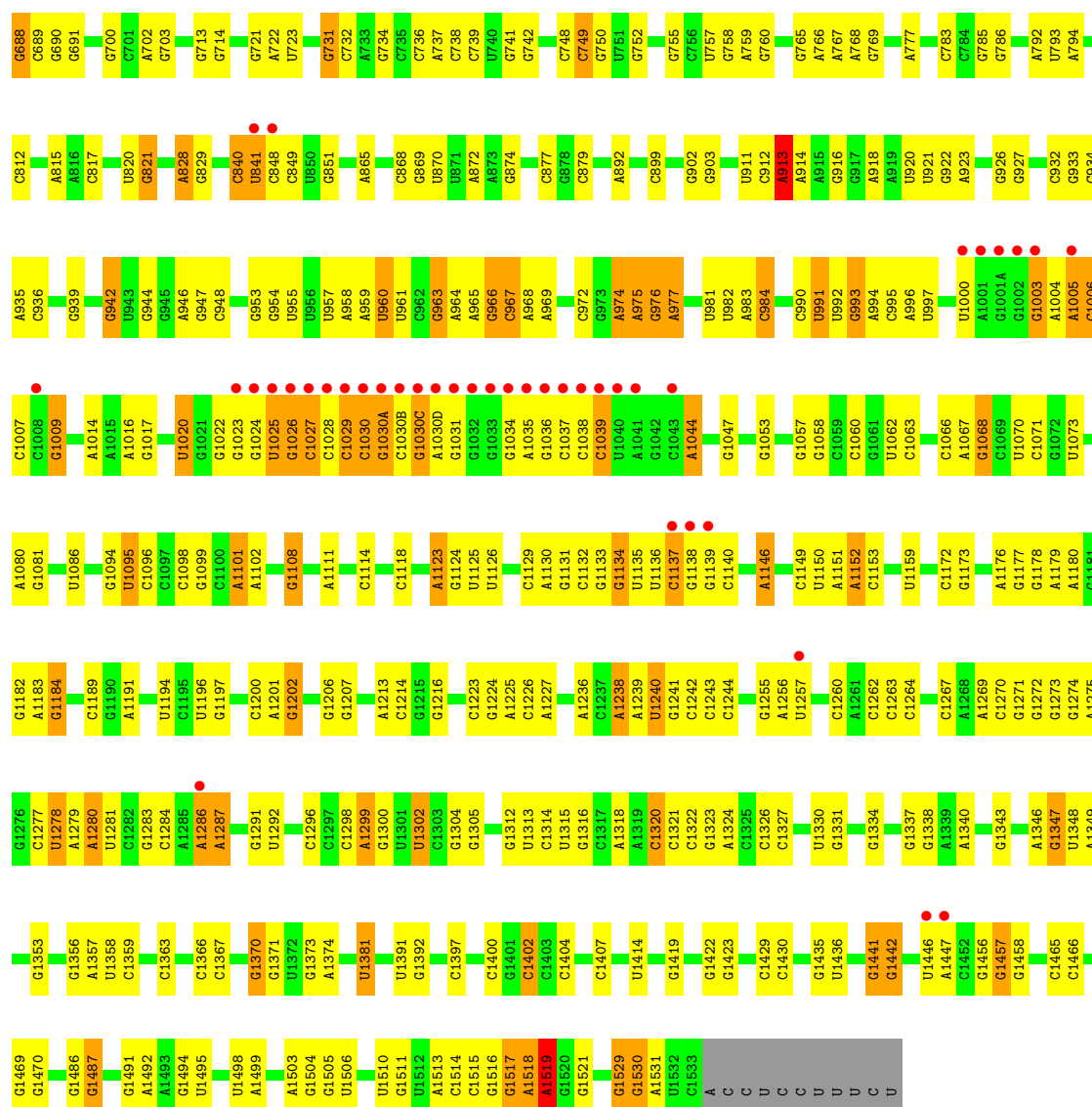


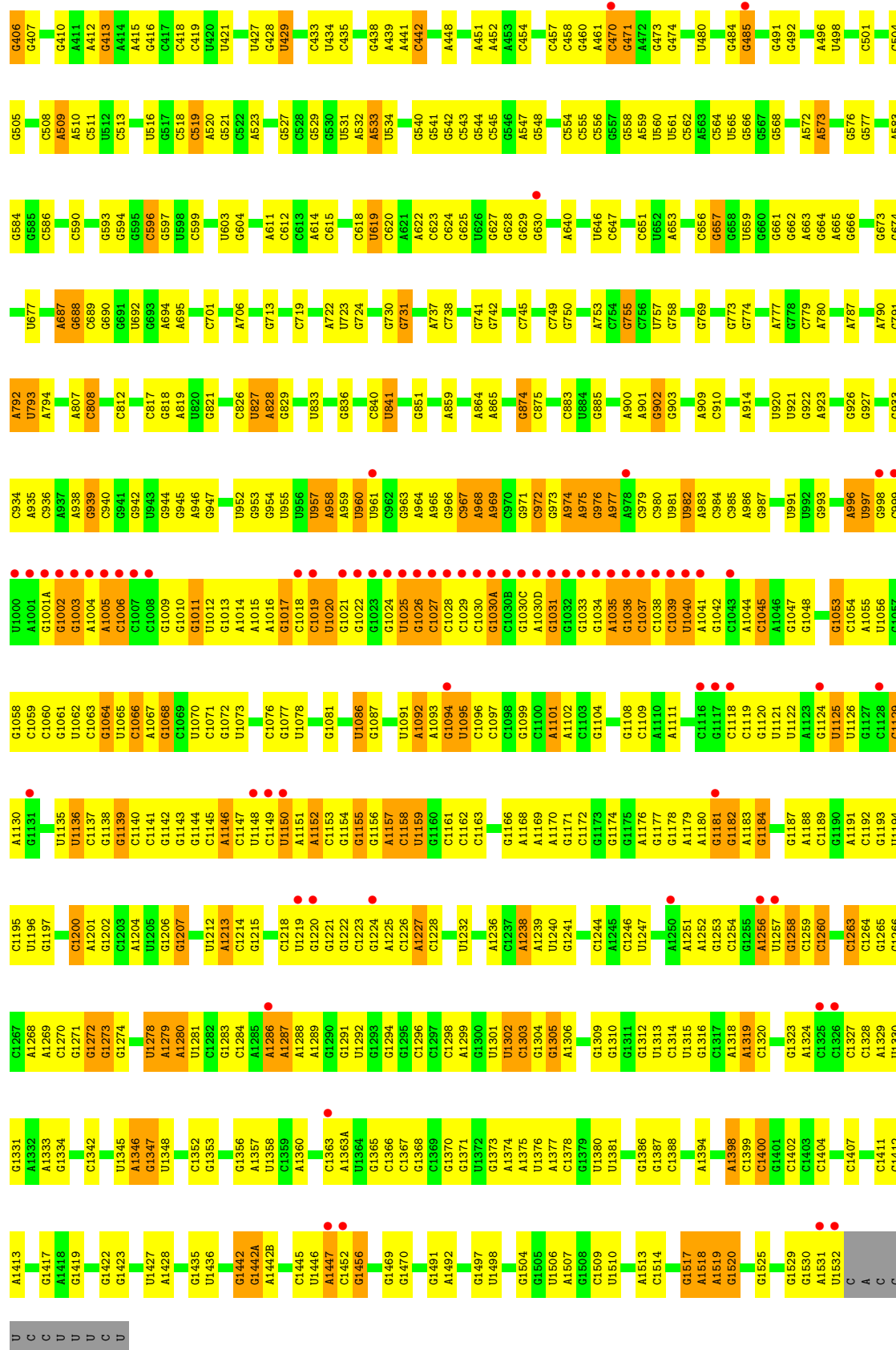
- Molecule 31: 50S ribosomal protein L36



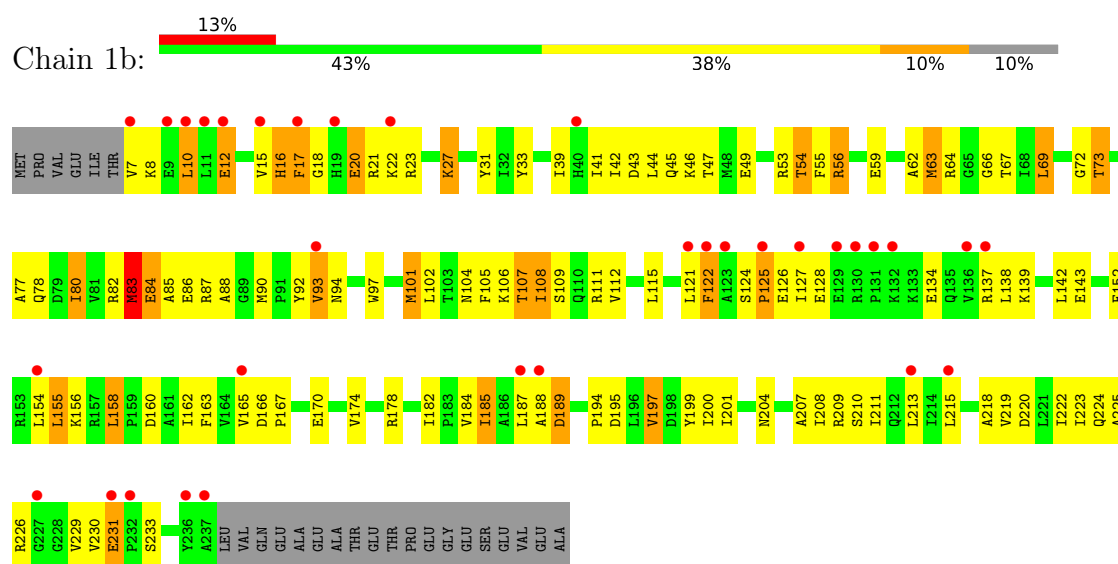
- Molecule 32: 16S Ribosomal RNA



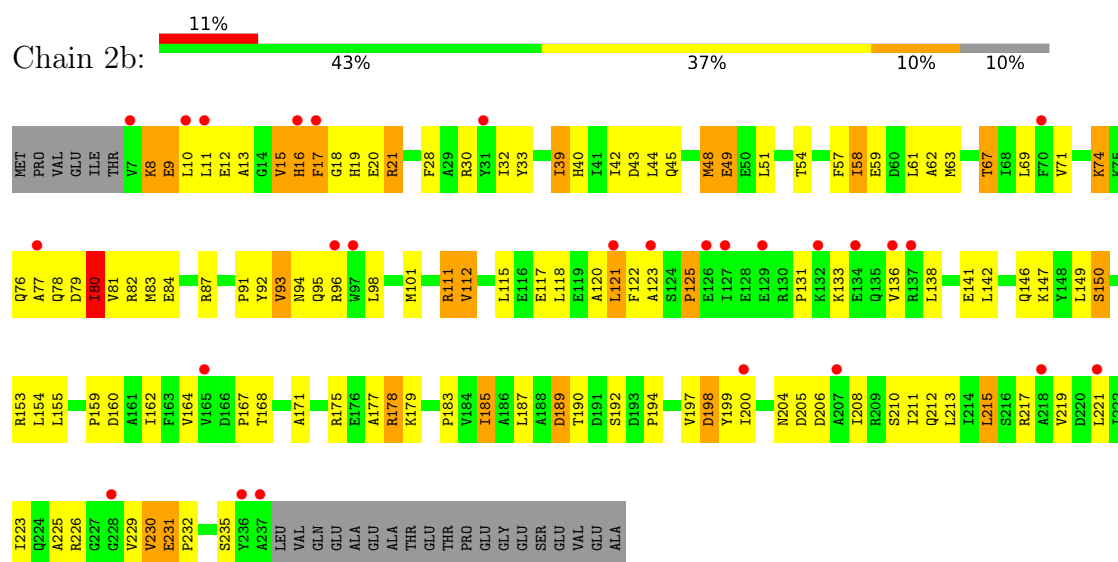




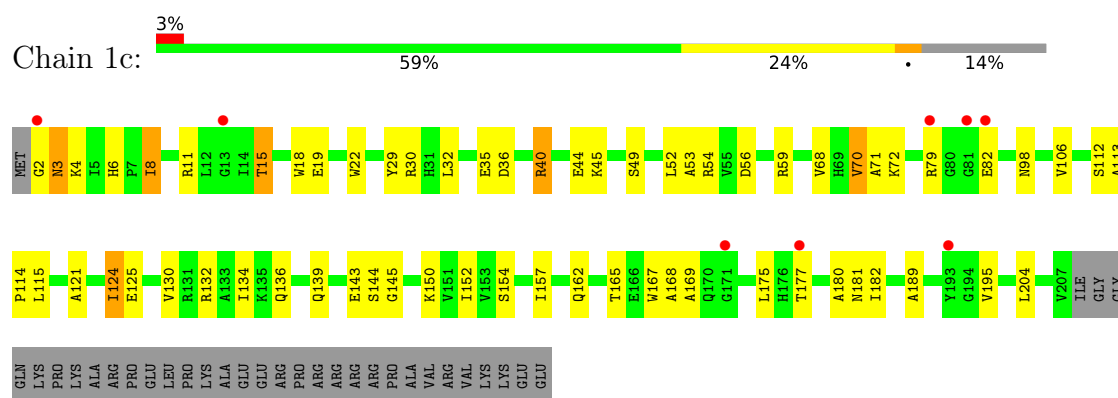
- Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2



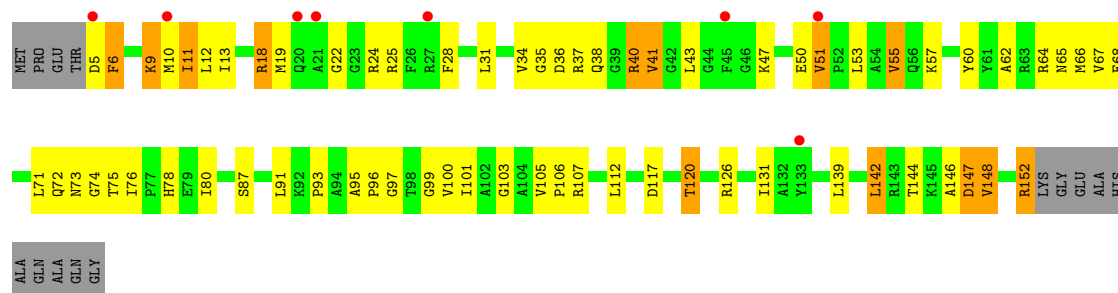
• Molecule 34: 30S ribosomal protein S3



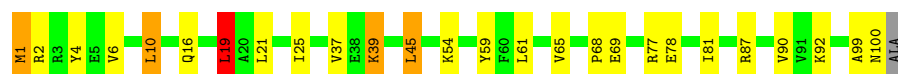
• Molecule 34: 30S ribosomal protein S3



- Molecule 36: 30S ribosomal protein S5



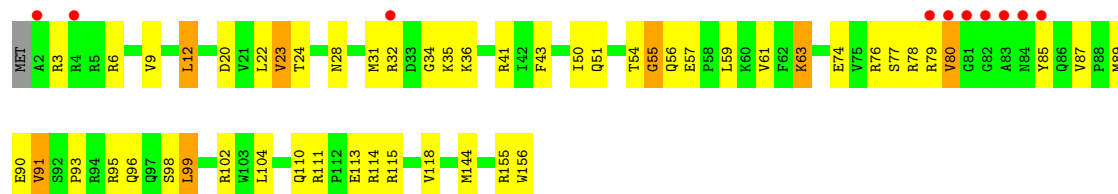
- Molecule 37: 30S ribosomal protein S6



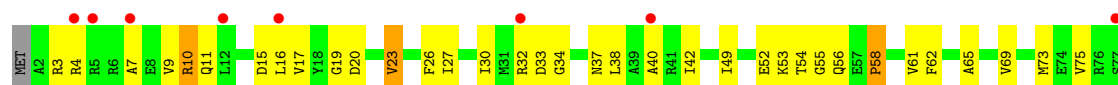
- Molecule 37: 30S ribosomal protein S6



- 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

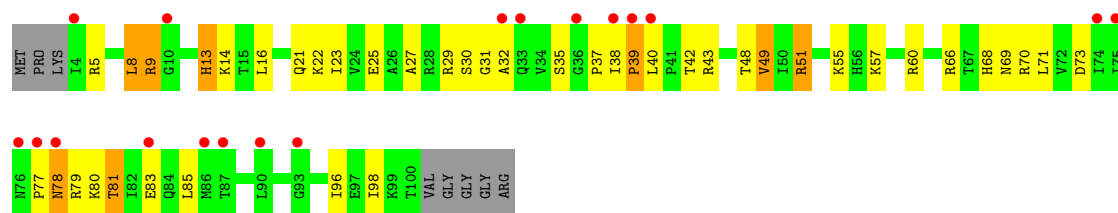


• Molecule 40: 30S ribosomal protein S9

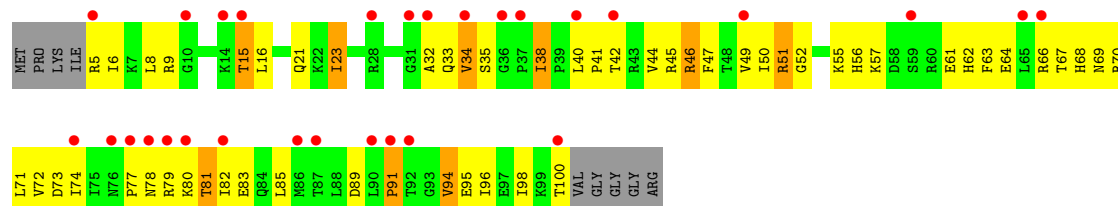


• Molecule 41: 30S ribosomal protein S10

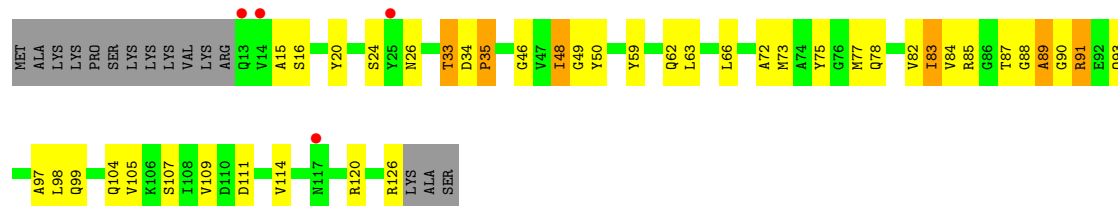




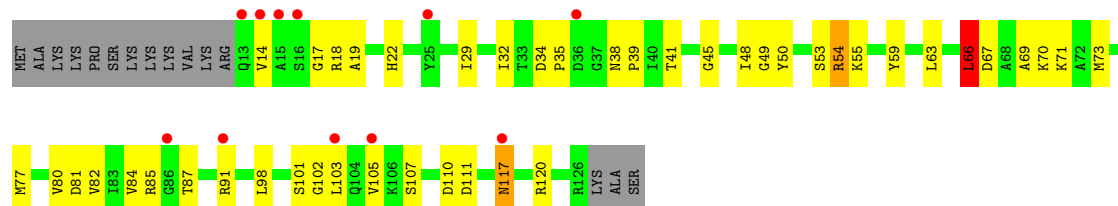
• Molecule 41: 30S ribosomal protein S10



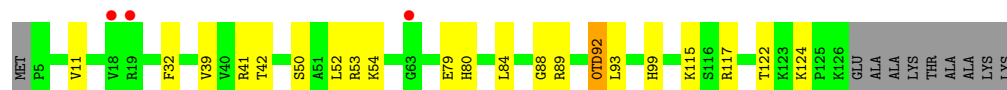
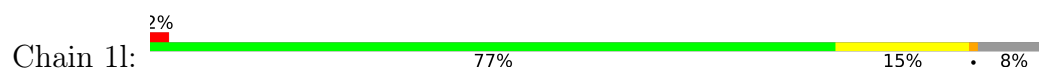
• Molecule 42: 30S ribosomal protein S11



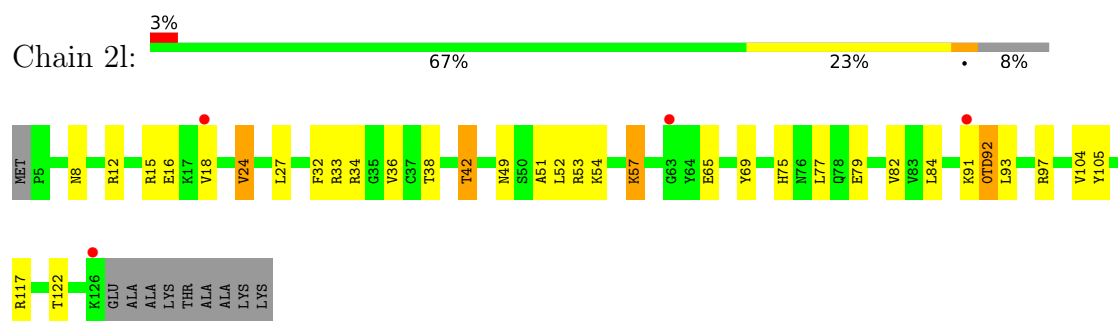
• Molecule 42: 30S ribosomal protein S11



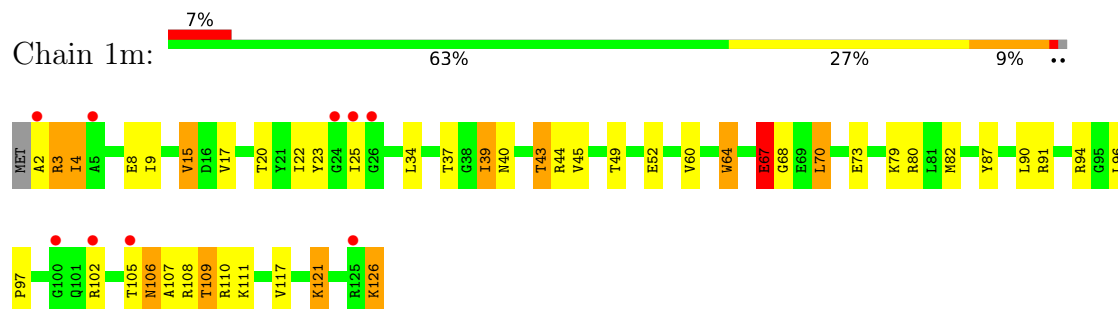
• Molecule 43: 30S ribosomal protein S12



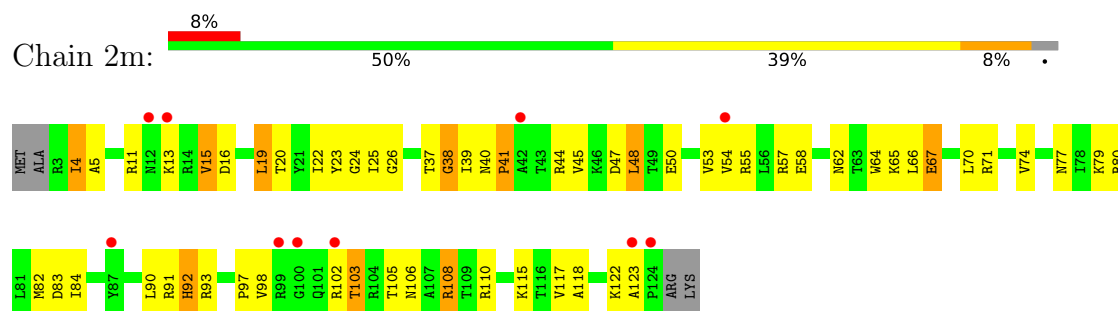
• Molecule 43: 30S ribosomal protein S12



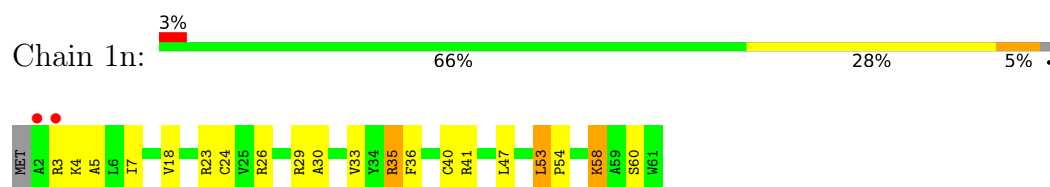
- Molecule 44: 30S ribosomal protein S13



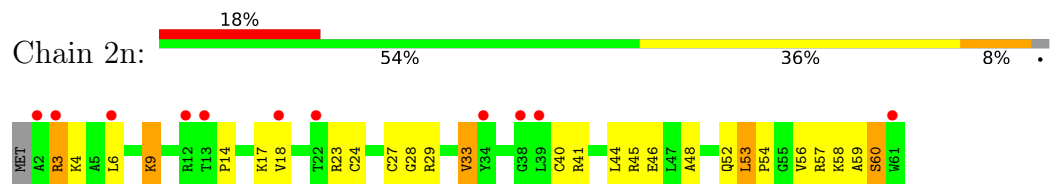
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

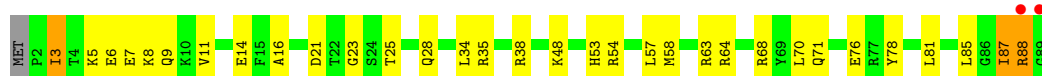


- Molecule 46: 30S ribosomal protein S15





- Molecule 46: 30S ribosomal protein S15

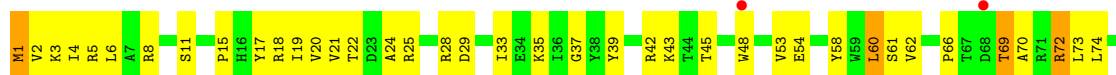


- Molecule 47: 30S ribosomal protein S16



GLY
ALA

- Molecule 47: 30S ribosomal protein S16



V79
Q82
GLU
ALA
ARG
GLY
GLY
ALA

- Molecule 48: 30S ribosomal protein S17

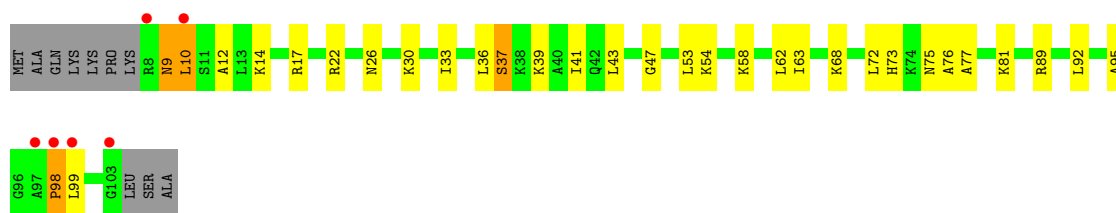


- Molecule 48: 30S ribosomal protein S17

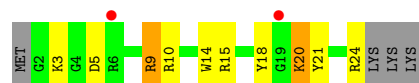


K100
ARG
GLY
GLY
LYS
ALA

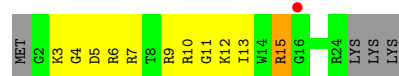
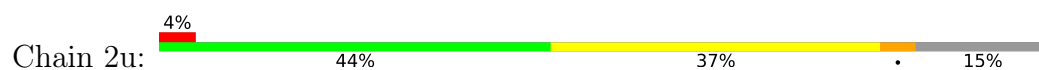
- Chain 2t:



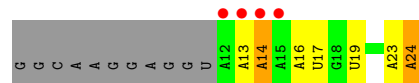
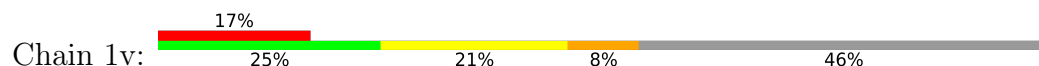
- Molecule 52: 30S ribosomal protein Thx



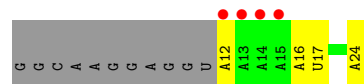
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: MET-PHE-mRNA



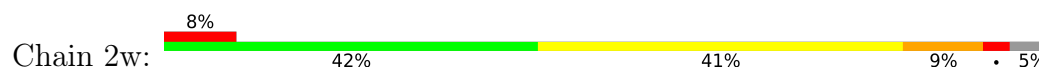
- Molecule 53: MET-PHE-mRNA

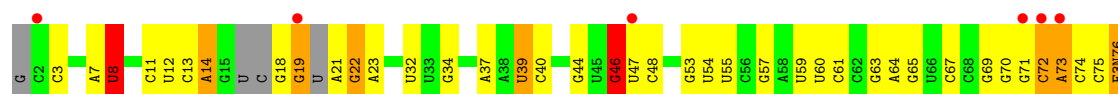


- Molecule 54: A-site Aminoacylated Phe-tRNAphe

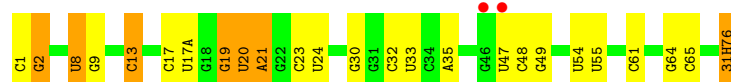


- Molecule 54: A-site Aminoacylated Phe-tRNAphe





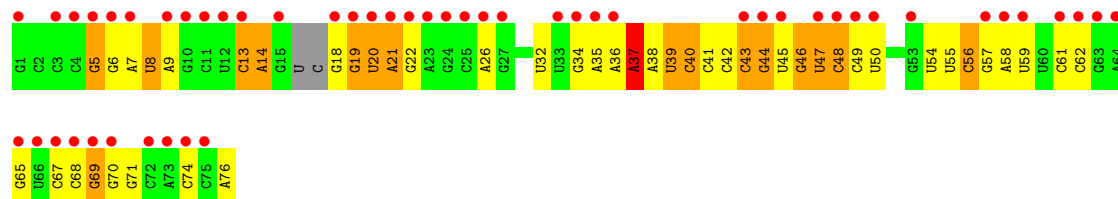
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



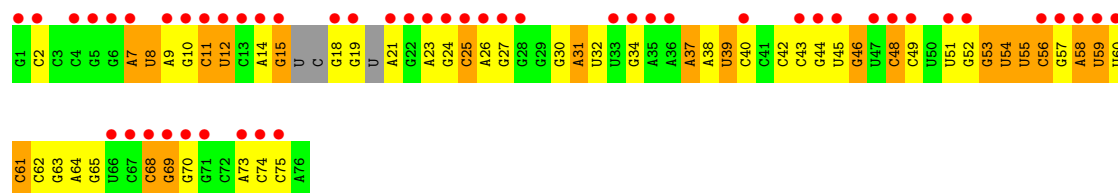
- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



- Molecule 56: E-site Deacylated tRNA^{phe}



- Molecule 56: E-site Deacylated tRNA^{phe}



- Molecule 57: Lasso peptide lariocidin B



- Molecule 57: Lasso peptide lariocidin B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.29Å 450.05Å 626.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	365.48 – 2.60 365.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (365.48-2.60) 99.8 (365.48-2.60)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.215 , 0.266 0.218 , 0.266	Depositor DCC
R_{free} test set	89929 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	300583	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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: K, M2G, 5MC, OMU, UR3, MIA, F3N, MG, 4OC, ZN, 5MU, SF4, MA6, PSU, 0TD, OMC, 31H, G7M, 4SU, 2MA, OMG, 2MG

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	0.54	0/69011	0.71	9/107720 (0.0%)
1	2A	0.43	0/67295	0.62	6/105042 (0.0%)
2	1B	0.44	0/2882	0.66	0/4494
2	2B	0.37	0/2879	0.58	0/4487
3	1D	0.52	0/2186	0.72	0/2944
3	2D	0.46	0/2186	0.66	0/2944
4	1E	0.50	0/1592	0.72	0/2149
4	2E	0.39	0/1592	0.60	0/2149
5	1F	0.51	0/1619	0.78	2/2193 (0.1%)
5	2F	0.42	0/1615	0.65	2/2188 (0.1%)
6	1G	0.44	0/1448	0.64	0/1957
6	2G	0.36	0/1453	0.59	0/1963
7	1H	0.45	0/1356	0.64	0/1834
7	2H	0.35	0/1356	0.53	0/1834
8	1I	0.39	0/1112	0.57	0/1514
8	2I	0.37	0/1079	0.61	0/1475
9	1N	0.52	0/1144	0.69	0/1543
9	2N	0.39	0/1144	0.61	0/1543
10	1O	0.50	0/943	0.66	0/1269
10	2O	0.38	0/943	0.59	0/1269
11	1P	0.51	0/1152	0.78	2/1533 (0.1%)
11	2P	0.43	0/1152	0.73	2/1533 (0.1%)
12	1Q	0.51	0/1143	0.69	0/1527
12	2Q	0.41	0/1143	0.57	0/1527
13	1R	0.57	0/982	0.77	0/1312
13	2R	0.41	0/982	0.63	0/1312
14	1S	0.45	0/883	0.69	0/1176
14	2S	0.39	0/880	0.61	0/1172
15	1T	0.48	0/1105	0.71	0/1477
15	2T	0.39	0/1097	0.61	0/1468
16	1U	0.57	0/977	0.73	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.41	0/977	0.60	0/1301
17	1V	0.52	0/782	0.71	0/1049
17	2V	0.38	0/782	0.63	0/1049
18	1W	0.57	0/897	0.70	0/1205
18	2W	0.45	0/897	0.58	0/1205
19	1X	0.56	0/764	0.76	2/1025 (0.2%)
19	2X	0.42	0/764	0.68	2/1025 (0.2%)
20	1Y	0.45	0/819	0.70	0/1095
20	2Y	0.40	0/819	0.65	0/1095
21	1Z	0.45	0/1267	0.66	0/1717
21	2Z	0.38	0/1299	0.61	0/1763
22	10	0.52	0/662	0.73	0/881
22	20	0.40	0/662	0.67	0/881
23	11	0.53	0/762	0.63	0/1014
23	21	0.42	0/762	0.56	0/1014
24	12	0.53	0/590	0.66	0/781
24	22	0.37	0/590	0.60	0/781
25	13	0.53	0/474	0.70	0/635
25	23	0.38	0/469	0.67	0/630
26	14	0.48	0/565	0.70	0/761
26	24	0.40	0/545	0.71	0/737
27	15	0.55	0/469	0.76	0/635
27	25	0.42	0/469	0.62	0/635
28	16	0.50	0/460	0.64	0/613
28	26	0.44	0/456	0.60	0/608
29	17	0.60	0/426	0.76	0/561
29	27	0.54	0/426	0.71	0/561
30	18	0.49	0/525	0.72	0/691
30	28	0.45	0/525	0.63	0/691
31	19	0.53	0/310	0.81	1/407 (0.2%)
31	29	0.38	0/310	0.65	0/407
32	1a	0.40	0/35795	0.60	3/55864 (0.0%)
32	2a	0.37	1/35886 (0.0%)	0.57	3/56005 (0.0%)
33	1b	0.37	0/1881	0.66	0/2542
33	2b	0.41	0/1860	0.60	0/2518
34	1c	0.39	0/1572	0.61	0/2126
34	2c	0.38	0/1566	0.57	1/2119 (0.0%)
35	1d	0.37	0/1685	0.61	0/2262
35	2d	0.37	0/1704	0.59	0/2284
36	1e	0.40	0/1145	0.62	0/1543
36	2e	0.40	0/1149	0.59	0/1548
37	1f	0.39	0/823	0.56	0/1115
37	2f	0.39	0/829	0.59	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.36	0/1250	0.59	0/1679
38	2g	0.38	0/1254	0.58	0/1683
39	1h	0.36	0/1108	0.57	0/1494
39	2h	0.33	0/1108	0.55	0/1494
40	1i	0.36	0/1002	0.61	1/1346 (0.1%)
40	2i	0.38	0/997	0.59	0/1343
41	1j	0.43	0/722	0.62	0/982
41	2j	0.40	0/727	0.68	1/988 (0.1%)
42	1k	0.39	0/844	0.59	0/1145
42	2k	0.39	0/848	0.60	0/1149
43	1l	0.43	0/937	0.62	0/1260
43	2l	0.39	0/937	0.60	0/1260
44	1m	0.41	0/990	0.68	0/1327
44	2m	0.37	0/961	0.62	0/1291
45	1n	0.39	0/501	0.60	0/664
45	2n	0.38	0/501	0.63	0/664
46	1o	0.39	0/739	0.53	0/985
46	2o	0.38	0/739	0.52	0/985
47	1p	0.39	0/697	0.62	0/939
47	2p	0.35	0/693	0.62	0/935
48	1q	0.40	0/836	0.56	0/1117
48	2q	0.37	0/836	0.57	0/1117
49	1r	0.39	0/560	0.60	0/746
49	2r	0.39	0/560	0.56	0/746
50	1s	0.36	0/667	0.66	0/900
50	2s	0.39	0/661	0.72	2/893 (0.2%)
51	1t	0.39	0/730	0.69	0/965
51	2t	0.40	0/729	0.60	0/965
52	1u	0.34	0/203	0.54	0/266
52	2u	0.35	0/203	0.53	0/266
53	1v	0.46	0/310	0.60	0/480
53	2v	0.43	0/310	0.52	0/480
54	1w	0.49	2/1603 (0.1%)	0.63	0/2492
54	2w	0.46	1/1531 (0.1%)	0.60	0/2379
55	1x	0.48	0/1723	0.62	0/2684
55	2x	0.40	0/1723	0.58	0/2684
56	1y	0.58	2/1606 (0.1%)	0.56	0/2497
56	2y	0.60	2/1583 (0.1%)	0.60	0/2459
57	1z	0.40	0/128	0.82	0/163
57	2z	0.37	0/128	0.77	0/163
All	All	0.45	8/316935 (0.0%)	0.64	39/474426 (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
15	1T	0	1
21	1Z	0	1
26	14	0	1
26	24	0	1
33	1b	0	1
40	2i	0	1
44	2m	0	1
47	1p	0	1
All	All	0	8

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	O3'-P	6.51	1.62	1.56
56	2y	8	4SU	O3'-P	6.11	1.62	1.56
54	1w	46	G7M	O3'-P	5.87	1.62	1.56
56	1y	8	4SU	O3'-P	5.47	1.61	1.56
32	2a	1498	UR3	O3'-P	5.45	1.61	1.56

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	9.78	124.16	109.50
11	1P	35	HIS	CA-C-N	-7.85	106.55	121.54
11	1P	35	HIS	C-N-CA	-7.85	106.55	121.54
1	2A	1992	G	C2'-C3'-O3'	7.07	120.10	109.50
32	2a	1272	G	N1-C2-N2	-7.00	95.19	116.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
15	1T	128	GLU	Peptide
21	1Z	136	PHE	Peptide
33	1b	122	PHE	Peptide
47	1p	4	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31193	646	0
1	2A	60322	0	30427	689	0
2	1B	2577	0	1305	23	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	51	0
3	2D	2136	0	2218	43	0
4	1E	1559	0	1618	35	0
4	2E	1559	0	1618	43	0
5	1F	1584	0	1625	40	0
5	2F	1580	0	1619	52	0
6	1G	1423	0	1436	44	0
6	2G	1428	0	1438	59	0
7	1H	1330	0	1407	29	0
7	2H	1330	0	1407	46	0
8	1I	1097	0	1140	37	1
8	2I	1064	0	1082	44	0
9	1N	1117	0	1184	15	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	23	0
10	2O	933	0	996	22	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	45	0
12	1Q	1122	0	1179	17	0
12	2Q	1122	0	1179	48	0
13	1R	968	0	1033	19	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	22	0
14	2S	870	0	923	29	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	18	0
17	1V	771	0	830	14	0
17	2V	771	0	830	15	0
18	1W	886	0	940	15	0
18	2W	886	0	940	13	0
19	1X	750	0	814	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	20	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	23	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	62	0
22	10	653	0	674	7	0
22	20	653	0	674	14	0
23	11	755	0	826	19	0
23	21	755	0	826	23	0
24	12	588	0	643	14	0
24	22	588	0	643	16	0
25	13	469	0	518	14	0
25	23	464	0	514	19	0
26	14	552	0	533	32	0
26	24	532	0	503	36	0
27	15	455	0	465	7	0
27	25	455	0	465	7	0
28	16	453	0	473	9	0
28	26	449	0	469	11	0
29	17	418	0	467	7	0
29	27	418	0	467	9	0
30	18	517	0	582	12	0
30	28	517	0	582	12	0
31	19	307	0	335	3	0
31	29	307	0	335	4	0
32	1a	32246	0	16295	471	0
32	2a	32327	0	16338	523	1
33	1b	1846	0	1867	87	0
33	2b	1825	0	1828	91	0
34	1c	1548	0	1535	42	0
34	2c	1542	0	1517	57	0
35	1d	1655	0	1672	59	0
35	2d	1674	0	1714	53	0
36	1e	1129	0	1185	42	0
36	2e	1133	0	1191	47	0
37	1f	810	0	804	16	0
37	2f	816	0	808	31	0
38	1g	1231	0	1238	31	0
38	2g	1235	0	1249	45	0
39	1h	1088	0	1126	31	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	37	0
41	1j	709	0	650	36	0
41	2j	714	0	672	45	0
42	1k	829	0	825	21	0
42	2k	833	0	836	28	0
43	1l	932	0	981	14	0
43	2l	932	0	980	20	0
44	1m	979	0	1028	38	0
44	2m	950	0	988	41	0
45	1n	492	0	529	14	0
45	2n	492	0	529	24	0
46	1o	728	0	760	22	0
46	2o	728	0	760	20	0
47	1p	681	0	697	35	0
47	2p	677	0	686	29	0
48	1q	823	0	891	17	0
48	2q	823	0	891	16	0
49	1r	555	0	618	11	0
49	2r	555	0	618	15	0
50	1s	652	0	662	34	0
50	2s	646	0	644	28	0
51	1t	728	0	798	23	0
51	2t	727	0	796	24	0
52	1u	199	0	208	10	0
52	2u	199	0	208	9	0
53	1v	277	0	140	5	0
53	2v	277	0	140	2	0
54	1w	1623	0	839	21	0
54	2w	1555	0	798	23	0
55	1x	1656	0	848	15	0
55	2x	1656	0	849	12	0
56	1y	1585	0	803	36	0
56	2y	1565	0	794	38	0
57	1z	127	0	139	7	0
57	2z	127	0	140	4	0
58	10	9	0	0	0	0
58	11	6	0	0	0	0
58	12	2	0	0	0	0
58	13	3	0	0	0	0
58	15	9	0	0	0	0
58	16	2	0	0	0	0
58	17	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	18	5	0	0	0	0
58	19	1	0	0	0	0
58	1A	1105	0	0	0	0
58	1B	37	0	0	0	0
58	1D	12	0	0	0	0
58	1E	14	0	0	0	0
58	1F	13	0	0	0	0
58	1G	5	0	0	0	0
58	1I	1	0	0	0	0
58	1N	7	0	0	0	0
58	1O	5	0	0	0	0
58	1P	4	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	4	0	0	0	0
58	1S	3	0	0	0	0
58	1T	3	0	0	0	0
58	1U	11	0	0	0	0
58	1V	7	0	0	0	0
58	1W	8	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	3	0	0	0	0
58	1Z	3	0	0	0	0
58	1a	218	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1h	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	1	0	0	0	0
58	1p	1	0	0	0	0
58	1s	1	0	0	0	0
58	1t	1	0	0	0	0
58	1v	2	0	0	0	0
58	1w	8	0	0	0	0
58	1x	13	0	0	0	0
58	1y	1	0	0	0	0
58	21	1	0	0	0	0
58	23	1	0	0	0	0
58	25	4	0	0	0	0
58	26	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	27	3	0	0	0	0
58	28	4	0	0	0	0
58	29	1	0	0	0	0
58	2A	883	0	0	0	0
58	2B	19	0	0	0	0
58	2D	7	0	0	0	0
58	2E	11	0	0	0	0
58	2F	9	0	0	0	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0
58	2O	1	0	0	0	0
58	2Q	3	0	0	0	0
58	2R	3	0	0	0	0
58	2S	1	0	0	0	0
58	2T	3	0	0	0	0
58	2U	2	0	0	0	0
58	2V	2	0	0	0	0
58	2W	2	0	0	0	0
58	2X	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	242	0	0	0	0
58	2d	1	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2i	1	0	0	0	0
58	2j	1	0	0	0	0
58	2l	5	0	0	0	0
58	2p	1	0	0	0	0
58	2q	2	0	0	0	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	3	0	0	0	0
58	2w	12	0	0	0	0
58	2x	5	0	0	0	0
58	2y	6	0	0	0	0
59	1A	1	0	0	0	0
59	2x	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	2	0
61	2d	8	0	0	0	0
62	10	13	0	0	1	0
62	11	11	0	0	0	0
62	12	4	0	0	0	0
62	13	5	0	0	0	0
62	14	1	0	0	0	0
62	15	5	0	0	0	0
62	16	4	0	0	0	0
62	17	7	0	0	1	0
62	18	9	0	0	1	0
62	1A	2019	0	0	73	0
62	1B	63	0	0	2	0
62	1D	24	0	0	1	0
62	1E	24	0	0	2	0
62	1F	15	0	0	1	0
62	1G	2	0	0	0	0
62	1H	2	0	0	0	0
62	1I	1	0	0	1	0
62	1N	5	0	0	0	0
62	1O	6	0	0	0	0
62	1P	19	0	0	0	0
62	1Q	8	0	0	0	0
62	1R	12	0	0	2	0
62	1S	5	0	0	0	0
62	1T	9	0	0	1	0
62	1U	15	0	0	1	0
62	1V	8	0	0	0	0
62	1W	9	0	0	1	0
62	1X	4	0	0	0	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	388	0	0	28	0
62	1b	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1f	1	0	0	0	0
62	1l	8	0	0	0	0
62	1m	2	0	0	0	0
62	1n	1	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	6	0	0	0	0
62	1w	20	0	0	1	0
62	1x	15	0	0	0	0
62	1y	2	0	0	0	0
62	1z	1	0	0	0	0
62	20	3	0	0	0	0
62	21	13	0	0	1	0
62	23	1	0	0	0	0
62	25	1	0	0	0	0
62	27	5	0	0	0	0
62	28	4	0	0	1	0
62	29	1	0	0	0	0
62	2A	1153	0	0	74	0
62	2B	23	0	0	2	0
62	2D	24	0	0	0	0
62	2E	14	0	0	0	0
62	2F	13	0	0	0	0
62	2I	2	0	0	0	0
62	2N	3	0	0	0	0
62	2O	3	0	0	0	0
62	2P	14	0	0	2	0
62	2Q	3	0	0	0	0
62	2R	3	0	0	0	0
62	2T	4	0	0	0	0
62	2U	2	0	0	0	0
62	2W	2	0	0	0	0
62	2X	2	0	0	0	0
62	2Y	1	0	0	0	0
62	2Z	1	0	0	0	0
62	2a	283	0	0	20	0
62	2c	2	0	0	0	0
62	2d	2	0	0	0	0
62	2e	1	0	0	0	0
62	2j	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2l	6	0	0	1	0
62	2p	1	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	0	0
62	2v	2	0	0	0	0
62	2w	10	0	0	0	0
62	2x	6	0	0	0	0
62	2y	9	0	0	0	0
All	All	300583	0	197064	4696	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 4696 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	1.31	1.29
1:1A:2136:C:N4	1:1A:2155:G:H1	1.49	1.08
1:1A:1054:A:N6	1:1A:1105:U:H3	1.55	1.04
1:2A:1604:C:OP2	62:2A:3903:HOH:O	1.77	1.03
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.40	1.03

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:87:LYS:NZ	32:2a:358:U:O3'[3_654]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	14 (5%)	2 (1%)	18	38
3	2D	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30	51
4	1E	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	12	28
4	2E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	12	28
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	46
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	6	12
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	11	25
6	2G	179/182 (98%)	151 (84%)	24 (13%)	4 (2%)	5	10
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	5	9
8	1I	144/148 (97%)	120 (83%)	20 (14%)	4 (3%)	4	6
8	2I	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9	19
9	1N	138/140 (99%)	133 (96%)	3 (2%)	2 (1%)	9	19
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16	34
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	19
11	2P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	12
12	1Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
12	2Q	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	9	19
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
14	1S	108/112 (96%)	97 (90%)	11 (10%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	8 (7%)	3 (3%)	4	6
15	1T	129/146 (88%)	119 (92%)	7 (5%)	3 (2%)	5	9
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	12
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	12
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	25
19	2X	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	11	25
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	28
20	2Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	28
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	6	12
21	2Z	156/206 (76%)	130 (83%)	22 (14%)	4 (3%)	4	7
22	10	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	23
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	10	23
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	25
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	8	18
24	22	68/72 (94%)	66 (97%)	2 (3%)	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%)	51 (76%)	10 (15%)	6 (9%)	0	0
26	24	67/71 (94%)	48 (72%)	12 (18%)	7 (10%)	0	0
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	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%)	58 (94%)	3 (5%)	1 (2%)	7	16
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	183 (80%)	32 (14%)	14 (6%)	1	1
33	2b	229/256 (90%)	185 (81%)	29 (13%)	15 (7%)	1	1
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	12	28
34	2c	204/239 (85%)	162 (79%)	32 (16%)	10 (5%)	1	2
35	1d	206/209 (99%)	184 (89%)	19 (9%)	3 (2%)	8	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	184 (89%)	20 (10%)	2 (1%)	12	28
36	1e	146/162 (90%)	133 (91%)	8 (6%)	5 (3%)	3	4
36	2e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	5	11
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	28
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	12
38	2g	153/156 (98%)	130 (85%)	15 (10%)	8 (5%)	1	2
39	1h	135/138 (98%)	121 (90%)	11 (8%)	3 (2%)	5	10
39	2h	135/138 (98%)	124 (92%)	9 (7%)	2 (2%)	8	18
40	1i	125/128 (98%)	105 (84%)	17 (14%)	3 (2%)	4	9
40	2i	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	16	34
41	1j	95/105 (90%)	81 (85%)	8 (8%)	6 (6%)	1	1
41	2j	94/105 (90%)	74 (79%)	15 (16%)	5 (5%)	1	1
42	1k	112/129 (87%)	100 (89%)	8 (7%)	4 (4%)	2	4
42	2k	112/129 (87%)	99 (88%)	9 (8%)	4 (4%)	2	4
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	9 (8%)	2 (2%)	7	15
44	1m	123/126 (98%)	110 (89%)	11 (9%)	2 (2%)	7	16
44	2m	120/126 (95%)	100 (83%)	16 (13%)	4 (3%)	3	5
45	1n	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	7	15
45	2n	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	4
46	1o	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	10	23
46	2o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10	23
47	1p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9	21
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9	21
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	28
49	1r	66/88 (75%)	57 (86%)	8 (12%)	1 (2%)	8	18
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	6 (7%)	5 (6%)	1	1
50	2s	81/93 (87%)	67 (83%)	11 (14%)	3 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	2
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	2
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
57	1z	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
57	2z	15/17 (88%)	10 (67%)	5 (33%)	0	100	100
All	All	11402/12162 (94%)	10291 (90%)	906 (8%)	205 (2%)	6	14

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	50	ALA
15	1T	55	ASN
23	11	3	LYS
33	1b	8	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	200 (93%)	15 (7%)	14	31
3	2D	215/218 (99%)	198 (92%)	17 (8%)	11	26
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	26
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10	22
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	16
5	2F	159/166 (96%)	147 (92%)	12 (8%)	12	28
6	1G	143/156 (92%)	128 (90%)	15 (10%)	6	14
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	9
7	1H	144/148 (97%)	125 (87%)	19 (13%)	4	8
7	2H	144/148 (97%)	122 (85%)	22 (15%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1I	113/124 (91%)	93 (82%)	20 (18%)	2	3
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	2
9	1N	118/119 (99%)	105 (89%)	13 (11%)	6	13
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	18
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	46
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14	31
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11	26
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	26
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	42
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	50
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	64
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14	32
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	24
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	3
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	44
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	25
16	1U	93/94 (99%)	83 (89%)	10 (11%)	6	13
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	28
17	1V	80/82 (98%)	72 (90%)	8 (10%)	7	16
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	16
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	33
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	20
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	35
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	8
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	6
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6	12
21	2Z	137/179 (76%)	110 (80%)	27 (20%)	1	2
22	10	65/67 (97%)	61 (94%)	4 (6%)	16	36
22	20	65/67 (97%)	62 (95%)	3 (5%)	24	49
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	28
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	13
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	36
25	13	51/52 (98%)	46 (90%)	5 (10%)	7	17
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	25
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	7
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	2
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	25
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	55
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	38
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	10
29	17	41/42 (98%)	35 (85%)	6 (15%)	3	6
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	18
30	28	54/55 (98%)	47 (87%)	7 (13%)	4	8
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	21
33	1b	192/220 (87%)	160 (83%)	32 (17%)	2	4
33	2b	187/220 (85%)	157 (84%)	30 (16%)	2	4
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	9
34	2c	140/188 (74%)	112 (80%)	28 (20%)	1	2
35	1d	169/181 (93%)	144 (85%)	25 (15%)	3	6
35	2d	173/181 (96%)	149 (86%)	24 (14%)	3	7
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	21
36	2e	114/123 (93%)	95 (83%)	19 (17%)	2	4
37	1f	84/90 (93%)	77 (92%)	7 (8%)	10	23
37	2f	85/90 (94%)	73 (86%)	12 (14%)	3	6
38	1g	119/127 (94%)	99 (83%)	20 (17%)	2	4
38	2g	120/127 (94%)	106 (88%)	14 (12%)	5	11
39	1h	114/119 (96%)	108 (95%)	6 (5%)	20	43
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	10
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4	9
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2	4
41	2j	69/92 (75%)	55 (80%)	14 (20%)	1	2
42	1k	82/99 (83%)	70 (85%)	12 (15%)	3	6
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	30
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	73
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16	36
44	1m	95/101 (94%)	81 (85%)	14 (15%)	3	6
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	10
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	15
45	2n	49/50 (98%)	41 (84%)	8 (16%)	2	4
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	35
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	35
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	6
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	4
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	29
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	22
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3	7
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	10
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	8
50	2s	67/80 (84%)	54 (81%)	13 (19%)	1	2
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	8
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	51
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	12
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	40
57	1z	13/13 (100%)	9 (69%)	4 (31%)	0	0
57	2z	13/13 (100%)	8 (62%)	5 (38%)	0	0
All	All	9331/10090 (92%)	8326 (89%)	1005 (11%)	6	13

5 of 1005 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	1t	37	SER
39	2h	29	SER
8	2l	108	THR
38	2g	85	TYR
45	2n	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
34	2c	6	HIS
49	2r	63	GLN
35	2d	77	ASN
41	2j	33	GLN
35	1d	201	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	477 (16%)	35 (1%)
1	2A	2791/2915 (95%)	482 (17%)	30 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	19 (16%)	0
32	1a	1497/1521 (98%)	237 (15%)	0
32	2a	1501/1521 (98%)	263 (17%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	72/76 (94%)	16 (22%)	0
54	2w	68/76 (89%)	22 (32%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	11 (14%)	0
56	1y	72/76 (94%)	25 (34%)	0
56	2y	70/76 (92%)	29 (41%)	0
All	All	9346/9620 (97%)	1608 (17%)	65 (0%)

5 of 1608 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	34	C
1	1A	45	C
1	1A	58	G

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Mol	Chain	Res	Type
1	1A	69	C

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1653	G
1	2A	1992	G
1	1A	1508	A
1	1A	1420	U
1	2A	2119	A

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

88 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$
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.51	2 (9%)
55	PSU	2x	55	55	18,21,22	1.36	3 (16%)	21,30,33	1.99	5 (23%)
32	4OC	2a	1402	32	20,23,24	0.82	0	25,32,35	0.93	1 (4%)
32	M2G	2a	966	32	24,27,28	1.27	4 (16%)	33,40,43	1.89	5 (15%)
56	4SU	1y	8	56	18,21,22	1.56	5 (27%)	25,30,33	1.51	4 (16%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.28	4 (19%)
32	5MC	2a	967	32	19,22,23	1.59	2 (10%)	26,32,35	1.30	4 (15%)
32	2MG	2a	1207	58,32	23,26,27	1.28	3 (13%)	33,38,41	2.29	8 (24%)
32	5MC	2a	1407	58,32	19,22,23	1.59	3 (15%)	26,32,35	1.45	4 (15%)
56	PSU	1y	32	56	18,21,22	1.43	2 (11%)	21,30,33	1.80	4 (19%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	21,30,33	2.06	5 (23%)
32	5MC	1a	1400	32	19,22,23	1.38	3 (15%)	26,32,35	1.34	4 (15%)
55	PSU	1x	55	55	18,21,22	1.47	3 (16%)	21,30,33	1.78	4 (19%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	1.20	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	31H	2x	76	58,55,59	31,34,35	1.37	2 (6%)	35,47,50	2.47	13 (37%)
55	4SU	2x	8	55	18,21,22	1.92	5 (27%)	25,30,33	1.18	3 (12%)
1	5MU	2A	1939	58,1	19,22,23	1.52	4 (21%)	27,32,35	2.31	7 (25%)
32	UR3	1a	1498	32	19,22,23	0.95	1 (5%)	26,32,35	1.73	5 (19%)
54	F3N	1w	76	1	33,36,37	1.49	6 (18%)	41,51,54	1.85	11 (26%)
54	5MU	2w	54	54	19,22,23	1.22	3 (15%)	27,32,35	2.37	8 (29%)
32	G7M	2a	527	58,32	23,26,27	1.50	5 (21%)	34,39,42	1.66	5 (14%)
1	OMC	2A	1920	1	19,22,23	0.86	1 (5%)	25,31,34	1.11	2 (8%)
54	G7M	1w	46	54	23,26,27	1.56	3 (13%)	34,39,42	1.80	4 (11%)
1	PSU	1A	2605	58,1	18,21,22	1.54	5 (27%)	21,30,33	1.96	5 (23%)
32	UR3	2a	1498	32	19,22,23	1.29	2 (10%)	26,32,35	1.84	5 (19%)
1	PSU	1A	1911	1	18,21,22	1.43	3 (16%)	21,30,33	2.04	3 (14%)
56	5MU	2y	54	56	19,22,23	1.56	3 (15%)	27,32,35	2.14	8 (29%)
54	F3N	2w	76	1	33,36,37	1.53	5 (15%)	41,51,54	1.78	9 (21%)
32	5MC	2a	1404	32	19,22,23	1.87	3 (15%)	26,32,35	1.21	4 (15%)
32	MA6	1a	1518	32	23,26,27	0.50	0	33,38,41	1.97	9 (27%)
56	4SU	2y	8	56,58	18,21,22	1.71	5 (27%)	25,30,33	2.10	5 (20%)
1	5MC	2A	1942	1	19,22,23	1.20	3 (15%)	26,32,35	1.10	2 (7%)
54	4SU	2w	8	54	18,21,22	1.84	4 (22%)	25,30,33	2.43	5 (20%)
55	5MU	2x	54	55	19,22,23	1.37	2 (10%)	27,32,35	2.26	6 (22%)
55	5MC	1x	32	55	19,22,23	1.78	3 (15%)	26,32,35	1.44	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.05	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.43	6 (22%)
56	G7M	1y	46	56	23,26,27	1.44	3 (13%)	34,39,42	1.76	5 (14%)
1	5MC	2A	1962	58,1	19,22,23	1.49	3 (15%)	26,32,35	1.11	2 (7%)
1	OMU	1A	2552	58,1	19,22,23	1.30	3 (15%)	25,31,34	2.05	5 (20%)
1	5MU	1A	1939	58,1	19,22,23	1.70	6 (31%)	27,32,35	2.33	6 (22%)
43	0TD	1l	92	43	8,9,10	3.92	2 (25%)	6,11,13	5.45	2 (33%)
32	5MC	1a	967	32	19,22,23	1.77	2 (10%)	26,32,35	1.29	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.16	3 (15%)	26,32,35	1.25	3 (11%)
56	MIA	1y	37	56	21,24,32	1.82	3 (14%)	30,35,47	2.02	9 (30%)
54	PSU	2w	55	54	18,21,22	1.47	2 (11%)	21,30,33	2.06	4 (19%)
55	31H	1x	76	58,55	31,34,35	1.36	4 (12%)	35,47,50	2.07	11 (31%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.10	10 (30%)
1	5MC	1A	1962	58,1	19,22,23	1.90	4 (21%)	26,32,35	1.39	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	39	54	18,21,22	1.42	3 (16%)	21,30,33	2.03	4 (19%)
1	OMG	1A	2251	58,55,1	23,26,27	1.38	3 (13%)	32,38,41	1.95	7 (21%)
56	PSU	2y	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.92	3 (14%)
1	OMG	2A	2251	58,55,1	23,26,27	1.32	3 (13%)	32,38,41	1.96	7 (21%)
54	4SU	1w	8	54	18,21,22	1.89	4 (22%)	25,30,33	1.87	6 (24%)
54	MIA	2w	37	54	24,27,32	2.14	6 (25%)	32,39,47	2.44	10 (31%)
1	OMU	2A	2552	58,1	19,22,23	1.10	2 (10%)	25,31,34	1.81	5 (20%)
1	PSU	2A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	1.81	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.51	0	33,38,41	2.14	9 (27%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.82	4 (19%)
56	PSU	1y	39	56	18,21,22	1.55	2 (11%)	21,30,33	1.74	3 (14%)
1	2MA	1A	2503	58,1	22,25,26	1.38	4 (18%)	32,37,40	2.41	8 (25%)
32	5MC	1a	1407	32	19,22,23	1.43	2 (10%)	26,32,35	1.07	4 (15%)
1	5MU	1A	1915	1	19,22,23	1.39	4 (21%)	27,32,35	2.67	10 (37%)
56	PSU	1y	55	56	18,21,22	1.51	3 (16%)	21,30,33	2.02	4 (19%)
54	PSU	1w	32	54	18,21,22	1.35	3 (16%)	21,30,33	1.81	4 (19%)
1	PSU	1A	1917	1	18,21,22	1.33	3 (16%)	21,30,33	2.06	5 (23%)
32	5MC	2a	1400	32	19,22,23	1.74	3 (15%)	26,32,35	1.38	2 (7%)
32	G7M	1a	527	32	23,26,27	1.58	4 (17%)	34,39,42	1.45	3 (8%)
32	M2G	1a	966	32	24,27,28	1.37	4 (16%)	33,40,43	2.05	6 (18%)
54	5MU	1w	54	54	19,22,23	1.48	4 (21%)	27,32,35	2.14	5 (18%)
56	5MU	1y	54	56	19,22,23	1.58	4 (21%)	27,32,35	1.87	7 (25%)
56	G7M	2y	46	56	23,26,27	1.68	5 (21%)	34,39,42	2.01	4 (11%)
32	MA6	2a	1519	32	23,26,27	0.49	0	33,38,41	2.09	10 (30%)
54	G7M	2w	46	54	23,26,27	1.49	3 (13%)	34,39,42	1.64	5 (14%)
55	5MC	2x	32	55	19,22,23	1.57	3 (15%)	26,32,35	1.56	6 (23%)
56	PSU	2y	39	56	18,21,22	1.41	2 (11%)	21,30,33	1.58	3 (14%)
56	MIA	2y	37	56	21,24,32	1.67	3 (14%)	30,35,47	2.12	7 (23%)
54	PSU	2w	32	54	18,21,22	1.41	2 (11%)	21,30,33	2.06	5 (23%)
32	2MG	1a	1207	58,32	23,26,27	1.27	2 (8%)	33,38,41	2.25	9 (27%)
54	MIA	1w	37	54	28,31,32	2.38	6 (21%)	38,44,47	2.76	14 (36%)
56	PSU	2y	55	56	18,21,22	1.43	2 (11%)	21,30,33	2.17	4 (19%)
1	2MA	2A	2503	58,1	22,25,26	1.46	5 (22%)	32,37,40	2.25	9 (28%)
32	PSU	1a	516	32	18,21,22	1.46	3 (16%)	21,30,33	1.79	4 (19%)
55	5MU	1x	54	55	19,22,23	1.49	5 (26%)	27,32,35	2.04	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1942	58,1	19,22,23	1.26	2 (10%)	26,32,35	1.50	5 (19%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	1.08	2 (8%)
43	0TD	2l	92	43	8,9,10	5.12	2 (25%)	6,11,13	2.48	1 (16%)
55	4SU	1x	8	55	18,21,22	2.24	5 (27%)	25,30,33	1.80	6 (24%)

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
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
56	4SU	1y	8	56	-	0/7/25/26	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	2MG	2a	1207	58,32	-	1/9/27/28	0/3/3/3
32	5MC	2a	1407	58,32	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
55	31H	2x	76	58,55,59	-	4/22/40/41	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	58,1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	1	-	2/19/37/38	0/4/4/4
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	2/7/25/26	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
54	F3N	2w	76	1	-	4/19/37/38	0/4/4/4
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	2y	8	56,58	-	1/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/7/25/26	0/3/3/3
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	4/7/12/14	-
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	3/7/25/34	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	58,55	-	4/22/40/41	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1962	58,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	58,55,1	-	1/9/27/28	0/3/3/3
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	58,55,1	-	0/9/27/28	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	1/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	2/7/25/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	58,32	-	0/9/27/28	0/3/3/3
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
56	PSU	2y	55	56	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	1/7/25/26	0/3/3/3
32	PSU	1a	516	32	-	1/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	58,1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2

The worst 5 of 262 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-13.70	1.68	1.82
43	1l	92	0TD	CB-SB	-10.44	1.71	1.82
54	1w	37	MIA	C2-S10	-7.76	1.69	1.75
1	1A	1962	5MC	C5-C4	6.84	1.49	1.44
54	1w	37	MIA	C13-C14	6.80	1.52	1.32

The worst 5 of 473 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.53	79.84	102.36
54	1w	37	MIA	C12-C13-C14	-9.06	110.74	127.01
1	2A	2503	2MA	C5-C4-N3	-8.40	118.33	127.18
1	1A	2503	2MA	C5-C4-N3	-8.24	118.50	127.18
54	2w	37	MIA	C5-C4-N3	-7.76	119.00	127.18

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C5-C6-N6-C12

There are no ring outliers.

38 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	39	PSU	2	0
56	1y	8	4SU	1	0
32	2a	967	5MC	2	0
32	2a	1207	2MG	1	0
32	1a	1402	4OC	1	0
55	2x	76	31H	1	0
55	2x	8	4SU	1	0
1	2A	1939	5MU	1	0
54	1w	76	F3N	4	0
54	1w	46	G7M	1	0
54	2w	76	F3N	3	0
32	1a	1518	MA6	2	0
56	2y	8	4SU	2	0
54	2w	8	4SU	1	0
55	2x	54	5MU	3	0
1	1A	2552	OMU	1	0
1	1A	1939	5MU	1	0
43	1l	92	0TD	1	0
32	1a	967	5MC	1	0
56	1y	37	MIA	2	0
55	1x	76	31H	1	0
32	2a	1518	MA6	3	0
1	1A	2251	OMG	1	0
54	1w	8	4SU	1	0
1	2A	2552	OMU	1	0
32	1a	1519	MA6	1	0
56	1y	39	PSU	1	0
1	1A	1917	PSU	1	0
32	2a	1400	5MC	2	0
32	1a	527	G7M	1	0
32	1a	966	M2G	3	0
56	2y	46	G7M	3	0
32	2a	1519	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	46	G7M	2	0
56	2y	39	PSU	2	0
1	1A	1920	OMC	1	0
43	2l	92	0TD	1	0
55	1x	8	4SU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2820 ligands modelled in this entry, 2818 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	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
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	1d	302	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	2w	1
54	1w	1
17	1V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2w	75:C	O3'	76:F3N	P	2.56
1	1w	75:C	O3'	76:F3N	P	2.32
1	1V	34:GLU	C	35:LEU	N	1.14

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%)	-0.59	187 (6%) 25 19	11, 27, 82, 92	0
1	2A	2789/2915 (95%)	-0.11	162 (5%) 29 23	23, 44, 80, 96	0
2	1B	120/121 (99%)	-0.43	0 100 100	21, 39, 54, 74	0
2	2B	120/121 (99%)	0.26	1 (0%) 82 80	43, 57, 66, 80	0
3	1D	275/276 (99%)	-0.37	2 (0%) 84 82	13, 28, 42, 71	0
3	2D	275/276 (99%)	-0.09	5 (1%) 67 63	21, 38, 50, 68	0
4	1E	204/206 (99%)	-0.36	0 100 100	12, 30, 49, 65	0
4	2E	204/206 (99%)	0.19	2 (0%) 79 76	26, 48, 60, 69	0
5	1F	203/210 (96%)	-0.32	0 100 100	12, 31, 54, 69	0
5	2F	203/210 (96%)	0.33	5 (2%) 58 52	24, 52, 65, 71	0
6	1G	181/182 (99%)	0.27	8 (4%) 39 33	28, 44, 59, 72	0
6	2G	181/182 (99%)	0.68	9 (4%) 34 28	48, 58, 68, 76	0
7	1H	174/180 (96%)	0.15	5 (2%) 53 48	29, 43, 55, 64	0
7	2H	174/180 (96%)	1.48	43 (24%) 2 1	59, 71, 78, 88	0
8	1I	146/148 (98%)	0.58	2 (1%) 73 69	34, 59, 67, 70	0
8	2I	146/148 (98%)	0.76	8 (5%) 30 25	42, 59, 69, 73	0
9	1N	140/140 (100%)	-0.31	0 100 100	18, 28, 46, 61	0
9	2N	140/140 (100%)	0.51	6 (4%) 40 34	36, 50, 67, 73	0
10	1O	122/122 (100%)	-0.28	0 100 100	19, 31, 48, 53	0
10	2O	122/122 (100%)	0.25	2 (1%) 70 66	35, 48, 58, 62	0
11	1P	149/150 (99%)	-0.14	0 100 100	14, 37, 55, 62	0
11	2P	149/150 (99%)	0.38	3 (2%) 65 60	28, 52, 66, 73	0
12	1Q	141/141 (100%)	-0.17	1 (0%) 84 82	17, 30, 48, 62	0
12	2Q	141/141 (100%)	0.44	4 (2%) 55 49	34, 50, 62, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.53	0 100 100	17, 25, 38, 44	0
13	2R	118/118 (100%)	0.04	0 100 100	31, 42, 54, 61	0
14	1S	110/112 (98%)	-0.04	0 100 100	26, 39, 51, 53	0
14	2S	110/112 (98%)	0.51	1 (0%) 81 78	45, 54, 62, 68	0
15	1T	131/146 (89%)	-0.14	2 (1%) 72 68	23, 35, 56, 69	0
15	2T	131/146 (89%)	0.47	3 (2%) 61 55	40, 50, 62, 68	0
16	1U	116/118 (98%)	-0.60	0 100 100	15, 21, 34, 47	0
16	2U	116/118 (98%)	0.33	3 (2%) 57 51	30, 47, 59, 64	0
17	1V	101/101 (100%)	-0.41	0 100 100	14, 27, 47, 56	0
17	2V	101/101 (100%)	0.53	0 100 100	29, 56, 62, 66	0
18	1W	112/113 (99%)	-0.52	1 (0%) 81 78	13, 22, 39, 66	0
18	2W	112/113 (99%)	-0.02	1 (0%) 81 78	30, 38, 56, 75	0
19	1X	95/96 (98%)	-0.28	1 (1%) 78 74	16, 29, 50, 65	0
19	2X	95/96 (98%)	0.21	2 (2%) 63 58	34, 44, 61, 71	0
20	1Y	107/110 (97%)	0.01	1 (0%) 81 78	24, 39, 55, 65	0
20	2Y	107/110 (97%)	0.83	12 (11%) 10 8	45, 57, 69, 75	0
21	1Z	154/206 (74%)	0.65	5 (3%) 50 44	26, 52, 70, 76	0
21	2Z	160/206 (77%)	1.26	33 (20%) 2 2	53, 66, 76, 79	0
22	10	83/85 (97%)	-0.24	1 (1%) 76 73	15, 26, 40, 51	0
22	20	83/85 (97%)	0.42	2 (2%) 59 54	35, 45, 54, 62	0
23	11	97/98 (98%)	0.08	2 (2%) 63 58	19, 37, 58, 65	0
23	21	97/98 (98%)	0.37	5 (5%) 33 27	29, 45, 61, 67	0
24	12	70/72 (97%)	-0.04	1 (1%) 73 69	23, 37, 47, 63	0
24	22	70/72 (97%)	0.66	2 (2%) 53 48	42, 54, 64, 70	0
25	13	59/60 (98%)	-0.19	0 100 100	15, 26, 49, 62	0
25	23	59/60 (98%)	0.44	2 (3%) 48 42	40, 50, 61, 68	0
26	14	69/71 (97%)	0.73	7 (10%) 12 9	38, 59, 74, 78	0
26	24	69/71 (97%)	1.17	10 (14%) 6 4	56, 68, 76, 79	0
27	15	59/60 (98%)	-0.49	0 100 100	12, 22, 39, 46	0
27	25	59/60 (98%)	0.08	0 100 100	28, 39, 54, 70	0
28	16	53/54 (98%)	-0.20	0 100 100	24, 32, 47, 53	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.38	1 (1%) 66 61	37, 46, 54, 60	0
29	17	48/49 (97%)	-0.50	2 (4%) 40 35	14, 19, 43, 50	0
29	27	48/49 (97%)	0.00	4 (8%) 17 13	24, 31, 51, 59	0
30	18	64/65 (98%)	-0.54	0 100 100	20, 25, 32, 46	0
30	28	64/65 (98%)	0.07	1 (1%) 70 66	33, 40, 46, 54	0
31	19	37/37 (100%)	-0.31	0 100 100	19, 29, 45, 51	0
31	29	37/37 (100%)	0.81	2 (5%) 31 26	44, 54, 66, 68	0
32	1a	1488/1521 (97%)	0.19	67 (4%) 38 32	25, 52, 79, 94	0
32	2a	1491/1521 (98%)	0.39	74 (4%) 34 28	34, 58, 79, 96	0
33	1b	231/256 (90%)	1.03	33 (14%) 6 5	50, 64, 74, 78	0
33	2b	231/256 (90%)	1.15	27 (11%) 9 7	51, 68, 75, 79	0
34	1c	206/239 (86%)	0.68	8 (3%) 43 38	43, 56, 69, 75	0
34	2c	206/239 (86%)	1.14	23 (11%) 10 8	56, 64, 73, 77	0
35	1d	208/209 (99%)	1.10	30 (14%) 6 5	44, 56, 66, 75	0
35	2d	208/209 (99%)	0.69	11 (5%) 32 26	45, 54, 63, 71	0
36	1e	148/162 (91%)	0.42	1 (0%) 84 82	35, 51, 61, 68	0
36	2e	148/162 (91%)	0.62	8 (5%) 31 26	45, 57, 65, 75	0
37	1f	100/101 (99%)	0.58	0 100 100	43, 55, 63, 68	0
37	2f	100/101 (99%)	0.49	1 (1%) 79 76	41, 52, 60, 70	0
38	1g	155/156 (99%)	0.68	10 (6%) 25 19	47, 57, 72, 77	0
38	2g	155/156 (99%)	0.92	17 (10%) 10 8	54, 63, 72, 76	0
39	1h	137/138 (99%)	0.43	3 (2%) 62 57	42, 53, 59, 65	0
39	2h	137/138 (99%)	0.48	2 (1%) 72 68	49, 58, 64, 69	0
40	1i	127/128 (99%)	0.96	12 (9%) 14 11	41, 61, 70, 74	0
40	2i	127/128 (99%)	1.38	28 (22%) 2 2	52, 68, 73, 75	0
41	1j	97/105 (92%)	1.23	18 (18%) 3 3	43, 63, 71, 76	0
41	2j	96/105 (91%)	1.62	29 (30%) 1 1	55, 68, 76, 78	0
42	1k	114/129 (88%)	0.46	4 (3%) 47 41	33, 52, 63, 67	0
42	2k	114/129 (88%)	0.87	11 (9%) 13 10	38, 56, 67, 74	0
43	1l	121/132 (91%)	0.10	3 (2%) 58 52	33, 40, 53, 64	0
43	2l	121/132 (91%)	0.54	4 (3%) 49 43	42, 50, 61, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	125/126 (99%)	0.58	9 (7%) 21 17	38, 52, 61, 66	0
44	2m	122/126 (96%)	0.89	10 (8%) 17 14	47, 61, 67, 69	0
45	1n	60/61 (98%)	0.73	2 (3%) 49 43	45, 52, 58, 64	0
45	2n	60/61 (98%)	1.39	11 (18%) 3 3	59, 63, 69, 75	0
46	1o	88/89 (98%)	0.30	2 (2%) 61 55	36, 51, 63, 66	0
46	2o	88/89 (98%)	0.51	2 (2%) 61 55	45, 54, 67, 69	0
47	1p	82/88 (93%)	0.95	7 (8%) 16 13	41, 56, 64, 70	0
47	2p	82/88 (93%)	0.68	3 (3%) 45 39	47, 56, 64, 66	0
48	1q	99/105 (94%)	0.56	2 (2%) 65 60	41, 54, 63, 64	0
48	2q	99/105 (94%)	0.62	2 (2%) 65 60	48, 57, 66, 68	0
49	1r	68/88 (77%)	0.59	1 (1%) 72 68	44, 52, 64, 67	0
49	2r	68/88 (77%)	0.31	1 (1%) 72 68	46, 52, 61, 67	0
50	1s	83/93 (89%)	0.67	4 (4%) 35 30	46, 54, 64, 68	0
50	2s	83/93 (89%)	1.16	7 (8%) 17 13	53, 64, 73, 76	0
51	1t	96/106 (90%)	0.71	3 (3%) 51 45	46, 57, 68, 71	0
51	2t	96/106 (90%)	0.67	6 (6%) 26 20	47, 56, 67, 72	0
52	1u	23/27 (85%)	0.92	2 (8%) 16 12	46, 52, 57, 58	0
52	2u	23/27 (85%)	1.14	1 (4%) 40 34	54, 62, 65, 72	0
53	1v	13/24 (54%)	0.58	4 (30%) 1 1	32, 39, 82, 89	0
53	2v	13/24 (54%)	0.90	4 (30%) 1 1	47, 53, 81, 93	0
54	1w	67/76 (88%)	0.51	5 (7%) 20 16	18, 63, 78, 85	0
54	2w	64/76 (84%)	0.91	6 (9%) 14 11	36, 71, 80, 87	0
55	1x	72/77 (93%)	-0.03	2 (2%) 55 49	16, 48, 66, 79	0
55	2x	72/77 (93%)	0.26	1 (1%) 73 69	31, 56, 70, 87	0
56	1y	67/76 (88%)	2.43	51 (76%) 0 0	50, 85, 89, 90	0
56	2y	66/76 (86%)	2.53	50 (75%) 0 0	56, 86, 91, 93	0
57	1z	17/17 (100%)	0.16	0 100 100	40, 45, 51, 52	0
57	2z	17/17 (100%)	0.76	1 (5%) 28 23	56, 59, 65, 68	0
All	All	20910/21782 (95%)	0.20	1185 (5%) 29 24	11, 49, 74, 96	0

The worst 5 of 1185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2174	C	8.9
45	1n	2	ALA	8.6
1	1A	2174	C	8.1
1	1A	2129	C	7.9
1	1A	2130	U	7.7

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
56	4SU	2y	8	20/21	0.45	0.20	84,89,100,114	0
56	G7M	2y	46	24/25	0.47	0.18	75,85,92,101	0
56	5MU	2y	54	21/22	0.48	0.17	78,86,96,113	0
56	5MU	1y	54	21/22	0.51	0.18	77,85,93,112	0
56	G7M	1y	46	24/25	0.52	0.19	81,86,94,100	0
56	4SU	1y	8	20/21	0.57	0.18	83,88,92,103	0
56	PSU	1y	55	20/21	0.66	0.18	83,87,96,107	0
56	MIA	1y	37	22/30	0.67	0.18	74,79,86,90	0
56	PSU	2y	39	20/21	0.67	0.16	76,80,88,100	0
56	MIA	2y	37	22/30	0.68	0.17	65,84,90,108	0
56	PSU	2y	32	20/21	0.71	0.16	79,83,88,104	0
56	PSU	2y	55	20/21	0.74	0.14	79,86,95,97	0
54	G7M	1w	46	24/25	0.77	0.14	58,66,85,96	0
56	PSU	1y	39	20/21	0.80	0.13	68,76,80,85	0
54	G7M	2w	46	24/25	0.82	0.12	69,73,87,98	0
56	PSU	1y	32	20/21	0.82	0.14	72,76,84,94	0
54	PSU	2w	55	20/21	0.86	0.13	63,68,77,78	0
54	4SU	2w	8	20/21	0.88	0.11	68,73,76,88	0
55	PSU	2x	55	20/21	0.91	0.11	54,58,63,65	0
54	5MU	2w	54	21/22	0.91	0.11	55,61,67,72	0
54	PSU	1w	55	20/21	0.91	0.11	42,57,69,69	0
55	4SU	2x	8	20/21	0.91	0.12	55,64,69,81	0
54	PSU	2w	32	20/21	0.92	0.12	47,58,63,66	0
55	5MU	2x	54	21/22	0.92	0.15	55,61,63,65	0
32	2MG	2a	1207	24/25	0.92	0.10	53,61,65,68	0
43	0TD	2l	92	10/11	0.92	0.16	45,53,56,61	0
55	5MU	1x	54	21/22	0.92	0.13	48,54,59,60	0
43	0TD	1l	92	10/11	0.93	0.11	35,41,45,48	0
32	5MC	2a	1400	21/22	0.93	0.11	43,50,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	2a	516	20/21	0.93	0.09	46,56,61,62	0
54	PSU	1w	32	20/21	0.94	0.09	38,41,47,49	0
55	PSU	1x	55	20/21	0.94	0.09	38,46,56,61	0
32	G7M	2a	527	24/25	0.94	0.10	47,52,59,60	0
32	M2G	2a	966	25/26	0.94	0.10	43,48,60,65	0
55	5MC	2x	32	21/22	0.94	0.11	45,52,57,59	0
32	5MC	2a	967	21/22	0.94	0.10	45,52,60,61	0
54	MIA	2w	37	25/30	0.94	0.09	29,50,59,65	0
55	5MC	1x	32	21/22	0.95	0.10	37,43,47,57	0
54	4SU	1w	8	20/21	0.95	0.09	55,63,67,67	0
32	5MC	1a	967	21/22	0.95	0.09	35,40,49,53	0
1	5MU	2A	1915	21/22	0.95	0.09	40,47,52,53	0
1	PSU	2A	1917	20/21	0.95	0.08	46,50,57,66	0
1	5MC	2A	1942	21/22	0.95	0.11	39,46,50,59	0
32	2MG	1a	1207	24/25	0.95	0.08	41,53,57,57	0
54	5MU	1w	54	21/22	0.95	0.10	38,46,51,52	0
1	PSU	1A	1917	20/21	0.95	0.10	34,38,46,47	0
55	4SU	1x	8	20/21	0.95	0.10	45,49,55,58	0
1	5MU	1A	1915	21/22	0.96	0.09	29,38,41,43	0
32	4OC	2a	1402	22/23	0.96	0.08	37,44,47,49	0
32	5MC	2a	1407	21/22	0.96	0.07	33,39,42,45	0
32	UR3	2a	1498	21/22	0.96	0.09	37,41,46,49	0
55	31H	2x	76	32/33	0.96	0.09	27,32,37,40	0
1	5MC	2A	1962	21/22	0.96	0.09	35,41,48,56	0
1	OMU	2A	2552	21/22	0.96	0.08	29,34,39,41	0
1	PSU	2A	1911	20/21	0.96	0.08	36,44,48,53	0
32	G7M	1a	527	24/25	0.96	0.07	32,37,41,44	0
32	M2G	1a	966	25/26	0.96	0.08	34,39,46,48	0
1	OMC	2A	1920	21/22	0.96	0.09	40,45,49,52	0
1	5MU	2A	1939	21/22	0.96	0.08	29,32,37,38	0
32	PSU	1a	516	20/21	0.97	0.07	32,41,45,46	0
32	MA6	2a	1518	24/25	0.97	0.08	35,43,48,49	0
32	MA6	2a	1519	24/25	0.97	0.09	31,43,47,49	0
32	5MC	1a	1400	21/22	0.97	0.10	32,36,40,42	0
54	MIA	1w	37	29/30	0.97	0.08	25,37,48,53	0
32	4OC	1a	1402	22/23	0.97	0.07	26,31,35,40	0
55	31H	1x	76	32/33	0.97	0.07	10,14,18,23	10
54	PSU	2w	39	20/21	0.97	0.08	37,49,59,61	0
32	5MC	1a	1407	21/22	0.97	0.09	26,32,35,40	0
32	5MC	2a	1404	21/22	0.97	0.07	34,37,40,42	0
1	5MC	1A	1942	21/22	0.97	0.08	23,28,31,35	0
54	F3N	2w	76	33/34	0.97	0.09	22,31,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	2MA	2A	2503	23/24	0.98	0.07	19,28,33,33	0
1	PSU	1A	1911	20/21	0.98	0.07	26,35,39,42	0
1	PSU	2A	2605	20/21	0.98	0.06	24,26,30,30	0
1	5MC	1A	1962	21/22	0.98	0.06	20,26,30,34	0
32	5MC	1a	1404	21/22	0.98	0.06	23,27,30,35	0
54	PSU	1w	39	20/21	0.98	0.07	28,39,42,45	0
1	2MA	1A	2503	23/24	0.98	0.05	10,15,18,20	0
32	UR3	1a	1498	21/22	0.98	0.06	22,32,34,40	0
32	MA6	1a	1519	24/25	0.98	0.07	24,28,30,31	0
54	F3N	1w	76	33/34	0.98	0.07	10,14,18,25	0
1	OMC	1A	1920	21/22	0.98	0.07	27,33,37,39	0
1	OMG	2A	2251	24/25	0.98	0.06	24,27,32,39	0
1	PSU	1A	2605	20/21	0.99	0.05	13,16,21,23	0
1	OMG	1A	2251	24/25	0.99	0.05	11,15,18,18	0
1	5MU	1A	1939	21/22	0.99	0.05	14,19,23,27	0
32	MA6	1a	1518	24/25	0.99	0.06	19,27,30,31	0
1	OMU	1A	2552	21/22	0.99	0.05	15,18,21,24	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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(\AA^2)	Q<0.9
58	MG	2A	3686	1/1	0.28	0.25	77,77,77,77	0
58	MG	2A	3253	1/1	0.41	0.15	76,76,76,76	0
58	MG	2A	3272	1/1	0.42	0.32	78,78,78,78	0
58	MG	2B	219	1/1	0.47	0.27	78,78,78,78	0
58	MG	18	105	1/1	0.48	0.24	70,70,70,70	0
58	MG	1A	3988	1/1	0.60	0.17	66,66,66,66	0
58	MG	2a	1626	1/1	0.62	0.26	65,65,65,65	0
58	MG	2a	1780	1/1	0.62	0.21	66,66,66,66	0
58	MG	2w	102	1/1	0.62	0.16	73,73,73,73	0
58	MG	2a	1631	1/1	0.63	0.16	78,78,78,78	0
58	MG	1A	4094	1/1	0.64	0.18	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1741	1/1	0.64	0.20	67,67,67,67	0
58	MG	1B	222	1/1	0.65	0.18	57,57,57,57	0
58	MG	2A	3810	1/1	0.65	0.26	62,62,62,62	0
58	MG	2a	1749	1/1	0.65	0.17	66,66,66,66	0
58	MG	2A	3850	1/1	0.65	0.38	65,65,65,65	0
58	MG	2a	1817	1/1	0.65	0.25	66,66,66,66	0
58	MG	1y	101	1/1	0.65	0.15	78,78,78,78	0
58	MG	1D	311	1/1	0.66	0.24	59,59,59,59	0
58	MG	2A	3608	1/1	0.67	0.23	73,73,73,73	0
58	MG	2a	1810	1/1	0.67	0.16	76,76,76,76	0
58	MG	1A	3478	1/1	0.68	0.14	52,52,52,52	0
58	MG	2A	3701	1/1	0.68	0.16	69,69,69,69	0
58	MG	1a	1779	1/1	0.68	0.14	48,48,48,48	0
58	MG	2A	3681	1/1	0.69	0.20	58,58,58,58	0
58	MG	1A	4038	1/1	0.69	0.18	49,49,49,49	0
58	MG	1O	205	1/1	0.69	0.26	62,62,62,62	0
58	MG	2A	3176	1/1	0.69	0.32	60,60,60,60	0
58	MG	2a	1745	1/1	0.69	0.15	71,71,71,71	0
58	MG	2y	104	1/1	0.69	0.28	80,80,80,80	0
58	MG	1a	1714	1/1	0.70	0.30	57,57,57,57	0
58	MG	2A	3291	1/1	0.70	0.23	64,64,64,64	0
58	MG	1A	3793	1/1	0.70	0.21	72,72,72,72	0
58	MG	29	101	1/1	0.71	0.57	63,63,63,63	0
58	MG	1A	3684	1/1	0.71	0.25	67,67,67,67	0
58	MG	2A	3344	1/1	0.72	0.15	72,72,72,72	0
58	MG	2A	3361	1/1	0.72	0.26	70,70,70,70	0
58	MG	1A	3750	1/1	0.72	0.18	60,60,60,60	0
58	MG	2a	1796	1/1	0.72	0.20	69,69,69,69	0
58	MG	1A	4023	1/1	0.73	0.20	55,55,55,55	0
58	MG	2A	3390	1/1	0.73	0.18	62,62,62,62	0
58	MG	2A	3404	1/1	0.73	0.17	64,64,64,64	0
58	MG	2a	1779	1/1	0.73	0.16	68,68,68,68	0
58	MG	10	107	1/1	0.73	0.31	59,59,59,59	0
58	MG	1A	4100	1/1	0.74	0.14	60,60,60,60	0
58	MG	2A	3373	1/1	0.74	0.22	76,76,76,76	0
58	MG	2A	3710	1/1	0.74	0.17	50,50,50,50	0
58	MG	2A	3768	1/1	0.74	0.18	48,48,48,48	0
58	MG	2A	3769	1/1	0.74	0.23	58,58,58,58	0
58	MG	2A	3800	1/1	0.74	0.15	52,52,52,52	0
58	MG	2A	3266	1/1	0.74	0.14	70,70,70,70	0
58	MG	1A	3803	1/1	0.74	0.20	54,54,54,54	0
58	MG	2A	3118	1/1	0.74	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2r	101	1/1	0.74	0.13	65,65,65,65	0
58	MG	1a	1769	1/1	0.74	0.15	70,70,70,70	0
58	MG	2w	103	1/1	0.74	0.19	73,73,73,73	0
58	MG	2a	1610	1/1	0.74	0.11	54,54,54,54	0
58	MG	2A	3340	1/1	0.75	0.18	58,58,58,58	0
58	MG	2l	201	1/1	0.75	0.25	63,63,63,63	0
58	MG	2A	3724	1/1	0.75	0.17	69,69,69,69	0
58	MG	2A	3752	1/1	0.76	0.18	61,61,61,61	0
58	MG	2A	3690	1/1	0.76	0.14	46,46,46,46	0
58	MG	1a	1814	1/1	0.76	0.29	64,64,64,64	0
58	MG	2A	3281	1/1	0.76	0.19	66,66,66,66	0
58	MG	2A	3074	1/1	0.76	0.24	66,66,66,66	0
58	MG	2A	3838	1/1	0.76	0.16	33,33,33,33	0
58	MG	2a	1708	1/1	0.77	0.20	59,59,59,59	0
58	MG	1a	1705	1/1	0.77	0.19	51,51,51,51	0
58	MG	2j	201	1/1	0.77	0.14	64,64,64,64	0
58	MG	2A	3761	1/1	0.77	0.12	42,42,42,42	0
58	MG	2A	3302	1/1	0.77	0.17	55,55,55,55	0
58	MG	1A	4093	1/1	0.77	0.21	55,55,55,55	0
58	MG	2B	202	1/1	0.77	0.19	69,69,69,69	0
58	MG	2a	1804	1/1	0.77	0.22	64,64,64,64	0
58	MG	2A	3755	1/1	0.78	0.13	33,33,33,33	0
58	MG	1a	1761	1/1	0.78	0.15	51,51,51,51	0
58	MG	1A	3688	1/1	0.78	0.12	49,49,49,49	0
58	MG	2A	3238	1/1	0.78	0.14	70,70,70,70	0
58	MG	2A	3775	1/1	0.78	0.17	71,71,71,71	0
58	MG	2a	1835	1/1	0.78	0.22	51,51,51,51	0
58	MG	2e	201	1/1	0.78	0.10	59,59,59,59	0
58	MG	2A	3778	1/1	0.78	0.23	51,51,51,51	0
58	MG	1A	3773	1/1	0.78	0.12	16,16,16,16	0
58	MG	2A	3307	1/1	0.78	0.22	61,61,61,61	0
58	MG	2A	3556	1/1	0.78	0.17	59,59,59,59	0
58	MG	2a	1757	1/1	0.78	0.16	68,68,68,68	0
58	MG	2w	105	1/1	0.78	0.12	61,61,61,61	0
58	MG	2A	3097	1/1	0.78	0.14	61,61,61,61	0
58	MG	2A	3582	1/1	0.79	0.24	70,70,70,70	0
58	MG	1A	3549	1/1	0.79	0.15	53,53,53,53	0
58	MG	2A	3658	1/1	0.79	0.17	41,41,41,41	0
58	MG	1A	4010	1/1	0.79	0.11	73,73,73,73	0
58	MG	2E	301	1/1	0.79	0.21	57,57,57,57	0
58	MG	1A	3951	1/1	0.79	0.13	57,57,57,57	0
58	MG	2y	101	1/1	0.79	0.18	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3576	1/1	0.79	0.14	43,43,43,43	0
58	MG	2A	3101	1/1	0.80	0.23	64,64,64,64	0
58	MG	1A	3062	1/1	0.80	0.13	56,56,56,56	0
58	MG	1A	3199	1/1	0.80	0.22	44,44,44,44	0
58	MG	2A	3773	1/1	0.80	0.15	38,38,38,38	0
58	MG	1a	1797	1/1	0.80	0.12	55,55,55,55	0
58	MG	1A	3212	1/1	0.80	0.24	66,66,66,66	0
58	MG	2a	1696	1/1	0.80	0.19	64,64,64,64	0
58	MG	2a	1698	1/1	0.80	0.17	47,47,47,47	0
58	MG	1t	201	1/1	0.80	0.12	51,51,51,51	0
58	MG	1x	105	1/1	0.80	0.21	59,59,59,59	0
58	MG	1B	230	1/1	0.80	0.17	69,69,69,69	0
58	MG	1A	3426	1/1	0.80	0.33	58,58,58,58	0
58	MG	2A	3869	1/1	0.80	0.14	52,52,52,52	0
58	MG	1A	3740	1/1	0.80	0.11	51,51,51,51	0
58	MG	2A	3597	1/1	0.81	0.20	62,62,62,62	0
58	MG	1A	3665	1/1	0.81	0.14	47,47,47,47	0
58	MG	1A	3548	1/1	0.81	0.50	52,52,52,52	0
58	MG	1A	3831	1/1	0.81	0.12	38,38,38,38	0
58	MG	2A	3682	1/1	0.81	0.21	60,60,60,60	0
58	MG	1A	4046	1/1	0.81	0.10	44,44,44,44	0
58	MG	2A	3846	1/1	0.81	0.13	60,60,60,60	0
58	MG	2a	1795	1/1	0.81	0.15	64,64,64,64	0
58	MG	2A	3848	1/1	0.81	0.14	61,61,61,61	0
58	MG	2A	3221	1/1	0.81	0.16	49,49,49,49	0
58	MG	2A	3860	1/1	0.81	0.22	56,56,56,56	0
58	MG	1Y	202	1/1	0.81	0.09	57,57,57,57	0
58	MG	2a	1818	1/1	0.81	0.16	63,63,63,63	0
58	MG	2a	1820	1/1	0.81	0.20	66,66,66,66	0
58	MG	2A	3871	1/1	0.81	0.11	62,62,62,62	0
58	MG	2A	3708	1/1	0.81	0.11	29,29,29,29	0
58	MG	1A	3848	1/1	0.81	0.12	41,41,41,41	0
58	MG	1A	3585	1/1	0.81	0.18	66,66,66,66	0
58	MG	2A	3411	1/1	0.81	0.11	49,49,49,49	0
58	MG	1A	3774	1/1	0.81	0.13	54,54,54,54	0
58	MG	2a	1616	1/1	0.81	0.14	60,60,60,60	0
58	MG	2A	3575	1/1	0.81	0.18	64,64,64,64	0
58	MG	1B	208	1/1	0.81	0.13	60,60,60,60	0
58	MG	1a	1733	1/1	0.81	0.15	50,50,50,50	0
58	MG	2A	3645	1/1	0.82	0.19	46,46,46,46	0
58	MG	16	102	1/1	0.82	0.12	40,40,40,40	0
58	MG	1A	4009	1/1	0.82	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1B	203	1/1	0.82	0.25	51,51,51,51	0
58	MG	2A	3088	1/1	0.82	0.26	62,62,62,62	0
58	MG	1A	3836	1/1	0.82	0.12	57,57,57,57	0
58	MG	1B	212	1/1	0.82	0.27	46,46,46,46	0
58	MG	1A	3841	1/1	0.82	0.16	50,50,50,50	0
58	MG	2a	1808	1/1	0.82	0.12	51,51,51,51	0
58	MG	2A	3709	1/1	0.82	0.22	62,62,62,62	0
58	MG	1A	4034	1/1	0.82	0.13	35,35,35,35	0
58	MG	2A	3720	1/1	0.82	0.14	44,44,44,44	0
58	MG	1A	3421	1/1	0.82	0.17	54,54,54,54	0
58	MG	2A	3234	1/1	0.82	0.15	50,50,50,50	0
58	MG	1A	3506	1/1	0.82	0.18	63,63,63,63	0
58	MG	1a	1790	1/1	0.82	0.15	74,74,74,74	0
58	MG	2A	3257	1/1	0.82	0.14	55,55,55,55	0
58	MG	1W	208	1/1	0.82	0.18	33,33,33,33	0
58	MG	2a	1649	1/1	0.82	0.19	70,70,70,70	0
58	MG	2a	1651	1/1	0.82	0.13	50,50,50,50	0
58	MG	1A	3957	1/1	0.82	0.20	69,69,69,69	0
58	MG	1A	3330	1/1	0.82	0.16	55,55,55,55	0
58	MG	2A	3629	1/1	0.82	0.11	52,52,52,52	0
58	MG	2A	3488	1/1	0.83	0.16	63,63,63,63	0
58	MG	2A	3491	1/1	0.83	0.17	58,58,58,58	0
58	MG	1a	1747	1/1	0.83	0.17	60,60,60,60	0
58	MG	1S	203	1/1	0.83	0.09	61,61,61,61	0
58	MG	2a	1704	1/1	0.83	0.14	52,52,52,52	0
58	MG	1U	211	1/1	0.83	0.69	64,64,64,64	0
58	MG	1A	3568	1/1	0.83	0.36	48,48,48,48	0
58	MG	2a	1748	1/1	0.83	0.19	75,75,75,75	0
58	MG	1Y	201	1/1	0.83	0.18	58,58,58,58	0
58	MG	1A	3489	1/1	0.83	0.12	53,53,53,53	0
58	MG	2A	3616	1/1	0.83	0.14	31,31,31,31	0
58	MG	1A	3089	1/1	0.83	0.10	30,30,30,30	0
58	MG	11	103	1/1	0.83	0.23	56,56,56,56	0
58	MG	1A	3544	1/1	0.83	0.32	56,56,56,56	0
58	MG	2A	3670	1/1	0.83	0.21	55,55,55,55	0
58	MG	2A	3853	1/1	0.83	0.16	60,60,60,60	0
58	MG	2A	3295	1/1	0.83	0.16	56,56,56,56	0
58	MG	1B	215	1/1	0.83	0.11	44,44,44,44	0
58	MG	1a	1625	1/1	0.83	0.26	61,61,61,61	0
58	MG	2A	3877	1/1	0.83	0.11	71,71,71,71	0
58	MG	1A	4043	1/1	0.83	0.11	27,27,27,27	0
58	MG	1a	1713	1/1	0.83	0.20	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3459	1/1	0.83	0.23	41,41,41,41	0
58	MG	1A	3828	1/1	0.83	0.09	25,25,25,25	0
58	MG	2a	1609	1/1	0.83	0.12	64,64,64,64	0
58	MG	2A	3172	1/1	0.83	0.11	71,71,71,71	0
58	MG	1A	3260	1/1	0.83	0.09	57,57,57,57	0
58	MG	2a	1625	1/1	0.83	0.14	63,63,63,63	0
58	MG	2A	3405	1/1	0.83	0.18	56,56,56,56	0
58	MG	2A	3204	1/1	0.83	0.31	66,66,66,66	0
58	MG	2A	3444	1/1	0.84	0.11	68,68,68,68	0
58	MG	2A	3472	1/1	0.84	0.14	67,67,67,67	0
58	MG	2a	1632	1/1	0.84	0.41	71,71,71,71	0
58	MG	2a	1633	1/1	0.84	0.20	60,60,60,60	0
58	MG	2A	3477	1/1	0.84	0.26	68,68,68,68	0
58	MG	2A	3767	1/1	0.84	0.15	48,48,48,48	0
58	MG	2a	1655	1/1	0.84	0.13	66,66,66,66	0
58	MG	1A	3725	1/1	0.84	0.19	48,48,48,48	0
58	MG	1A	3505	1/1	0.84	0.15	49,49,49,49	0
58	MG	2A	3070	1/1	0.84	0.24	47,47,47,47	0
58	MG	2A	3268	1/1	0.84	0.19	56,56,56,56	0
58	MG	2A	3271	1/1	0.84	0.11	52,52,52,52	0
58	MG	1A	3474	1/1	0.84	0.21	52,52,52,52	0
58	MG	1A	3837	1/1	0.84	0.11	30,30,30,30	0
58	MG	2A	3822	1/1	0.84	0.11	42,42,42,42	0
58	MG	2a	1762	1/1	0.84	0.11	76,76,76,76	0
58	MG	2A	3283	1/1	0.84	0.28	54,54,54,54	0
58	MG	2A	3286	1/1	0.84	0.23	58,58,58,58	0
58	MG	2a	1793	1/1	0.84	0.15	56,56,56,56	0
58	MG	2A	3626	1/1	0.84	0.15	55,55,55,55	0
58	MG	1a	1751	1/1	0.84	0.08	50,50,50,50	0
58	MG	2A	3293	1/1	0.84	0.11	53,53,53,53	0
58	MG	1A	3476	1/1	0.84	0.27	66,66,66,66	0
58	MG	1A	3401	1/1	0.84	0.22	64,64,64,64	0
58	MG	1A	3924	1/1	0.84	0.17	68,68,68,68	0
58	MG	2A	3872	1/1	0.84	0.13	62,62,62,62	0
58	MG	1A	3358	1/1	0.84	0.21	58,58,58,58	0
58	MG	2A	3191	1/1	0.84	0.12	52,52,52,52	0
58	MG	2A	3195	1/1	0.84	0.17	62,62,62,62	0
58	MG	1a	1687	1/1	0.84	0.17	62,62,62,62	0
58	MG	2U	202	1/1	0.84	0.08	40,40,40,40	0
58	MG	28	101	1/1	0.84	0.34	60,60,60,60	0
58	MG	2A	3383	1/1	0.84	0.17	54,54,54,54	0
58	MG	2A	3209	1/1	0.84	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1798	1/1	0.84	0.18	66,66,66,66	0
58	MG	2x	105	1/1	0.84	0.40	58,58,58,58	0
58	MG	1A	3711	1/1	0.84	0.14	31,31,31,31	0
58	MG	1A	3805	1/1	0.84	0.12	47,47,47,47	0
58	MG	1A	3368	1/1	0.85	0.10	42,42,42,42	0
58	MG	2A	3697	1/1	0.85	0.13	57,57,57,57	0
58	MG	1A	3970	1/1	0.85	0.15	34,34,34,34	0
58	MG	1A	3527	1/1	0.85	0.29	61,61,61,61	0
58	MG	1A	3475	1/1	0.85	0.17	46,46,46,46	0
58	MG	2A	3393	1/1	0.85	0.21	61,61,61,61	0
58	MG	2A	3401	1/1	0.85	0.12	57,57,57,57	0
58	MG	2A	3721	1/1	0.85	0.11	43,43,43,43	0
58	MG	1A	3274	1/1	0.85	0.23	62,62,62,62	0
58	MG	2A	3733	1/1	0.85	0.16	59,59,59,59	0
58	MG	1A	3334	1/1	0.85	0.09	41,41,41,41	0
58	MG	2a	1661	1/1	0.85	0.15	55,55,55,55	0
58	MG	1A	3554	1/1	0.85	0.17	60,60,60,60	0
58	MG	1A	3840	1/1	0.85	0.13	43,43,43,43	0
58	MG	1W	202	1/1	0.85	0.17	40,40,40,40	0
58	MG	1A	3566	1/1	0.85	0.08	44,44,44,44	0
58	MG	2a	1726	1/1	0.85	0.14	65,65,65,65	0
58	MG	1A	3842	1/1	0.85	0.12	42,42,42,42	0
58	MG	1A	4058	1/1	0.85	0.11	13,13,13,13	0
58	MG	2A	3493	1/1	0.85	0.12	44,44,44,44	0
58	MG	2A	3504	1/1	0.85	0.19	57,57,57,57	0
58	MG	2A	3519	1/1	0.85	0.18	57,57,57,57	0
58	MG	1A	4068	1/1	0.85	0.11	41,41,41,41	0
58	MG	2A	3817	1/1	0.85	0.13	51,51,51,51	0
58	MG	1A	4090	1/1	0.85	0.25	46,46,46,46	0
58	MG	2a	1794	1/1	0.85	0.16	42,42,42,42	0
58	MG	2A	3275	1/1	0.85	0.10	55,55,55,55	0
58	MG	1A	3356	1/1	0.85	0.15	53,53,53,53	0
58	MG	1A	3856	1/1	0.85	0.16	59,59,59,59	0
58	MG	1a	1605	1/1	0.85	0.13	62,62,62,62	0
58	MG	2a	1809	1/1	0.85	0.19	58,58,58,58	0
58	MG	1A	3303	1/1	0.85	0.29	52,52,52,52	0
58	MG	1a	1641	1/1	0.85	0.16	60,60,60,60	0
58	MG	2A	3096	1/1	0.85	0.15	61,61,61,61	0
58	MG	1a	1645	1/1	0.85	0.11	55,55,55,55	0
58	MG	2a	1827	1/1	0.85	0.26	66,66,66,66	0
58	MG	2A	3655	1/1	0.85	0.20	44,44,44,44	0
58	MG	2d	301	1/1	0.85	0.32	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3303	1/1	0.85	0.33	56,56,56,56	0
58	MG	2A	3879	1/1	0.85	0.15	49,49,49,49	0
58	MG	2A	3883	1/1	0.85	0.16	59,59,59,59	0
58	MG	2A	3660	1/1	0.85	0.12	62,62,62,62	0
58	MG	1A	3943	1/1	0.85	0.14	51,51,51,51	0
58	MG	2A	3675	1/1	0.85	0.15	46,46,46,46	0
58	MG	1a	1688	1/1	0.85	0.20	52,52,52,52	0
58	MG	2A	3342	1/1	0.85	0.30	68,68,68,68	0
58	MG	1A	3589	1/1	0.85	0.49	54,54,54,54	0
58	MG	2y	103	1/1	0.85	0.21	70,70,70,70	0
58	MG	2a	1602	1/1	0.85	0.14	68,68,68,68	0
58	MG	2a	1666	1/1	0.86	0.20	53,53,53,53	0
58	MG	1A	3995	1/1	0.86	0.08	25,25,25,25	0
58	MG	1A	3839	1/1	0.86	0.13	45,45,45,45	0
58	MG	2A	3403	1/1	0.86	0.16	65,65,65,65	0
58	MG	1A	3555	1/1	0.86	0.08	51,51,51,51	0
58	MG	2A	3212	1/1	0.86	0.12	64,64,64,64	0
58	MG	2A	3218	1/1	0.86	0.14	53,53,53,53	0
58	MG	1a	1644	1/1	0.86	0.15	47,47,47,47	0
58	MG	2A	3465	1/1	0.86	0.14	62,62,62,62	0
58	MG	2a	1755	1/1	0.86	0.11	68,68,68,68	0
58	MG	1B	221	1/1	0.86	0.10	39,39,39,39	0
58	MG	2A	3473	1/1	0.86	0.09	52,52,52,52	0
58	MG	2A	3236	1/1	0.86	0.15	57,57,57,57	0
58	MG	2A	3237	1/1	0.86	0.21	53,53,53,53	0
58	MG	2a	1785	1/1	0.86	0.11	33,33,33,33	0
58	MG	1a	1674	1/1	0.86	0.20	52,52,52,52	0
58	MG	2A	3320	1/1	0.86	0.17	65,65,65,65	0
58	MG	2A	3718	1/1	0.86	0.16	50,50,50,50	0
58	MG	2A	3334	1/1	0.86	0.14	60,60,60,60	0
58	MG	2A	3338	1/1	0.86	0.10	63,63,63,63	0
58	MG	2A	3542	1/1	0.86	0.17	45,45,45,45	0
58	MG	2A	3243	1/1	0.86	0.14	59,59,59,59	0
58	MG	2E	311	1/1	0.86	0.14	57,57,57,57	0
58	MG	2T	202	1/1	0.86	0.14	61,61,61,61	0
58	MG	2A	3734	1/1	0.86	0.13	51,51,51,51	0
58	MG	2A	3736	1/1	0.86	0.10	37,37,37,37	0
58	MG	2a	1825	1/1	0.86	0.14	62,62,62,62	0
58	MG	2A	3742	1/1	0.86	0.12	32,32,32,32	0
58	MG	2A	3745	1/1	0.86	0.11	39,39,39,39	0
58	MG	1h	201	1/1	0.86	0.09	55,55,55,55	0
58	MG	2A	3113	1/1	0.86	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2g	201	1/1	0.86	0.14	63,63,63,63	0
58	MG	2A	3357	1/1	0.86	0.16	52,52,52,52	0
58	MG	2A	3763	1/1	0.86	0.12	47,47,47,47	0
58	MG	1s	101	1/1	0.86	0.17	54,54,54,54	0
58	MG	2A	3363	1/1	0.86	0.11	51,51,51,51	0
58	MG	1A	3362	1/1	0.86	0.11	56,56,56,56	0
58	MG	1v	101	1/1	0.86	0.23	65,65,65,65	0
58	MG	2A	3385	1/1	0.86	0.12	61,61,61,61	0
58	MG	2A	3777	1/1	0.86	0.14	60,60,60,60	0
58	MG	1A	3359	1/1	0.86	0.19	64,64,64,64	0
58	MG	2A	3797	1/1	0.86	0.12	56,56,56,56	0
58	MG	2y	105	1/1	0.86	0.23	68,68,68,68	0
58	MG	1A	3540	1/1	0.87	0.21	46,46,46,46	0
58	MG	1a	1802	1/1	0.87	0.08	46,46,46,46	0
58	MG	2A	3882	1/1	0.87	0.14	59,59,59,59	0
58	MG	2A	3244	1/1	0.87	0.14	56,56,56,56	0
58	MG	2A	3250	1/1	0.87	0.12	57,57,57,57	0
58	MG	2B	211	1/1	0.87	0.16	64,64,64,64	0
58	MG	1a	1809	1/1	0.87	0.11	63,63,63,63	0
58	MG	2A	3256	1/1	0.87	0.23	49,49,49,49	0
58	MG	1A	3985	1/1	0.87	0.15	58,58,58,58	0
58	MG	1a	1602	1/1	0.87	0.17	57,57,57,57	0
58	MG	1l	201	1/1	0.87	0.15	64,64,64,64	0
58	MG	2W	201	1/1	0.87	0.22	67,67,67,67	0
58	MG	25	104	1/1	0.87	0.10	55,55,55,55	0
58	MG	1A	3543	1/1	0.87	0.21	46,46,46,46	0
58	MG	1a	1607	1/1	0.87	0.08	50,50,50,50	0
58	MG	1A	3266	1/1	0.87	0.19	60,60,60,60	0
58	MG	2a	1606	1/1	0.87	0.17	49,49,49,49	0
58	MG	2A	3647	1/1	0.87	0.16	53,53,53,53	0
58	MG	2A	3278	1/1	0.87	0.12	51,51,51,51	0
58	MG	1a	1635	1/1	0.87	0.14	48,48,48,48	0
58	MG	2a	1620	1/1	0.87	0.16	80,80,80,80	0
58	MG	1x	106	1/1	0.87	0.27	51,51,51,51	0
58	MG	1A	3191	1/1	0.87	0.10	43,43,43,43	0
58	MG	2a	1629	1/1	0.87	0.12	59,59,59,59	0
58	MG	2A	3039	1/1	0.87	0.11	50,50,50,50	0
58	MG	2A	3051	1/1	0.87	0.09	35,35,35,35	0
58	MG	2A	3058	1/1	0.87	0.12	60,60,60,60	0
58	MG	2A	3298	1/1	0.87	0.13	61,61,61,61	0
58	MG	1A	3669	1/1	0.87	0.09	25,25,25,25	0
58	MG	2A	3073	1/1	0.87	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3405	1/1	0.87	0.18	38,38,38,38	0
58	MG	2A	3702	1/1	0.87	0.11	43,43,43,43	0
58	MG	2A	3704	1/1	0.87	0.09	65,65,65,65	0
58	MG	2A	3310	1/1	0.87	0.24	53,53,53,53	0
58	MG	2a	1700	1/1	0.87	0.12	62,62,62,62	0
58	MG	2A	3316	1/1	0.87	0.22	67,67,67,67	0
58	MG	1a	1670	1/1	0.87	0.26	60,60,60,60	0
58	MG	2A	3090	1/1	0.87	0.11	65,65,65,65	0
58	MG	2a	1733	1/1	0.87	0.14	62,62,62,62	0
58	MG	2A	3336	1/1	0.87	0.30	52,52,52,52	0
58	MG	1A	3852	1/1	0.87	0.16	53,53,53,53	0
58	MG	1a	1676	1/1	0.87	0.09	54,54,54,54	0
58	MG	2a	1752	1/1	0.87	0.13	61,61,61,61	0
58	MG	1B	234	1/1	0.87	0.12	63,63,63,63	0
58	MG	2A	3105	1/1	0.87	0.15	51,51,51,51	0
58	MG	1A	4035	1/1	0.87	0.10	35,35,35,35	0
58	MG	2A	3358	1/1	0.87	0.20	54,54,54,54	0
58	MG	2A	3114	1/1	0.87	0.17	57,57,57,57	0
58	MG	1O	201	1/1	0.87	0.15	62,62,62,62	0
58	MG	2A	3364	1/1	0.87	0.10	46,46,46,46	0
58	MG	2A	3759	1/1	0.87	0.14	47,47,47,47	0
58	MG	2A	3127	1/1	0.87	0.08	55,55,55,55	0
58	MG	2A	3154	1/1	0.87	0.13	61,61,61,61	0
58	MG	2a	1799	1/1	0.87	0.14	51,51,51,51	0
58	MG	1A	3407	1/1	0.87	0.19	56,56,56,56	0
58	MG	1S	201	1/1	0.87	0.45	43,43,43,43	0
58	MG	1A	3861	1/1	0.87	0.13	53,53,53,53	0
58	MG	2A	3192	1/1	0.87	0.19	62,62,62,62	0
58	MG	1U	210	1/1	0.87	0.16	43,43,43,43	0
58	MG	2A	3202	1/1	0.87	0.19	50,50,50,50	0
58	MG	1A	3872	1/1	0.87	0.15	34,34,34,34	0
58	MG	2a	1824	1/1	0.87	0.12	59,59,59,59	0
58	MG	2A	3781	1/1	0.87	0.12	61,61,61,61	0
58	MG	2A	3406	1/1	0.87	0.12	52,52,52,52	0
58	MG	2A	3206	1/1	0.87	0.11	45,45,45,45	0
58	MG	2A	3809	1/1	0.87	0.12	63,63,63,63	0
58	MG	2A	3432	1/1	0.87	0.27	60,60,60,60	0
58	MG	2A	3207	1/1	0.87	0.20	65,65,65,65	0
58	MG	2A	3819	1/1	0.87	0.10	74,74,74,74	0
58	MG	2A	3445	1/1	0.87	0.14	44,44,44,44	0
58	MG	2l	205	1/1	0.87	0.14	52,52,52,52	0
58	MG	1A	4056	1/1	0.87	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2v	102	1/1	0.87	0.11	42,42,42,42	0
58	MG	1a	1758	1/1	0.87	0.11	40,40,40,40	0
58	MG	1A	3511	1/1	0.87	0.10	59,59,59,59	0
58	MG	1A	3830	1/1	0.87	0.12	40,40,40,40	0
58	MG	2A	3224	1/1	0.87	0.12	56,56,56,56	0
58	MG	1A	3074	1/1	0.87	0.23	54,54,54,54	0
58	MG	1A	3955	1/1	0.87	0.11	53,53,53,53	0
58	MG	2A	3498	1/1	0.87	0.19	42,42,42,42	0
58	MG	1A	3726	1/1	0.87	0.09	33,33,33,33	0
58	MG	2A	3351	1/1	0.88	0.19	52,52,52,52	0
58	MG	1B	214	1/1	0.88	0.25	56,56,56,56	0
58	MG	1A	3611	1/1	0.88	0.10	43,43,43,43	0
58	MG	2A	3214	1/1	0.88	0.21	60,60,60,60	0
58	MG	2A	3215	1/1	0.88	0.15	56,56,56,56	0
58	MG	2a	1621	1/1	0.88	0.15	52,52,52,52	0
58	MG	2A	3216	1/1	0.88	0.12	52,52,52,52	0
58	MG	1A	3850	1/1	0.88	0.09	49,49,49,49	0
58	MG	1x	101	1/1	0.88	0.21	48,48,48,48	0
58	MG	2A	3384	1/1	0.88	0.11	50,50,50,50	0
58	MG	2A	3222	1/1	0.88	0.25	55,55,55,55	0
58	MG	1A	3612	1/1	0.88	0.10	19,19,19,19	0
58	MG	2a	1640	1/1	0.88	0.18	53,53,53,53	0
58	MG	2A	3391	1/1	0.88	0.12	53,53,53,53	0
58	MG	1A	4027	1/1	0.88	0.10	53,53,53,53	0
58	MG	1B	232	1/1	0.88	0.36	58,58,58,58	0
58	MG	1A	4032	1/1	0.88	0.11	42,42,42,42	0
58	MG	2A	3744	1/1	0.88	0.21	56,56,56,56	0
58	MG	1B	235	1/1	0.88	0.20	56,56,56,56	0
58	MG	2A	3750	1/1	0.88	0.12	67,67,67,67	0
58	MG	2A	3054	1/1	0.88	0.27	53,53,53,53	0
58	MG	2a	1701	1/1	0.88	0.28	66,66,66,66	0
58	MG	1A	3619	1/1	0.88	0.09	5,5,5,5	0
58	MG	2A	3409	1/1	0.88	0.12	54,54,54,54	0
58	MG	2a	1722	1/1	0.88	0.26	66,66,66,66	0
58	MG	2A	3064	1/1	0.88	0.08	56,56,56,56	0
58	MG	2A	3420	1/1	0.88	0.18	45,45,45,45	0
58	MG	2A	3251	1/1	0.88	0.14	57,57,57,57	0
58	MG	2A	3252	1/1	0.88	0.18	62,62,62,62	0
58	MG	1G	204	1/1	0.88	0.12	47,47,47,47	0
58	MG	1A	3658	1/1	0.88	0.08	36,36,36,36	0
58	MG	1a	1710	1/1	0.88	0.15	49,49,49,49	0
58	MG	1A	3865	1/1	0.88	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4042	1/1	0.88	0.10	35,35,35,35	0
58	MG	1A	3470	1/1	0.88	0.14	53,53,53,53	0
58	MG	1a	1738	1/1	0.88	0.15	47,47,47,47	0
58	MG	2A	3100	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3895	1/1	0.88	0.11	24,24,24,24	0
58	MG	1A	4051	1/1	0.88	0.08	26,26,26,26	0
58	MG	1A	3906	1/1	0.88	0.12	49,49,49,49	0
58	MG	2A	3524	1/1	0.88	0.13	52,52,52,52	0
58	MG	2A	3526	1/1	0.88	0.10	51,51,51,51	0
58	MG	2A	3825	1/1	0.88	0.10	42,42,42,42	0
58	MG	1A	3416	1/1	0.88	0.10	46,46,46,46	0
58	MG	2A	3116	1/1	0.88	0.13	48,48,48,48	0
58	MG	1A	3381	1/1	0.88	0.22	45,45,45,45	0
58	MG	2A	3122	1/1	0.88	0.18	70,70,70,70	0
58	MG	1A	3026	1/1	0.88	0.12	45,45,45,45	0
58	MG	2A	3593	1/1	0.88	0.08	46,46,46,46	0
58	MG	2A	3300	1/1	0.88	0.09	44,44,44,44	0
58	MG	1A	3537	1/1	0.88	0.15	51,51,51,51	0
58	MG	2A	3163	1/1	0.88	0.18	45,45,45,45	0
58	MG	2A	3170	1/1	0.88	0.10	60,60,60,60	0
58	MG	2A	3627	1/1	0.88	0.14	42,42,42,42	0
58	MG	1a	1782	1/1	0.88	0.12	49,49,49,49	0
58	MG	2A	3636	1/1	0.88	0.14	31,31,31,31	0
58	MG	2A	3314	1/1	0.88	0.14	49,49,49,49	0
58	MG	1A	3438	1/1	0.88	0.09	40,40,40,40	0
58	MG	11	105	1/1	0.88	0.08	59,59,59,59	0
58	MG	2A	3322	1/1	0.88	0.13	56,56,56,56	0
58	MG	2t	201	1/1	0.88	0.09	52,52,52,52	0
58	MG	2A	3326	1/1	0.88	0.11	58,58,58,58	0
58	MG	1A	3480	1/1	0.88	0.11	50,50,50,50	0
58	MG	2A	3674	1/1	0.88	0.14	38,38,38,38	0
58	MG	1A	3412	1/1	0.88	0.14	53,53,53,53	0
58	MG	2w	112	1/1	0.88	0.12	56,56,56,56	0
58	MG	21	101	1/1	0.88	0.11	59,59,59,59	0
58	MG	1A	3603	1/1	0.88	0.09	31,31,31,31	0
58	MG	1B	209	1/1	0.88	0.10	54,54,54,54	0
58	MG	1A	3752	1/1	0.88	0.07	27,27,27,27	0
58	MG	1a	1612	1/1	0.88	0.11	58,58,58,58	0
58	MG	1a	1702	1/1	0.89	0.15	52,52,52,52	0
58	MG	1G	203	1/1	0.89	0.10	51,51,51,51	0
58	MG	2A	3534	1/1	0.89	0.09	24,24,24,24	0
58	MG	2A	3292	1/1	0.89	0.30	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3167	1/1	0.89	0.12	39,39,39,39	0
58	MG	1A	3413	1/1	0.89	0.33	46,46,46,46	0
58	MG	1A	3876	1/1	0.89	0.18	22,22,22,22	0
58	MG	2B	204	1/1	0.89	0.15	62,62,62,62	0
58	MG	1A	3881	1/1	0.89	0.16	24,24,24,24	0
58	MG	2A	3589	1/1	0.89	0.08	25,25,25,25	0
58	MG	1a	1734	1/1	0.89	0.10	53,53,53,53	0
58	MG	2E	303	1/1	0.89	0.08	46,46,46,46	0
58	MG	1A	3251	1/1	0.89	0.12	51,51,51,51	0
58	MG	2G	201	1/1	0.89	0.18	59,59,59,59	0
58	MG	2Q	202	1/1	0.89	0.13	38,38,38,38	0
58	MG	2Q	203	1/1	0.89	0.33	56,56,56,56	0
58	MG	2A	3600	1/1	0.89	0.13	42,42,42,42	0
58	MG	2A	3306	1/1	0.89	0.09	47,47,47,47	0
58	MG	2V	202	1/1	0.89	0.08	54,54,54,54	0
58	MG	1A	3901	1/1	0.89	0.15	26,26,26,26	0
58	MG	2A	3622	1/1	0.89	0.10	34,34,34,34	0
58	MG	1A	3904	1/1	0.89	0.10	37,37,37,37	0
58	MG	1A	3378	1/1	0.89	0.14	41,41,41,41	0
58	MG	1A	4063	1/1	0.89	0.18	30,30,30,30	0
58	MG	1A	3811	1/1	0.89	0.09	37,37,37,37	0
58	MG	2a	1604	1/1	0.89	0.15	56,56,56,56	0
58	MG	2A	3179	1/1	0.89	0.22	41,41,41,41	0
58	MG	2a	1607	1/1	0.89	0.25	63,63,63,63	0
58	MG	2A	3324	1/1	0.89	0.16	59,59,59,59	0
58	MG	1A	3933	1/1	0.89	0.07	25,25,25,25	0
58	MG	2a	1612	1/1	0.89	0.22	58,58,58,58	0
58	MG	2A	3656	1/1	0.89	0.12	42,42,42,42	0
58	MG	1Z	3700	1/1	0.89	0.08	44,44,44,44	0
58	MG	10	106	1/1	0.89	0.10	48,48,48,48	0
58	MG	2A	3337	1/1	0.89	0.16	60,60,60,60	0
58	MG	2A	3671	1/1	0.89	0.11	65,65,65,65	0
58	MG	1A	3666	1/1	0.89	0.13	36,36,36,36	0
58	MG	2A	3203	1/1	0.89	0.13	39,39,39,39	0
58	MG	2A	3679	1/1	0.89	0.11	49,49,49,49	0
58	MG	10	108	1/1	0.89	0.12	51,51,51,51	0
58	MG	1A	3552	1/1	0.89	0.18	45,45,45,45	0
58	MG	2a	1646	1/1	0.89	0.26	56,56,56,56	0
58	MG	1A	3172	1/1	0.89	0.15	48,48,48,48	0
58	MG	2A	3355	1/1	0.89	0.11	56,56,56,56	0
58	MG	2A	3691	1/1	0.89	0.12	49,49,49,49	0
58	MG	2A	3694	1/1	0.89	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3356	1/1	0.89	0.09	51,51,51,51	0
58	MG	2a	1679	1/1	0.89	0.16	43,43,43,43	0
58	MG	2a	1684	1/1	0.89	0.12	43,43,43,43	0
58	MG	2A	3208	1/1	0.89	0.09	53,53,53,53	0
58	MG	11	106	1/1	0.89	0.10	45,45,45,45	0
58	MG	2A	3703	1/1	0.89	0.12	59,59,59,59	0
58	MG	1A	3388	1/1	0.89	0.09	55,55,55,55	0
58	MG	1A	3455	1/1	0.89	0.22	51,51,51,51	0
58	MG	2a	1706	1/1	0.89	0.10	60,60,60,60	0
58	MG	1A	3714	1/1	0.89	0.12	40,40,40,40	0
58	MG	2A	3365	1/1	0.89	0.09	57,57,57,57	0
58	MG	2A	3366	1/1	0.89	0.10	51,51,51,51	0
58	MG	2a	1730	1/1	0.89	0.32	60,60,60,60	0
58	MG	2A	3719	1/1	0.89	0.07	38,38,38,38	0
58	MG	2a	1734	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	3987	1/1	0.89	0.21	58,58,58,58	0
58	MG	1A	3508	1/1	0.89	0.12	58,58,58,58	0
58	MG	2A	3723	1/1	0.89	0.09	46,46,46,46	0
58	MG	1A	3457	1/1	0.89	0.28	41,41,41,41	0
58	MG	1w	107	1/1	0.89	0.14	51,51,51,51	0
58	MG	2A	3388	1/1	0.89	0.30	56,56,56,56	0
58	MG	1A	3998	1/1	0.89	0.22	53,53,53,53	0
58	MG	2a	1764	1/1	0.89	0.13	67,67,67,67	0
58	MG	2A	3225	1/1	0.89	0.10	47,47,47,47	0
58	MG	1A	3735	1/1	0.89	0.15	63,63,63,63	0
58	MG	2A	3400	1/1	0.89	0.09	59,59,59,59	0
58	MG	2A	3746	1/1	0.89	0.10	62,62,62,62	0
58	MG	1a	1638	1/1	0.89	0.12	61,61,61,61	0
58	MG	1B	223	1/1	0.89	0.10	40,40,40,40	0
58	MG	2A	3036	1/1	0.89	0.14	51,51,51,51	0
58	MG	2A	3241	1/1	0.89	0.14	50,50,50,50	0
58	MG	2a	1800	1/1	0.89	0.10	59,59,59,59	0
58	MG	1B	226	1/1	0.89	0.10	49,49,49,49	0
58	MG	2a	1805	1/1	0.89	0.14	63,63,63,63	0
58	MG	1A	3736	1/1	0.89	0.08	40,40,40,40	0
58	MG	1a	1651	1/1	0.89	0.15	55,55,55,55	0
58	MG	1A	3029	1/1	0.89	0.08	30,30,30,30	0
58	MG	2A	3421	1/1	0.89	0.23	38,38,38,38	0
58	MG	1A	3598	1/1	0.89	0.22	53,53,53,53	0
58	MG	2A	3434	1/1	0.89	0.17	58,58,58,58	0
58	MG	2A	3065	1/1	0.89	0.13	44,44,44,44	0
58	MG	1A	3272	1/1	0.89	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3449	1/1	0.89	0.15	52,52,52,52	0
58	MG	2A	3792	1/1	0.89	0.11	46,46,46,46	0
58	MG	2a	1841	1/1	0.89	0.20	60,60,60,60	0
58	MG	1a	1679	1/1	0.89	0.22	48,48,48,48	0
58	MG	1a	1685	1/1	0.89	0.10	47,47,47,47	0
58	MG	2A	3079	1/1	0.89	0.10	37,37,37,37	0
58	MG	2A	3082	1/1	0.89	0.12	50,50,50,50	0
58	MG	2A	3484	1/1	0.89	0.12	51,51,51,51	0
58	MG	2A	3487	1/1	0.89	0.10	51,51,51,51	0
58	MG	1A	3102	1/1	0.89	0.15	50,50,50,50	0
58	MG	2A	3490	1/1	0.89	0.07	44,44,44,44	0
58	MG	2A	3837	1/1	0.89	0.10	47,47,47,47	0
58	MG	1E	309	1/1	0.89	0.12	48,48,48,48	0
58	MG	2A	3277	1/1	0.89	0.16	58,58,58,58	0
58	MG	1a	1689	1/1	0.89	0.08	50,50,50,50	0
58	MG	2w	107	1/1	0.89	0.21	60,60,60,60	0
58	MG	2w	109	1/1	0.89	0.31	66,66,66,66	0
58	MG	2A	3849	1/1	0.89	0.09	22,22,22,22	0
58	MG	2x	102	1/1	0.89	0.23	40,40,40,40	0
58	MG	1a	1692	1/1	0.89	0.34	61,61,61,61	0
58	MG	2A	3516	1/1	0.89	0.16	49,49,49,49	0
58	MG	1a	1695	1/1	0.89	0.30	48,48,48,48	0
58	MG	2A	3520	1/1	0.89	0.12	52,52,52,52	0
58	MG	2A	3870	1/1	0.89	0.09	52,52,52,52	0
58	MG	1A	3599	1/1	0.90	0.16	61,61,61,61	0
58	MG	2B	207	1/1	0.90	0.11	53,53,53,53	0
58	MG	2B	210	1/1	0.90	0.06	56,56,56,56	0
58	MG	1A	4024	1/1	0.90	0.11	51,51,51,51	0
58	MG	2A	3309	1/1	0.90	0.33	39,39,39,39	0
58	MG	1E	312	1/1	0.90	0.15	44,44,44,44	0
58	MG	1F	312	1/1	0.90	0.13	39,39,39,39	0
58	MG	2E	306	1/1	0.90	0.14	46,46,46,46	0
58	MG	2E	309	1/1	0.90	0.09	38,38,38,38	0
58	MG	1A	3541	1/1	0.90	0.13	32,32,32,32	0
58	MG	2F	301	1/1	0.90	0.12	37,37,37,37	0
58	MG	2A	3621	1/1	0.90	0.14	60,60,60,60	0
58	MG	2N	201	1/1	0.90	0.19	55,55,55,55	0
58	MG	1A	3433	1/1	0.90	0.14	35,35,35,35	0
58	MG	1A	3867	1/1	0.90	0.11	43,43,43,43	0
58	MG	2A	3137	1/1	0.90	0.11	49,49,49,49	0
58	MG	2A	3147	1/1	0.90	0.15	47,47,47,47	0
58	MG	2V	201	1/1	0.90	0.36	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3332	1/1	0.90	0.32	59,59,59,59	0
58	MG	2A	3642	1/1	0.90	0.12	55,55,55,55	0
58	MG	1O	204	1/1	0.90	0.16	49,49,49,49	0
58	MG	1A	3757	1/1	0.90	0.08	18,18,18,18	0
58	MG	1A	3259	1/1	0.90	0.12	55,55,55,55	0
58	MG	1A	3298	1/1	0.90	0.19	57,57,57,57	0
58	MG	2A	3657	1/1	0.90	0.16	58,58,58,58	0
58	MG	2A	3174	1/1	0.90	0.16	63,63,63,63	0
58	MG	2A	3659	1/1	0.90	0.07	53,53,53,53	0
58	MG	1A	3888	1/1	0.90	0.06	15,15,15,15	0
58	MG	2A	3664	1/1	0.90	0.13	55,55,55,55	0
58	MG	1A	4045	1/1	0.90	0.21	45,45,45,45	0
58	MG	2A	3347	1/1	0.90	0.11	58,58,58,58	0
58	MG	2a	1614	1/1	0.90	0.18	53,53,53,53	0
58	MG	2a	1615	1/1	0.90	0.20	62,62,62,62	0
58	MG	2A	3350	1/1	0.90	0.13	53,53,53,53	0
58	MG	2A	3182	1/1	0.90	0.16	38,38,38,38	0
58	MG	2A	3353	1/1	0.90	0.10	47,47,47,47	0
58	MG	2a	1624	1/1	0.90	0.12	56,56,56,56	0
58	MG	1a	1742	1/1	0.90	0.12	45,45,45,45	0
58	MG	1A	3639	1/1	0.90	0.08	43,43,43,43	0
58	MG	1a	1750	1/1	0.90	0.12	45,45,45,45	0
58	MG	2A	3201	1/1	0.90	0.16	47,47,47,47	0
58	MG	1A	3644	1/1	0.90	0.13	53,53,53,53	0
58	MG	1A	3494	1/1	0.90	0.09	45,45,45,45	0
58	MG	2a	1639	1/1	0.90	0.14	48,48,48,48	0
58	MG	1a	1759	1/1	0.90	0.14	55,55,55,55	0
58	MG	2A	3699	1/1	0.90	0.16	44,44,44,44	0
58	MG	2A	3700	1/1	0.90	0.14	52,52,52,52	0
58	MG	1A	3659	1/1	0.90	0.12	45,45,45,45	0
58	MG	1A	3913	1/1	0.90	0.17	48,48,48,48	0
58	MG	2A	3372	1/1	0.90	0.17	46,46,46,46	0
58	MG	2a	1662	1/1	0.90	0.22	56,56,56,56	0
58	MG	1A	3816	1/1	0.90	0.13	54,54,54,54	0
58	MG	2a	1670	1/1	0.90	0.18	51,51,51,51	0
58	MG	2a	1678	1/1	0.90	0.17	50,50,50,50	0
58	MG	2A	3375	1/1	0.90	0.30	62,62,62,62	0
58	MG	1A	4075	1/1	0.90	0.10	13,13,13,13	0
58	MG	2A	3210	1/1	0.90	0.11	64,64,64,64	0
58	MG	1A	4085	1/1	0.90	0.09	23,23,23,23	0
58	MG	1O	109	1/1	0.90	0.08	42,42,42,42	0
58	MG	1A	3932	1/1	0.90	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3817	1/1	0.90	0.12	52,52,52,52	0
58	MG	1A	3551	1/1	0.90	0.15	46,46,46,46	0
58	MG	2A	3395	1/1	0.90	0.12	45,45,45,45	0
58	MG	2a	1717	1/1	0.90	0.13	56,56,56,56	0
58	MG	2a	1718	1/1	0.90	0.11	51,51,51,51	0
58	MG	1A	4095	1/1	0.90	0.13	50,50,50,50	0
58	MG	2a	1725	1/1	0.90	0.11	54,54,54,54	0
58	MG	1b	301	1/1	0.90	0.09	53,53,53,53	0
58	MG	2A	3402	1/1	0.90	0.09	63,63,63,63	0
58	MG	17	103	1/1	0.90	0.08	49,49,49,49	0
58	MG	1A	4099	1/1	0.90	0.09	41,41,41,41	0
58	MG	2a	1741	1/1	0.90	0.22	34,34,34,34	0
58	MG	2A	3228	1/1	0.90	0.12	52,52,52,52	0
58	MG	1A	3115	1/1	0.90	0.19	32,32,32,32	0
58	MG	1a	1604	1/1	0.90	0.08	48,48,48,48	0
58	MG	1A	3458	1/1	0.90	0.10	56,56,56,56	0
58	MG	1A	3364	1/1	0.90	0.15	56,56,56,56	0
58	MG	1w	108	1/1	0.90	0.13	60,60,60,60	0
58	MG	2A	3760	1/1	0.90	0.19	40,40,40,40	0
58	MG	1A	3966	1/1	0.90	0.13	38,38,38,38	0
58	MG	1a	1617	1/1	0.90	0.11	53,53,53,53	0
58	MG	2A	3437	1/1	0.90	0.20	42,42,42,42	0
58	MG	1A	3235	1/1	0.90	0.14	43,43,43,43	0
58	MG	2a	1788	1/1	0.90	0.10	37,37,37,37	0
58	MG	1a	1627	1/1	0.90	0.15	42,42,42,42	0
58	MG	1A	3973	1/1	0.90	0.11	34,34,34,34	0
58	MG	2A	3451	1/1	0.90	0.22	47,47,47,47	0
58	MG	2A	3776	1/1	0.90	0.18	63,63,63,63	0
58	MG	2A	3452	1/1	0.90	0.27	50,50,50,50	0
58	MG	2A	3455	1/1	0.90	0.22	58,58,58,58	0
58	MG	1A	3979	1/1	0.90	0.11	62,62,62,62	0
58	MG	2A	3788	1/1	0.90	0.15	60,60,60,60	0
58	MG	1B	218	1/1	0.90	0.09	43,43,43,43	0
58	MG	1A	3567	1/1	0.90	0.11	45,45,45,45	0
58	MG	2A	3799	1/1	0.90	0.11	71,71,71,71	0
58	MG	2A	3057	1/1	0.90	0.12	43,43,43,43	0
58	MG	2A	3482	1/1	0.90	0.13	38,38,38,38	0
58	MG	1A	3267	1/1	0.90	0.16	49,49,49,49	0
58	MG	2A	3811	1/1	0.90	0.09	63,63,63,63	0
58	MG	2A	3812	1/1	0.90	0.10	60,60,60,60	0
58	MG	2A	3485	1/1	0.90	0.14	44,44,44,44	0
58	MG	2a	1829	1/1	0.90	0.14	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1834	1/1	0.90	0.19	68,68,68,68	0
58	MG	1A	3582	1/1	0.90	0.08	28,28,28,28	0
58	MG	1a	1656	1/1	0.90	0.16	52,52,52,52	0
58	MG	2A	3273	1/1	0.90	0.17	54,54,54,54	0
58	MG	2A	3826	1/1	0.90	0.08	31,31,31,31	0
58	MG	2A	3067	1/1	0.90	0.12	52,52,52,52	0
58	MG	1a	1663	1/1	0.90	0.12	53,53,53,53	0
58	MG	1a	1665	1/1	0.90	0.09	56,56,56,56	0
58	MG	1a	1666	1/1	0.90	0.12	45,45,45,45	0
58	MG	2A	3077	1/1	0.90	0.15	43,43,43,43	0
58	MG	1A	3531	1/1	0.90	0.34	50,50,50,50	0
58	MG	2A	3289	1/1	0.90	0.18	57,57,57,57	0
58	MG	1B	229	1/1	0.90	0.10	44,44,44,44	0
58	MG	2A	3868	1/1	0.90	0.11	39,39,39,39	0
58	MG	1a	1675	1/1	0.90	0.24	56,56,56,56	0
58	MG	1A	3728	1/1	0.90	0.10	47,47,47,47	0
58	MG	2A	3091	1/1	0.90	0.15	54,54,54,54	0
58	MG	2w	110	1/1	0.90	0.10	58,58,58,58	0
58	MG	2A	3552	1/1	0.90	0.08	33,33,33,33	0
58	MG	1a	1678	1/1	0.90	0.19	51,51,51,51	0
58	MG	1A	4003	1/1	0.90	0.12	23,23,23,23	0
58	MG	1A	3342	1/1	0.90	0.07	40,40,40,40	0
58	MG	2A	3581	1/1	0.90	0.09	48,48,48,48	0
58	MG	2B	201	1/1	0.90	0.13	56,56,56,56	0
58	MG	1A	3211	1/1	0.90	0.09	39,39,39,39	0
58	MG	2y	106	1/1	0.90	0.17	66,66,66,66	0
58	MG	1a	1693	1/1	0.91	0.20	41,41,41,41	0
58	MG	1A	3103	1/1	0.91	0.07	46,46,46,46	0
58	MG	1T	203	1/1	0.91	0.20	44,44,44,44	0
58	MG	2E	308	1/1	0.91	0.07	54,54,54,54	0
58	MG	1a	1704	1/1	0.91	0.12	41,41,41,41	0
58	MG	2A	3610	1/1	0.91	0.08	26,26,26,26	0
58	MG	1U	202	1/1	0.91	0.15	47,47,47,47	0
58	MG	2F	306	1/1	0.91	0.09	44,44,44,44	0
58	MG	1a	1707	1/1	0.91	0.14	48,48,48,48	0
58	MG	2A	3312	1/1	0.91	0.09	55,55,55,55	0
58	MG	2A	3624	1/1	0.91	0.06	23,23,23,23	0
58	MG	2A	3111	1/1	0.91	0.09	46,46,46,46	0
58	MG	2S	201	1/1	0.91	0.20	64,64,64,64	0
58	MG	1A	3878	1/1	0.91	0.23	27,27,27,27	0
58	MG	2A	3318	1/1	0.91	0.12	49,49,49,49	0
58	MG	2A	3630	1/1	0.91	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3335	1/1	0.91	0.09	47,47,47,47	0
58	MG	1V	207	1/1	0.91	0.11	43,43,43,43	0
58	MG	2W	202	1/1	0.91	0.11	61,61,61,61	0
58	MG	1a	1715	1/1	0.91	0.16	37,37,37,37	0
58	MG	1a	1716	1/1	0.91	0.26	48,48,48,48	0
58	MG	26	101	1/1	0.91	0.12	45,45,45,45	0
58	MG	2A	3328	1/1	0.91	0.15	46,46,46,46	0
58	MG	28	104	1/1	0.91	0.14	44,44,44,44	0
58	MG	2A	3330	1/1	0.91	0.11	55,55,55,55	0
58	MG	1a	1720	1/1	0.91	0.09	48,48,48,48	0
58	MG	2A	3333	1/1	0.91	0.12	57,57,57,57	0
58	MG	1a	1722	1/1	0.91	0.26	52,52,52,52	0
58	MG	2A	3144	1/1	0.91	0.14	29,29,29,29	0
58	MG	2A	3146	1/1	0.91	0.22	60,60,60,60	0
58	MG	1a	1726	1/1	0.91	0.25	56,56,56,56	0
58	MG	1a	1729	1/1	0.91	0.10	53,53,53,53	0
58	MG	2a	1613	1/1	0.91	0.24	61,61,61,61	0
58	MG	1A	3885	1/1	0.91	0.09	33,33,33,33	0
58	MG	1A	4052	1/1	0.91	0.06	40,40,40,40	0
58	MG	1A	3574	1/1	0.91	0.14	46,46,46,46	0
58	MG	2a	1617	1/1	0.91	0.08	57,57,57,57	0
58	MG	1A	3889	1/1	0.91	0.07	20,20,20,20	0
58	MG	1A	3409	1/1	0.91	0.13	39,39,39,39	0
58	MG	1A	3069	1/1	0.91	0.08	36,36,36,36	0
58	MG	2A	3181	1/1	0.91	0.21	58,58,58,58	0
58	MG	1A	3346	1/1	0.91	0.08	37,37,37,37	0
58	MG	2A	3692	1/1	0.91	0.08	43,43,43,43	0
58	MG	2A	3186	1/1	0.91	0.11	49,49,49,49	0
58	MG	2A	3190	1/1	0.91	0.13	58,58,58,58	0
58	MG	2A	3359	1/1	0.91	0.23	56,56,56,56	0
58	MG	1A	4076	1/1	0.91	0.10	55,55,55,55	0
58	MG	1a	1757	1/1	0.91	0.08	47,47,47,47	0
58	MG	2a	1641	1/1	0.91	0.23	53,53,53,53	0
58	MG	2a	1644	1/1	0.91	0.10	54,54,54,54	0
58	MG	1A	3594	1/1	0.91	0.13	30,30,30,30	0
58	MG	2a	1647	1/1	0.91	0.13	50,50,50,50	0
58	MG	2A	3199	1/1	0.91	0.21	51,51,51,51	0
58	MG	1A	3911	1/1	0.91	0.09	41,41,41,41	0
58	MG	2A	3369	1/1	0.91	0.08	52,52,52,52	0
58	MG	1A	3349	1/1	0.91	0.25	65,65,65,65	0
58	MG	1A	3268	1/1	0.91	0.06	37,37,37,37	0
58	MG	2A	3711	1/1	0.91	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1773	1/1	0.91	0.09	57,57,57,57	0
58	MG	1A	3927	1/1	0.91	0.10	46,46,46,46	0
58	MG	1A	4096	1/1	0.91	0.11	45,45,45,45	0
58	MG	1A	3795	1/1	0.91	0.12	38,38,38,38	0
58	MG	1A	3424	1/1	0.91	0.08	39,39,39,39	0
58	MG	1A	3804	1/1	0.91	0.09	27,27,27,27	0
58	MG	1A	3604	1/1	0.91	0.10	28,28,28,28	0
58	MG	2A	3213	1/1	0.91	0.23	53,53,53,53	0
58	MG	2a	1702	1/1	0.91	0.26	51,51,51,51	0
58	MG	2A	3394	1/1	0.91	0.25	64,64,64,64	0
58	MG	1A	3516	1/1	0.91	0.16	47,47,47,47	0
58	MG	1a	1810	1/1	0.91	0.14	48,48,48,48	0
58	MG	2a	1715	1/1	0.91	0.14	53,53,53,53	0
58	MG	1a	1811	1/1	0.91	0.10	53,53,53,53	0
58	MG	1A	3523	1/1	0.91	0.13	55,55,55,55	0
58	MG	1a	1615	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3357	1/1	0.91	0.09	44,44,44,44	0
58	MG	2A	3223	1/1	0.91	0.35	52,52,52,52	0
58	MG	1A	3429	1/1	0.91	0.16	41,41,41,41	0
58	MG	1A	3641	1/1	0.91	0.14	42,42,42,42	0
58	MG	1a	1630	1/1	0.91	0.23	39,39,39,39	0
58	MG	2a	1739	1/1	0.91	0.12	66,66,66,66	0
58	MG	2A	3416	1/1	0.91	0.23	44,44,44,44	0
58	MG	2A	3766	1/1	0.91	0.10	46,46,46,46	0
58	MG	2A	3230	1/1	0.91	0.16	40,40,40,40	0
58	MG	1A	3533	1/1	0.91	0.07	41,41,41,41	0
58	MG	2A	3431	1/1	0.91	0.10	43,43,43,43	0
58	MG	2a	1753	1/1	0.91	0.12	77,77,77,77	0
58	MG	1A	3981	1/1	0.91	0.09	35,35,35,35	0
58	MG	1A	3834	1/1	0.91	0.10	55,55,55,55	0
58	MG	1A	3001	1/1	0.91	0.07	29,29,29,29	0
58	MG	2A	3442	1/1	0.91	0.17	49,49,49,49	0
58	MG	1x	103	1/1	0.91	0.12	46,46,46,46	0
58	MG	2A	3780	1/1	0.91	0.08	39,39,39,39	0
58	MG	1A	3002	1/1	0.91	0.10	41,41,41,41	0
58	MG	1A	3448	1/1	0.91	0.12	35,35,35,35	0
58	MG	1a	1652	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3794	1/1	0.91	0.16	73,73,73,73	0
58	MG	2A	3007	1/1	0.91	0.09	44,44,44,44	0
58	MG	2A	3024	1/1	0.91	0.10	36,36,36,36	0
58	MG	2A	3464	1/1	0.91	0.12	43,43,43,43	0
58	MG	2A	3802	1/1	0.91	0.10	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3454	1/1	0.91	0.12	31,31,31,31	0
58	MG	2A	3255	1/1	0.91	0.16	61,61,61,61	0
58	MG	1A	3100	1/1	0.91	0.10	44,44,44,44	0
58	MG	2A	3474	1/1	0.91	0.24	45,45,45,45	0
58	MG	2A	3813	1/1	0.91	0.08	35,35,35,35	0
58	MG	2a	1813	1/1	0.91	0.21	50,50,50,50	0
58	MG	2a	1815	1/1	0.91	0.10	43,43,43,43	0
58	MG	2A	3045	1/1	0.91	0.08	55,55,55,55	0
58	MG	2A	3481	1/1	0.91	0.24	51,51,51,51	0
58	MG	2A	3261	1/1	0.91	0.22	55,55,55,55	0
58	MG	2a	1822	1/1	0.91	0.20	55,55,55,55	0
58	MG	2A	3047	1/1	0.91	0.14	53,53,53,53	0
58	MG	2A	3267	1/1	0.91	0.14	53,53,53,53	0
58	MG	1A	3363	1/1	0.91	0.11	49,49,49,49	0
58	MG	2a	1828	1/1	0.91	0.16	50,50,50,50	0
58	MG	1A	3025	1/1	0.91	0.26	35,35,35,35	0
58	MG	2A	3840	1/1	0.91	0.07	31,31,31,31	0
58	MG	1E	306	1/1	0.91	0.10	38,38,38,38	0
58	MG	2a	1839	1/1	0.91	0.17	50,50,50,50	0
58	MG	1a	1671	1/1	0.91	0.13	50,50,50,50	0
58	MG	1A	3702	1/1	0.91	0.10	47,47,47,47	0
58	MG	2A	3276	1/1	0.91	0.14	54,54,54,54	0
58	MG	1E	311	1/1	0.91	0.07	16,16,16,16	0
58	MG	1A	3313	1/1	0.91	0.17	61,61,61,61	0
58	MG	2A	3867	1/1	0.91	0.09	49,49,49,49	0
58	MG	2l	204	1/1	0.91	0.09	52,52,52,52	0
58	MG	2A	3280	1/1	0.91	0.14	59,59,59,59	0
58	MG	2A	3068	1/1	0.91	0.07	36,36,36,36	0
58	MG	1A	3314	1/1	0.91	0.09	47,47,47,47	0
58	MG	2v	101	1/1	0.91	0.20	56,56,56,56	0
58	MG	2A	3071	1/1	0.91	0.13	46,46,46,46	0
58	MG	1A	4031	1/1	0.91	0.10	56,56,56,56	0
58	MG	2A	3290	1/1	0.91	0.21	53,53,53,53	0
58	MG	1a	1680	1/1	0.91	0.13	47,47,47,47	0
58	MG	2w	106	1/1	0.91	0.11	36,36,36,36	0
58	MG	1A	3859	1/1	0.91	0.12	19,19,19,19	0
58	MG	1A	3715	1/1	0.91	0.10	49,49,49,49	0
58	MG	1A	3316	1/1	0.91	0.18	47,47,47,47	0
58	MG	2w	111	1/1	0.91	0.13	60,60,60,60	0
58	MG	1A	3321	1/1	0.91	0.18	49,49,49,49	0
58	MG	1A	3265	1/1	0.91	0.11	50,50,50,50	0
58	MG	2x	104	1/1	0.91	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3584	1/1	0.91	0.10	48,48,48,48	0
58	MG	2A	3586	1/1	0.91	0.10	43,43,43,43	0
58	MG	2A	3301	1/1	0.91	0.20	40,40,40,40	0
58	MG	2B	212	1/1	0.91	0.20	56,56,56,56	0
58	MG	2A	3592	1/1	0.91	0.09	58,58,58,58	0
58	MG	2D	307	1/1	0.91	0.22	44,44,44,44	0
58	MG	2A	3327	1/1	0.92	0.23	44,44,44,44	0
58	MG	1A	3385	1/1	0.92	0.12	43,43,43,43	0
58	MG	1A	3327	1/1	0.92	0.10	47,47,47,47	0
58	MG	2A	3161	1/1	0.92	0.11	44,44,44,44	0
58	MG	1A	3682	1/1	0.92	0.10	47,47,47,47	0
58	MG	2A	3166	1/1	0.92	0.25	65,65,65,65	0
58	MG	2A	3168	1/1	0.92	0.14	35,35,35,35	0
58	MG	1A	3396	1/1	0.92	0.40	41,41,41,41	0
58	MG	1A	3846	1/1	0.92	0.10	62,62,62,62	0
58	MG	2Z	301	1/1	0.92	0.10	58,58,58,58	0
58	MG	2A	3637	1/1	0.92	0.12	37,37,37,37	0
58	MG	1A	3473	1/1	0.92	0.17	47,47,47,47	0
58	MG	2A	3341	1/1	0.92	0.34	72,72,72,72	0
58	MG	1A	3195	1/1	0.92	0.08	43,43,43,43	0
58	MG	2A	3343	1/1	0.92	0.20	55,55,55,55	0
58	MG	1A	3095	1/1	0.92	0.16	47,47,47,47	0
58	MG	1A	4040	1/1	0.92	0.06	26,26,26,26	0
58	MG	1A	3713	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3140	1/1	0.92	0.22	36,36,36,36	0
58	MG	2A	3352	1/1	0.92	0.13	51,51,51,51	0
58	MG	2A	3663	1/1	0.92	0.07	55,55,55,55	0
58	MG	1A	3269	1/1	0.92	0.11	45,45,45,45	0
58	MG	2A	3354	1/1	0.92	0.14	56,56,56,56	0
58	MG	1a	1760	1/1	0.92	0.10	47,47,47,47	0
58	MG	1A	3716	1/1	0.92	0.19	44,44,44,44	0
58	MG	1A	3719	1/1	0.92	0.10	26,26,26,26	0
58	MG	2A	3198	1/1	0.92	0.15	60,60,60,60	0
58	MG	1A	3868	1/1	0.92	0.16	65,65,65,65	0
58	MG	15	103	1/1	0.92	0.29	37,37,37,37	0
58	MG	2A	3683	1/1	0.92	0.17	59,59,59,59	0
58	MG	15	109	1/1	0.92	0.10	42,42,42,42	0
58	MG	2A	3687	1/1	0.92	0.11	39,39,39,39	0
58	MG	1A	3870	1/1	0.92	0.14	34,34,34,34	0
58	MG	2a	1628	1/1	0.92	0.09	53,53,53,53	0
58	MG	1A	3871	1/1	0.92	0.08	34,34,34,34	0
58	MG	2a	1630	1/1	0.92	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4062	1/1	0.92	0.09	49,49,49,49	0
58	MG	1A	3723	1/1	0.92	0.11	28,28,28,28	0
58	MG	1a	1804	1/1	0.92	0.08	62,62,62,62	0
58	MG	1A	4067	1/1	0.92	0.08	35,35,35,35	0
58	MG	1A	3271	1/1	0.92	0.17	33,33,33,33	0
58	MG	1A	3483	1/1	0.92	0.06	32,32,32,32	0
58	MG	1a	1608	1/1	0.92	0.23	44,44,44,44	0
58	MG	1A	3488	1/1	0.92	0.19	24,24,24,24	0
58	MG	1a	1614	1/1	0.92	0.08	48,48,48,48	0
58	MG	2a	1648	1/1	0.92	0.13	56,56,56,56	0
58	MG	1A	4083	1/1	0.92	0.07	37,37,37,37	0
58	MG	2a	1650	1/1	0.92	0.08	51,51,51,51	0
58	MG	1l	202	1/1	0.92	0.08	49,49,49,49	0
58	MG	2a	1654	1/1	0.92	0.15	47,47,47,47	0
58	MG	1A	3146	1/1	0.92	0.13	34,34,34,34	0
58	MG	2a	1658	1/1	0.92	0.11	55,55,55,55	0
58	MG	1A	3051	1/1	0.92	0.13	20,20,20,20	0
58	MG	1A	3737	1/1	0.92	0.08	58,58,58,58	0
58	MG	2A	3397	1/1	0.92	0.15	53,53,53,53	0
58	MG	2A	3399	1/1	0.92	0.08	52,52,52,52	0
58	MG	1w	101	1/1	0.92	0.10	43,43,43,43	0
58	MG	1A	3890	1/1	0.92	0.12	27,27,27,27	0
58	MG	2a	1682	1/1	0.92	0.11	51,51,51,51	0
58	MG	1a	1632	1/1	0.92	0.13	53,53,53,53	0
58	MG	2a	1686	1/1	0.92	0.15	42,42,42,42	0
58	MG	2A	3727	1/1	0.92	0.14	52,52,52,52	0
58	MG	1A	3496	1/1	0.92	0.07	39,39,39,39	0
58	MG	1A	3900	1/1	0.92	0.07	20,20,20,20	0
58	MG	1x	104	1/1	0.92	0.24	45,45,45,45	0
58	MG	1a	1640	1/1	0.92	0.08	51,51,51,51	0
58	MG	1A	3744	1/1	0.92	0.06	11,11,11,11	0
58	MG	2A	3240	1/1	0.92	0.12	34,34,34,34	0
58	MG	2a	1707	1/1	0.92	0.13	45,45,45,45	0
58	MG	1x	108	1/1	0.92	0.10	18,18,18,18	0
58	MG	2a	1713	1/1	0.92	0.16	59,59,59,59	0
58	MG	1A	3275	1/1	0.92	0.10	35,35,35,35	0
58	MG	2A	3005	1/1	0.92	0.25	55,55,55,55	0
58	MG	2A	3426	1/1	0.92	0.13	46,46,46,46	0
58	MG	2A	3427	1/1	0.92	0.17	45,45,45,45	0
58	MG	1A	4103	1/1	0.92	0.09	40,40,40,40	0
58	MG	2A	3017	1/1	0.92	0.13	28,28,28,28	0
58	MG	2A	3433	1/1	0.92	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3023	1/1	0.92	0.08	51,51,51,51	0
58	MG	1a	1647	1/1	0.92	0.26	60,60,60,60	0
58	MG	2a	1737	1/1	0.92	0.20	40,40,40,40	0
58	MG	2A	3438	1/1	0.92	0.19	47,47,47,47	0
58	MG	2A	3441	1/1	0.92	0.15	43,43,43,43	0
58	MG	2a	1743	1/1	0.92	0.16	52,52,52,52	0
58	MG	2A	3032	1/1	0.92	0.10	30,30,30,30	0
58	MG	2a	1747	1/1	0.92	0.18	51,51,51,51	0
58	MG	1A	3236	1/1	0.92	0.24	42,42,42,42	0
58	MG	1A	3908	1/1	0.92	0.08	24,24,24,24	0
58	MG	1A	3425	1/1	0.92	0.14	34,34,34,34	0
58	MG	2A	3265	1/1	0.92	0.12	47,47,47,47	0
58	MG	1A	3760	1/1	0.92	0.08	32,32,32,32	0
58	MG	2A	3454	1/1	0.92	0.16	48,48,48,48	0
58	MG	1A	3920	1/1	0.92	0.07	18,18,18,18	0
58	MG	2A	3790	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3921	1/1	0.92	0.11	32,32,32,32	0
58	MG	2A	3270	1/1	0.92	0.11	56,56,56,56	0
58	MG	2A	3468	1/1	0.92	0.12	63,63,63,63	0
58	MG	1B	216	1/1	0.92	0.07	38,38,38,38	0
58	MG	1A	3764	1/1	0.92	0.07	13,13,13,13	0
58	MG	1A	3250	1/1	0.92	0.25	45,45,45,45	0
58	MG	2A	3806	1/1	0.92	0.08	48,48,48,48	0
58	MG	2A	3475	1/1	0.92	0.15	53,53,53,53	0
58	MG	2a	1798	1/1	0.92	0.11	36,36,36,36	0
58	MG	1A	3929	1/1	0.92	0.11	18,18,18,18	0
58	MG	2A	3479	1/1	0.92	0.11	54,54,54,54	0
58	MG	2a	1802	1/1	0.92	0.08	49,49,49,49	0
58	MG	2a	1803	1/1	0.92	0.22	53,53,53,53	0
58	MG	1A	3428	1/1	0.92	0.28	41,41,41,41	0
58	MG	1A	3307	1/1	0.92	0.14	36,36,36,36	0
58	MG	1A	3312	1/1	0.92	0.15	39,39,39,39	0
58	MG	1A	3945	1/1	0.92	0.08	19,19,19,19	0
58	MG	1a	1683	1/1	0.92	0.17	54,54,54,54	0
58	MG	1A	3615	1/1	0.92	0.09	40,40,40,40	0
58	MG	1A	3530	1/1	0.92	0.26	55,55,55,55	0
58	MG	2a	1816	1/1	0.92	0.20	54,54,54,54	0
58	MG	2A	3835	1/1	0.92	0.06	43,43,43,43	0
58	MG	1A	3628	1/1	0.92	0.08	31,31,31,31	0
58	MG	1A	3171	1/1	0.92	0.21	27,27,27,27	0
58	MG	1A	3968	1/1	0.92	0.06	31,31,31,31	0
58	MG	2A	3841	1/1	0.92	0.09	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3500	1/1	0.92	0.10	39,39,39,39	0
58	MG	1A	3020	1/1	0.92	0.08	37,37,37,37	0
58	MG	2A	3509	1/1	0.92	0.11	38,38,38,38	0
58	MG	1A	3453	1/1	0.92	0.14	49,49,49,49	0
58	MG	2a	1830	1/1	0.92	0.11	52,52,52,52	0
58	MG	1a	1696	1/1	0.92	0.20	38,38,38,38	0
58	MG	1A	3822	1/1	0.92	0.09	31,31,31,31	0
58	MG	1F	310	1/1	0.92	0.10	51,51,51,51	0
58	MG	2A	3525	1/1	0.92	0.08	34,34,34,34	0
58	MG	2a	1842	1/1	0.92	0.10	64,64,64,64	0
58	MG	1A	3823	1/1	0.92	0.08	22,22,22,22	0
58	MG	2A	3102	1/1	0.92	0.21	50,50,50,50	0
58	MG	2A	3535	1/1	0.92	0.12	45,45,45,45	0
58	MG	2A	3538	1/1	0.92	0.09	45,45,45,45	0
58	MG	2A	3540	1/1	0.92	0.13	36,36,36,36	0
58	MG	1a	1706	1/1	0.92	0.19	61,61,61,61	0
58	MG	1A	3645	1/1	0.92	0.09	69,69,69,69	0
58	MG	1a	1709	1/1	0.92	0.17	56,56,56,56	0
58	MG	2A	3559	1/1	0.92	0.15	25,25,25,25	0
58	MG	2A	3562	1/1	0.92	0.10	42,42,42,42	0
58	MG	2A	3572	1/1	0.92	0.15	46,46,46,46	0
58	MG	2w	101	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3648	1/1	0.92	0.08	27,27,27,27	0
58	MG	1A	3654	1/1	0.92	0.09	34,34,34,34	0
58	MG	2w	104	1/1	0.92	0.09	65,65,65,65	0
58	MG	2A	3311	1/1	0.92	0.13	60,60,60,60	0
58	MG	1A	3833	1/1	0.92	0.10	44,44,44,44	0
58	MG	2A	3313	1/1	0.92	0.12	49,49,49,49	0
58	MG	1A	3997	1/1	0.92	0.15	40,40,40,40	0
58	MG	1A	3185	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3133	1/1	0.92	0.09	53,53,53,53	0
58	MG	1A	3835	1/1	0.92	0.07	39,39,39,39	0
58	MG	1A	3379	1/1	0.92	0.09	41,41,41,41	0
58	MG	2x	103	1/1	0.92	0.33	65,65,65,65	0
58	MG	2A	3145	1/1	0.92	0.13	37,37,37,37	0
58	MG	2A	3601	1/1	0.92	0.14	44,44,44,44	0
58	MG	2A	3607	1/1	0.92	0.11	41,41,41,41	0
58	MG	2y	102	1/1	0.92	0.12	62,62,62,62	0
58	MG	2A	3325	1/1	0.92	0.08	60,60,60,60	0
58	MG	2F	309	1/1	0.92	0.10	47,47,47,47	0
58	MG	2A	3609	1/1	0.92	0.08	43,43,43,43	0
58	MG	1A	3066	1/1	0.92	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2B	203	1/1	0.93	0.11	57,57,57,57	0
58	MG	1A	3829	1/1	0.93	0.14	27,27,27,27	0
58	MG	2B	206	1/1	0.93	0.16	53,53,53,53	0
58	MG	1A	3386	1/1	0.93	0.14	37,37,37,37	0
58	MG	2B	209	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3961	1/1	0.93	0.06	34,34,34,34	0
58	MG	2A	3008	1/1	0.93	0.17	44,44,44,44	0
58	MG	2A	3010	1/1	0.93	0.13	41,41,41,41	0
58	MG	1A	3964	1/1	0.93	0.07	12,12,12,12	0
58	MG	2D	304	1/1	0.93	0.06	39,39,39,39	0
58	MG	1a	1658	1/1	0.93	0.17	41,41,41,41	0
58	MG	1a	1662	1/1	0.93	0.22	44,44,44,44	0
58	MG	2A	3029	1/1	0.93	0.17	49,49,49,49	0
58	MG	2A	3031	1/1	0.93	0.11	38,38,38,38	0
58	MG	1A	3535	1/1	0.93	0.29	28,28,28,28	0
58	MG	2A	3549	1/1	0.93	0.10	35,35,35,35	0
58	MG	1a	1664	1/1	0.93	0.14	46,46,46,46	0
58	MG	1A	3254	1/1	0.93	0.08	45,45,45,45	0
58	MG	2A	3557	1/1	0.93	0.06	27,27,27,27	0
58	MG	2A	3042	1/1	0.93	0.12	38,38,38,38	0
58	MG	1B	225	1/1	0.93	0.08	40,40,40,40	0
58	MG	2A	3563	1/1	0.93	0.13	48,48,48,48	0
58	MG	1a	1669	1/1	0.93	0.15	42,42,42,42	0
58	MG	2A	3048	1/1	0.93	0.14	39,39,39,39	0
58	MG	2R	201	1/1	0.93	0.11	57,57,57,57	0
58	MG	2R	203	1/1	0.93	0.12	42,42,42,42	0
58	MG	1A	3169	1/1	0.93	0.19	30,30,30,30	0
58	MG	1A	3353	1/1	0.93	0.08	34,34,34,34	0
58	MG	1a	1673	1/1	0.93	0.10	49,49,49,49	0
58	MG	2A	3297	1/1	0.93	0.28	52,52,52,52	0
58	MG	1A	3202	1/1	0.93	0.10	25,25,25,25	0
58	MG	2A	3299	1/1	0.93	0.13	64,64,64,64	0
58	MG	2A	3061	1/1	0.93	0.11	37,37,37,37	0
58	MG	2A	3063	1/1	0.93	0.08	69,69,69,69	0
58	MG	2A	3594	1/1	0.93	0.12	43,43,43,43	0
58	MG	1A	3980	1/1	0.93	0.10	62,62,62,62	0
58	MG	1B	233	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3304	1/1	0.93	0.10	46,46,46,46	0
58	MG	2A	3604	1/1	0.93	0.09	54,54,54,54	0
58	MG	1a	1677	1/1	0.93	0.09	52,52,52,52	0
58	MG	1A	3464	1/1	0.93	0.13	37,37,37,37	0
58	MG	1A	3983	1/1	0.93	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1605	1/1	0.93	0.13	52,52,52,52	0
58	MG	1A	3693	1/1	0.93	0.08	15,15,15,15	0
58	MG	1a	1682	1/1	0.93	0.10	63,63,63,63	0
58	MG	1A	3986	1/1	0.93	0.09	48,48,48,48	0
58	MG	2A	3075	1/1	0.93	0.15	40,40,40,40	0
58	MG	2A	3623	1/1	0.93	0.13	53,53,53,53	0
58	MG	1E	307	1/1	0.93	0.06	24,24,24,24	0
58	MG	1a	1686	1/1	0.93	0.25	46,46,46,46	0
58	MG	1A	3695	1/1	0.93	0.06	56,56,56,56	0
58	MG	2A	3319	1/1	0.93	0.27	64,64,64,64	0
58	MG	1E	310	1/1	0.93	0.07	21,21,21,21	0
58	MG	1A	3468	1/1	0.93	0.12	45,45,45,45	0
58	MG	1a	1690	1/1	0.93	0.21	39,39,39,39	0
58	MG	1A	3053	1/1	0.93	0.26	48,48,48,48	0
58	MG	2A	3644	1/1	0.93	0.11	36,36,36,36	0
58	MG	1A	3996	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3646	1/1	0.93	0.09	28,28,28,28	0
58	MG	1A	3117	1/1	0.93	0.17	28,28,28,28	0
58	MG	2A	3649	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3410	1/1	0.93	0.09	37,37,37,37	0
58	MG	1a	1698	1/1	0.93	0.11	56,56,56,56	0
58	MG	1A	4000	1/1	0.93	0.11	38,38,38,38	0
58	MG	2a	1635	1/1	0.93	0.18	40,40,40,40	0
58	MG	2a	1636	1/1	0.93	0.22	44,44,44,44	0
58	MG	2a	1637	1/1	0.93	0.14	52,52,52,52	0
58	MG	2A	3106	1/1	0.93	0.21	57,57,57,57	0
58	MG	2A	3110	1/1	0.93	0.07	58,58,58,58	0
58	MG	2A	3335	1/1	0.93	0.15	45,45,45,45	0
58	MG	2a	1642	1/1	0.93	0.37	58,58,58,58	0
58	MG	2A	3662	1/1	0.93	0.12	43,43,43,43	0
58	MG	2a	1645	1/1	0.93	0.08	52,52,52,52	0
58	MG	1N	203	1/1	0.93	0.13	40,40,40,40	0
58	MG	1A	3228	1/1	0.93	0.08	34,34,34,34	0
58	MG	2A	3669	1/1	0.93	0.10	47,47,47,47	0
58	MG	1A	4008	1/1	0.93	0.08	51,51,51,51	0
58	MG	1A	3175	1/1	0.93	0.13	30,30,30,30	0
58	MG	1A	3557	1/1	0.93	0.18	48,48,48,48	0
58	MG	2a	1653	1/1	0.93	0.30	54,54,54,54	0
58	MG	1A	4021	1/1	0.93	0.09	30,30,30,30	0
58	MG	2A	3123	1/1	0.93	0.07	43,43,43,43	0
58	MG	1T	201	1/1	0.93	0.16	46,46,46,46	0
58	MG	2A	3128	1/1	0.93	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1T	202	1/1	0.93	0.13	47,47,47,47	0
58	MG	2a	1664	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3720	1/1	0.93	0.12	47,47,47,47	0
58	MG	2A	3143	1/1	0.93	0.09	38,38,38,38	0
58	MG	2a	1671	1/1	0.93	0.21	46,46,46,46	0
58	MG	2a	1677	1/1	0.93	0.15	50,50,50,50	0
58	MG	2A	3688	1/1	0.93	0.14	51,51,51,51	0
58	MG	1A	3860	1/1	0.93	0.06	24,24,24,24	0
58	MG	1A	4025	1/1	0.93	0.16	44,44,44,44	0
58	MG	1A	3477	1/1	0.93	0.22	43,43,43,43	0
58	MG	1A	3101	1/1	0.93	0.14	48,48,48,48	0
58	MG	2a	1687	1/1	0.93	0.11	38,38,38,38	0
58	MG	2a	1688	1/1	0.93	0.07	42,42,42,42	0
58	MG	2a	1691	1/1	0.93	0.24	49,49,49,49	0
58	MG	2a	1692	1/1	0.93	0.15	48,48,48,48	0
58	MG	2a	1695	1/1	0.93	0.09	56,56,56,56	0
58	MG	2A	3151	1/1	0.93	0.14	34,34,34,34	0
58	MG	2A	3152	1/1	0.93	0.14	49,49,49,49	0
58	MG	2a	1699	1/1	0.93	0.24	57,57,57,57	0
58	MG	1A	3479	1/1	0.93	0.12	47,47,47,47	0
58	MG	2A	3155	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3727	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3249	1/1	0.93	0.13	41,41,41,41	0
58	MG	2A	3165	1/1	0.93	0.12	40,40,40,40	0
58	MG	1A	3423	1/1	0.93	0.08	38,38,38,38	0
58	MG	2A	3167	1/1	0.93	0.12	44,44,44,44	0
58	MG	2A	3371	1/1	0.93	0.11	48,48,48,48	0
58	MG	2a	1714	1/1	0.93	0.17	58,58,58,58	0
58	MG	1Y	203	1/1	0.93	0.21	47,47,47,47	0
58	MG	2A	3717	1/1	0.93	0.17	57,57,57,57	0
58	MG	1A	3367	1/1	0.93	0.09	46,46,46,46	0
58	MG	2a	1719	1/1	0.93	0.11	62,62,62,62	0
58	MG	2a	1720	1/1	0.93	0.20	34,34,34,34	0
58	MG	1a	1743	1/1	0.93	0.10	51,51,51,51	0
58	MG	1a	1746	1/1	0.93	0.08	37,37,37,37	0
58	MG	1Z	3701	1/1	0.93	0.07	45,45,45,45	0
58	MG	2a	1728	1/1	0.93	0.21	52,52,52,52	0
58	MG	10	105	1/1	0.93	0.10	41,41,41,41	0
58	MG	2a	1731	1/1	0.93	0.26	48,48,48,48	0
58	MG	2A	3180	1/1	0.93	0.16	50,50,50,50	0
58	MG	1A	3873	1/1	0.93	0.10	25,25,25,25	0
58	MG	2A	3730	1/1	0.93	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1752	1/1	0.93	0.12	53,53,53,53	0
58	MG	2a	1740	1/1	0.93	0.15	51,51,51,51	0
58	MG	2A	3183	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	3328	1/1	0.93	0.09	29,29,29,29	0
58	MG	2A	3741	1/1	0.93	0.07	42,42,42,42	0
58	MG	2a	1746	1/1	0.93	0.30	50,50,50,50	0
58	MG	2A	3188	1/1	0.93	0.12	54,54,54,54	0
58	MG	1A	3490	1/1	0.93	0.09	44,44,44,44	0
58	MG	2A	3398	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3491	1/1	0.93	0.08	33,33,33,33	0
58	MG	1A	4049	1/1	0.93	0.08	25,25,25,25	0
58	MG	2a	1754	1/1	0.93	0.11	50,50,50,50	0
58	MG	2A	3194	1/1	0.93	0.19	55,55,55,55	0
58	MG	2a	1756	1/1	0.93	0.12	64,64,64,64	0
58	MG	2A	3753	1/1	0.93	0.10	47,47,47,47	0
58	MG	2a	1759	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3754	1/1	0.93	0.12	49,49,49,49	0
58	MG	1A	3747	1/1	0.93	0.05	12,12,12,12	0
58	MG	2a	1772	1/1	0.93	0.09	54,54,54,54	0
58	MG	2a	1777	1/1	0.93	0.08	59,59,59,59	0
58	MG	1a	1766	1/1	0.93	0.17	45,45,45,45	0
58	MG	1a	1768	1/1	0.93	0.10	54,54,54,54	0
58	MG	2A	3200	1/1	0.93	0.15	46,46,46,46	0
58	MG	1A	3369	1/1	0.93	0.08	42,42,42,42	0
58	MG	2A	3407	1/1	0.93	0.10	44,44,44,44	0
58	MG	1A	3751	1/1	0.93	0.12	31,31,31,31	0
58	MG	1A	3495	1/1	0.93	0.16	55,55,55,55	0
58	MG	2A	3413	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3770	1/1	0.93	0.08	41,41,41,41	0
58	MG	1a	1781	1/1	0.93	0.09	48,48,48,48	0
58	MG	1A	4061	1/1	0.93	0.12	34,34,34,34	0
58	MG	1a	1787	1/1	0.93	0.14	49,49,49,49	0
58	MG	1a	1788	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3891	1/1	0.93	0.08	28,28,28,28	0
58	MG	2A	3429	1/1	0.93	0.22	53,53,53,53	0
58	MG	1A	3077	1/1	0.93	0.19	30,30,30,30	0
58	MG	2A	3787	1/1	0.93	0.08	49,49,49,49	0
58	MG	2A	3211	1/1	0.93	0.09	44,44,44,44	0
58	MG	2A	3789	1/1	0.93	0.06	55,55,55,55	0
58	MG	1A	3607	1/1	0.93	0.09	39,39,39,39	0
58	MG	1A	3096	1/1	0.93	0.10	41,41,41,41	0
58	MG	1A	3380	1/1	0.93	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1807	1/1	0.93	0.15	38,38,38,38	0
58	MG	1A	3435	1/1	0.93	0.20	57,57,57,57	0
58	MG	1A	3786	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3801	1/1	0.93	0.09	38,38,38,38	0
58	MG	1A	3509	1/1	0.93	0.12	38,38,38,38	0
58	MG	2A	3803	1/1	0.93	0.14	45,45,45,45	0
58	MG	2A	3805	1/1	0.93	0.09	56,56,56,56	0
58	MG	1A	3252	1/1	0.93	0.08	37,37,37,37	0
58	MG	2A	3447	1/1	0.93	0.14	49,49,49,49	0
58	MG	1a	1817	1/1	0.93	0.10	47,47,47,47	0
58	MG	1A	3442	1/1	0.93	0.29	51,51,51,51	0
58	MG	2a	1837	1/1	0.93	0.17	42,42,42,42	0
58	MG	1e	201	1/1	0.93	0.10	54,54,54,54	0
58	MG	1A	3520	1/1	0.93	0.38	34,34,34,34	0
58	MG	1a	1619	1/1	0.93	0.10	36,36,36,36	0
58	MG	2A	3462	1/1	0.93	0.09	54,54,54,54	0
58	MG	1a	1622	1/1	0.93	0.09	41,41,41,41	0
58	MG	1A	3642	1/1	0.93	0.07	8,8,8,8	0
58	MG	1A	3445	1/1	0.93	0.13	39,39,39,39	0
58	MG	1A	3928	1/1	0.93	0.08	37,37,37,37	0
58	MG	2l	202	1/1	0.93	0.10	48,48,48,48	0
58	MG	2A	3239	1/1	0.93	0.08	41,41,41,41	0
58	MG	1A	3815	1/1	0.93	0.07	42,42,42,42	0
58	MG	2p	101	1/1	0.93	0.23	57,57,57,57	0
58	MG	2A	3839	1/1	0.93	0.07	47,47,47,47	0
58	MG	1w	103	1/1	0.93	0.27	50,50,50,50	0
58	MG	1w	106	1/1	0.93	0.12	44,44,44,44	0
58	MG	2A	3844	1/1	0.93	0.12	61,61,61,61	0
58	MG	1a	1634	1/1	0.93	0.18	53,53,53,53	0
58	MG	2A	3246	1/1	0.93	0.07	45,45,45,45	0
58	MG	1A	3931	1/1	0.93	0.08	36,36,36,36	0
58	MG	2A	3483	1/1	0.93	0.09	50,50,50,50	0
58	MG	1A	3382	1/1	0.93	0.07	40,40,40,40	0
58	MG	2A	3855	1/1	0.93	0.10	35,35,35,35	0
58	MG	1x	102	1/1	0.93	0.22	51,51,51,51	0
58	MG	2A	3863	1/1	0.93	0.08	36,36,36,36	0
58	MG	1A	3529	1/1	0.93	0.07	37,37,37,37	0
58	MG	1A	3651	1/1	0.93	0.09	41,41,41,41	0
58	MG	1a	1642	1/1	0.93	0.24	54,54,54,54	0
58	MG	1A	3449	1/1	0.93	0.15	34,34,34,34	0
58	MG	2A	3258	1/1	0.93	0.14	44,44,44,44	0
58	MG	2A	3494	1/1	0.93	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3260	1/1	0.93	0.11	47,47,47,47	0
58	MG	2A	3878	1/1	0.93	0.12	52,52,52,52	0
58	MG	1x	107	1/1	0.93	0.19	49,49,49,49	0
58	MG	2A	3502	1/1	0.93	0.15	37,37,37,37	0
58	MG	1A	3297	1/1	0.93	0.20	37,37,37,37	0
58	MG	2A	3508	1/1	0.93	0.09	39,39,39,39	0
58	MG	1x	109	1/1	0.93	0.08	43,43,43,43	0
60	ZN	24	501	1/1	0.93	0.10	113,113,113,113	0
58	MG	2B	214	1/1	0.94	0.09	43,43,43,43	0
58	MG	2A	3043	1/1	0.94	0.11	52,52,52,52	0
58	MG	2A	3279	1/1	0.94	0.20	56,56,56,56	0
58	MG	2A	3544	1/1	0.94	0.08	28,28,28,28	0
58	MG	1a	1661	1/1	0.94	0.12	46,46,46,46	0
58	MG	2E	302	1/1	0.94	0.12	47,47,47,47	0
58	MG	2A	3046	1/1	0.94	0.07	38,38,38,38	0
58	MG	1A	3722	1/1	0.94	0.08	35,35,35,35	0
58	MG	1A	4101	1/1	0.94	0.07	41,41,41,41	0
58	MG	2A	3050	1/1	0.94	0.25	53,53,53,53	0
58	MG	2A	3560	1/1	0.94	0.08	42,42,42,42	0
58	MG	2A	3561	1/1	0.94	0.06	24,24,24,24	0
58	MG	2F	303	1/1	0.94	0.10	59,59,59,59	0
58	MG	2F	304	1/1	0.94	0.23	48,48,48,48	0
58	MG	2F	305	1/1	0.94	0.11	40,40,40,40	0
58	MG	1A	4102	1/1	0.94	0.11	39,39,39,39	0
58	MG	2A	3052	1/1	0.94	0.07	44,44,44,44	0
58	MG	2A	3569	1/1	0.94	0.14	22,22,22,22	0
58	MG	2A	3571	1/1	0.94	0.06	28,28,28,28	0
58	MG	2O	201	1/1	0.94	0.19	43,43,43,43	0
58	MG	1A	3899	1/1	0.94	0.14	55,55,55,55	0
58	MG	1A	3443	1/1	0.94	0.14	52,52,52,52	0
58	MG	2A	3294	1/1	0.94	0.14	49,49,49,49	0
58	MG	1A	3444	1/1	0.94	0.24	55,55,55,55	0
58	MG	1A	3050	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3203	1/1	0.94	0.16	18,18,18,18	0
58	MG	2U	201	1/1	0.94	0.28	41,41,41,41	0
58	MG	1B	213	1/1	0.94	0.18	43,43,43,43	0
58	MG	1A	3209	1/1	0.94	0.12	33,33,33,33	0
58	MG	2A	3066	1/1	0.94	0.18	49,49,49,49	0
58	MG	1A	3909	1/1	0.94	0.28	15,15,15,15	0
58	MG	1A	3550	1/1	0.94	0.18	48,48,48,48	0
58	MG	1A	3452	1/1	0.94	0.10	32,32,32,32	0
58	MG	2A	3598	1/1	0.94	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3919	1/1	0.94	0.06	15,15,15,15	0
58	MG	1A	3088	1/1	0.94	0.21	29,29,29,29	0
58	MG	2A	3308	1/1	0.94	0.08	47,47,47,47	0
58	MG	1A	3280	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3741	1/1	0.94	0.09	40,40,40,40	0
58	MG	2a	1601	1/1	0.94	0.10	54,54,54,54	0
58	MG	1A	3925	1/1	0.94	0.10	39,39,39,39	0
58	MG	1a	1684	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3611	1/1	0.94	0.08	45,45,45,45	0
58	MG	2A	3615	1/1	0.94	0.10	24,24,24,24	0
58	MG	1A	3371	1/1	0.94	0.21	38,38,38,38	0
58	MG	2a	1608	1/1	0.94	0.18	47,47,47,47	0
58	MG	1A	3374	1/1	0.94	0.08	39,39,39,39	0
58	MG	2A	3089	1/1	0.94	0.10	44,44,44,44	0
58	MG	2A	3317	1/1	0.94	0.06	37,37,37,37	0
58	MG	1A	3748	1/1	0.94	0.11	39,39,39,39	0
58	MG	1A	3563	1/1	0.94	0.17	34,34,34,34	0
58	MG	1A	3377	1/1	0.94	0.13	43,43,43,43	0
58	MG	1A	3126	1/1	0.94	0.08	43,43,43,43	0
58	MG	1A	3462	1/1	0.94	0.09	53,53,53,53	0
58	MG	1A	3759	1/1	0.94	0.09	33,33,33,33	0
58	MG	1A	3946	1/1	0.94	0.08	17,17,17,17	0
58	MG	2A	3641	1/1	0.94	0.08	37,37,37,37	0
58	MG	2A	3104	1/1	0.94	0.07	39,39,39,39	0
58	MG	1A	3948	1/1	0.94	0.14	54,54,54,54	0
58	MG	2A	3329	1/1	0.94	0.23	46,46,46,46	0
58	MG	1a	1697	1/1	0.94	0.13	45,45,45,45	0
58	MG	2A	3108	1/1	0.94	0.24	40,40,40,40	0
58	MG	1A	3024	1/1	0.94	0.09	39,39,39,39	0
58	MG	1a	1701	1/1	0.94	0.15	44,44,44,44	0
58	MG	2A	3112	1/1	0.94	0.14	28,28,28,28	0
58	MG	1A	3580	1/1	0.94	0.25	32,32,32,32	0
58	MG	1A	3300	1/1	0.94	0.07	39,39,39,39	0
58	MG	1E	314	1/1	0.94	0.18	45,45,45,45	0
58	MG	2A	3339	1/1	0.94	0.08	52,52,52,52	0
58	MG	1F	307	1/1	0.94	0.09	19,19,19,19	0
58	MG	1A	3960	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	3302	1/1	0.94	0.10	36,36,36,36	0
58	MG	2a	1643	1/1	0.94	0.18	54,54,54,54	0
58	MG	2A	3668	1/1	0.94	0.05	37,37,37,37	0
58	MG	2A	3125	1/1	0.94	0.09	37,37,37,37	0
58	MG	1A	3784	1/1	0.94	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3230	1/1	0.94	0.15	51,51,51,51	0
58	MG	2A	3349	1/1	0.94	0.20	52,52,52,52	0
58	MG	2A	3131	1/1	0.94	0.10	39,39,39,39	0
58	MG	2A	3676	1/1	0.94	0.17	53,53,53,53	0
58	MG	2A	3677	1/1	0.94	0.14	26,26,26,26	0
58	MG	1A	3787	1/1	0.94	0.11	33,33,33,33	0
58	MG	1N	206	1/1	0.94	0.24	38,38,38,38	0
58	MG	1A	3234	1/1	0.94	0.12	34,34,34,34	0
58	MG	2a	1657	1/1	0.94	0.07	46,46,46,46	0
58	MG	1O	203	1/1	0.94	0.11	34,34,34,34	0
58	MG	1A	3972	1/1	0.94	0.09	42,42,42,42	0
58	MG	1A	3595	1/1	0.94	0.06	31,31,31,31	0
58	MG	1a	1728	1/1	0.94	0.09	49,49,49,49	0
58	MG	2A	3148	1/1	0.94	0.15	34,34,34,34	0
58	MG	2a	1668	1/1	0.94	0.10	48,48,48,48	0
58	MG	1P	201	1/1	0.94	0.35	30,30,30,30	0
58	MG	2A	3360	1/1	0.94	0.09	53,53,53,53	0
58	MG	1Q	207	1/1	0.94	0.09	30,30,30,30	0
58	MG	2A	3362	1/1	0.94	0.18	56,56,56,56	0
58	MG	1R	201	1/1	0.94	0.06	38,38,38,38	0
58	MG	1a	1737	1/1	0.94	0.15	53,53,53,53	0
58	MG	2A	3157	1/1	0.94	0.14	38,38,38,38	0
58	MG	2A	3158	1/1	0.94	0.13	32,32,32,32	0
58	MG	1A	3976	1/1	0.94	0.10	44,44,44,44	0
58	MG	2A	3162	1/1	0.94	0.28	56,56,56,56	0
58	MG	2a	1689	1/1	0.94	0.12	47,47,47,47	0
58	MG	2a	1690	1/1	0.94	0.19	33,33,33,33	0
58	MG	2A	3705	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3707	1/1	0.94	0.08	55,55,55,55	0
58	MG	1S	202	1/1	0.94	0.11	39,39,39,39	0
58	MG	1A	3977	1/1	0.94	0.12	55,55,55,55	0
58	MG	1A	3091	1/1	0.94	0.10	44,44,44,44	0
58	MG	2A	3380	1/1	0.94	0.07	51,51,51,51	0
58	MG	2A	3712	1/1	0.94	0.11	40,40,40,40	0
58	MG	2A	3382	1/1	0.94	0.27	42,42,42,42	0
58	MG	1A	3153	1/1	0.94	0.17	31,31,31,31	0
58	MG	1A	3601	1/1	0.94	0.14	36,36,36,36	0
58	MG	2A	3169	1/1	0.94	0.08	43,43,43,43	0
58	MG	1A	3391	1/1	0.94	0.06	39,39,39,39	0
58	MG	2A	3171	1/1	0.94	0.06	50,50,50,50	0
58	MG	1U	204	1/1	0.94	0.12	27,27,27,27	0
58	MG	1A	3395	1/1	0.94	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1753	1/1	0.94	0.09	59,59,59,59	0
58	MG	2a	1716	1/1	0.94	0.18	49,49,49,49	0
58	MG	2A	3177	1/1	0.94	0.12	52,52,52,52	0
58	MG	1a	1756	1/1	0.94	0.13	41,41,41,41	0
58	MG	1A	3247	1/1	0.94	0.17	38,38,38,38	0
58	MG	2A	3737	1/1	0.94	0.11	53,53,53,53	0
58	MG	2a	1721	1/1	0.94	0.15	43,43,43,43	0
58	MG	1V	206	1/1	0.94	0.10	39,39,39,39	0
58	MG	2a	1724	1/1	0.94	0.24	45,45,45,45	0
58	MG	1A	3398	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3400	1/1	0.94	0.23	50,50,50,50	0
58	MG	1A	3487	1/1	0.94	0.09	29,29,29,29	0
58	MG	1a	1763	1/1	0.94	0.07	49,49,49,49	0
58	MG	1A	3825	1/1	0.94	0.09	24,24,24,24	0
58	MG	1A	3248	1/1	0.94	0.10	35,35,35,35	0
58	MG	1A	3623	1/1	0.94	0.11	23,23,23,23	0
58	MG	2a	1736	1/1	0.94	0.27	47,47,47,47	0
58	MG	1A	3624	1/1	0.94	0.07	24,24,24,24	0
58	MG	2a	1738	1/1	0.94	0.10	59,59,59,59	0
58	MG	1A	3402	1/1	0.94	0.27	30,30,30,30	0
58	MG	2A	3756	1/1	0.94	0.06	40,40,40,40	0
58	MG	2A	3758	1/1	0.94	0.09	20,20,20,20	0
58	MG	1A	4005	1/1	0.94	0.22	22,22,22,22	0
58	MG	1A	3166	1/1	0.94	0.15	44,44,44,44	0
58	MG	1A	3640	1/1	0.94	0.09	30,30,30,30	0
58	MG	2A	3762	1/1	0.94	0.08	46,46,46,46	0
58	MG	2A	3419	1/1	0.94	0.15	28,28,28,28	0
58	MG	1A	3326	1/1	0.94	0.07	34,34,34,34	0
58	MG	1A	3492	1/1	0.94	0.30	38,38,38,38	0
58	MG	1A	3092	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3838	1/1	0.94	0.06	22,22,22,22	0
58	MG	1A	3005	1/1	0.94	0.07	36,36,36,36	0
58	MG	2A	3772	1/1	0.94	0.06	31,31,31,31	0
58	MG	1A	4026	1/1	0.94	0.12	43,43,43,43	0
58	MG	15	106	1/1	0.94	0.16	37,37,37,37	0
58	MG	15	108	1/1	0.94	0.13	34,34,34,34	0
58	MG	1A	3060	1/1	0.94	0.14	41,41,41,41	0
58	MG	2a	1771	1/1	0.94	0.07	57,57,57,57	0
58	MG	2A	3436	1/1	0.94	0.20	39,39,39,39	0
58	MG	2a	1776	1/1	0.94	0.17	43,43,43,43	0
58	MG	2A	3779	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	3502	1/1	0.94	0.21	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1812	1/1	0.94	0.14	42,42,42,42	0
58	MG	2a	1782	1/1	0.94	0.11	57,57,57,57	0
58	MG	2A	3440	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3332	1/1	0.94	0.07	41,41,41,41	0
58	MG	2a	1789	1/1	0.94	0.13	52,52,52,52	0
58	MG	2a	1790	1/1	0.94	0.22	54,54,54,54	0
58	MG	1A	3844	1/1	0.94	0.12	42,42,42,42	0
58	MG	2A	3443	1/1	0.94	0.15	42,42,42,42	0
58	MG	1A	3019	1/1	0.94	0.09	30,30,30,30	0
58	MG	1A	3847	1/1	0.94	0.06	50,50,50,50	0
58	MG	1f	202	1/1	0.94	0.13	44,44,44,44	0
58	MG	2A	3219	1/1	0.94	0.14	44,44,44,44	0
58	MG	1A	3419	1/1	0.94	0.07	42,42,42,42	0
58	MG	1a	1606	1/1	0.94	0.10	60,60,60,60	0
58	MG	2A	3453	1/1	0.94	0.21	40,40,40,40	0
58	MG	1A	3255	1/1	0.94	0.10	46,46,46,46	0
58	MG	2A	3804	1/1	0.94	0.10	43,43,43,43	0
58	MG	2a	1807	1/1	0.94	0.18	54,54,54,54	0
58	MG	1n	101	1/1	0.94	0.07	34,34,34,34	0
58	MG	2A	3456	1/1	0.94	0.22	49,49,49,49	0
58	MG	1A	3337	1/1	0.94	0.22	53,53,53,53	0
58	MG	2a	1811	1/1	0.94	0.13	48,48,48,48	0
58	MG	2a	1812	1/1	0.94	0.07	45,45,45,45	0
58	MG	2A	3463	1/1	0.94	0.14	57,57,57,57	0
58	MG	2A	3227	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3668	1/1	0.94	0.06	17,17,17,17	0
58	MG	2A	3467	1/1	0.94	0.12	49,49,49,49	0
58	MG	2A	3815	1/1	0.94	0.08	57,57,57,57	0
58	MG	1A	3858	1/1	0.94	0.09	13,13,13,13	0
58	MG	2A	3470	1/1	0.94	0.09	34,34,34,34	0
58	MG	2A	3820	1/1	0.94	0.09	32,32,32,32	0
58	MG	1A	3256	1/1	0.94	0.08	49,49,49,49	0
58	MG	2a	1826	1/1	0.94	0.11	55,55,55,55	0
58	MG	1A	3672	1/1	0.94	0.06	20,20,20,20	0
58	MG	1a	1618	1/1	0.94	0.08	43,43,43,43	0
58	MG	2A	3827	1/1	0.94	0.09	36,36,36,36	0
58	MG	2A	3832	1/1	0.94	0.07	56,56,56,56	0
58	MG	1A	3517	1/1	0.94	0.07	54,54,54,54	0
58	MG	1a	1621	1/1	0.94	0.11	45,45,45,45	0
58	MG	2a	1836	1/1	0.94	0.06	52,52,52,52	0
58	MG	1A	3863	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3027	1/1	0.94	0.09	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1840	1/1	0.94	0.12	69,69,69,69	0
58	MG	1a	1626	1/1	0.94	0.13	50,50,50,50	0
58	MG	1A	3176	1/1	0.94	0.11	28,28,28,28	0
58	MG	2A	3842	1/1	0.94	0.10	32,32,32,32	0
58	MG	1a	1628	1/1	0.94	0.14	50,50,50,50	0
58	MG	2f	202	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3845	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3524	1/1	0.94	0.07	47,47,47,47	0
58	MG	2A	3486	1/1	0.94	0.07	32,32,32,32	0
58	MG	1A	3526	1/1	0.94	0.26	54,54,54,54	0
58	MG	1A	3699	1/1	0.94	0.08	20,20,20,20	0
58	MG	1A	3263	1/1	0.94	0.08	29,29,29,29	0
58	MG	1A	3709	1/1	0.94	0.10	39,39,39,39	0
58	MG	1A	3875	1/1	0.94	0.04	27,27,27,27	0
58	MG	1A	4079	1/1	0.94	0.07	37,37,37,37	0
58	MG	1A	3004	1/1	0.94	0.11	18,18,18,18	0
58	MG	1A	3431	1/1	0.94	0.10	24,24,24,24	0
58	MG	1A	3189	1/1	0.94	0.09	24,24,24,24	0
58	MG	2A	3262	1/1	0.94	0.11	52,52,52,52	0
58	MG	2A	3505	1/1	0.94	0.06	40,40,40,40	0
58	MG	2A	3018	1/1	0.94	0.15	48,48,48,48	0
58	MG	1A	3049	1/1	0.94	0.06	8,8,8,8	0
58	MG	2A	3511	1/1	0.94	0.12	42,42,42,42	0
58	MG	1a	1650	1/1	0.94	0.12	45,45,45,45	0
58	MG	2w	108	1/1	0.94	0.07	53,53,53,53	0
58	MG	2A	3881	1/1	0.94	0.08	48,48,48,48	0
58	MG	2A	3028	1/1	0.94	0.18	45,45,45,45	0
58	MG	1A	3437	1/1	0.94	0.05	36,36,36,36	0
58	MG	2A	3522	1/1	0.94	0.07	49,49,49,49	0
58	MG	1A	3718	1/1	0.94	0.14	47,47,47,47	0
58	MG	1A	3106	1/1	0.94	0.29	40,40,40,40	0
58	MG	2A	3035	1/1	0.94	0.12	23,23,23,23	0
58	MG	2B	205	1/1	0.94	0.14	51,51,51,51	0
58	MG	2x	106	1/1	0.94	0.14	43,43,43,43	0
58	MG	1A	3109	1/1	0.94	0.17	37,37,37,37	0
58	MG	1a	1659	1/1	0.94	0.21	47,47,47,47	0
58	MG	2B	208	1/1	0.94	0.24	50,50,50,50	0
58	MG	2A	3536	1/1	0.94	0.15	48,48,48,48	0
58	MG	2A	3537	1/1	0.94	0.09	50,50,50,50	0
58	MG	1a	1660	1/1	0.94	0.15	53,53,53,53	0
58	MG	2A	3539	1/1	0.94	0.12	41,41,41,41	0
58	MG	2A	3220	1/1	0.95	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3874	1/1	0.95	0.17	45,45,45,45	0
58	MG	2A	3876	1/1	0.95	0.13	36,36,36,36	0
58	MG	1X	101	1/1	0.95	0.12	28,28,28,28	0
58	MG	1A	3991	1/1	0.95	0.05	23,23,23,23	0
58	MG	1A	3993	1/1	0.95	0.05	11,11,11,11	0
58	MG	2A	3880	1/1	0.95	0.08	53,53,53,53	0
58	MG	2A	3489	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3819	1/1	0.95	0.06	46,46,46,46	0
58	MG	1A	3820	1/1	0.95	0.32	26,26,26,26	0
58	MG	1A	3340	1/1	0.95	0.15	41,41,41,41	0
58	MG	10	102	1/1	0.95	0.13	39,39,39,39	0
58	MG	2A	3229	1/1	0.95	0.07	47,47,47,47	0
58	MG	2A	3499	1/1	0.95	0.21	44,44,44,44	0
58	MG	1a	1813	1/1	0.95	0.09	52,52,52,52	0
58	MG	2A	3231	1/1	0.95	0.14	46,46,46,46	0
58	MG	2A	3503	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3116	1/1	0.95	0.05	30,30,30,30	0
58	MG	1a	1815	1/1	0.95	0.09	44,44,44,44	0
58	MG	1a	1816	1/1	0.95	0.09	43,43,43,43	0
58	MG	1A	3622	1/1	0.95	0.11	38,38,38,38	0
58	MG	1a	1818	1/1	0.95	0.12	42,42,42,42	0
58	MG	2A	3512	1/1	0.95	0.07	50,50,50,50	0
58	MG	2B	217	1/1	0.95	0.07	47,47,47,47	0
58	MG	2B	218	1/1	0.95	0.11	53,53,53,53	0
58	MG	2A	3515	1/1	0.95	0.09	12,12,12,12	0
58	MG	2D	301	1/1	0.95	0.10	35,35,35,35	0
58	MG	2D	303	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3826	1/1	0.95	0.05	24,24,24,24	0
58	MG	1A	3343	1/1	0.95	0.17	42,42,42,42	0
58	MG	2A	3242	1/1	0.95	0.28	32,32,32,32	0
58	MG	1e	202	1/1	0.95	0.18	55,55,55,55	0
58	MG	1A	3222	1/1	0.95	0.08	31,31,31,31	0
58	MG	1A	3348	1/1	0.95	0.11	43,43,43,43	0
58	MG	2A	3249	1/1	0.95	0.09	54,54,54,54	0
58	MG	2A	3529	1/1	0.95	0.07	28,28,28,28	0
58	MG	1A	3227	1/1	0.95	0.11	31,31,31,31	0
58	MG	1A	4012	1/1	0.95	0.05	23,23,23,23	0
58	MG	2F	302	1/1	0.95	0.13	45,45,45,45	0
58	MG	1m	3001	1/1	0.95	0.07	38,38,38,38	0
58	MG	15	102	1/1	0.95	0.12	23,23,23,23	0
58	MG	1A	4017	1/1	0.95	0.06	29,29,29,29	0
58	MG	1A	4018	1/1	0.95	0.04	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3499	1/1	0.95	0.08	38,38,38,38	0
58	MG	1A	4022	1/1	0.95	0.05	40,40,40,40	0
58	MG	2A	3543	1/1	0.95	0.08	43,43,43,43	0
58	MG	1A	3422	1/1	0.95	0.06	35,35,35,35	0
58	MG	2Q	201	1/1	0.95	0.17	48,48,48,48	0
58	MG	1A	3084	1/1	0.95	0.12	22,22,22,22	0
58	MG	2A	3550	1/1	0.95	0.07	34,34,34,34	0
58	MG	18	101	1/1	0.95	0.36	49,49,49,49	0
58	MG	2R	202	1/1	0.95	0.17	38,38,38,38	0
58	MG	2A	3264	1/1	0.95	0.25	49,49,49,49	0
58	MG	1A	3273	1/1	0.95	0.24	41,41,41,41	0
58	MG	2T	201	1/1	0.95	0.10	52,52,52,52	0
58	MG	1a	1601	1/1	0.95	0.27	48,48,48,48	0
58	MG	1A	3507	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3121	1/1	0.95	0.14	35,35,35,35	0
58	MG	1A	3174	1/1	0.95	0.16	41,41,41,41	0
58	MG	1A	3122	1/1	0.95	0.11	28,28,28,28	0
58	MG	1A	3657	1/1	0.95	0.06	28,28,28,28	0
58	MG	1A	3512	1/1	0.95	0.08	46,46,46,46	0
58	MG	2X	101	1/1	0.95	0.08	51,51,51,51	0
58	MG	1a	1609	1/1	0.95	0.22	56,56,56,56	0
58	MG	1A	3360	1/1	0.95	0.10	32,32,32,32	0
58	MG	23	101	1/1	0.95	0.17	47,47,47,47	0
58	MG	25	102	1/1	0.95	0.07	38,38,38,38	0
58	MG	25	103	1/1	0.95	0.05	34,34,34,34	0
58	MG	1x	111	1/1	0.95	0.09	39,39,39,39	0
58	MG	2A	3580	1/1	0.95	0.11	36,36,36,36	0
58	MG	27	102	1/1	0.95	0.15	41,41,41,41	0
58	MG	27	103	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3660	1/1	0.95	0.05	20,20,20,20	0
58	MG	28	103	1/1	0.95	0.06	39,39,39,39	0
58	MG	2A	3001	1/1	0.95	0.16	37,37,37,37	0
58	MG	2A	3003	1/1	0.95	0.14	44,44,44,44	0
58	MG	1A	3664	1/1	0.95	0.04	12,12,12,12	0
58	MG	1a	1616	1/1	0.95	0.15	41,41,41,41	0
58	MG	2a	1603	1/1	0.95	0.07	56,56,56,56	0
58	MG	2A	3284	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3430	1/1	0.95	0.12	32,32,32,32	0
58	MG	2A	3287	1/1	0.95	0.05	55,55,55,55	0
58	MG	1A	4044	1/1	0.95	0.05	24,24,24,24	0
58	MG	2A	3016	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3361	1/1	0.95	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3292	1/1	0.95	0.13	33,33,33,33	0
58	MG	2a	1611	1/1	0.95	0.16	55,55,55,55	0
58	MG	2A	3603	1/1	0.95	0.10	49,49,49,49	0
58	MG	2A	3020	1/1	0.95	0.24	47,47,47,47	0
58	MG	2A	3605	1/1	0.95	0.15	47,47,47,47	0
58	MG	2A	3606	1/1	0.95	0.07	42,42,42,42	0
58	MG	2A	3022	1/1	0.95	0.11	37,37,37,37	0
58	MG	1A	4048	1/1	0.95	0.07	25,25,25,25	0
58	MG	2a	1618	1/1	0.95	0.20	58,58,58,58	0
58	MG	2a	1619	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3853	1/1	0.95	0.19	39,39,39,39	0
58	MG	1A	4050	1/1	0.95	0.06	14,14,14,14	0
58	MG	2a	1623	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3293	1/1	0.95	0.09	38,38,38,38	0
58	MG	2A	3612	1/1	0.95	0.07	51,51,51,51	0
58	MG	2A	3613	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3857	1/1	0.95	0.06	42,42,42,42	0
58	MG	1A	3047	1/1	0.95	0.05	27,27,27,27	0
58	MG	2A	3619	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3620	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3676	1/1	0.95	0.06	11,11,11,11	0
58	MG	1A	4059	1/1	0.95	0.11	55,55,55,55	0
58	MG	2a	1634	1/1	0.95	0.18	37,37,37,37	0
58	MG	1A	3681	1/1	0.95	0.13	37,37,37,37	0
58	MG	2A	3305	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3041	1/1	0.95	0.25	43,43,43,43	0
58	MG	1A	3237	1/1	0.95	0.31	39,39,39,39	0
58	MG	1A	3440	1/1	0.95	0.18	32,32,32,32	0
58	MG	1A	4064	1/1	0.95	0.06	44,44,44,44	0
58	MG	2A	3633	1/1	0.95	0.06	35,35,35,35	0
58	MG	2A	3634	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3441	1/1	0.95	0.16	31,31,31,31	0
58	MG	1A	3238	1/1	0.95	0.10	47,47,47,47	0
58	MG	1A	4072	1/1	0.95	0.06	29,29,29,29	0
58	MG	1A	3694	1/1	0.95	0.06	22,22,22,22	0
58	MG	1a	1649	1/1	0.95	0.10	47,47,47,47	0
58	MG	2A	3315	1/1	0.95	0.09	59,59,59,59	0
58	MG	1A	3181	1/1	0.95	0.11	16,16,16,16	0
58	MG	2A	3053	1/1	0.95	0.12	49,49,49,49	0
58	MG	2a	1652	1/1	0.95	0.06	57,57,57,57	0
58	MG	1A	4077	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3650	1/1	0.95	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3654	1/1	0.95	0.16	49,49,49,49	0
58	MG	2a	1656	1/1	0.95	0.07	64,64,64,64	0
58	MG	1A	3534	1/1	0.95	0.23	31,31,31,31	0
58	MG	1A	4082	1/1	0.95	0.08	36,36,36,36	0
58	MG	2A	3321	1/1	0.95	0.06	45,45,45,45	0
58	MG	2A	3060	1/1	0.95	0.17	44,44,44,44	0
58	MG	2a	1663	1/1	0.95	0.08	55,55,55,55	0
58	MG	2A	3323	1/1	0.95	0.06	35,35,35,35	0
58	MG	1A	3370	1/1	0.95	0.17	39,39,39,39	0
58	MG	2a	1667	1/1	0.95	0.15	28,28,28,28	0
58	MG	1A	3536	1/1	0.95	0.15	25,25,25,25	0
58	MG	1A	3874	1/1	0.95	0.14	23,23,23,23	0
58	MG	1A	3710	1/1	0.95	0.09	28,28,28,28	0
58	MG	2a	1672	1/1	0.95	0.15	45,45,45,45	0
58	MG	2A	3665	1/1	0.95	0.09	44,44,44,44	0
58	MG	2A	3666	1/1	0.95	0.10	47,47,47,47	0
58	MG	1A	3184	1/1	0.95	0.14	37,37,37,37	0
58	MG	1A	3712	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3539	1/1	0.95	0.17	41,41,41,41	0
58	MG	2a	1685	1/1	0.95	0.08	47,47,47,47	0
58	MG	1A	4097	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	4098	1/1	0.95	0.13	44,44,44,44	0
58	MG	2A	3072	1/1	0.95	0.05	42,42,42,42	0
58	MG	1a	1668	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3883	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3447	1/1	0.95	0.14	43,43,43,43	0
58	MG	2A	3680	1/1	0.95	0.13	50,50,50,50	0
58	MG	2a	1693	1/1	0.95	0.14	37,37,37,37	0
58	MG	1A	3131	1/1	0.95	0.11	52,52,52,52	0
58	MG	1A	3308	1/1	0.95	0.15	36,36,36,36	0
58	MG	2a	1697	1/1	0.95	0.18	30,30,30,30	0
58	MG	1A	3311	1/1	0.95	0.12	48,48,48,48	0
58	MG	2A	3084	1/1	0.95	0.09	42,42,42,42	0
58	MG	2A	3086	1/1	0.95	0.11	40,40,40,40	0
58	MG	1A	4104	1/1	0.95	0.27	44,44,44,44	0
58	MG	1A	3547	1/1	0.95	0.14	34,34,34,34	0
58	MG	2A	3346	1/1	0.95	0.08	54,54,54,54	0
58	MG	1B	204	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3187	1/1	0.95	0.11	49,49,49,49	0
58	MG	2A	3695	1/1	0.95	0.08	51,51,51,51	0
58	MG	2a	1710	1/1	0.95	0.05	38,38,38,38	0
58	MG	2a	1712	1/1	0.95	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3095	1/1	0.95	0.08	31,31,31,31	0
58	MG	2A	3698	1/1	0.95	0.06	48,48,48,48	0
58	MG	1A	3896	1/1	0.95	0.07	16,16,16,16	0
58	MG	1A	3897	1/1	0.95	0.05	12,12,12,12	0
58	MG	1a	1681	1/1	0.95	0.09	55,55,55,55	0
58	MG	1A	3188	1/1	0.95	0.05	28,28,28,28	0
58	MG	1A	3137	1/1	0.95	0.14	26,26,26,26	0
58	MG	1A	3456	1/1	0.95	0.06	40,40,40,40	0
58	MG	1A	3315	1/1	0.95	0.10	32,32,32,32	0
58	MG	1A	3553	1/1	0.95	0.10	38,38,38,38	0
58	MG	2A	3107	1/1	0.95	0.04	35,35,35,35	0
58	MG	1A	3384	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3138	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3461	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3560	1/1	0.95	0.10	41,41,41,41	0
58	MG	2A	3716	1/1	0.95	0.07	34,34,34,34	0
58	MG	2a	1732	1/1	0.95	0.10	42,42,42,42	0
58	MG	1a	1691	1/1	0.95	0.18	33,33,33,33	0
58	MG	1A	3319	1/1	0.95	0.06	28,28,28,28	0
58	MG	1A	3015	1/1	0.95	0.08	23,23,23,23	0
58	MG	1a	1694	1/1	0.95	0.17	30,30,30,30	0
58	MG	2A	3370	1/1	0.95	0.08	57,57,57,57	0
58	MG	2A	3119	1/1	0.95	0.17	53,53,53,53	0
58	MG	1A	3466	1/1	0.95	0.06	43,43,43,43	0
58	MG	1A	3923	1/1	0.95	0.06	17,17,17,17	0
58	MG	2a	1742	1/1	0.95	0.16	53,53,53,53	0
58	MG	2A	3374	1/1	0.95	0.22	67,67,67,67	0
58	MG	1A	3389	1/1	0.95	0.06	32,32,32,32	0
58	MG	2A	3376	1/1	0.95	0.10	38,38,38,38	0
58	MG	2A	3735	1/1	0.95	0.09	49,49,49,49	0
58	MG	2A	3378	1/1	0.95	0.19	48,48,48,48	0
58	MG	1A	3570	1/1	0.95	0.07	30,30,30,30	0
58	MG	1a	1700	1/1	0.95	0.11	48,48,48,48	0
58	MG	1A	3322	1/1	0.95	0.23	25,25,25,25	0
58	MG	2A	3743	1/1	0.95	0.09	47,47,47,47	0
58	MG	2A	3132	1/1	0.95	0.08	42,42,42,42	0
58	MG	1D	309	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3386	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3748	1/1	0.95	0.06	47,47,47,47	0
58	MG	2a	1761	1/1	0.95	0.08	71,71,71,71	0
58	MG	2A	3749	1/1	0.95	0.24	41,41,41,41	0
58	MG	2a	1763	1/1	0.95	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3387	1/1	0.95	0.08	58,58,58,58	0
58	MG	2A	3134	1/1	0.95	0.10	45,45,45,45	0
58	MG	2A	3135	1/1	0.95	0.18	37,37,37,37	0
58	MG	2a	1773	1/1	0.95	0.06	66,66,66,66	0
58	MG	1a	1703	1/1	0.95	0.11	36,36,36,36	0
58	MG	2A	3392	1/1	0.95	0.15	39,39,39,39	0
58	MG	2A	3140	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3757	1/1	0.95	0.08	43,43,43,43	0
58	MG	2a	1781	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3575	1/1	0.95	0.19	34,34,34,34	0
58	MG	2a	1784	1/1	0.95	0.07	59,59,59,59	0
58	MG	1D	312	1/1	0.95	0.14	23,23,23,23	0
58	MG	2a	1787	1/1	0.95	0.16	37,37,37,37	0
58	MG	1A	3393	1/1	0.95	0.16	15,15,15,15	0
58	MG	1A	3753	1/1	0.95	0.07	44,44,44,44	0
58	MG	1a	1708	1/1	0.95	0.11	45,45,45,45	0
58	MG	1A	3755	1/1	0.95	0.09	28,28,28,28	0
58	MG	1A	3061	1/1	0.95	0.10	25,25,25,25	0
58	MG	1a	1712	1/1	0.95	0.24	45,45,45,45	0
58	MG	1A	3257	1/1	0.95	0.21	36,36,36,36	0
58	MG	1A	3944	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3201	1/1	0.95	0.14	30,30,30,30	0
58	MG	1A	3762	1/1	0.95	0.09	37,37,37,37	0
58	MG	2a	1801	1/1	0.95	0.14	53,53,53,53	0
58	MG	1A	3592	1/1	0.95	0.23	37,37,37,37	0
58	MG	2A	3408	1/1	0.95	0.22	38,38,38,38	0
58	MG	1a	1721	1/1	0.95	0.13	48,48,48,48	0
58	MG	2A	3410	1/1	0.95	0.06	42,42,42,42	0
58	MG	1F	311	1/1	0.95	0.16	20,20,20,20	0
58	MG	1A	3765	1/1	0.95	0.06	19,19,19,19	0
58	MG	1F	313	1/1	0.95	0.13	42,42,42,42	0
58	MG	2A	3417	1/1	0.95	0.17	40,40,40,40	0
58	MG	2A	3785	1/1	0.95	0.13	50,50,50,50	0
58	MG	1A	3770	1/1	0.95	0.06	29,29,29,29	0
58	MG	1A	3956	1/1	0.95	0.07	30,30,30,30	0
58	MG	1G	205	1/1	0.95	0.09	44,44,44,44	0
58	MG	1a	1735	1/1	0.95	0.05	38,38,38,38	0
58	MG	1N	201	1/1	0.95	0.10	44,44,44,44	0
58	MG	2A	3793	1/1	0.95	0.11	58,58,58,58	0
58	MG	1A	3399	1/1	0.95	0.08	52,52,52,52	0
58	MG	2A	3430	1/1	0.95	0.12	40,40,40,40	0
58	MG	2A	3798	1/1	0.95	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3173	1/1	0.95	0.07	41,41,41,41	0
58	MG	1a	1739	1/1	0.95	0.05	22,22,22,22	0
58	MG	1A	3959	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	3329	1/1	0.95	0.11	35,35,35,35	0
58	MG	2A	3435	1/1	0.95	0.27	55,55,55,55	0
58	MG	1A	3776	1/1	0.95	0.05	14,14,14,14	0
58	MG	2a	1831	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3962	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	3151	1/1	0.95	0.31	32,32,32,32	0
58	MG	2A	3439	1/1	0.95	0.18	52,52,52,52	0
58	MG	1a	1748	1/1	0.95	0.17	38,38,38,38	0
58	MG	1A	3076	1/1	0.95	0.06	25,25,25,25	0
58	MG	2A	3184	1/1	0.95	0.09	39,39,39,39	0
58	MG	1Q	205	1/1	0.95	0.09	40,40,40,40	0
58	MG	2A	3814	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3481	1/1	0.95	0.14	32,32,32,32	0
58	MG	1A	3602	1/1	0.95	0.12	48,48,48,48	0
58	MG	2A	3446	1/1	0.95	0.06	33,33,33,33	0
58	MG	1R	202	1/1	0.95	0.11	36,36,36,36	0
58	MG	1A	3052	1/1	0.95	0.16	21,21,21,21	0
58	MG	1A	3796	1/1	0.95	0.08	36,36,36,36	0
58	MG	1A	3484	1/1	0.95	0.08	36,36,36,36	0
58	MG	1A	3606	1/1	0.95	0.05	23,23,23,23	0
58	MG	1A	3978	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3406	1/1	0.95	0.07	40,40,40,40	0
58	MG	2q	202	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3807	1/1	0.95	0.06	10,10,10,10	0
58	MG	2A	3457	1/1	0.95	0.21	50,50,50,50	0
58	MG	2A	3458	1/1	0.95	0.18	50,50,50,50	0
58	MG	2A	3461	1/1	0.95	0.21	32,32,32,32	0
58	MG	2v	103	1/1	0.95	0.13	41,41,41,41	0
58	MG	1U	203	1/1	0.95	0.12	21,21,21,21	0
58	MG	1A	3610	1/1	0.95	0.06	23,23,23,23	0
58	MG	1U	207	1/1	0.95	0.34	27,27,27,27	0
58	MG	2A	3205	1/1	0.95	0.09	53,53,53,53	0
58	MG	1a	1774	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3847	1/1	0.95	0.07	51,51,51,51	0
58	MG	1a	1778	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	3982	1/1	0.95	0.05	45,45,45,45	0
58	MG	1A	3812	1/1	0.95	0.09	35,35,35,35	0
58	MG	1A	3813	1/1	0.95	0.05	34,34,34,34	0
58	MG	2A	3854	1/1	0.95	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3210	1/1	0.95	0.07	29,29,29,29	0
58	MG	2A	3857	1/1	0.95	0.07	30,30,30,30	0
58	MG	2A	3859	1/1	0.95	0.04	46,46,46,46	0
58	MG	1A	3083	1/1	0.95	0.13	34,34,34,34	0
58	MG	2A	3861	1/1	0.95	0.14	60,60,60,60	0
58	MG	2A	3862	1/1	0.95	0.12	47,47,47,47	0
58	MG	1W	205	1/1	0.95	0.08	35,35,35,35	0
58	MG	2A	3866	1/1	0.95	0.12	43,43,43,43	0
58	MG	1a	1793	1/1	0.95	0.11	55,55,55,55	0
58	MG	1W	207	1/1	0.95	0.14	14,14,14,14	0
58	MG	1A	3613	1/1	0.95	0.09	41,41,41,41	0
58	MG	1a	1799	1/1	0.95	0.07	62,62,62,62	0
58	MG	1a	1801	1/1	0.95	0.09	62,62,62,62	0
58	MG	2A	3583	1/1	0.96	0.07	20,20,20,20	0
58	MG	1A	3079	1/1	0.96	0.05	18,18,18,18	0
58	MG	1a	1646	1/1	0.96	0.10	60,60,60,60	0
58	MG	2A	3587	1/1	0.96	0.14	40,40,40,40	0
58	MG	2A	3588	1/1	0.96	0.12	49,49,49,49	0
58	MG	2A	3040	1/1	0.96	0.07	42,42,42,42	0
58	MG	1A	4088	1/1	0.96	0.10	34,34,34,34	0
58	MG	1A	4089	1/1	0.96	0.07	33,33,33,33	0
58	MG	1A	3469	1/1	0.96	0.15	27,27,27,27	0
58	MG	1A	4091	1/1	0.96	0.06	30,30,30,30	0
58	MG	1A	4092	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3320	1/1	0.96	0.07	42,42,42,42	0
58	MG	1A	3081	1/1	0.96	0.09	23,23,23,23	0
58	MG	2A	3602	1/1	0.96	0.07	26,26,26,26	0
58	MG	1A	3893	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	3733	1/1	0.96	0.06	16,16,16,16	0
58	MG	1A	3139	1/1	0.96	0.15	22,22,22,22	0
58	MG	1A	3011	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3142	1/1	0.96	0.19	38,38,38,38	0
58	MG	2A	3055	1/1	0.96	0.05	38,38,38,38	0
58	MG	2T	203	1/1	0.96	0.14	46,46,46,46	0
58	MG	2A	3056	1/1	0.96	0.10	60,60,60,60	0
58	MG	1A	3738	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3200	1/1	0.96	0.07	25,25,25,25	0
58	MG	1A	3006	1/1	0.96	0.06	31,31,31,31	0
58	MG	1a	1667	1/1	0.96	0.11	38,38,38,38	0
58	MG	2A	3614	1/1	0.96	0.06	18,18,18,18	0
58	MG	2A	3062	1/1	0.96	0.20	52,52,52,52	0
58	MG	1A	3905	1/1	0.96	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3262	1/1	0.96	0.05	33,33,33,33	0
58	MG	1A	3745	1/1	0.96	0.12	24,24,24,24	0
58	MG	25	101	1/1	0.96	0.12	37,37,37,37	0
58	MG	1A	3404	1/1	0.96	0.15	25,25,25,25	0
58	MG	1a	1672	1/1	0.96	0.10	37,37,37,37	0
58	MG	1A	3590	1/1	0.96	0.08	41,41,41,41	0
58	MG	1A	3749	1/1	0.96	0.07	47,47,47,47	0
58	MG	27	101	1/1	0.96	0.13	28,28,28,28	0
58	MG	1A	3147	1/1	0.96	0.12	37,37,37,37	0
58	MG	1A	3593	1/1	0.96	0.24	27,27,27,27	0
58	MG	1A	3482	1/1	0.96	0.08	40,40,40,40	0
58	MG	1A	3264	1/1	0.96	0.10	36,36,36,36	0
58	MG	1A	3597	1/1	0.96	0.11	38,38,38,38	0
58	MG	1A	3016	1/1	0.96	0.07	34,34,34,34	0
58	MG	1A	3926	1/1	0.96	0.09	36,36,36,36	0
58	MG	2A	3080	1/1	0.96	0.09	41,41,41,41	0
58	MG	2A	3081	1/1	0.96	0.14	35,35,35,35	0
58	MG	1A	3758	1/1	0.96	0.09	51,51,51,51	0
58	MG	1A	3336	1/1	0.96	0.17	38,38,38,38	0
58	MG	2A	3085	1/1	0.96	0.16	40,40,40,40	0
58	MG	1A	3206	1/1	0.96	0.09	42,42,42,42	0
58	MG	2A	3087	1/1	0.96	0.05	36,36,36,36	0
58	MG	1A	3930	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3411	1/1	0.96	0.11	49,49,49,49	0
58	MG	2A	3651	1/1	0.96	0.22	37,37,37,37	0
58	MG	2A	3652	1/1	0.96	0.07	32,32,32,32	0
58	MG	2A	3653	1/1	0.96	0.10	44,44,44,44	0
58	MG	1A	3338	1/1	0.96	0.19	42,42,42,42	0
58	MG	1B	231	1/1	0.96	0.08	57,57,57,57	0
58	MG	2A	3345	1/1	0.96	0.05	35,35,35,35	0
58	MG	2A	3092	1/1	0.96	0.30	36,36,36,36	0
58	MG	1A	3207	1/1	0.96	0.07	13,13,13,13	0
58	MG	1A	3934	1/1	0.96	0.04	5,5,5,5	0
58	MG	1A	3935	1/1	0.96	0.05	21,21,21,21	0
58	MG	2A	3099	1/1	0.96	0.16	44,44,44,44	0
58	MG	1A	3940	1/1	0.96	0.07	41,41,41,41	0
58	MG	1D	307	1/1	0.96	0.08	23,23,23,23	0
58	MG	1A	3766	1/1	0.96	0.05	22,22,22,22	0
58	MG	1A	3767	1/1	0.96	0.06	25,25,25,25	0
58	MG	2a	1627	1/1	0.96	0.20	54,54,54,54	0
58	MG	1A	3768	1/1	0.96	0.07	18,18,18,18	0
58	MG	1A	3108	1/1	0.96	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3947	1/1	0.96	0.11	37,37,37,37	0
58	MG	1E	308	1/1	0.96	0.09	43,43,43,43	0
58	MG	2A	3109	1/1	0.96	0.10	32,32,32,32	0
58	MG	1A	3159	1/1	0.96	0.33	31,31,31,31	0
58	MG	1A	3161	1/1	0.96	0.04	43,43,43,43	0
58	MG	1A	3952	1/1	0.96	0.05	53,53,53,53	0
58	MG	1A	3775	1/1	0.96	0.06	23,23,23,23	0
58	MG	1A	3347	1/1	0.96	0.12	26,26,26,26	0
58	MG	2a	1638	1/1	0.96	0.13	53,53,53,53	0
58	MG	1A	3782	1/1	0.96	0.07	22,22,22,22	0
58	MG	2A	3367	1/1	0.96	0.15	41,41,41,41	0
58	MG	1A	3498	1/1	0.96	0.11	37,37,37,37	0
58	MG	2A	3685	1/1	0.96	0.10	36,36,36,36	0
58	MG	1A	3162	1/1	0.96	0.16	20,20,20,20	0
58	MG	1A	3500	1/1	0.96	0.08	31,31,31,31	0
58	MG	1A	3791	1/1	0.96	0.05	35,35,35,35	0
58	MG	1G	201	1/1	0.96	0.10	30,30,30,30	0
58	MG	1G	202	1/1	0.96	0.15	43,43,43,43	0
58	MG	1A	3963	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3616	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3618	1/1	0.96	0.05	26,26,26,26	0
58	MG	2A	3379	1/1	0.96	0.06	38,38,38,38	0
58	MG	1I	201	1/1	0.96	0.05	48,48,48,48	0
58	MG	1A	3214	1/1	0.96	0.14	34,34,34,34	0
58	MG	1N	202	1/1	0.96	0.12	31,31,31,31	0
58	MG	1a	1725	1/1	0.96	0.11	54,54,54,54	0
58	MG	1A	3800	1/1	0.96	0.06	11,11,11,11	0
58	MG	2A	3142	1/1	0.96	0.12	40,40,40,40	0
58	MG	1A	3802	1/1	0.96	0.11	30,30,30,30	0
58	MG	1N	207	1/1	0.96	0.09	40,40,40,40	0
58	MG	2A	3706	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3389	1/1	0.96	0.07	36,36,36,36	0
58	MG	1a	1732	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3503	1/1	0.96	0.05	38,38,38,38	0
58	MG	1O	202	1/1	0.96	0.10	42,42,42,42	0
58	MG	1A	3974	1/1	0.96	0.10	36,36,36,36	0
58	MG	1A	3975	1/1	0.96	0.05	41,41,41,41	0
58	MG	2A	3715	1/1	0.96	0.07	20,20,20,20	0
58	MG	1A	3504	1/1	0.96	0.14	31,31,31,31	0
58	MG	2A	3396	1/1	0.96	0.16	50,50,50,50	0
58	MG	1A	3350	1/1	0.96	0.13	33,33,33,33	0
58	MG	1P	203	1/1	0.96	0.28	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1681	1/1	0.96	0.06	41,41,41,41	0
58	MG	1Q	204	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3806	1/1	0.96	0.04	13,13,13,13	0
58	MG	2A	3159	1/1	0.96	0.12	42,42,42,42	0
58	MG	1a	1744	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3626	1/1	0.96	0.04	29,29,29,29	0
58	MG	1A	3221	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3630	1/1	0.96	0.07	39,39,39,39	0
58	MG	1A	3636	1/1	0.96	0.11	44,44,44,44	0
58	MG	1A	3427	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3355	1/1	0.96	0.18	29,29,29,29	0
58	MG	1A	3165	1/1	0.96	0.25	26,26,26,26	0
58	MG	2a	1694	1/1	0.96	0.25	35,35,35,35	0
58	MG	1a	1755	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3818	1/1	0.96	0.08	22,22,22,22	0
58	MG	1A	3067	1/1	0.96	0.09	30,30,30,30	0
58	MG	1A	3281	1/1	0.96	0.08	25,25,25,25	0
58	MG	1A	3432	1/1	0.96	0.07	32,32,32,32	0
58	MG	2A	3418	1/1	0.96	0.16	34,34,34,34	0
58	MG	1A	3647	1/1	0.96	0.06	24,24,24,24	0
58	MG	1U	205	1/1	0.96	0.20	27,27,27,27	0
58	MG	1A	3283	1/1	0.96	0.13	22,22,22,22	0
58	MG	2A	3423	1/1	0.96	0.20	52,52,52,52	0
58	MG	1A	3289	1/1	0.96	0.09	37,37,37,37	0
58	MG	1a	1767	1/1	0.96	0.14	60,60,60,60	0
58	MG	2a	1709	1/1	0.96	0.07	50,50,50,50	0
58	MG	2A	3428	1/1	0.96	0.15	41,41,41,41	0
58	MG	2a	1711	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3521	1/1	0.96	0.15	27,27,27,27	0
58	MG	1V	203	1/1	0.96	0.18	24,24,24,24	0
58	MG	1A	3999	1/1	0.96	0.07	35,35,35,35	0
58	MG	1A	3655	1/1	0.96	0.06	22,22,22,22	0
58	MG	1A	4002	1/1	0.96	0.08	48,48,48,48	0
58	MG	1A	3436	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	4004	1/1	0.96	0.05	9,9,9,9	0
58	MG	1A	3290	1/1	0.96	0.10	26,26,26,26	0
58	MG	2A	3764	1/1	0.96	0.05	46,46,46,46	0
58	MG	2A	3193	1/1	0.96	0.08	46,46,46,46	0
58	MG	1a	1783	1/1	0.96	0.05	36,36,36,36	0
58	MG	2a	1723	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3832	1/1	0.96	0.10	31,31,31,31	0
58	MG	2A	3196	1/1	0.96	0.10	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3197	1/1	0.96	0.26	43,43,43,43	0
58	MG	1X	103	1/1	0.96	0.16	29,29,29,29	0
58	MG	1A	3525	1/1	0.96	0.07	35,35,35,35	0
58	MG	2A	3774	1/1	0.96	0.07	50,50,50,50	0
58	MG	1A	3090	1/1	0.96	0.13	43,43,43,43	0
58	MG	1a	1795	1/1	0.96	0.13	67,67,67,67	0
58	MG	1A	4011	1/1	0.96	0.11	31,31,31,31	0
58	MG	2a	1735	1/1	0.96	0.20	48,48,48,48	0
58	MG	1A	3663	1/1	0.96	0.06	19,19,19,19	0
58	MG	1A	4013	1/1	0.96	0.05	17,17,17,17	0
58	MG	1Z	3702	1/1	0.96	0.07	34,34,34,34	0
58	MG	1A	4015	1/1	0.96	0.07	20,20,20,20	0
58	MG	2A	3783	1/1	0.96	0.06	61,61,61,61	0
58	MG	2A	3784	1/1	0.96	0.16	46,46,46,46	0
58	MG	1a	1803	1/1	0.96	0.06	37,37,37,37	0
58	MG	10	104	1/1	0.96	0.15	39,39,39,39	0
58	MG	2a	1744	1/1	0.96	0.23	48,48,48,48	0
58	MG	1a	1806	1/1	0.96	0.14	35,35,35,35	0
58	MG	1A	3439	1/1	0.96	0.24	28,28,28,28	0
58	MG	1A	3528	1/1	0.96	0.10	66,66,66,66	0
58	MG	2A	3791	1/1	0.96	0.07	21,21,21,21	0
58	MG	1A	3054	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3459	1/1	0.96	0.07	32,32,32,32	0
58	MG	2A	3460	1/1	0.96	0.10	47,47,47,47	0
58	MG	2A	3795	1/1	0.96	0.05	32,32,32,32	0
58	MG	1A	3294	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3366	1/1	0.96	0.08	39,39,39,39	0
58	MG	11	102	1/1	0.96	0.07	36,36,36,36	0
58	MG	1A	3232	1/1	0.96	0.19	25,25,25,25	0
58	MG	1A	3057	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3843	1/1	0.96	0.05	31,31,31,31	0
58	MG	12	101	1/1	0.96	0.06	43,43,43,43	0
58	MG	2A	3469	1/1	0.96	0.23	36,36,36,36	0
58	MG	2a	1765	1/1	0.96	0.06	55,55,55,55	0
58	MG	12	102	1/1	0.96	0.10	33,33,33,33	0
58	MG	2A	3471	1/1	0.96	0.12	45,45,45,45	0
58	MG	2A	3807	1/1	0.96	0.12	49,49,49,49	0
58	MG	1A	3299	1/1	0.96	0.06	43,43,43,43	0
58	MG	1d	301	1/1	0.96	0.28	49,49,49,49	0
58	MG	1A	4028	1/1	0.96	0.08	48,48,48,48	0
58	MG	15	105	1/1	0.96	0.26	41,41,41,41	0
58	MG	1f	201	1/1	0.96	0.15	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4029	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	4030	1/1	0.96	0.07	62,62,62,62	0
58	MG	2A	3816	1/1	0.96	0.04	41,41,41,41	0
58	MG	1A	3845	1/1	0.96	0.08	27,27,27,27	0
58	MG	2A	3818	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	3446	1/1	0.96	0.15	26,26,26,26	0
58	MG	2A	3232	1/1	0.96	0.09	39,39,39,39	0
58	MG	2a	1791	1/1	0.96	0.14	47,47,47,47	0
58	MG	1A	3118	1/1	0.96	0.27	31,31,31,31	0
58	MG	2A	3235	1/1	0.96	0.15	41,41,41,41	0
58	MG	1A	3686	1/1	0.96	0.08	27,27,27,27	0
58	MG	1p	101	1/1	0.96	0.10	54,54,54,54	0
58	MG	2a	1797	1/1	0.96	0.06	55,55,55,55	0
58	MG	2A	3828	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3829	1/1	0.96	0.07	28,28,28,28	0
58	MG	1A	3538	1/1	0.96	0.19	35,35,35,35	0
58	MG	2A	3834	1/1	0.96	0.08	45,45,45,45	0
58	MG	19	101	1/1	0.96	0.10	38,38,38,38	0
58	MG	1A	3691	1/1	0.96	0.09	29,29,29,29	0
58	MG	1A	3093	1/1	0.96	0.07	42,42,42,42	0
58	MG	1a	1603	1/1	0.96	0.07	38,38,38,38	0
58	MG	2A	3495	1/1	0.96	0.11	29,29,29,29	0
58	MG	1A	3372	1/1	0.96	0.09	45,45,45,45	0
58	MG	1A	3451	1/1	0.96	0.19	33,33,33,33	0
58	MG	1A	3698	1/1	0.96	0.10	34,34,34,34	0
58	MG	2A	3247	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3094	1/1	0.96	0.07	17,17,17,17	0
58	MG	1A	4047	1/1	0.96	0.04	27,27,27,27	0
58	MG	2a	1814	1/1	0.96	0.06	46,46,46,46	0
58	MG	1A	3123	1/1	0.96	0.20	37,37,37,37	0
58	MG	2A	3507	1/1	0.96	0.07	50,50,50,50	0
58	MG	1a	1611	1/1	0.96	0.07	34,34,34,34	0
58	MG	1A	3704	1/1	0.96	0.05	14,14,14,14	0
58	MG	2a	1819	1/1	0.96	0.14	51,51,51,51	0
58	MG	2A	3510	1/1	0.96	0.09	22,22,22,22	0
58	MG	2a	1821	1/1	0.96	0.06	58,58,58,58	0
58	MG	2A	3254	1/1	0.96	0.08	45,45,45,45	0
58	MG	1A	3707	1/1	0.96	0.06	18,18,18,18	0
58	MG	2A	3858	1/1	0.96	0.13	43,43,43,43	0
58	MG	1A	3708	1/1	0.96	0.10	19,19,19,19	0
58	MG	1A	3866	1/1	0.96	0.05	34,34,34,34	0
58	MG	2A	3518	1/1	0.96	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4054	1/1	0.96	0.07	34,34,34,34	0
58	MG	1A	3545	1/1	0.96	0.12	27,27,27,27	0
58	MG	2A	3864	1/1	0.96	0.08	45,45,45,45	0
58	MG	2a	1832	1/1	0.96	0.16	44,44,44,44	0
58	MG	2A	3865	1/1	0.96	0.08	40,40,40,40	0
58	MG	1x	112	1/1	0.96	0.15	39,39,39,39	0
58	MG	1x	113	1/1	0.96	0.17	45,45,45,45	0
58	MG	1A	3240	1/1	0.96	0.11	22,22,22,22	0
58	MG	1a	1620	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3528	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3310	1/1	0.96	0.07	25,25,25,25	0
58	MG	2A	3531	1/1	0.96	0.06	22,22,22,22	0
58	MG	2A	3873	1/1	0.96	0.06	37,37,37,37	0
58	MG	2A	3533	1/1	0.96	0.10	46,46,46,46	0
58	MG	2A	3004	1/1	0.96	0.14	41,41,41,41	0
58	MG	1A	3246	1/1	0.96	0.22	31,31,31,31	0
58	MG	2i	201	1/1	0.96	0.05	41,41,41,41	0
58	MG	2A	3006	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3059	1/1	0.96	0.06	32,32,32,32	0
58	MG	1A	3183	1/1	0.96	0.10	29,29,29,29	0
58	MG	2l	203	1/1	0.96	0.06	42,42,42,42	0
58	MG	1A	3028	1/1	0.96	0.17	15,15,15,15	0
58	MG	2A	3274	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3011	1/1	0.96	0.06	36,36,36,36	0
58	MG	2q	201	1/1	0.96	0.06	55,55,55,55	0
58	MG	2A	3012	1/1	0.96	0.05	30,30,30,30	0
58	MG	2A	3014	1/1	0.96	0.06	30,30,30,30	0
58	MG	2A	3546	1/1	0.96	0.05	32,32,32,32	0
58	MG	1A	3132	1/1	0.96	0.04	25,25,25,25	0
58	MG	1a	1629	1/1	0.96	0.30	45,45,45,45	0
58	MG	1A	3134	1/1	0.96	0.09	25,25,25,25	0
58	MG	1a	1631	1/1	0.96	0.15	42,42,42,42	0
58	MG	2A	3282	1/1	0.96	0.16	46,46,46,46	0
58	MG	1A	3317	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3318	1/1	0.96	0.17	43,43,43,43	0
58	MG	1A	3882	1/1	0.96	0.11	23,23,23,23	0
58	MG	2A	3025	1/1	0.96	0.07	35,35,35,35	0
58	MG	2B	213	1/1	0.96	0.04	40,40,40,40	0
58	MG	2A	3288	1/1	0.96	0.18	54,54,54,54	0
58	MG	2B	216	1/1	0.96	0.14	54,54,54,54	0
58	MG	2A	3566	1/1	0.96	0.04	38,38,38,38	0
58	MG	2A	3026	1/1	0.96	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3467	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3884	1/1	0.96	0.05	28,28,28,28	0
58	MG	2A	3573	1/1	0.96	0.14	52,52,52,52	0
58	MG	2A	3574	1/1	0.96	0.05	37,37,37,37	0
58	MG	1A	4081	1/1	0.96	0.09	31,31,31,31	0
58	MG	1A	3562	1/1	0.96	0.18	18,18,18,18	0
58	MG	2A	3577	1/1	0.96	0.10	36,36,36,36	0
58	MG	2A	3578	1/1	0.96	0.08	26,26,26,26	0
58	MG	2E	304	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3033	1/1	0.96	0.12	32,32,32,32	0
58	MG	2E	307	1/1	0.96	0.07	29,29,29,29	0
58	MG	1A	3887	1/1	0.96	0.05	11,11,11,11	0
58	MG	2A	3296	1/1	0.96	0.11	54,54,54,54	0
58	MG	1N	205	1/1	0.97	0.27	41,41,41,41	0
58	MG	1A	3683	1/1	0.97	0.04	16,16,16,16	0
58	MG	2A	3631	1/1	0.97	0.07	39,39,39,39	0
58	MG	2A	3632	1/1	0.97	0.07	26,26,26,26	0
58	MG	1A	3465	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3994	1/1	0.97	0.05	16,16,16,16	0
58	MG	1a	1717	1/1	0.97	0.14	40,40,40,40	0
58	MG	1a	1718	1/1	0.97	0.14	32,32,32,32	0
58	MG	2A	3638	1/1	0.97	0.04	27,27,27,27	0
58	MG	2A	3639	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3258	1/1	0.97	0.09	21,21,21,21	0
58	MG	1A	3390	1/1	0.97	0.10	42,42,42,42	0
58	MG	2A	3643	1/1	0.97	0.07	20,20,20,20	0
58	MG	1A	3104	1/1	0.97	0.07	15,15,15,15	0
58	MG	2A	3115	1/1	0.97	0.11	36,36,36,36	0
58	MG	1a	1724	1/1	0.97	0.12	49,49,49,49	0
58	MG	1A	3041	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	3394	1/1	0.97	0.13	16,16,16,16	0
58	MG	2A	3121	1/1	0.97	0.17	39,39,39,39	0
58	MG	1a	1727	1/1	0.97	0.05	44,44,44,44	0
58	MG	1P	202	1/1	0.97	0.23	20,20,20,20	0
58	MG	1A	3471	1/1	0.97	0.38	35,35,35,35	0
58	MG	1Q	201	1/1	0.97	0.08	29,29,29,29	0
58	MG	1Q	203	1/1	0.97	0.09	26,26,26,26	0
58	MG	2A	3368	1/1	0.97	0.07	43,43,43,43	0
58	MG	28	102	1/1	0.97	0.13	39,39,39,39	0
58	MG	2A	3129	1/1	0.97	0.15	47,47,47,47	0
58	MG	2A	3130	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	4001	1/1	0.97	0.04	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3697	1/1	0.97	0.07	35,35,35,35	0
58	MG	2A	3661	1/1	0.97	0.06	47,47,47,47	0
58	MG	1a	1736	1/1	0.97	0.07	46,46,46,46	0
58	MG	1Q	206	1/1	0.97	0.09	45,45,45,45	0
58	MG	1A	3472	1/1	0.97	0.12	33,33,33,33	0
58	MG	1A	3556	1/1	0.97	0.09	48,48,48,48	0
58	MG	2A	3138	1/1	0.97	0.21	34,34,34,34	0
58	MG	2A	3667	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3701	1/1	0.97	0.06	12,12,12,12	0
58	MG	2A	3141	1/1	0.97	0.16	31,31,31,31	0
58	MG	2A	3381	1/1	0.97	0.17	31,31,31,31	0
58	MG	1R	203	1/1	0.97	0.16	27,27,27,27	0
58	MG	2A	3673	1/1	0.97	0.06	37,37,37,37	0
58	MG	1R	204	1/1	0.97	0.16	29,29,29,29	0
58	MG	1A	4006	1/1	0.97	0.05	13,13,13,13	0
58	MG	1A	3323	1/1	0.97	0.14	23,23,23,23	0
58	MG	1A	3703	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3849	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3558	1/1	0.97	0.12	26,26,26,26	0
58	MG	2A	3150	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3851	1/1	0.97	0.05	40,40,40,40	0
58	MG	2a	1622	1/1	0.97	0.06	60,60,60,60	0
58	MG	1A	3324	1/1	0.97	0.07	50,50,50,50	0
58	MG	2A	3684	1/1	0.97	0.08	32,32,32,32	0
58	MG	2A	3153	1/1	0.97	0.16	53,53,53,53	0
58	MG	1A	3261	1/1	0.97	0.12	16,16,16,16	0
58	MG	1A	3107	1/1	0.97	0.11	23,23,23,23	0
58	MG	2A	3156	1/1	0.97	0.04	43,43,43,43	0
58	MG	2A	3689	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3565	1/1	0.97	0.14	23,23,23,23	0
58	MG	1A	4019	1/1	0.97	0.04	30,30,30,30	0
58	MG	1A	3150	1/1	0.97	0.07	27,27,27,27	0
58	MG	2A	3693	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3012	1/1	0.97	0.06	23,23,23,23	0
58	MG	1V	201	1/1	0.97	0.14	15,15,15,15	0
58	MG	1A	3205	1/1	0.97	0.15	30,30,30,30	0
58	MG	2A	3164	1/1	0.97	0.08	43,43,43,43	0
58	MG	1a	1762	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3331	1/1	0.97	0.21	36,36,36,36	0
58	MG	1a	1764	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3571	1/1	0.97	0.12	21,21,21,21	0
58	MG	1W	201	1/1	0.97	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3022	1/1	0.97	0.15	27,27,27,27	0
58	MG	1W	203	1/1	0.97	0.09	42,42,42,42	0
58	MG	1a	1770	1/1	0.97	0.06	49,49,49,49	0
58	MG	1a	1772	1/1	0.97	0.05	58,58,58,58	0
58	MG	1W	204	1/1	0.97	0.09	22,22,22,22	0
58	MG	2A	3414	1/1	0.97	0.19	35,35,35,35	0
58	MG	2A	3415	1/1	0.97	0.14	38,38,38,38	0
58	MG	2A	3175	1/1	0.97	0.12	43,43,43,43	0
58	MG	1A	3155	1/1	0.97	0.12	23,23,23,23	0
58	MG	2A	3713	1/1	0.97	0.08	38,38,38,38	0
58	MG	1a	1776	1/1	0.97	0.05	56,56,56,56	0
58	MG	1A	3577	1/1	0.97	0.13	32,32,32,32	0
58	MG	1A	3208	1/1	0.97	0.12	23,23,23,23	0
58	MG	1A	3721	1/1	0.97	0.07	36,36,36,36	0
58	MG	2A	3422	1/1	0.97	0.28	40,40,40,40	0
58	MG	1X	102	1/1	0.97	0.08	27,27,27,27	0
58	MG	2a	1659	1/1	0.97	0.28	44,44,44,44	0
58	MG	1A	3581	1/1	0.97	0.07	27,27,27,27	0
58	MG	1X	106	1/1	0.97	0.06	57,57,57,57	0
58	MG	2A	3185	1/1	0.97	0.08	24,24,24,24	0
58	MG	2A	3725	1/1	0.97	0.10	29,29,29,29	0
58	MG	2a	1665	1/1	0.97	0.07	54,54,54,54	0
58	MG	1A	3158	1/1	0.97	0.09	37,37,37,37	0
58	MG	2A	3187	1/1	0.97	0.09	40,40,40,40	0
58	MG	2A	3732	1/1	0.97	0.10	37,37,37,37	0
58	MG	2a	1669	1/1	0.97	0.06	44,44,44,44	0
58	MG	1a	1789	1/1	0.97	0.04	36,36,36,36	0
58	MG	1A	4033	1/1	0.97	0.04	31,31,31,31	0
58	MG	1A	3485	1/1	0.97	0.05	33,33,33,33	0
58	MG	2a	1673	1/1	0.97	0.06	32,32,32,32	0
58	MG	2a	1674	1/1	0.97	0.05	29,29,29,29	0
58	MG	2a	1676	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3587	1/1	0.97	0.06	25,25,25,25	0
58	MG	1a	1796	1/1	0.97	0.04	54,54,54,54	0
58	MG	2A	3738	1/1	0.97	0.20	64,64,64,64	0
58	MG	1A	4037	1/1	0.97	0.04	38,38,38,38	0
58	MG	1A	3588	1/1	0.97	0.08	37,37,37,37	0
58	MG	2a	1683	1/1	0.97	0.06	40,40,40,40	0
58	MG	10	101	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	4039	1/1	0.97	0.12	27,27,27,27	0
58	MG	1A	3110	1/1	0.97	0.30	27,27,27,27	0
58	MG	1A	4041	1/1	0.97	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3877	1/1	0.97	0.17	21,21,21,21	0
58	MG	1A	3729	1/1	0.97	0.04	24,24,24,24	0
58	MG	1A	3879	1/1	0.97	0.22	25,25,25,25	0
58	MG	2A	3751	1/1	0.97	0.10	40,40,40,40	0
58	MG	1a	1808	1/1	0.97	0.16	51,51,51,51	0
58	MG	1A	3880	1/1	0.97	0.10	35,35,35,35	0
58	MG	1A	3730	1/1	0.97	0.12	45,45,45,45	0
58	MG	1A	3114	1/1	0.97	0.14	21,21,21,21	0
58	MG	1A	3339	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3086	1/1	0.97	0.35	26,26,26,26	0
58	MG	1A	3341	1/1	0.97	0.04	34,34,34,34	0
58	MG	1A	3886	1/1	0.97	0.06	38,38,38,38	0
58	MG	13	102	1/1	0.97	0.12	32,32,32,32	0
58	MG	1A	3417	1/1	0.97	0.15	32,32,32,32	0
58	MG	1A	4053	1/1	0.97	0.04	25,25,25,25	0
58	MG	2a	1703	1/1	0.97	0.12	42,42,42,42	0
58	MG	1A	3596	1/1	0.97	0.12	23,23,23,23	0
58	MG	1A	3493	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3418	1/1	0.97	0.11	23,23,23,23	0
58	MG	1A	3063	1/1	0.97	0.26	44,44,44,44	0
58	MG	1A	3600	1/1	0.97	0.12	37,37,37,37	0
58	MG	1A	3894	1/1	0.97	0.09	12,12,12,12	0
58	MG	1A	3220	1/1	0.97	0.12	20,20,20,20	0
58	MG	2A	3771	1/1	0.97	0.08	30,30,30,30	0
58	MG	18	103	1/1	0.97	0.09	33,33,33,33	0
58	MG	1A	3497	1/1	0.97	0.15	35,35,35,35	0
58	MG	1A	4065	1/1	0.97	0.04	26,26,26,26	0
58	MG	1A	4066	1/1	0.97	0.05	13,13,13,13	0
58	MG	2A	3226	1/1	0.97	0.19	30,30,30,30	0
58	MG	1A	3276	1/1	0.97	0.04	31,31,31,31	0
58	MG	1A	3898	1/1	0.97	0.06	11,11,11,11	0
58	MG	1A	3277	1/1	0.97	0.14	21,21,21,21	0
58	MG	1A	4074	1/1	0.97	0.10	27,27,27,27	0
58	MG	1A	3605	1/1	0.97	0.05	16,16,16,16	0
58	MG	2A	3782	1/1	0.97	0.09	33,33,33,33	0
58	MG	1w	102	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3478	1/1	0.97	0.07	16,16,16,16	0
58	MG	1A	3064	1/1	0.97	0.09	33,33,33,33	0
58	MG	2a	1727	1/1	0.97	0.10	39,39,39,39	0
58	MG	2A	3786	1/1	0.97	0.04	30,30,30,30	0
58	MG	2A	3480	1/1	0.97	0.08	35,35,35,35	0
58	MG	1w	105	1/1	0.97	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3501	1/1	0.97	0.12	24,24,24,24	0
58	MG	1A	3608	1/1	0.97	0.07	17,17,17,17	0
58	MG	1A	4080	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3065	1/1	0.97	0.07	30,30,30,30	0
58	MG	1a	1613	1/1	0.97	0.12	21,21,21,21	0
58	MG	1A	3223	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3352	1/1	0.97	0.18	28,28,28,28	0
58	MG	1A	4084	1/1	0.97	0.08	22,22,22,22	0
58	MG	1A	3910	1/1	0.97	0.05	46,46,46,46	0
58	MG	2A	3245	1/1	0.97	0.18	37,37,37,37	0
58	MG	2A	3492	1/1	0.97	0.13	45,45,45,45	0
58	MG	1A	4087	1/1	0.97	0.05	30,30,30,30	0
58	MG	1A	3284	1/1	0.97	0.25	37,37,37,37	0
58	MG	2A	3248	1/1	0.97	0.06	47,47,47,47	0
58	MG	2A	3497	1/1	0.97	0.11	32,32,32,32	0
58	MG	1A	3286	1/1	0.97	0.24	25,25,25,25	0
58	MG	1A	3915	1/1	0.97	0.19	21,21,21,21	0
58	MG	1A	3916	1/1	0.97	0.14	15,15,15,15	0
58	MG	2a	1750	1/1	0.97	0.06	42,42,42,42	0
58	MG	2a	1751	1/1	0.97	0.05	58,58,58,58	0
58	MG	2A	3501	1/1	0.97	0.05	61,61,61,61	0
58	MG	1a	1623	1/1	0.97	0.05	37,37,37,37	0
58	MG	1a	1624	1/1	0.97	0.15	42,42,42,42	0
58	MG	1A	3225	1/1	0.97	0.09	22,22,22,22	0
58	MG	1A	3617	1/1	0.97	0.05	13,13,13,13	0
58	MG	2A	3506	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3017	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3291	1/1	0.97	0.10	30,30,30,30	0
58	MG	1A	3170	1/1	0.97	0.06	31,31,31,31	0
58	MG	1A	3008	1/1	0.97	0.05	13,13,13,13	0
58	MG	1A	3514	1/1	0.97	0.12	37,37,37,37	0
58	MG	1A	3515	1/1	0.97	0.32	34,34,34,34	0
58	MG	2a	1770	1/1	0.97	0.05	46,46,46,46	0
58	MG	2A	3514	1/1	0.97	0.07	36,36,36,36	0
58	MG	2A	3824	1/1	0.97	0.07	19,19,19,19	0
58	MG	1a	1633	1/1	0.97	0.09	45,45,45,45	0
58	MG	2a	1774	1/1	0.97	0.10	43,43,43,43	0
58	MG	2a	1775	1/1	0.97	0.04	56,56,56,56	0
58	MG	1A	3030	1/1	0.97	0.16	14,14,14,14	0
58	MG	2A	3013	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3779	1/1	0.97	0.06	31,31,31,31	0
58	MG	1a	1637	1/1	0.97	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3269	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3296	1/1	0.97	0.07	23,23,23,23	0
58	MG	2a	1783	1/1	0.97	0.07	39,39,39,39	0
58	MG	1a	1639	1/1	0.97	0.06	34,34,34,34	0
58	MG	2A	3836	1/1	0.97	0.05	54,54,54,54	0
58	MG	2a	1786	1/1	0.97	0.04	45,45,45,45	0
58	MG	2A	3019	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3783	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3631	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	4105	1/1	0.97	0.19	41,41,41,41	0
58	MG	1a	1643	1/1	0.97	0.12	41,41,41,41	0
58	MG	1A	3632	1/1	0.97	0.03	25,25,25,25	0
58	MG	1A	3635	1/1	0.97	0.04	13,13,13,13	0
58	MG	1B	205	1/1	0.97	0.24	47,47,47,47	0
58	MG	1B	207	1/1	0.97	0.20	33,33,33,33	0
58	MG	1a	1648	1/1	0.97	0.09	41,41,41,41	0
58	MG	1A	3788	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3938	1/1	0.97	0.06	30,30,30,30	0
58	MG	2A	3541	1/1	0.97	0.06	38,38,38,38	0
58	MG	2A	3851	1/1	0.97	0.04	36,36,36,36	0
58	MG	2A	3852	1/1	0.97	0.07	21,21,21,21	0
58	MG	1B	210	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3789	1/1	0.97	0.05	28,28,28,28	0
58	MG	2A	3037	1/1	0.97	0.06	31,31,31,31	0
58	MG	2a	1806	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3545	1/1	0.97	0.05	41,41,41,41	0
58	MG	1A	3070	1/1	0.97	0.09	14,14,14,14	0
58	MG	2A	3547	1/1	0.97	0.05	31,31,31,31	0
58	MG	2A	3548	1/1	0.97	0.06	37,37,37,37	0
58	MG	1a	1657	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3127	1/1	0.97	0.18	26,26,26,26	0
58	MG	1A	3128	1/1	0.97	0.11	25,25,25,25	0
58	MG	2A	3553	1/1	0.97	0.09	27,27,27,27	0
58	MG	2A	3555	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3178	1/1	0.97	0.22	25,25,25,25	0
58	MG	1B	217	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3797	1/1	0.97	0.05	15,15,15,15	0
58	MG	1B	219	1/1	0.97	0.08	21,21,21,21	0
58	MG	1A	3798	1/1	0.97	0.04	17,17,17,17	0
58	MG	1A	3949	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3301	1/1	0.97	0.11	28,28,28,28	0
58	MG	2a	1823	1/1	0.97	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3564	1/1	0.97	0.06	41,41,41,41	0
58	MG	1B	224	1/1	0.97	0.06	45,45,45,45	0
58	MG	2A	3875	1/1	0.97	0.18	53,53,53,53	0
58	MG	2A	3568	1/1	0.97	0.06	26,26,26,26	0
58	MG	1A	3071	1/1	0.97	0.04	6,6,6,6	0
58	MG	1A	3953	1/1	0.97	0.05	48,48,48,48	0
58	MG	1B	228	1/1	0.97	0.05	30,30,30,30	0
58	MG	1A	3954	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3032	1/1	0.97	0.18	20,20,20,20	0
58	MG	2a	1833	1/1	0.97	0.10	57,57,57,57	0
58	MG	1A	3304	1/1	0.97	0.07	36,36,36,36	0
58	MG	2A	3059	1/1	0.97	0.10	35,35,35,35	0
58	MG	1A	3245	1/1	0.97	0.14	18,18,18,18	0
58	MG	1A	3958	1/1	0.97	0.10	43,43,43,43	0
58	MG	2A	3579	1/1	0.97	0.05	26,26,26,26	0
58	MG	1A	3649	1/1	0.97	0.06	10,10,10,10	0
58	MG	1A	3373	1/1	0.97	0.17	35,35,35,35	0
58	MG	1B	237	1/1	0.97	0.04	25,25,25,25	0
58	MG	1D	305	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3808	1/1	0.97	0.04	33,33,33,33	0
58	MG	2f	201	1/1	0.97	0.18	35,35,35,35	0
58	MG	2A	3585	1/1	0.97	0.15	37,37,37,37	0
58	MG	1D	308	1/1	0.97	0.14	38,38,38,38	0
58	MG	1A	3133	1/1	0.97	0.12	48,48,48,48	0
58	MG	1A	3375	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3656	1/1	0.97	0.04	17,17,17,17	0
58	MG	1A	3965	1/1	0.97	0.10	51,51,51,51	0
58	MG	2B	215	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3814	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3967	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3376	1/1	0.97	0.06	31,31,31,31	0
58	MG	1A	3098	1/1	0.97	0.06	25,25,25,25	0
58	MG	1A	3186	1/1	0.97	0.05	46,46,46,46	0
58	MG	1A	3033	1/1	0.97	0.22	20,20,20,20	0
58	MG	1A	3661	1/1	0.97	0.06	18,18,18,18	0
58	MG	1F	303	1/1	0.97	0.16	26,26,26,26	0
58	MG	1F	304	1/1	0.97	0.05	43,43,43,43	0
58	MG	1A	3034	1/1	0.97	0.20	25,25,25,25	0
58	MG	1F	309	1/1	0.97	0.05	32,32,32,32	0
58	MG	1A	3040	1/1	0.97	0.12	43,43,43,43	0
58	MG	1A	3080	1/1	0.97	0.10	40,40,40,40	0
58	MG	1a	1699	1/1	0.97	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3193	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	3542	1/1	0.97	0.18	33,33,33,33	0
58	MG	2E	310	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3827	1/1	0.97	0.05	29,29,29,29	0
58	MG	2A	3093	1/1	0.97	0.18	36,36,36,36	0
58	MG	1A	3141	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3196	1/1	0.97	0.27	27,27,27,27	0
58	MG	1A	3675	1/1	0.97	0.07	16,16,16,16	0
58	MG	2A	3617	1/1	0.97	0.05	38,38,38,38	0
58	MG	2A	3618	1/1	0.97	0.12	28,28,28,28	0
58	MG	2F	307	1/1	0.97	0.21	35,35,35,35	0
58	MG	2F	308	1/1	0.97	0.11	35,35,35,35	0
58	MG	2A	3098	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3387	1/1	0.97	0.19	18,18,18,18	0
58	MG	1A	3677	1/1	0.97	0.07	12,12,12,12	0
58	MG	1A	3546	1/1	0.97	0.05	18,18,18,18	0
58	MG	1A	3197	1/1	0.97	0.30	18,18,18,18	0
58	MG	1A	3989	1/1	0.97	0.10	47,47,47,47	0
58	MG	1N	204	1/1	0.97	0.04	27,27,27,27	0
59	K	2x	101	1/1	0.97	0.05	41,41,41,41	0
58	MG	2A	3348	1/1	0.97	0.07	44,44,44,44	0
58	MG	2A	3425	1/1	0.98	0.09	27,27,27,27	0
58	MG	1A	3785	1/1	0.98	0.04	17,17,17,17	0
58	MG	1A	3239	1/1	0.98	0.12	21,21,21,21	0
58	MG	1A	3305	1/1	0.98	0.04	19,19,19,19	0
58	MG	1A	3936	1/1	0.98	0.08	57,57,57,57	0
58	MG	1A	3646	1/1	0.98	0.06	12,12,12,12	0
58	MG	1a	1610	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3939	1/1	0.98	0.07	18,18,18,18	0
58	MG	1A	3144	1/1	0.98	0.04	5,5,5,5	0
58	MG	1A	3942	1/1	0.98	0.03	48,48,48,48	0
58	MG	1A	3241	1/1	0.98	0.07	31,31,31,31	0
58	MG	1B	206	1/1	0.98	0.04	41,41,41,41	0
58	MG	1A	3792	1/1	0.98	0.05	14,14,14,14	0
58	MG	1A	3309	1/1	0.98	0.10	41,41,41,41	0
58	MG	1A	3794	1/1	0.98	0.10	38,38,38,38	0
58	MG	1A	3650	1/1	0.98	0.04	18,18,18,18	0
58	MG	1B	211	1/1	0.98	0.26	34,34,34,34	0
58	MG	1A	3242	1/1	0.98	0.07	22,22,22,22	0
58	MG	1A	3652	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3950	1/1	0.98	0.04	33,33,33,33	0
58	MG	1v	102	1/1	0.98	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3243	1/1	0.98	0.04	23,23,23,23	0
58	MG	1A	3799	1/1	0.98	0.07	10,10,10,10	0
58	MG	2A	3448	1/1	0.98	0.19	40,40,40,40	0
58	MG	1A	3145	1/1	0.98	0.05	38,38,38,38	0
58	MG	2A	3450	1/1	0.98	0.19	28,28,28,28	0
58	MG	1w	104	1/1	0.98	0.05	51,51,51,51	0
58	MG	1A	3801	1/1	0.98	0.05	24,24,24,24	0
58	MG	1A	3097	1/1	0.98	0.09	28,28,28,28	0
58	MG	2A	3217	1/1	0.98	0.14	37,37,37,37	0
58	MG	1B	220	1/1	0.98	0.04	24,24,24,24	0
58	MG	2A	3722	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3463	1/1	0.98	0.10	30,30,30,30	0
58	MG	1A	3021	1/1	0.98	0.10	15,15,15,15	0
58	MG	1A	3149	1/1	0.98	0.22	18,18,18,18	0
58	MG	1A	3190	1/1	0.98	0.14	23,23,23,23	0
58	MG	2A	3728	1/1	0.98	0.04	28,28,28,28	0
58	MG	2A	3729	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3119	1/1	0.98	0.15	22,22,22,22	0
58	MG	1A	3662	1/1	0.98	0.05	14,14,14,14	0
58	MG	1a	1636	1/1	0.98	0.08	23,23,23,23	0
58	MG	1B	227	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3810	1/1	0.98	0.21	18,18,18,18	0
58	MG	1A	3192	1/1	0.98	0.15	30,30,30,30	0
58	MG	1x	110	1/1	0.98	0.11	43,43,43,43	0
58	MG	1A	3099	1/1	0.98	0.12	10,10,10,10	0
58	MG	2A	3740	1/1	0.98	0.05	36,36,36,36	0
58	MG	1A	3253	1/1	0.98	0.26	31,31,31,31	0
58	MG	1A	3194	1/1	0.98	0.21	20,20,20,20	0
58	MG	2A	3233	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3392	1/1	0.98	0.21	18,18,18,18	0
58	MG	1A	3152	1/1	0.98	0.24	23,23,23,23	0
58	MG	2A	3002	1/1	0.98	0.23	35,35,35,35	0
58	MG	2A	3747	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3969	1/1	0.98	0.08	17,17,17,17	0
58	MG	2A	3476	1/1	0.98	0.06	39,39,39,39	0
58	MG	2a	1660	1/1	0.98	0.05	52,52,52,52	0
58	MG	1B	236	1/1	0.98	0.05	35,35,35,35	0
58	MG	1A	3018	1/1	0.98	0.10	20,20,20,20	0
58	MG	1D	301	1/1	0.98	0.17	22,22,22,22	0
58	MG	1A	3971	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3154	1/1	0.98	0.27	20,20,20,20	0
58	MG	1A	3325	1/1	0.98	0.16	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3561	1/1	0.98	0.12	21,21,21,21	0
58	MG	1a	1653	1/1	0.98	0.03	36,36,36,36	0
58	MG	1a	1654	1/1	0.98	0.12	33,33,33,33	0
58	MG	1a	1655	1/1	0.98	0.09	39,39,39,39	0
58	MG	2A	3015	1/1	0.98	0.11	38,38,38,38	0
58	MG	1D	310	1/1	0.98	0.24	19,19,19,19	0
58	MG	1A	3821	1/1	0.98	0.06	35,35,35,35	0
58	MG	1A	3678	1/1	0.98	0.04	12,12,12,12	0
58	MG	2a	1675	1/1	0.98	0.14	35,35,35,35	0
58	MG	1E	302	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3765	1/1	0.98	0.04	39,39,39,39	0
58	MG	1E	303	1/1	0.98	0.08	18,18,18,18	0
58	MG	2A	3021	1/1	0.98	0.07	16,16,16,16	0
58	MG	2a	1680	1/1	0.98	0.09	37,37,37,37	0
58	MG	1A	3680	1/1	0.98	0.05	21,21,21,21	0
58	MG	1A	3198	1/1	0.98	0.15	28,28,28,28	0
58	MG	2A	3496	1/1	0.98	0.12	35,35,35,35	0
58	MG	1A	3085	1/1	0.98	0.10	22,22,22,22	0
58	MG	1A	3564	1/1	0.98	0.21	26,26,26,26	0
58	MG	2A	3259	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3156	1/1	0.98	0.04	26,26,26,26	0
58	MG	2A	3027	1/1	0.98	0.12	24,24,24,24	0
58	MG	1A	3685	1/1	0.98	0.06	11,11,11,11	0
58	MG	2A	3263	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3124	1/1	0.98	0.13	26,26,26,26	0
58	MG	2A	3030	1/1	0.98	0.12	33,33,33,33	0
58	MG	1A	3984	1/1	0.98	0.03	22,22,22,22	0
58	MG	1F	301	1/1	0.98	0.08	27,27,27,27	0
58	MG	1A	3125	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3160	1/1	0.98	0.09	29,29,29,29	0
58	MG	1F	305	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3692	1/1	0.98	0.09	9,9,9,9	0
58	MG	2A	3038	1/1	0.98	0.10	13,13,13,13	0
58	MG	2A	3513	1/1	0.98	0.07	24,24,24,24	0
58	MG	1F	308	1/1	0.98	0.17	18,18,18,18	0
58	MG	1A	3056	1/1	0.98	0.04	24,24,24,24	0
58	MG	1A	3333	1/1	0.98	0.05	31,31,31,31	0
58	MG	2A	3517	1/1	0.98	0.12	34,34,34,34	0
58	MG	2a	1705	1/1	0.98	0.05	49,49,49,49	0
58	MG	1A	3572	1/1	0.98	0.04	12,12,12,12	0
58	MG	1A	3696	1/1	0.98	0.06	12,12,12,12	0
58	MG	2A	3044	1/1	0.98	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3521	1/1	0.98	0.06	39,39,39,39	0
58	MG	2A	3796	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3087	1/1	0.98	0.23	30,30,30,30	0
58	MG	2A	3523	1/1	0.98	0.05	25,25,25,25	0
58	MG	1A	3486	1/1	0.98	0.05	21,21,21,21	0
58	MG	1A	3408	1/1	0.98	0.11	36,36,36,36	0
58	MG	1A	3700	1/1	0.98	0.11	16,16,16,16	0
58	MG	2A	3049	1/1	0.98	0.10	14,14,14,14	0
58	MG	1A	3578	1/1	0.98	0.11	24,24,24,24	0
58	MG	2A	3285	1/1	0.98	0.09	44,44,44,44	0
58	MG	2A	3532	1/1	0.98	0.06	39,39,39,39	0
58	MG	1A	3579	1/1	0.98	0.15	23,23,23,23	0
58	MG	1A	3163	1/1	0.98	0.15	25,25,25,25	0
58	MG	2A	3808	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3164	1/1	0.98	0.14	21,21,21,21	0
58	MG	1A	3706	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3043	1/1	0.98	0.23	29,29,29,29	0
58	MG	1A	3583	1/1	0.98	0.19	24,24,24,24	0
58	MG	1A	3584	1/1	0.98	0.34	30,30,30,30	0
58	MG	1A	3130	1/1	0.98	0.31	25,25,25,25	0
58	MG	2a	1729	1/1	0.98	0.13	33,33,33,33	0
58	MG	1A	3586	1/1	0.98	0.04	28,28,28,28	0
58	MG	1A	3105	1/1	0.98	0.12	31,31,31,31	0
58	MG	1A	3414	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3854	1/1	0.98	0.10	14,14,14,14	0
58	MG	1A	3855	1/1	0.98	0.10	30,30,30,30	0
58	MG	1A	3415	1/1	0.98	0.10	33,33,33,33	0
58	MG	2A	3821	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	4014	1/1	0.98	0.03	15,15,15,15	0
58	MG	1A	3168	1/1	0.98	0.12	26,26,26,26	0
58	MG	1A	4016	1/1	0.98	0.07	15,15,15,15	0
58	MG	1A	3591	1/1	0.98	0.06	35,35,35,35	0
58	MG	2A	3551	1/1	0.98	0.03	25,25,25,25	0
58	MG	2A	3069	1/1	0.98	0.04	23,23,23,23	0
58	MG	1A	3717	1/1	0.98	0.05	7,7,7,7	0
58	MG	2A	3554	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3213	1/1	0.98	0.06	32,32,32,32	0
58	MG	1A	3044	1/1	0.98	0.12	25,25,25,25	0
58	MG	1A	3862	1/1	0.98	0.18	29,29,29,29	0
58	MG	2A	3558	1/1	0.98	0.08	20,20,20,20	0
58	MG	1A	3215	1/1	0.98	0.21	23,23,23,23	0
58	MG	1A	3864	1/1	0.98	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3420	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3344	1/1	0.98	0.17	48,48,48,48	0
58	MG	1A	3345	1/1	0.98	0.09	31,31,31,31	0
58	MG	1A	3216	1/1	0.98	0.03	20,20,20,20	0
58	MG	1A	3869	1/1	0.98	0.11	19,19,19,19	0
58	MG	2A	3567	1/1	0.98	0.05	24,24,24,24	0
58	MG	1A	3217	1/1	0.98	0.11	36,36,36,36	0
58	MG	2a	1758	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3279	1/1	0.98	0.08	28,28,28,28	0
58	MG	2A	3570	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3218	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3219	1/1	0.98	0.13	32,32,32,32	0
58	MG	1A	3351	1/1	0.98	0.28	26,26,26,26	0
58	MG	1a	1719	1/1	0.98	0.07	30,30,30,30	0
58	MG	2a	1766	1/1	0.98	0.12	32,32,32,32	0
58	MG	2a	1768	1/1	0.98	0.12	44,44,44,44	0
58	MG	1A	3731	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3732	1/1	0.98	0.05	25,25,25,25	0
58	MG	2A	3856	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3046	1/1	0.98	0.03	18,18,18,18	0
58	MG	1U	206	1/1	0.98	0.12	29,29,29,29	0
58	MG	2A	3094	1/1	0.98	0.13	33,33,33,33	0
58	MG	1A	3734	1/1	0.98	0.03	13,13,13,13	0
58	MG	1U	208	1/1	0.98	0.12	21,21,21,21	0
58	MG	2a	1778	1/1	0.98	0.05	54,54,54,54	0
58	MG	1A	3010	1/1	0.98	0.05	18,18,18,18	0
58	MG	1A	3354	1/1	0.98	0.21	19,19,19,19	0
58	MG	2A	3331	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3285	1/1	0.98	0.11	16,16,16,16	0
58	MG	1V	202	1/1	0.98	0.18	30,30,30,30	0
58	MG	1A	3513	1/1	0.98	0.15	22,22,22,22	0
58	MG	1V	204	1/1	0.98	0.23	22,22,22,22	0
58	MG	2A	3103	1/1	0.98	0.09	22,22,22,22	0
58	MG	2A	3590	1/1	0.98	0.08	40,40,40,40	0
58	MG	2A	3591	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3739	1/1	0.98	0.08	30,30,30,30	0
58	MG	1A	3135	1/1	0.98	0.10	20,20,20,20	0
58	MG	1A	3287	1/1	0.98	0.27	20,20,20,20	0
58	MG	2a	1792	1/1	0.98	0.10	43,43,43,43	0
58	MG	1A	3742	1/1	0.98	0.06	50,50,50,50	0
58	MG	1A	3173	1/1	0.98	0.09	6,6,6,6	0
58	MG	2A	3599	1/1	0.98	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3224	1/1	0.98	0.08	25,25,25,25	0
58	MG	1A	3746	1/1	0.98	0.07	10,10,10,10	0
58	MG	1A	3518	1/1	0.98	0.35	21,21,21,21	0
58	MG	1A	3519	1/1	0.98	0.20	27,27,27,27	0
58	MG	1A	3892	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3136	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3226	1/1	0.98	0.06	30,30,30,30	0
58	MG	1a	1749	1/1	0.98	0.06	37,37,37,37	0
58	MG	2A	3117	1/1	0.98	0.05	39,39,39,39	0
58	MG	1X	104	1/1	0.98	0.15	33,33,33,33	0
58	MG	1X	105	1/1	0.98	0.03	25,25,25,25	0
58	MG	1A	3522	1/1	0.98	0.19	26,26,26,26	0
58	MG	1A	3620	1/1	0.98	0.04	18,18,18,18	0
58	MG	1a	1754	1/1	0.98	0.04	41,41,41,41	0
58	MG	2A	3124	1/1	0.98	0.12	45,45,45,45	0
58	MG	1A	4060	1/1	0.98	0.12	44,44,44,44	0
58	MG	2A	3126	1/1	0.98	0.03	36,36,36,36	0
58	MG	1A	3621	1/1	0.98	0.03	19,19,19,19	0
58	MG	1A	3754	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3009	1/1	0.98	0.03	18,18,18,18	0
58	MG	1A	3035	1/1	0.98	0.07	41,41,41,41	0
58	MG	1A	3295	1/1	0.98	0.16	15,15,15,15	0
58	MG	1A	3902	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3903	1/1	0.98	0.05	15,15,15,15	0
58	MG	1A	3625	1/1	0.98	0.04	18,18,18,18	0
58	MG	2A	3625	1/1	0.98	0.04	25,25,25,25	0
58	MG	2D	302	1/1	0.98	0.14	38,38,38,38	0
58	MG	1A	4071	1/1	0.98	0.07	6,6,6,6	0
58	MG	2A	3136	1/1	0.98	0.04	34,34,34,34	0
58	MG	2D	305	1/1	0.98	0.06	26,26,26,26	0
58	MG	2D	306	1/1	0.98	0.24	30,30,30,30	0
58	MG	2A	3628	1/1	0.98	0.04	29,29,29,29	0
58	MG	1a	1765	1/1	0.98	0.10	40,40,40,40	0
58	MG	1A	3365	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3761	1/1	0.98	0.09	8,8,8,8	0
58	MG	1A	3907	1/1	0.98	0.06	35,35,35,35	0
58	MG	2E	305	1/1	0.98	0.08	35,35,35,35	0
58	MG	1I	101	1/1	0.98	0.24	23,23,23,23	0
58	MG	1A	3177	1/1	0.98	0.14	21,21,21,21	0
58	MG	1a	1771	1/1	0.98	0.04	49,49,49,49	0
58	MG	1A	3763	1/1	0.98	0.04	20,20,20,20	0
58	MG	2A	3377	1/1	0.98	0.03	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1838	1/1	0.98	0.06	49,49,49,49	0
58	MG	1l	104	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	4078	1/1	0.98	0.03	19,19,19,19	0
58	MG	1A	3629	1/1	0.98	0.05	11,11,11,11	0
58	MG	2A	3149	1/1	0.98	0.11	27,27,27,27	0
58	MG	1a	1777	1/1	0.98	0.05	56,56,56,56	0
58	MG	1A	3113	1/1	0.98	0.12	25,25,25,25	0
58	MG	1A	3233	1/1	0.98	0.21	24,24,24,24	0
58	MG	1a	1780	1/1	0.98	0.05	40,40,40,40	0
58	MG	2A	3648	1/1	0.98	0.08	44,44,44,44	0
58	MG	13	101	1/1	0.98	0.11	18,18,18,18	0
58	MG	1A	3914	1/1	0.98	0.05	31,31,31,31	0
58	MG	13	103	1/1	0.98	0.07	33,33,33,33	0
58	MG	1a	1784	1/1	0.98	0.05	57,57,57,57	0
58	MG	1a	1785	1/1	0.98	0.05	40,40,40,40	0
58	MG	1a	1786	1/1	0.98	0.04	44,44,44,44	0
58	MG	2A	3160	1/1	0.98	0.12	37,37,37,37	0
58	MG	15	101	1/1	0.98	0.23	28,28,28,28	0
58	MG	1A	3179	1/1	0.98	0.07	19,19,19,19	0
58	MG	1A	3633	1/1	0.98	0.05	13,13,13,13	0
58	MG	15	104	1/1	0.98	0.15	20,20,20,20	0
58	MG	1a	1791	1/1	0.98	0.04	53,53,53,53	0
58	MG	1a	1792	1/1	0.98	0.03	33,33,33,33	0
58	MG	1A	3769	1/1	0.98	0.06	17,17,17,17	0
58	MG	1a	1794	1/1	0.98	0.03	51,51,51,51	0
58	MG	1A	3634	1/1	0.98	0.04	20,20,20,20	0
58	MG	15	107	1/1	0.98	0.04	18,18,18,18	0
58	MG	1A	3771	1/1	0.98	0.07	17,17,17,17	0
58	MG	1A	3922	1/1	0.98	0.09	42,42,42,42	0
58	MG	16	101	1/1	0.98	0.05	32,32,32,32	0
58	MG	1a	1800	1/1	0.98	0.07	52,52,52,52	0
58	MG	1A	3772	1/1	0.98	0.04	21,21,21,21	0
58	MG	17	101	1/1	0.98	0.11	23,23,23,23	0
58	MG	2A	3672	1/1	0.98	0.10	37,37,37,37	0
58	MG	17	102	1/1	0.98	0.20	31,31,31,31	0
58	MG	2A	3178	1/1	0.98	0.08	19,19,19,19	0
58	MG	1A	3036	1/1	0.98	0.09	21,21,21,21	0
58	MG	2A	3412	1/1	0.98	0.06	24,24,24,24	0
58	MG	1a	1805	1/1	0.98	0.06	47,47,47,47	0
58	MG	2A	3678	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3532	1/1	0.98	0.08	39,39,39,39	0
58	MG	1A	3637	1/1	0.98	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	18	104	1/1	0.98	0.04	28,28,28,28	0
58	MG	1A	3182	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3778	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	3450	1/1	0.98	0.18	27,27,27,27	0
58	MG	1A	3038	1/1	0.98	0.11	28,28,28,28	0
58	MG	1A	3082	1/1	0.98	0.15	22,22,22,22	0
59	K	1A	3569	1/1	0.98	0.04	29,29,29,29	0
58	MG	2A	3189	1/1	0.98	0.08	37,37,37,37	0
60	ZN	14	501	1/1	0.98	0.05	79,79,79,79	0
60	ZN	1n	102	1/1	0.98	0.03	47,47,47,47	0
60	ZN	2Y	501	1/1	0.98	0.04	70,70,70,70	0
58	MG	1A	3643	1/1	0.98	0.05	9,9,9,9	0
58	MG	2a	1760	1/1	0.99	0.04	62,62,62,62	0
58	MG	1A	3288	1/1	0.99	0.20	31,31,31,31	0
58	MG	2A	3739	1/1	0.99	0.05	38,38,38,38	0
58	MG	1A	3129	1/1	0.99	0.26	29,29,29,29	0
58	MG	1A	3638	1/1	0.99	0.03	12,12,12,12	0
58	MG	1A	3075	1/1	0.99	0.03	23,23,23,23	0
58	MG	1A	3229	1/1	0.99	0.12	30,30,30,30	0
58	MG	2a	1767	1/1	0.99	0.05	28,28,28,28	0
58	MG	1A	3510	1/1	0.99	0.04	26,26,26,26	0
58	MG	2a	1769	1/1	0.99	0.04	46,46,46,46	0
58	MG	18	102	1/1	0.99	0.10	24,24,24,24	0
58	MG	1A	4106	1/1	0.99	0.04	42,42,42,42	0
58	MG	1B	201	1/1	0.99	0.07	36,36,36,36	0
58	MG	1B	202	1/1	0.99	0.11	34,34,34,34	0
58	MG	1A	3824	1/1	0.99	0.06	25,25,25,25	0
58	MG	1A	3048	1/1	0.99	0.15	25,25,25,25	0
58	MG	1A	3231	1/1	0.99	0.14	19,19,19,19	0
58	MG	1A	3434	1/1	0.99	0.06	34,34,34,34	0
58	MG	1A	3397	1/1	0.99	0.10	22,22,22,22	0
58	MG	1Q	202	1/1	0.99	0.07	22,22,22,22	0
58	MG	1A	3204	1/1	0.99	0.08	24,24,24,24	0
58	MG	1A	3111	1/1	0.99	0.21	22,22,22,22	0
58	MG	1A	3705	1/1	0.99	0.03	5,5,5,5	0
58	MG	1A	3180	1/1	0.99	0.06	21,21,21,21	0
58	MG	1A	3112	1/1	0.99	0.04	29,29,29,29	0
58	MG	1A	3559	1/1	0.99	0.15	22,22,22,22	0
58	MG	1A	3157	1/1	0.99	0.13	22,22,22,22	0
58	MG	1a	1711	1/1	0.99	0.08	29,29,29,29	0
58	MG	1A	3403	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3653	1/1	0.99	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3640	1/1	0.99	0.06	26,26,26,26	0
58	MG	1A	3039	1/1	0.99	0.28	22,22,22,22	0
58	MG	1A	3078	1/1	0.99	0.17	24,24,24,24	0
58	MG	1A	3013	1/1	0.99	0.06	12,12,12,12	0
58	MG	1A	3609	1/1	0.99	0.08	31,31,31,31	0
58	MG	1A	3007	1/1	0.99	0.04	29,29,29,29	0
58	MG	1A	3270	1/1	0.99	0.05	30,30,30,30	0
58	MG	2A	3076	1/1	0.99	0.15	28,28,28,28	0
58	MG	2A	3527	1/1	0.99	0.03	20,20,20,20	0
58	MG	1U	201	1/1	0.99	0.19	16,16,16,16	0
58	MG	2A	3078	1/1	0.99	0.10	20,20,20,20	0
58	MG	2A	3530	1/1	0.99	0.06	30,30,30,30	0
58	MG	1A	3781	1/1	0.99	0.03	15,15,15,15	0
58	MG	1A	3042	1/1	0.99	0.12	13,13,13,13	0
58	MG	1a	1723	1/1	0.99	0.04	42,42,42,42	0
58	MG	1A	3003	1/1	0.99	0.05	19,19,19,19	0
58	MG	2A	3083	1/1	0.99	0.05	44,44,44,44	0
58	MG	1A	3614	1/1	0.99	0.08	25,25,25,25	0
58	MG	1A	3306	1/1	0.99	0.05	18,18,18,18	0
58	MG	1A	3912	1/1	0.99	0.03	32,32,32,32	0
58	MG	1A	3031	1/1	0.99	0.13	20,20,20,20	0
58	MG	2A	3424	1/1	0.99	0.05	25,25,25,25	0
58	MG	1U	209	1/1	0.99	0.22	24,24,24,24	0
58	MG	1a	1730	1/1	0.99	0.04	22,22,22,22	0
58	MG	1a	1731	1/1	0.99	0.10	25,25,25,25	0
58	MG	1A	4055	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3244	1/1	0.99	0.24	23,23,23,23	0
58	MG	1A	4057	1/1	0.99	0.07	43,43,43,43	0
58	MG	1A	3573	1/1	0.99	0.14	31,31,31,31	0
58	MG	1A	3667	1/1	0.99	0.06	21,21,21,21	0
58	MG	1A	3917	1/1	0.99	0.03	26,26,26,26	0
58	MG	1V	205	1/1	0.99	0.10	17,17,17,17	0
58	MG	1A	3918	1/1	0.99	0.03	20,20,20,20	0
58	MG	1a	1740	1/1	0.99	0.06	23,23,23,23	0
58	MG	1A	3790	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	3120	1/1	0.99	0.17	25,25,25,25	0
58	MG	1D	302	1/1	0.99	0.06	31,31,31,31	0
58	MG	1D	303	1/1	0.99	0.05	25,25,25,25	0
58	MG	1a	1745	1/1	0.99	0.03	44,44,44,44	0
58	MG	1D	304	1/1	0.99	0.04	7,7,7,7	0
58	MG	1A	3055	1/1	0.99	0.07	37,37,37,37	0
58	MG	1W	206	1/1	0.99	0.03	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1D	306	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3990	1/1	0.99	0.05	14,14,14,14	0
58	MG	1A	3670	1/1	0.99	0.03	10,10,10,10	0
58	MG	1A	3992	1/1	0.99	0.08	24,24,24,24	0
58	MG	2A	3565	1/1	0.99	0.06	24,24,24,24	0
58	MG	1A	3671	1/1	0.99	0.05	19,19,19,19	0
58	MG	1A	4069	1/1	0.99	0.03	27,27,27,27	0
58	MG	1A	4070	1/1	0.99	0.04	34,34,34,34	0
58	MG	1E	301	1/1	0.99	0.23	20,20,20,20	0
58	MG	1A	3576	1/1	0.99	0.18	32,32,32,32	0
58	MG	1A	3673	1/1	0.99	0.04	27,27,27,27	0
58	MG	1E	304	1/1	0.99	0.13	22,22,22,22	0
58	MG	2A	3009	1/1	0.99	0.05	29,29,29,29	0
58	MG	2A	3120	1/1	0.99	0.04	16,16,16,16	0
58	MG	2A	3696	1/1	0.99	0.10	21,21,21,21	0
58	MG	1E	305	1/1	0.99	0.14	21,21,21,21	0
58	MG	2A	3823	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	4073	1/1	0.99	0.04	12,12,12,12	0
58	MG	1A	3674	1/1	0.99	0.05	12,12,12,12	0
58	MG	1A	3143	1/1	0.99	0.10	20,20,20,20	0
58	MG	1A	3278	1/1	0.99	0.07	31,31,31,31	0
58	MG	10	103	1/1	0.99	0.14	28,28,28,28	0
58	MG	1A	3068	1/1	0.99	0.03	19,19,19,19	0
58	MG	2A	3830	1/1	0.99	0.07	25,25,25,25	0
58	MG	2A	3831	1/1	0.99	0.04	36,36,36,36	0
58	MG	1A	3045	1/1	0.99	0.06	23,23,23,23	0
58	MG	2A	3833	1/1	0.99	0.03	43,43,43,43	0
58	MG	2A	3466	1/1	0.99	0.06	14,14,14,14	0
58	MG	1A	3679	1/1	0.99	0.02	11,11,11,11	0
58	MG	1E	313	1/1	0.99	0.08	25,25,25,25	0
58	MG	1A	3383	1/1	0.99	0.15	21,21,21,21	0
58	MG	1A	3627	1/1	0.99	0.12	39,39,39,39	0
58	MG	1F	302	1/1	0.99	0.09	13,13,13,13	0
58	MG	1A	3037	1/1	0.99	0.09	15,15,15,15	0
58	MG	1A	3460	1/1	0.99	0.13	32,32,32,32	0
58	MG	1a	1775	1/1	0.99	0.03	42,42,42,42	0
58	MG	2A	3843	1/1	0.99	0.04	21,21,21,21	0
58	MG	1A	3743	1/1	0.99	0.03	39,39,39,39	0
58	MG	1F	306	1/1	0.99	0.03	28,28,28,28	0
58	MG	2A	3139	1/1	0.99	0.10	27,27,27,27	0
58	MG	2A	3595	1/1	0.99	0.06	29,29,29,29	0
58	MG	2A	3596	1/1	0.99	0.03	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4007	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	4086	1/1	0.99	0.03	16,16,16,16	0
58	MG	1A	3937	1/1	0.99	0.03	16,16,16,16	0
58	MG	1A	3282	1/1	0.99	0.14	21,21,21,21	0
58	MG	1A	3809	1/1	0.99	0.03	14,14,14,14	0
58	MG	1A	3058	1/1	0.99	0.02	16,16,16,16	0
58	MG	2A	3726	1/1	0.99	0.11	26,26,26,26	0
58	MG	2A	3034	1/1	0.99	0.10	32,32,32,32	0
58	MG	1A	3941	1/1	0.99	0.05	18,18,18,18	0
58	MG	1A	3148	1/1	0.99	0.13	14,14,14,14	0
58	MG	1A	3687	1/1	0.99	0.04	17,17,17,17	0
58	MG	2A	3731	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	3072	1/1	0.99	0.22	21,21,21,21	0
58	MG	1A	3689	1/1	0.99	0.03	11,11,11,11	0
60	ZN	1Y	204	1/1	0.99	0.02	54,54,54,54	0
58	MG	1A	3690	1/1	0.99	0.04	16,16,16,16	0
60	ZN	19	102	1/1	0.99	0.03	31,31,31,31	0
58	MG	1A	3073	1/1	0.99	0.04	8,8,8,8	0
58	MG	1A	3023	1/1	0.99	0.06	6,6,6,6	0
58	MG	1A	4020	1/1	0.99	0.02	21,21,21,21	0
60	ZN	25	105	1/1	0.99	0.06	50,50,50,50	0
60	ZN	29	102	1/1	0.99	0.03	62,62,62,62	0
60	ZN	2n	501	1/1	0.99	0.03	68,68,68,68	0
61	SF4	1d	302	8/8	0.99	0.04	45,51,56,57	0
61	SF4	2d	302	8/8	0.99	0.03	45,53,60,64	0
60	ZN	15	110	1/1	1.00	0.04	28,28,28,28	0
60	ZN	16	103	1/1	1.00	0.02	30,30,30,30	0
58	MG	1A	3724	1/1	1.00	0.04	5,5,5,5	0
58	MG	2A	3635	1/1	1.00	0.04	27,27,27,27	0
58	MG	1A	3780	1/1	1.00	0.02	21,21,21,21	0
58	MG	1P	204	1/1	1.00	0.05	23,23,23,23	0
58	MG	1A	4036	1/1	1.00	0.02	13,13,13,13	0
60	ZN	26	102	1/1	1.00	0.02	43,43,43,43	0
58	MG	1A	3014	1/1	1.00	0.08	16,16,16,16	0
58	MG	1A	3777	1/1	1.00	0.02	23,23,23,23	0
58	MG	1A	3756	1/1	1.00	0.04	10,10,10,10	0
58	MG	2A	3714	1/1	1.00	0.04	13,13,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.