



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:19 AM UTC

PDB ID : 9DFC / pdb_00009dfc
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with lasso peptide lariocidin, mRNA, aminoacylated A-site Phe-tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.50Å 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 : 2.50 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)

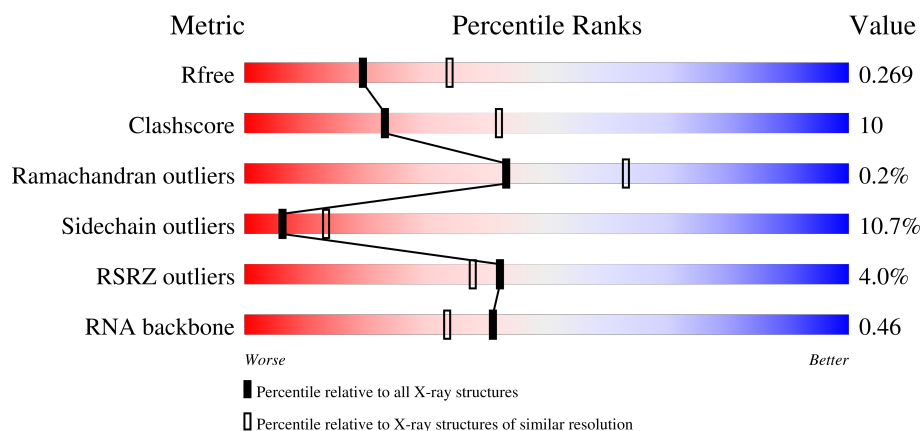
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)


























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>4%</div> <div>62%</div> <div>29%</div> <div>7%</div> <div>.</div> </div>
1	2A	2915	<div> <div>4%</div> <div>57%</div> <div>31%</div> <div>8%</div> <div>.</div> </div>

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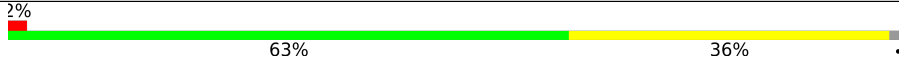
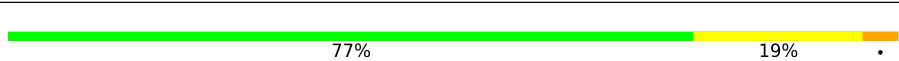
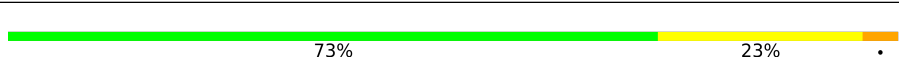
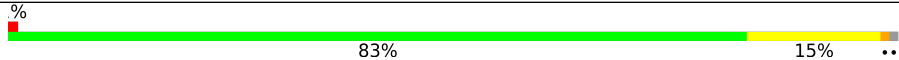
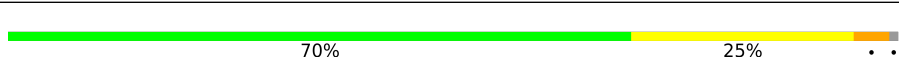
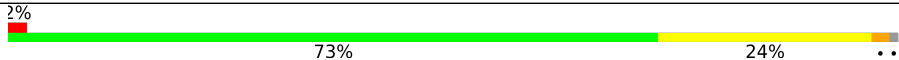
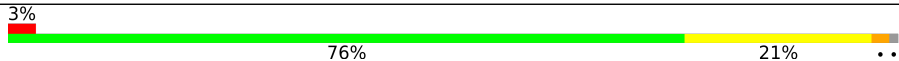
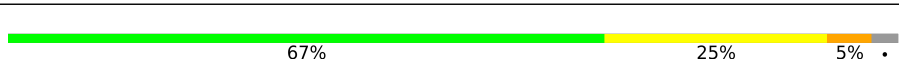

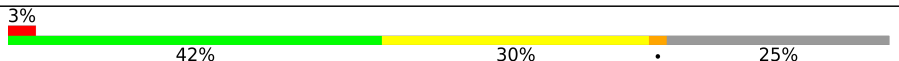
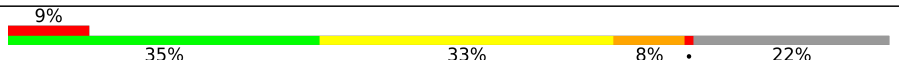
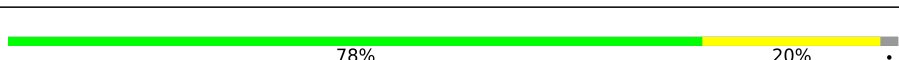
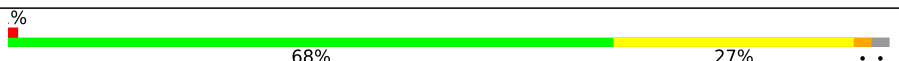
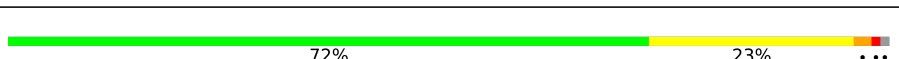
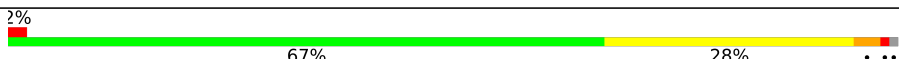

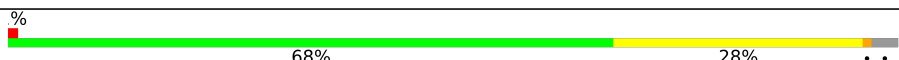
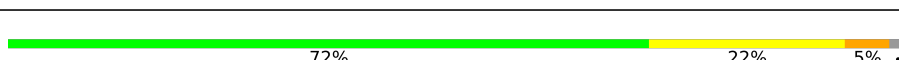
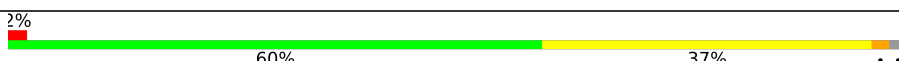
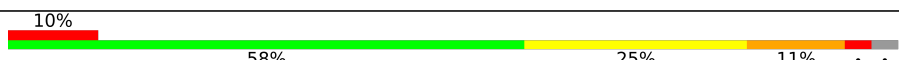
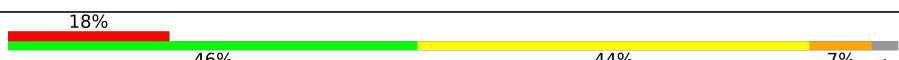
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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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	

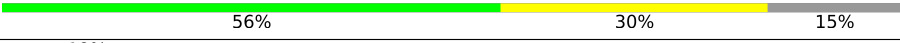

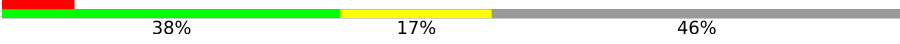
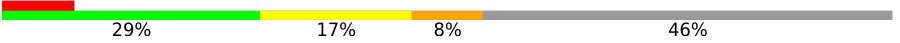

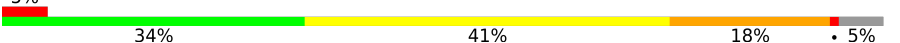


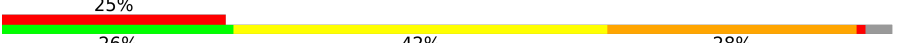
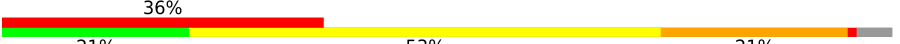

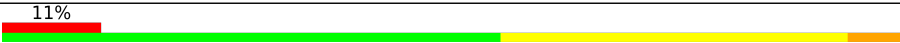
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Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	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	18	
57	2z	18	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1A	3418	-	-	-	X
58	MG	1U	211	-	-	-	X
58	MG	2a	1634	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300593 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	1z	18	Total	C	N	O	0	0	0
			132	81	29	22			
57	2z	18	Total	C	N	O	0	0	0
			132	81	29	22			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1108	Total	Mg	0	0
			1108	1108		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	39	Total 39	Mg 39	0	0
58	1D	13	Total 13	Mg 13	0	0
58	1E	14	Total 14	Mg 14	0	0
58	1F	12	Total 12	Mg 12	0	0
58	1G	5	Total 5	Mg 5	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	4	Total 4	Mg 4	0	0
58	1Q	6	Total 6	Mg 6	0	0
58	1R	5	Total 5	Mg 5	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	9	Total 9	Mg 9	0	0
58	1W	6	Total 6	Mg 6	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	10	Total 10	Mg 10	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	14	1	Total 1	Mg 1	0	0
58	15	7	Total 7	Mg 7	0	0
58	16	2	Total 2	Mg 2	0	0
58	17	4	Total 4	Mg 4	0	0
58	18	3	Total 3	Mg 3	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	216	Total 216	Mg 216	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	1t	1	Total 1	Mg 1	0	0
58	1v	2	Total 2	Mg 2	0	0
58	1w	9	Total 9	Mg 9	0	0
58	1x	13	Total 13	Mg 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1y	1	Total 1	Mg 1	0	0
58	1z	1	Total 1	Mg 1	0	0
58	2A	882	Total 882	Mg 882	0	0
58	2B	20	Total 20	Mg 20	0	0
58	2D	7	Total 7	Mg 7	0	0
58	2E	10	Total 10	Mg 10	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	2	Total 2	Mg 2	0	0
58	2T	4	Total 4	Mg 4	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	1	Total 1	Mg 1	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	3	Total 3	Mg 3	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	2	Total 2	Mg 2	0	0
58	28	4	Total 4	Mg 4	0	0
58	2a	240	Total 240	Mg 240	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2l	5	Total 5	Mg 5	0	0
58	2n	1	Total 1	Mg 1	0	0
58	2p	1	Total 1	Mg 1	0	0
58	2q	3	Total 3	Mg 3	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	8	Total 8	Mg 8	0	0
58	2y	6	Total 6	Mg 6	0	0

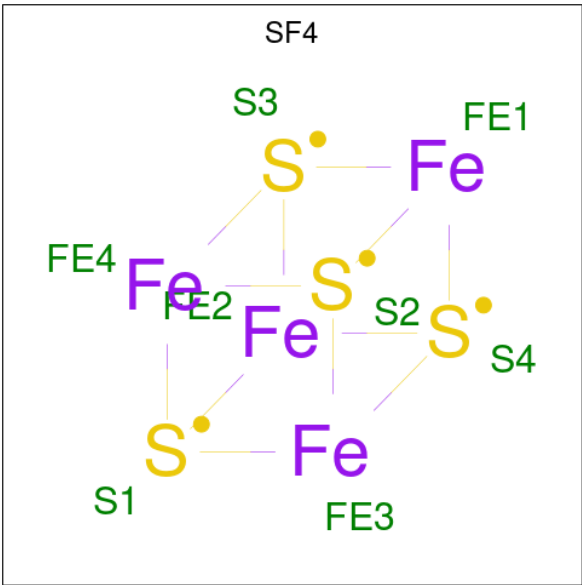
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

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

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	2017	Total	O	0	0
			2017	2017		
62	1B	63	Total	O	0	0
			63	63		
62	1D	28	Total	O	0	0
			28	28		
62	1E	29	Total	O	0	0
			29	29		
62	1F	14	Total	O	0	0
			14	14		
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	6	Total	O	0	0
			6	6		
62	1O	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1P	20	Total 20	O 20	0	0
62	1Q	7	Total 7	O 7	0	0
62	1R	11	Total 11	O 11	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	9	Total 9	O 9	0	0
62	1U	13	Total 13	O 13	0	0
62	1V	8	Total 8	O 8	0	0
62	1W	6	Total 6	O 6	0	0
62	1X	6	Total 6	O 6	0	0
62	1Y	2	Total 2	O 2	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	11	Total 11	O 11	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	9	Total 9	O 9	0	0
62	18	8	Total 8	O 8	0	0
62	1a	386	Total 386	O 386	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1b	1	Total 1	O 1	0	0
62	1g	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	9	Total 9	O 9	0	0
62	1m	1	Total 1	O 1	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	5	Total 5	O 5	0	0
62	1w	21	Total 21	O 21	0	0
62	1x	15	Total 15	O 15	0	0
62	1y	1	Total 1	O 1	0	0
62	1z	1	Total 1	O 1	0	0
62	2A	1165	Total 1165	O 1165	0	0
62	2B	22	Total 22	O 22	0	0
62	2D	22	Total 22	O 22	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2N	1	Total 1	O 1	0	0
62	2O	3	Total 3	O 3	0	0
62	2P	15	Total 15	O 15	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	4	Total 4	O 4	0	0
62	2T	4	Total 4	O 4	0	0
62	2U	2	Total 2	O 2	0	0
62	2V	1	Total 1	O 1	0	0
62	2X	1	Total 1	O 1	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	12	Total 12	O 12	0	0
62	23	2	Total 2	O 2	0	0
62	25	1	Total 1	O 1	0	0
62	27	5	Total 5	O 5	0	0
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	283	Total 283	O 283	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	2	Total 2	O 2	0	0

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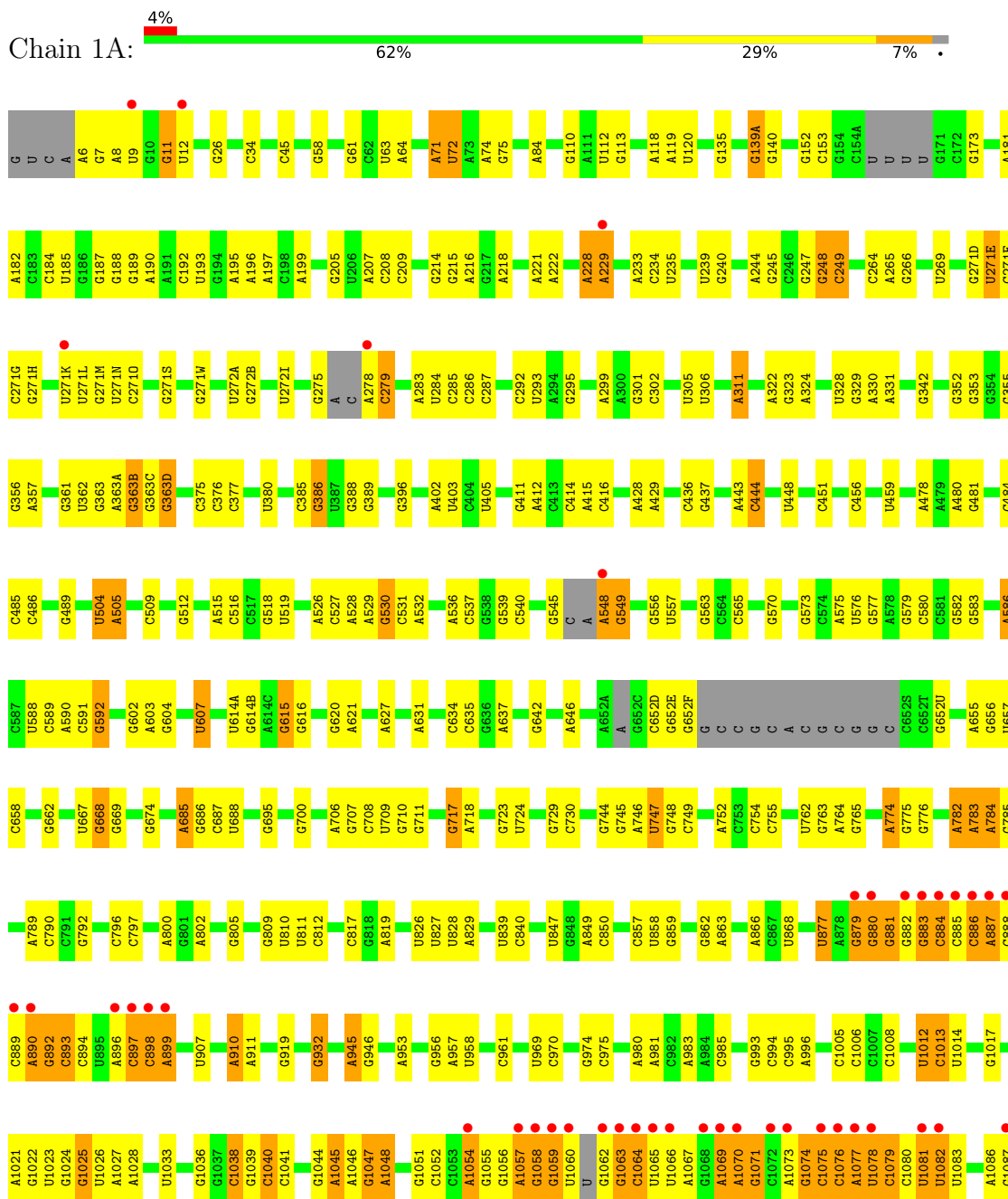
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2e	1	Total 1	O 1	0	0
62	2g	1	Total 1	O 1	0	0
62	2i	1	Total 1	O 1	0	0
62	2j	3	Total 3	O 3	0	0
62	2l	6	Total 6	O 6	0	0
62	2p	1	Total 1	O 1	0	0
62	2r	1	Total 1	O 1	0	0
62	2t	1	Total 1	O 1	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	7	Total 7	O 7	0	0
62	2x	8	Total 8	O 8	0	0
62	2y	6	Total 6	O 6	0	0

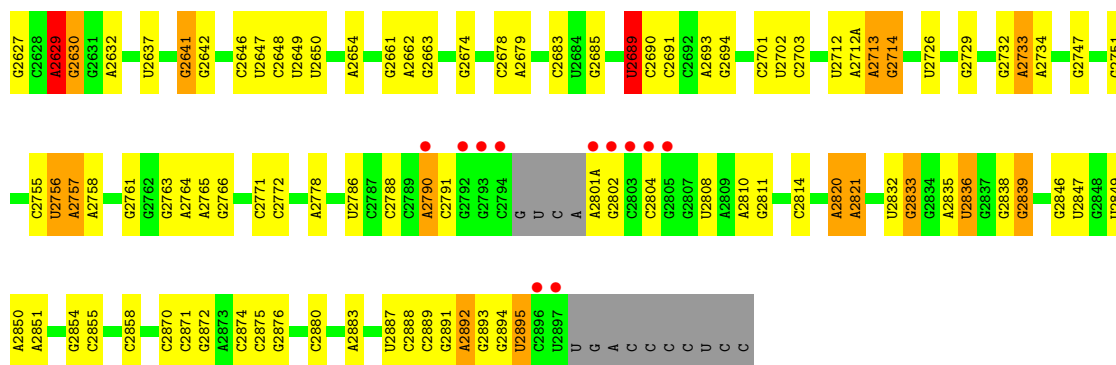
3 Residue-property plots

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.

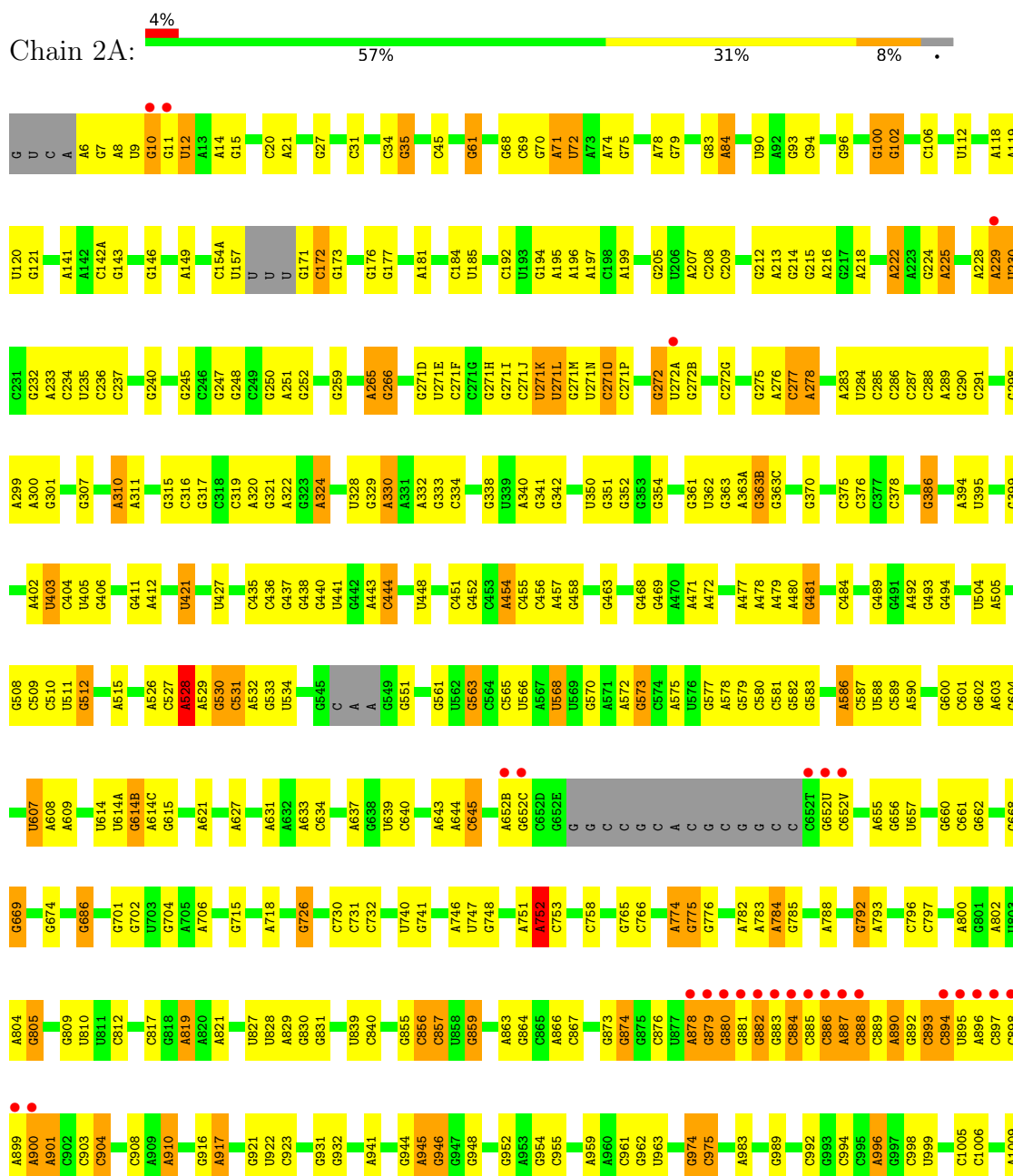
• Molecule 1: 23S Ribosomal RNA



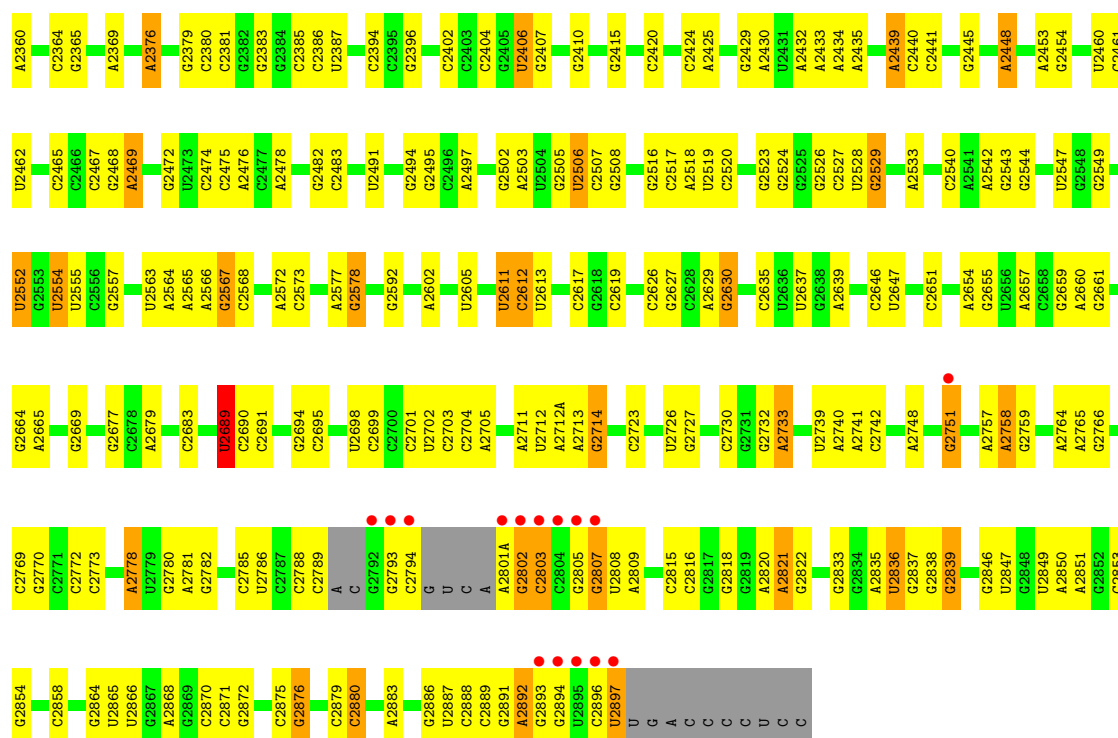
G2529	G2396	C2313	G2192	U2130	A2051	G1930	A1812	G1674	U	G1421	U1300	A1174	A1088
A2533	C2404	G2314	G2196	G2131	G2052	U1931	G1813	U1688	A	A1427	A1301	U1175	G1089
A2534	G2405	G2315	U2197	U2132	A1932	G1932	A1814	A1932	C	C1428	G1302	G1176	U1090
G2535	U2405	G2316	A2198	G2133	G2055	G1933	A1815	U1693	G1537	C1429	A1303	A1177	G1091
G2536	G2406	G2319	G2199	A2135	G2056	A1937	G1816	G1696	U1540	C1430	G1311	C1178	G1092
U2537	G2407	A2320	U2203	C2136	A2060	A1938	G1817	G1697	G1541	U1431	U1312	C1179	G1093
G2538	A2418	G2325	G2205	C2137	G2061	U1939	U1820	A1698	A1542	U1431	U1312	C1180	U1094
G2544	U2419	G2326	G2206	C2138	G2062	C1942	G1823	A1700	C1545	G1442	G1315	C1181	A1095
G2549	A2422	A2327	G2207	C2139	C2065	U1946	G1824	A1700	C1546	A1445	A1321	A1182	A1096
G2550	U2423	A2328	A2208	C2140	C2066	U1947	A1825	G1703	C1547	A1448	G1328	U1097	A1098
U2551	C2424	G2329	U2218	G2141	G2069	G1948	G1826	G1703	A1554	G1448	G1328	G1187	G1099
U2552	A2425	G2330	A2225	C2142	G2072	U1955	A1827	G1721	A1558	A1449	U1329	C1201	C1100
G2553	C2427	A2335	G2228	C2145	C2072	U1962	G1828	G1721	A1558	G1450	G1332	G1202	A1102
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G2557	G2429	A2337	G2243	G2148	U2075	U1964	C1830	G1756	A1578	U1452	G1338	A1220	U1104
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A2565	A2439	G2345	U2245	G2151	U2079	U1966	U1847	G1767	G1581	C1467	A1360	G1235	G1125
A2566	C2440	A2346	A2247	G2152	U2086	G1968	U1851	G1767	C1582	G1473	G1364	G1243	G1128
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G2626	G2513	G2385	G2307	G2187	G2125	A2033	C1926	U1808	C1670	G	U1420	G1173	
		U2387	G2308	C2188	A2126	C2039	U1926	U1808	C1670	G	U1420	G1173	
		U2390	A2311	U2189	G2127	C2039	U1926	U1808	C1670	G	U1420	G1173	
		G2391	U2312	C2191	C2129	C2043	G1929	U1808	C1670	G	U1420	G1173	



• Molecule 1: 23S Ribosomal RNA

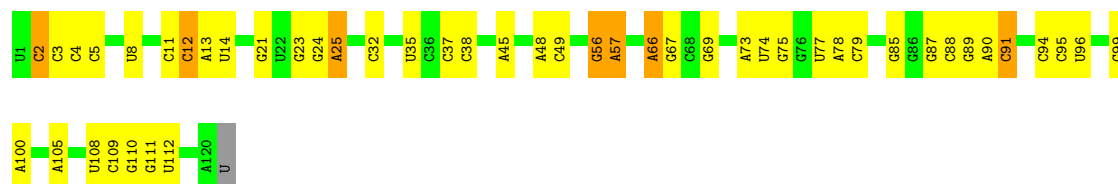






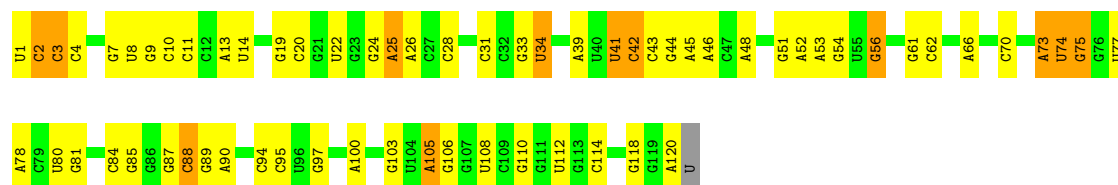
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 60% 34% 6% .



• Molecule 2: 5S Ribosomal RNA

Chain 2B: 46% 43% 10% .



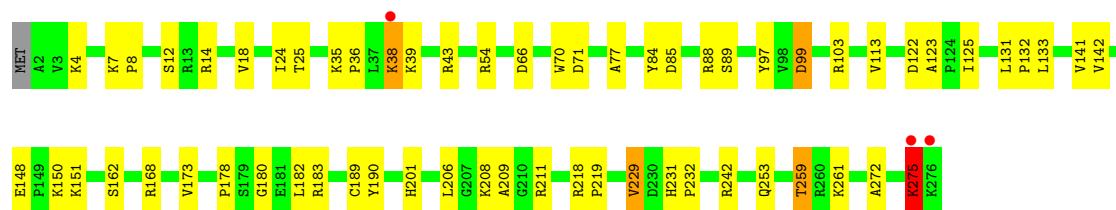
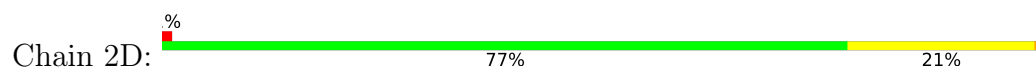
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 75% 21% .

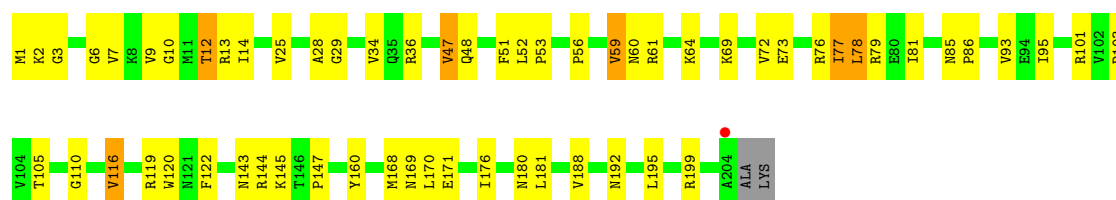




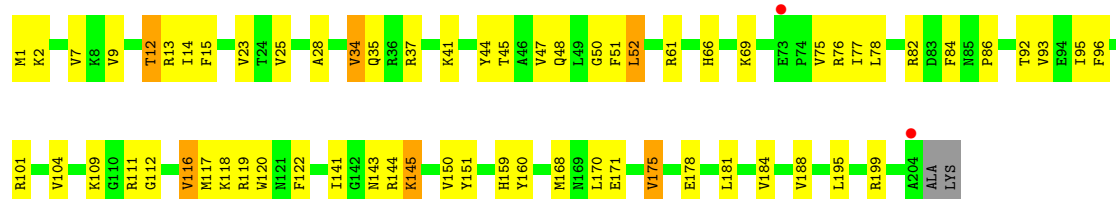
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3

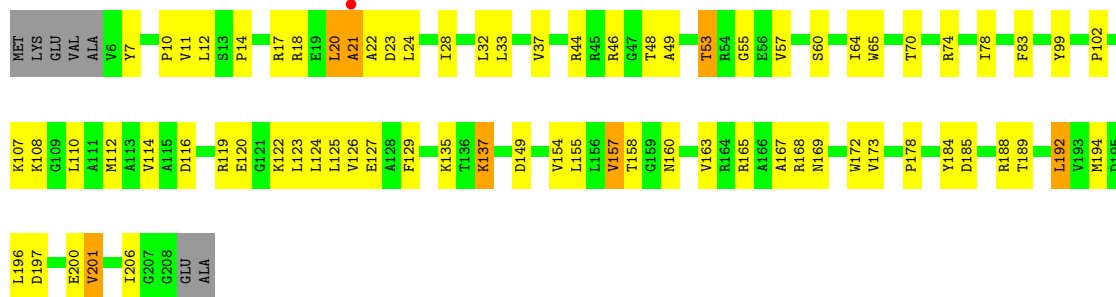


- Molecule 5: 50S ribosomal protein L4



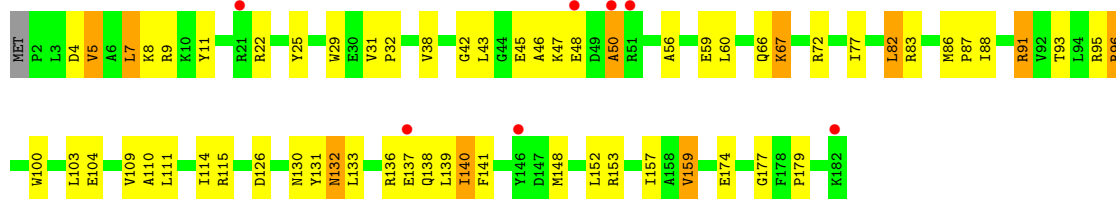
- Molecule 5: 50S ribosomal protein L4

Chain 2F:  61% 32% . .



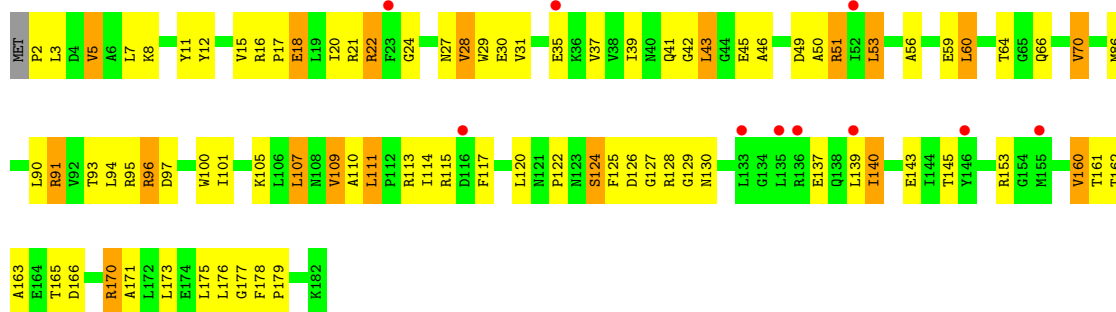
- Molecule 6: 50S ribosomal protein L5

Chain 1G:  4% 65% 29% 5% .



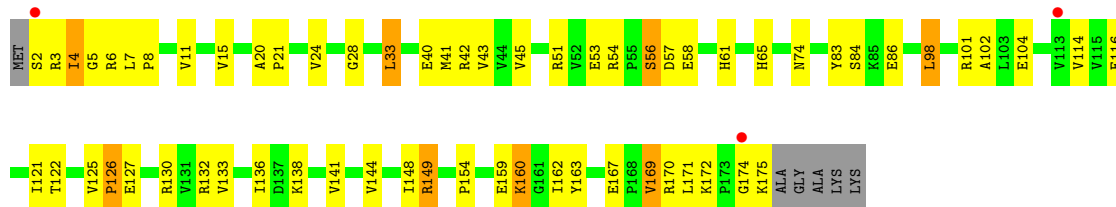
- Molecule 6: 50S ribosomal protein L5

Chain 2G:  5% 52% 37% 10% .

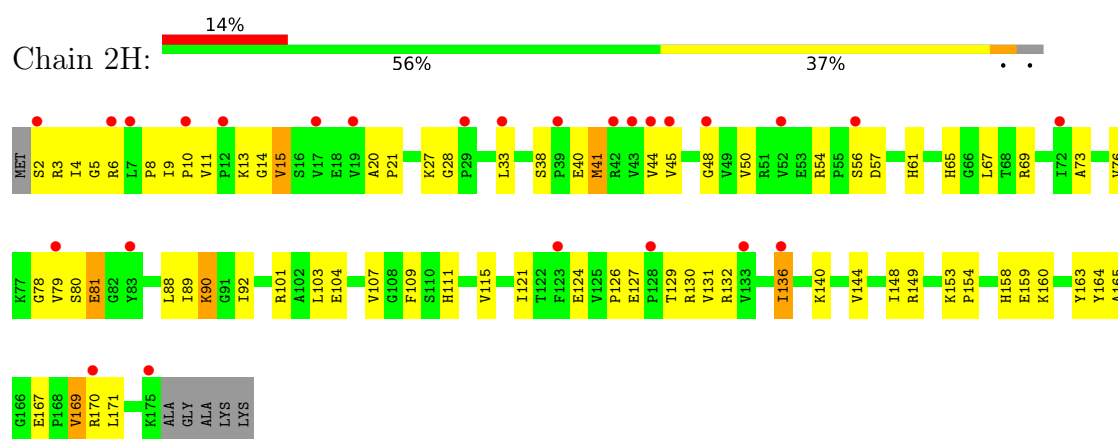


- Molecule 7: 50S ribosomal protein L6

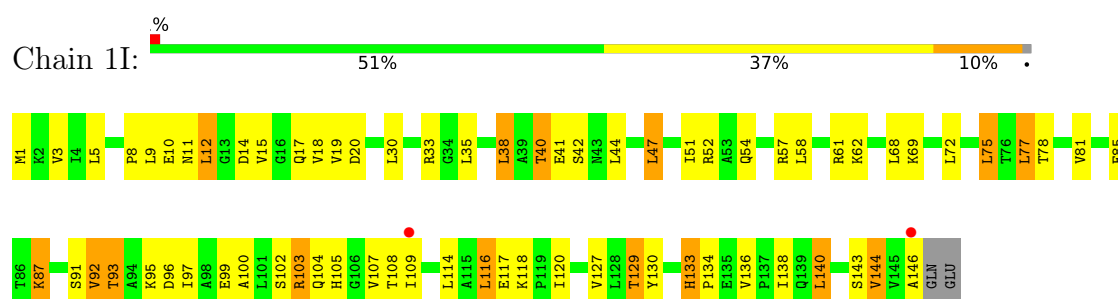
Chain 1H:  2% 62% 31% . .



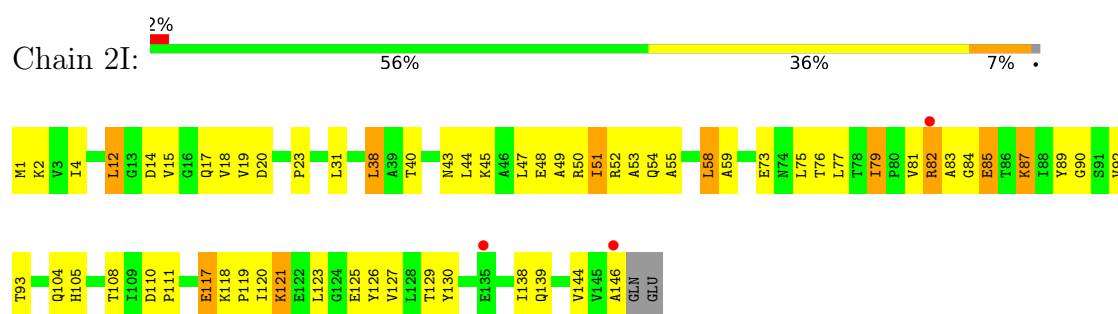
- Molecule 7: 50S ribosomal protein L6



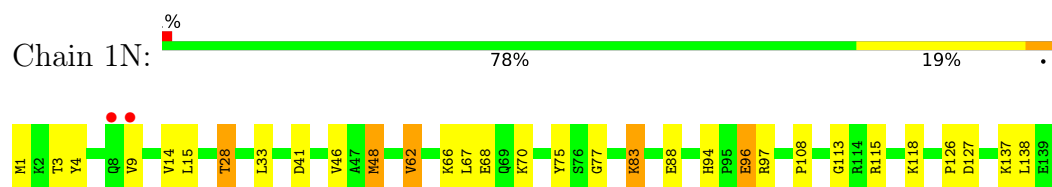
• Molecule 8: 50S ribosomal protein L9



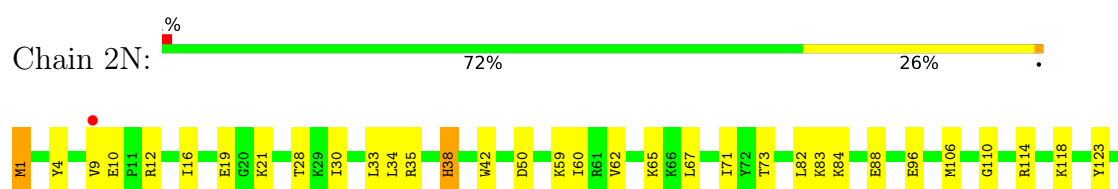
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

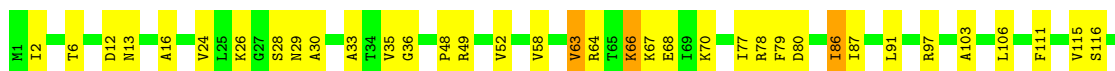




- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14



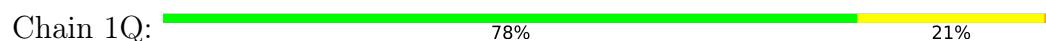
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

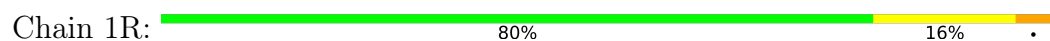




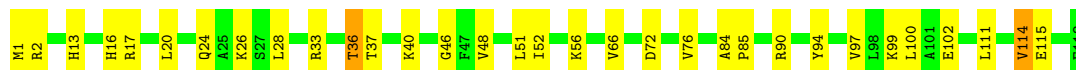
- Molecule 12: 50S ribosomal protein L16



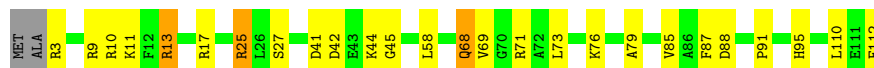
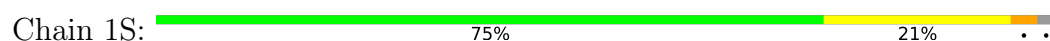
- Molecule 13: 50S ribosomal protein L17



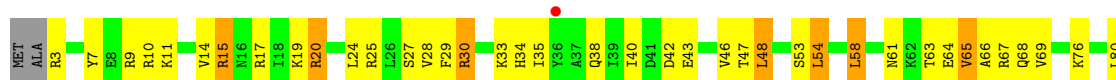
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

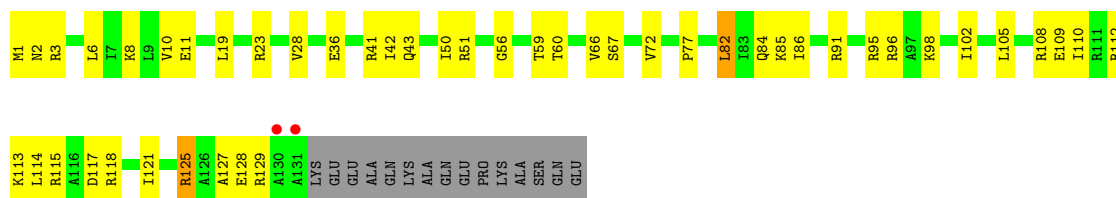


- Molecule 14: 50S ribosomal protein L18

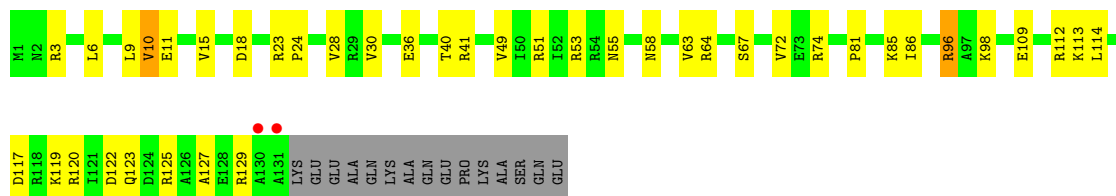


- Molecule 15: 50S ribosomal protein L19

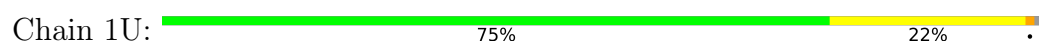




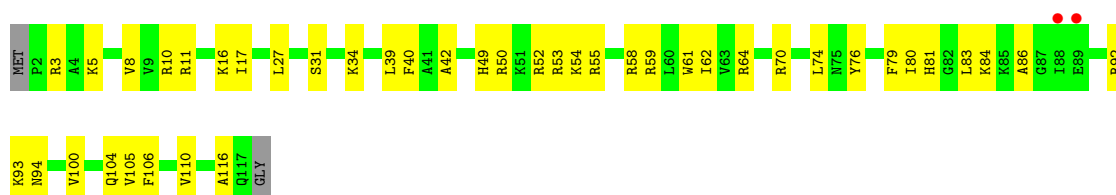
• Molecule 15: 50S ribosomal protein L19



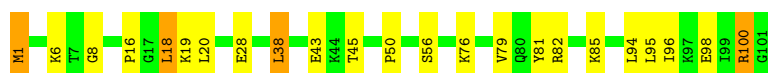
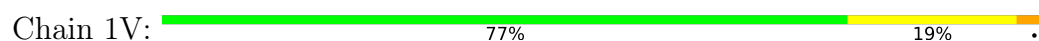
• Molecule 16: 50S ribosomal protein L20



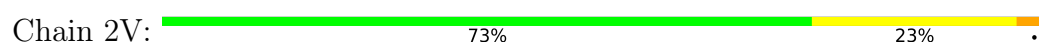
• Molecule 16: 50S ribosomal protein L20



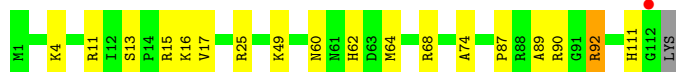
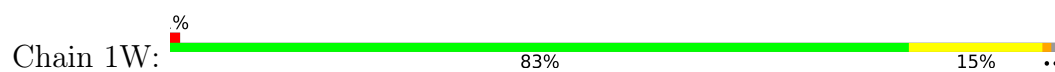
• Molecule 17: 50S ribosomal protein L21



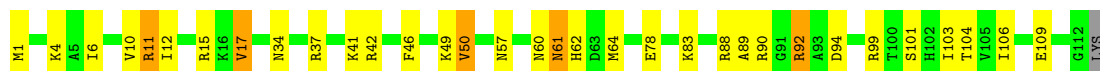
• Molecule 17: 50S ribosomal protein L21



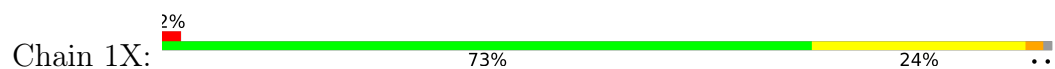
• Molecule 18: 50S ribosomal protein L22



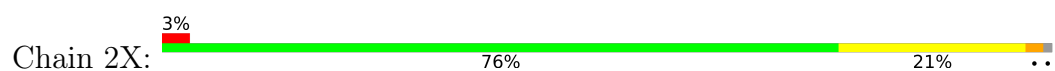
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



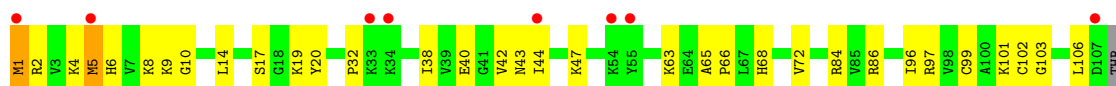
- Molecule 19: 50S ribosomal protein L23



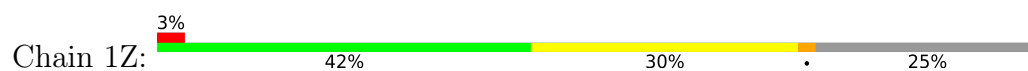
- Molecule 20: 50S ribosomal protein L24

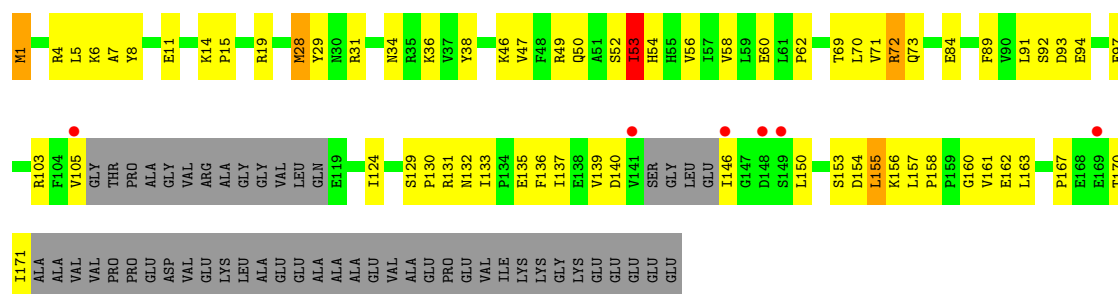


- Molecule 20: 50S ribosomal protein L24

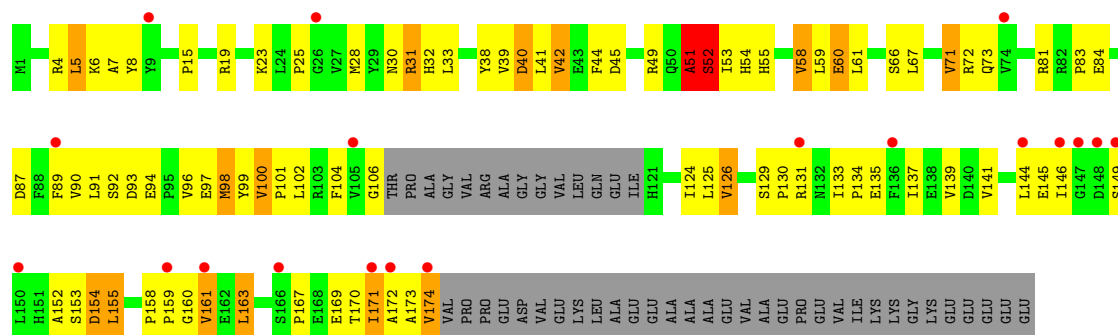


- Molecule 21: 50S ribosomal protein L25

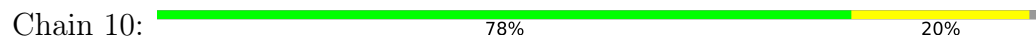




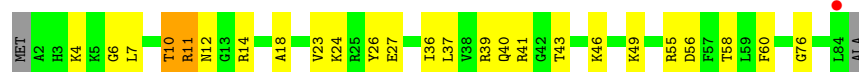
- Molecule 21: 50S ribosomal protein L25



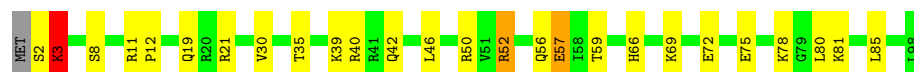
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

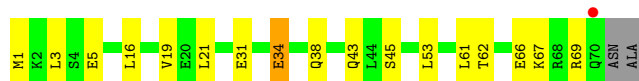
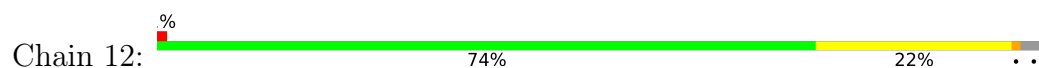


- Molecule 23: 50S ribosomal protein L28

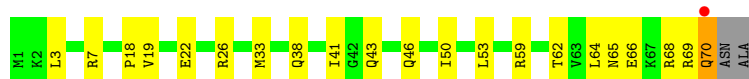




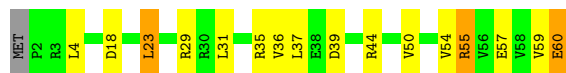
- Molecule 24: 50S ribosomal protein L29



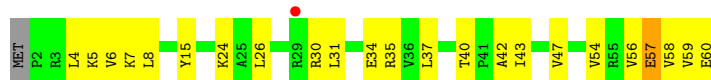
- Molecule 24: 50S ribosomal protein L29



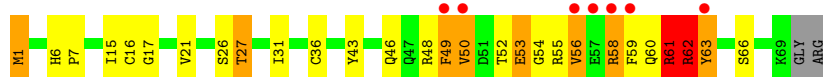
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30




- Molecule 26: 50S ribosomal protein L31

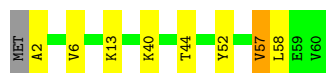


- Molecule 26: 50S ribosomal protein L31




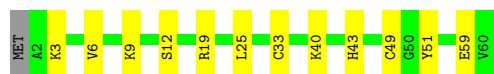
- Molecule 27: 50S ribosomal protein L32

Chain 15:  85% 12% ..



- Molecule 27: 50S ribosomal protein L32

Chain 25:  78% 20% .



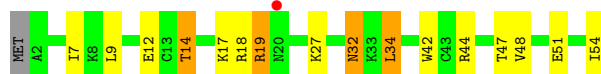
- Molecule 28: 50S ribosomal protein L33

Chain 16:  61% 33% . .




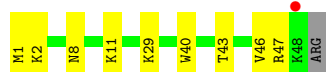
- Molecule 28: 50S ribosomal protein L33

Chain 26:  2% 69% 22% 7% .




- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 80% 18% .



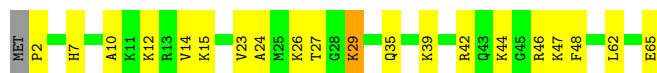
- Molecule 29: 50S ribosomal protein L34

Chain 27:  6% 80% 16% . .



- Molecule 30: 50S ribosomal protein L35

Chain 18:  68% 29% . .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  69% 29% .



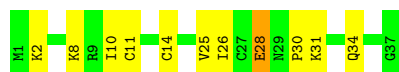
- Molecule 31: 50S ribosomal protein L36

Chain 19:  73% 27%



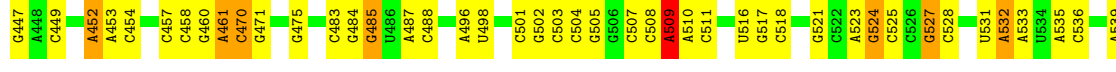
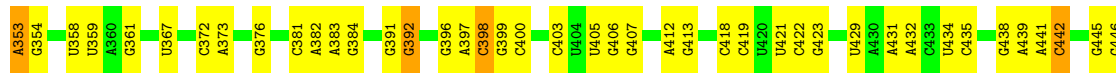
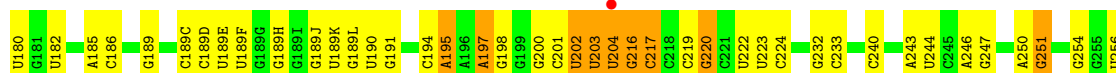
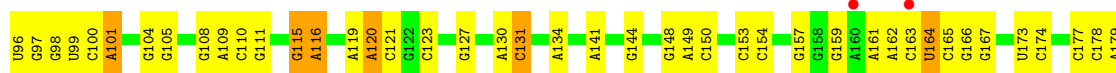
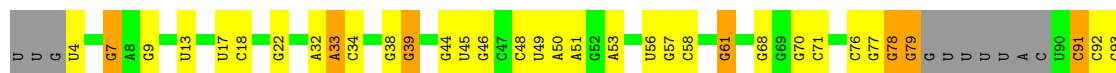
- Molecule 31: 50S ribosomal protein L36

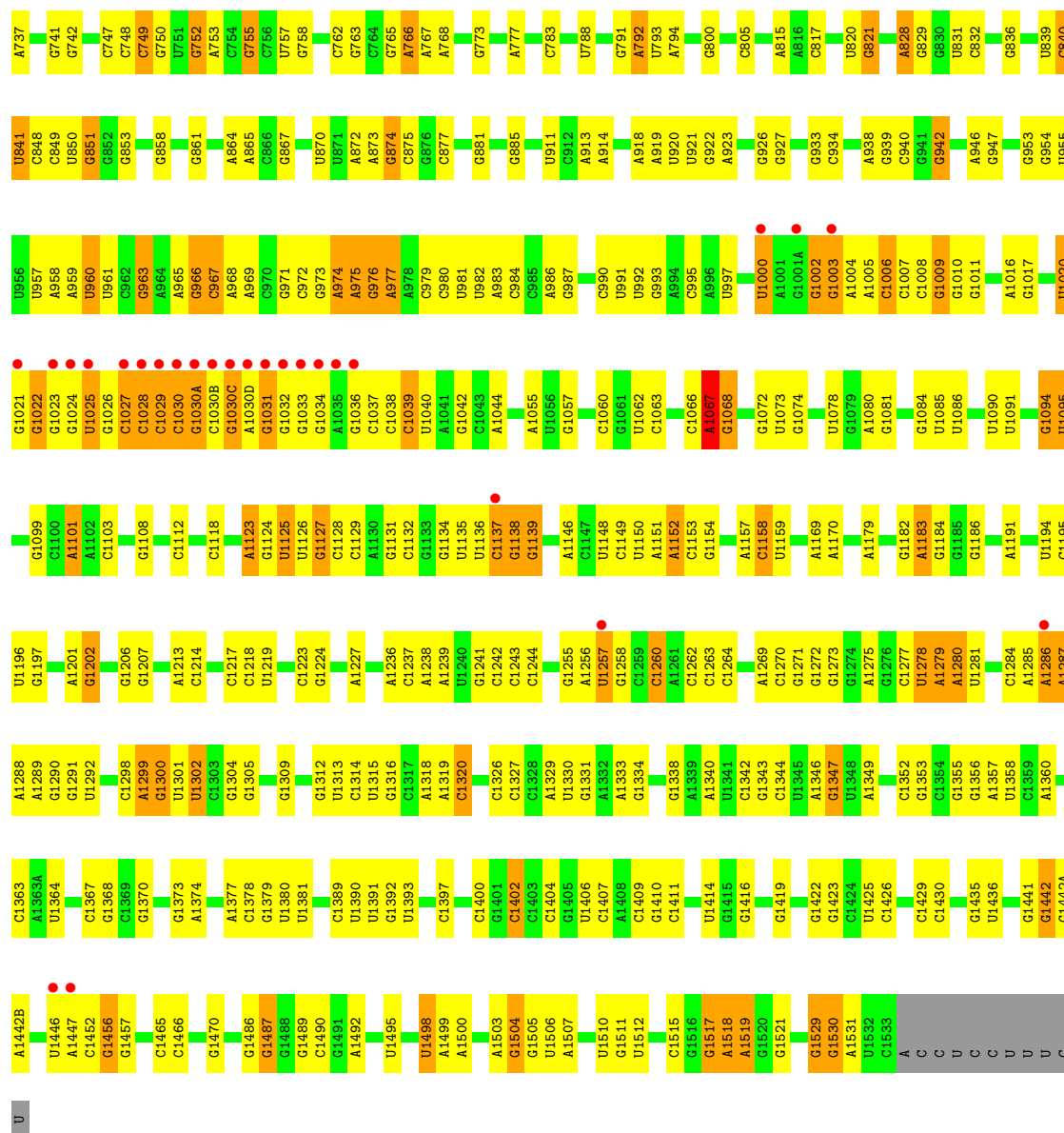
Chain 29:  70% 27% .



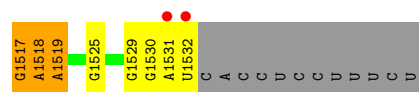
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  2% 52% 39% 8% .

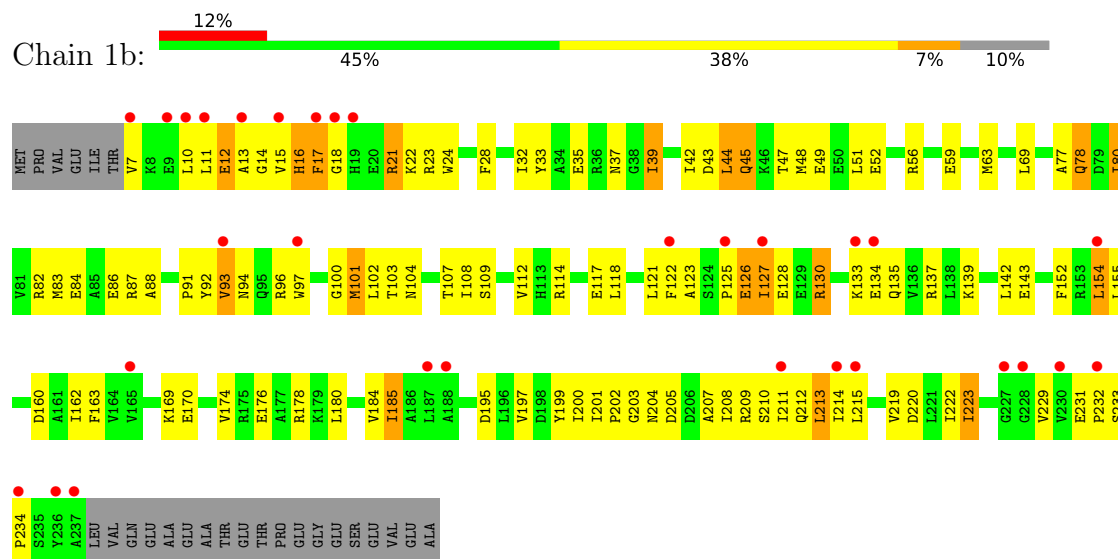




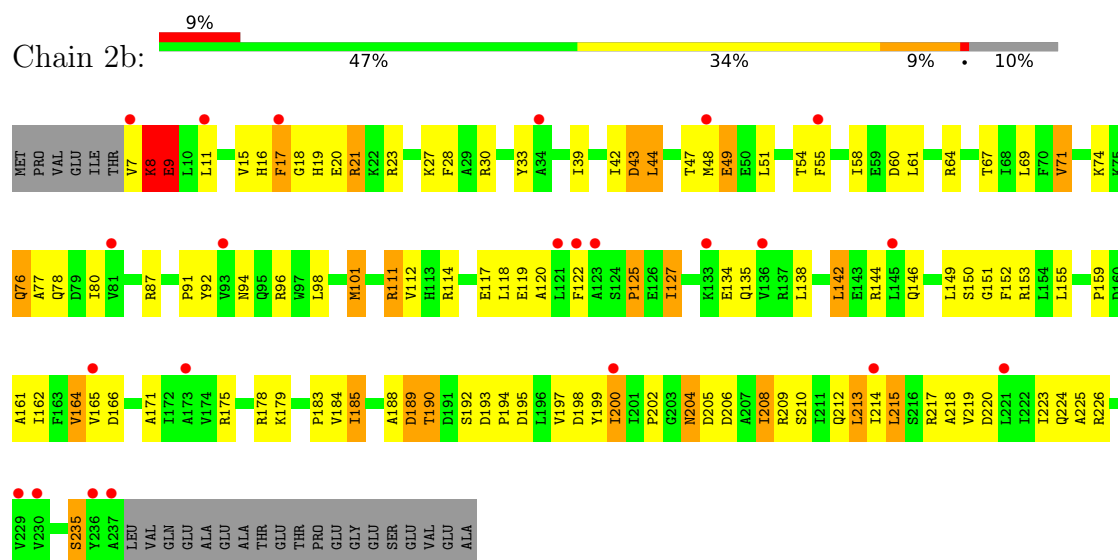
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C1325	C1328	A1329	U1330	G1331	A1332	G1333	G1334	G1338	A1339	A1340	U1341	G1342	G1343	G1344	U1345	A1346	G1347	C1352	G1353	G1354	G1355	G1356	A1357	G1358	G1359	A1360	G1361	C1362	C1363	G1365	C1366	C1367	G1370	G1371	U1372	G1373	A1374	A1375	U1376	C1377	G1379	G1386	U1390	U1391	C1397	A1398	C1399	G1400	A1513																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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C985	A986	G987	U991	U992	G993	A994	C995	U996	A997	G998	C999	G1001A	G1002	G1003	A1004	A1005	C1006	C1007	A995	G942	U943	G944	G945	G946	C948	U952	G953	G954	U955	U956	U957	A958	A959	U960	A864	A865	G963	A964	C965	G966	C967	A968	C962	A969	C970	U971	C972	A973	A974	G975	A976	C977	A977	U982	A983	C984																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C779	A780	C784	A787	A792	U793	A794	C806	G809	C817	G818	A819	U820	G821	C825	U827	A828	G836	G837	C838	U839	C840	U841	C848	C849	U850	U851	C859	A859	A864	A865	C875	C881	C882	U882	G885	G886	C887	G888	A889	A900	A901	G902	A903	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022	G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1031	G1032	G1033	G1034	G1035	G1036	G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068	G1069	G1070	G1071	G1072	G1073	G1074	G1075	G1076	G1077	G1078	G1079	G1080	G1081	G1082	G1083	G1084	G1085	G1086	G1087	G1088	G1089	G1090	G1091	G1092	G1093	G1094	G1095	G1096	G1097	G1098	G1099	G1100	G1101	G1102	G1103	G1104	G1105	G1106	G1107	G1108	G1109	G1110	G1111	G1112	G1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1123	G1124	G1125	G1126	G1127	G1128	G1129	G1130	G1131	G1132	G1133	G1134	G1135	G1136	G1137	G1138	G1139	G1140	G1141	G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201	G1202	G1203	G1204	G1205	G1206	G1207	G1208	G1209	G1210	G1211	G1212	G1213	G1214	G1215	G1216	G1217	G1218	G1219	G1220	G1221	G1222	G1223	G1224	G1225	G1226	G1227	G1228	G1229	G1230	G1231	G1232	G1233	G1234	G1235	G1236	G1237	G1238	G1239	G1240	G1241	G1242	G1243	G1244	G1245	G1246	G1247	G1248	G1249	G1250	G1251	G1252	G1253	G1254	G1255	G1256	G1257	G1258	G1259	G1260	G1261	G1262	G1263	G1264	G1265	G1266	G1267	G1268	G1269	G1270	G1271	G1272	G1273	G1274	G1275	G1276	G1277	G1278	G1279	G1280	G1281	G1282	G1283	G1284	G1285	G1286	G1287	G1288	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	G1300	G1301	G1302	G1303	G1304	G1305	G1306	G1307	G1308	G1309	G1310	G1311	G1312	G1313	G1314	G1315	G1316	G1317	G1318	G1319	G1320	G1321	G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381	G1382	G1383	G1384	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715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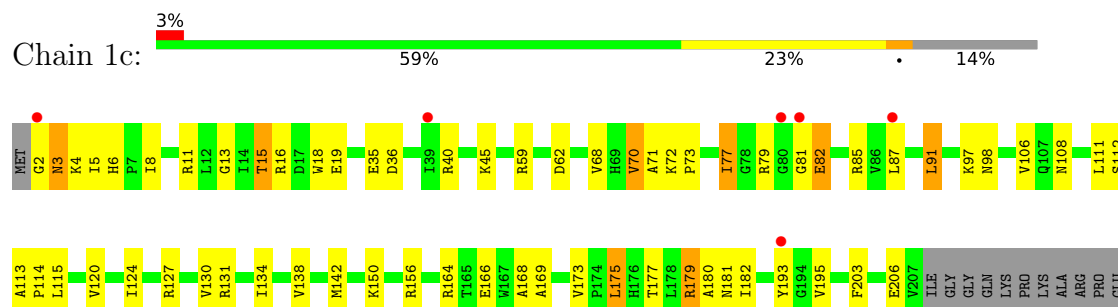
• Molecule 33: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S2

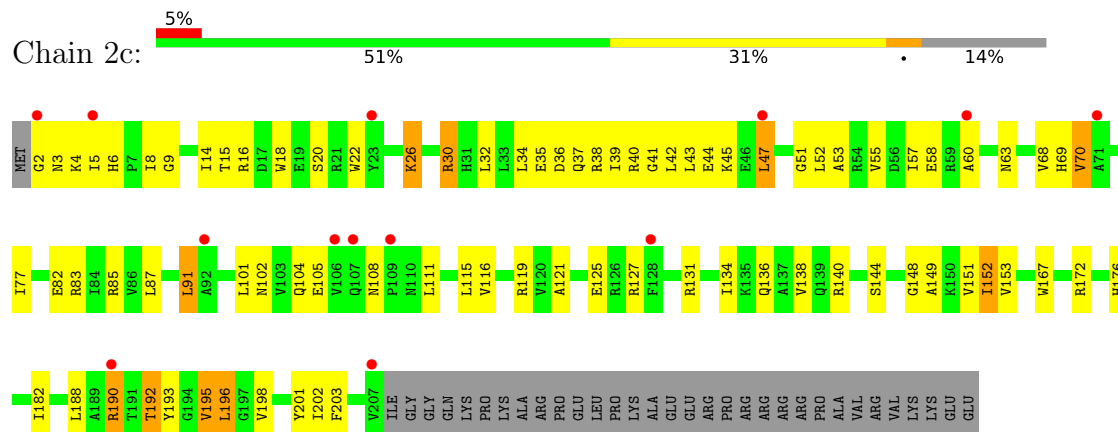


• Molecule 34: 30S ribosomal protein S3

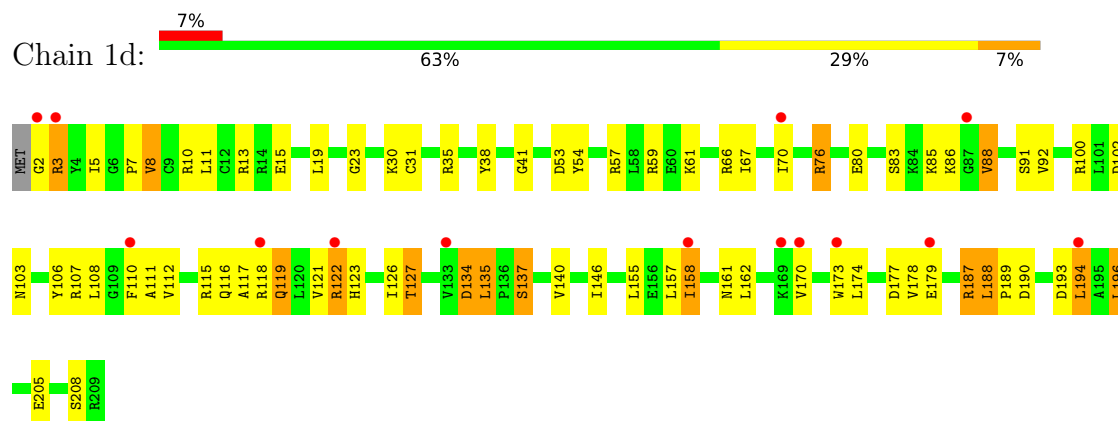


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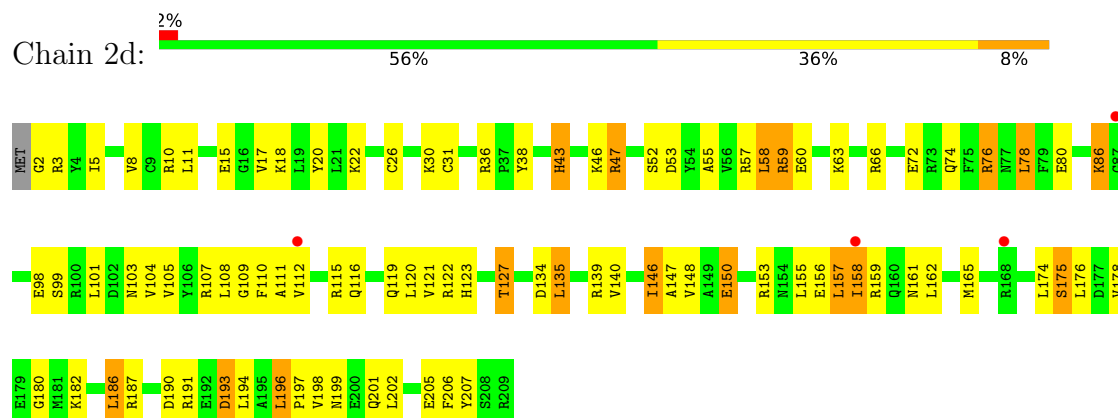
• Molecule 34: 30S ribosomal protein S3



• Molecule 35: 30S ribosomal protein S4

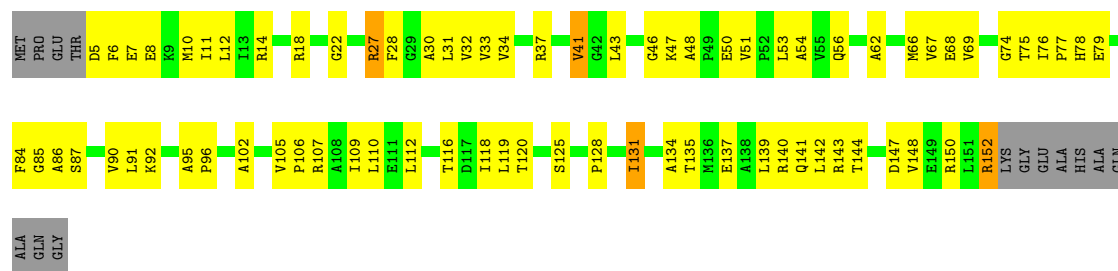


• Molecule 35: 30S ribosomal protein S4

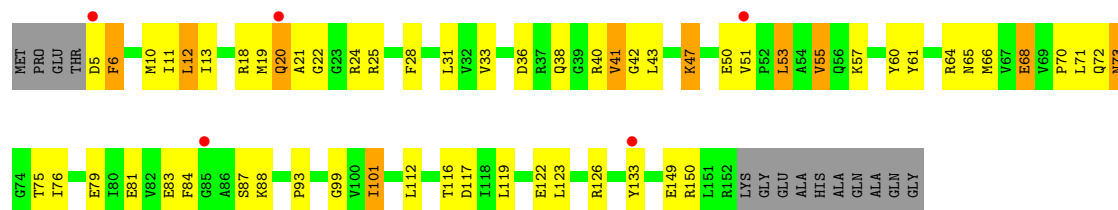


• Molecule 36: 30S ribosomal protein S5

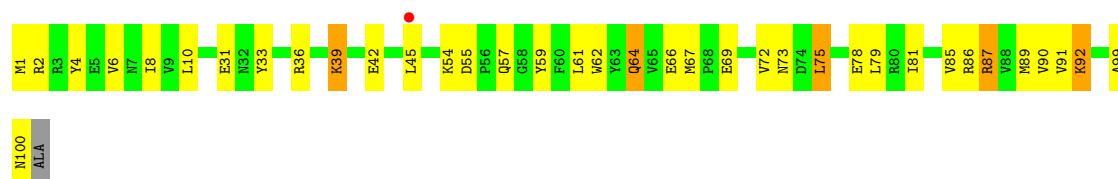




- Molecule 36: 30S ribosomal protein S5



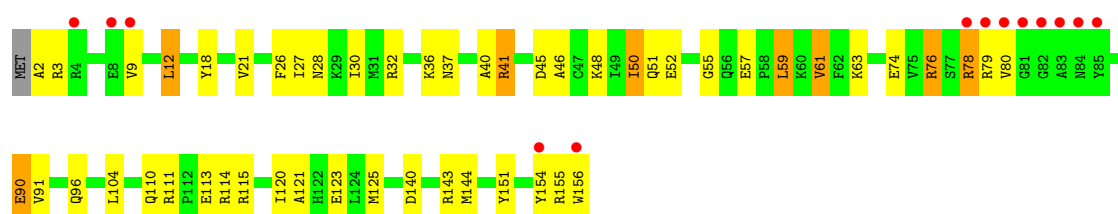
- Molecule 37: 30S ribosomal protein S6



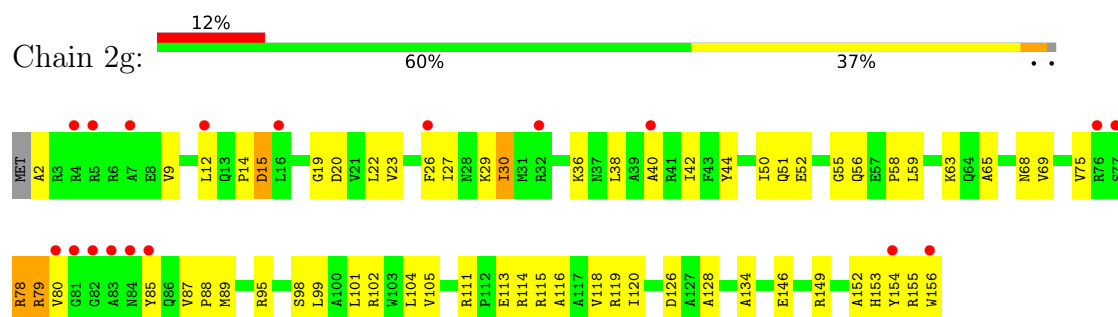
- Molecule 37: 30S ribosomal protein S6



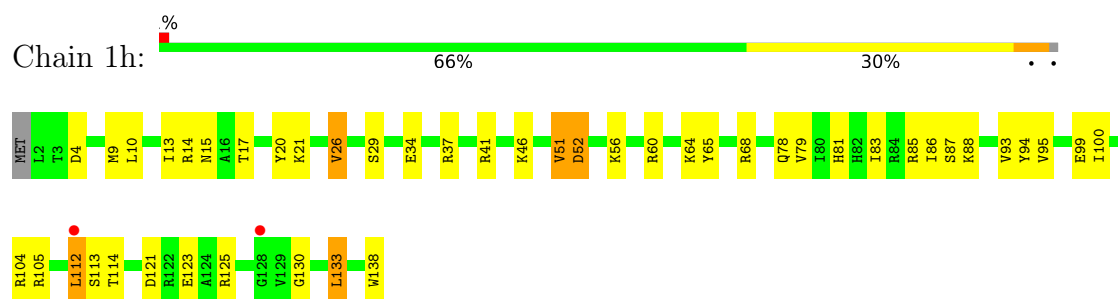
- Molecule 38: 30S ribosomal protein S7



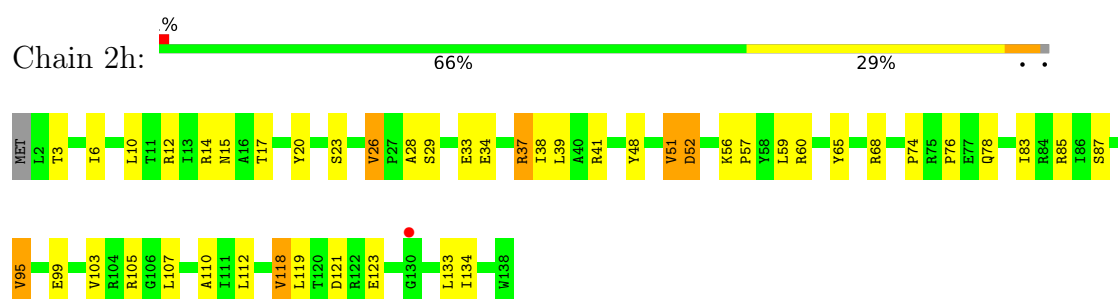
- Molecule 38: 30S ribosomal protein S7



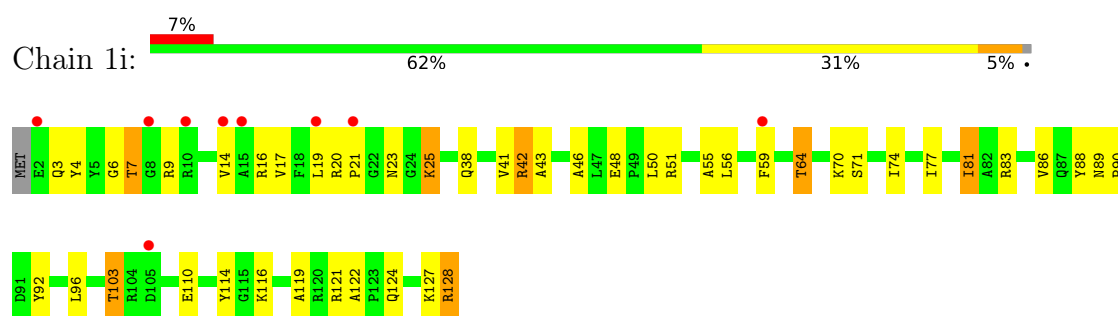
- Molecule 39: 30S ribosomal protein S8



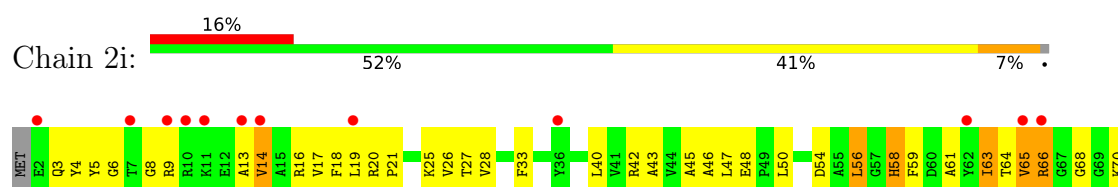
- Molecule 39: 30S ribosomal protein S8

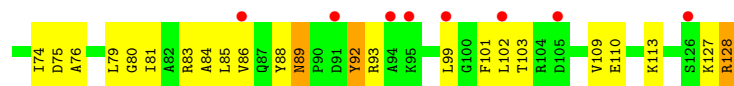


- Molecule 40: 30S ribosomal protein S9

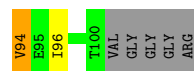


- Molecule 40: 30S ribosomal protein S9

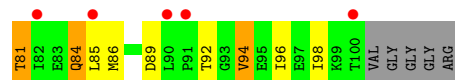
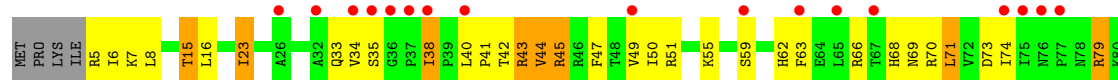




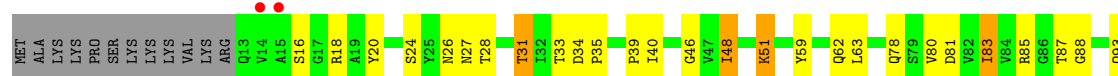
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11

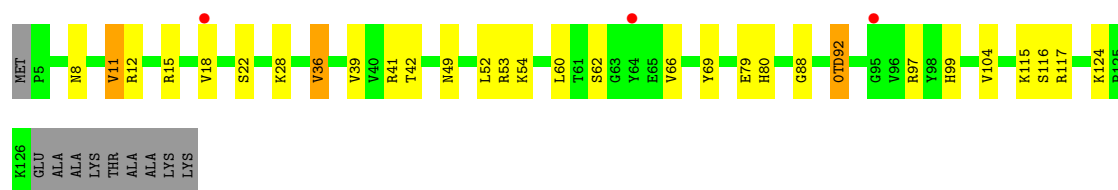


• Molecule 42: 30S ribosomal protein S11

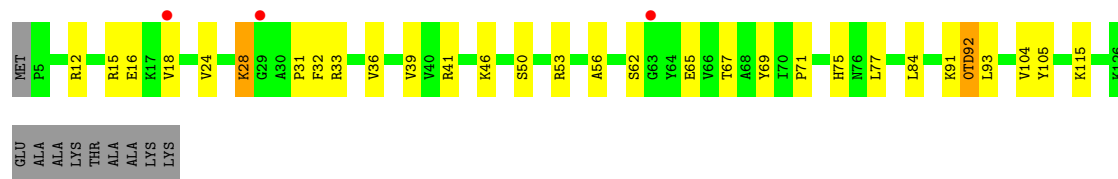


• Molecule 43: 30S ribosomal protein S12

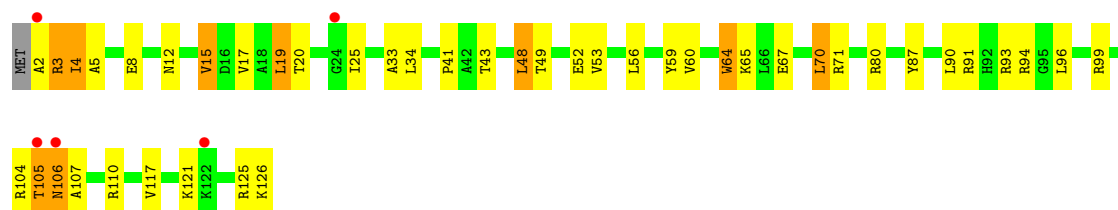




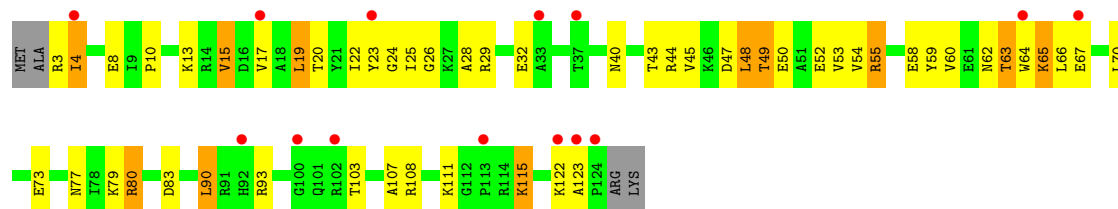
- Molecule 43: 30S ribosomal protein S12



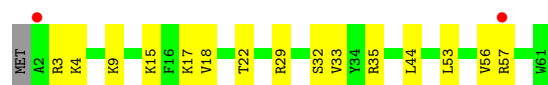
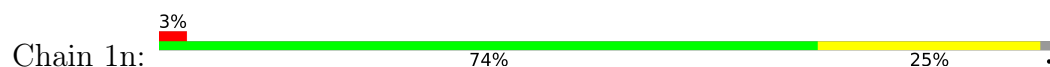
- Molecule 44: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S13

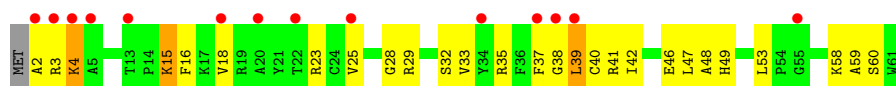


- Molecule 45: 30S ribosomal protein S14 type Z

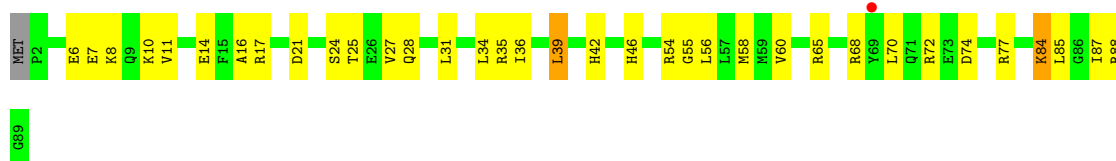


- Molecule 45: 30S ribosomal protein S14 type Z

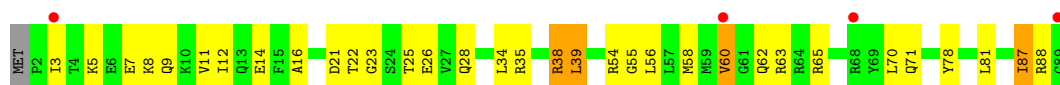




- Molecule 46: 30S ribosomal protein S15



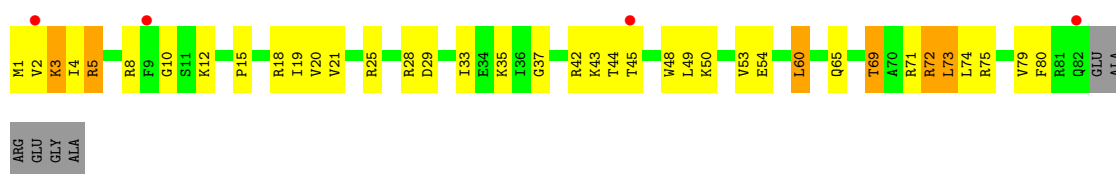
- Molecule 46: 30S ribosomal protein S15



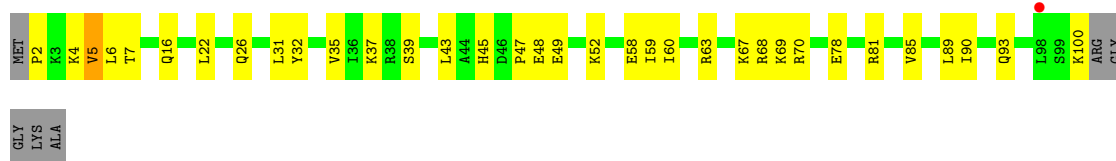
- Molecule 47: 30S ribosomal protein S16



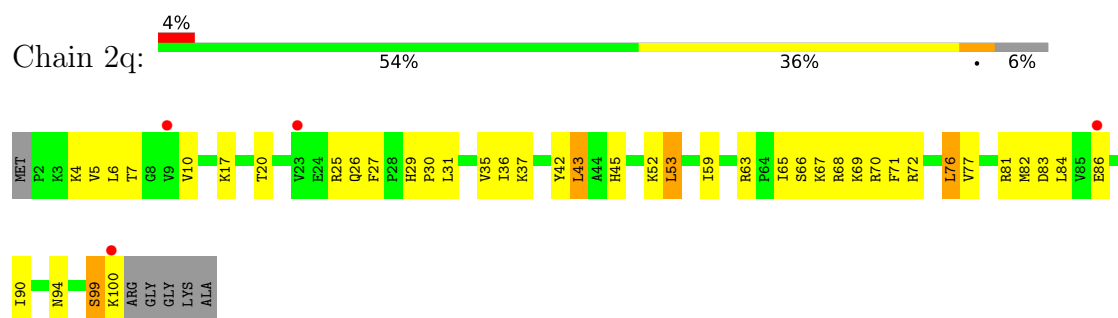
- Molecule 47: 30S ribosomal protein S16



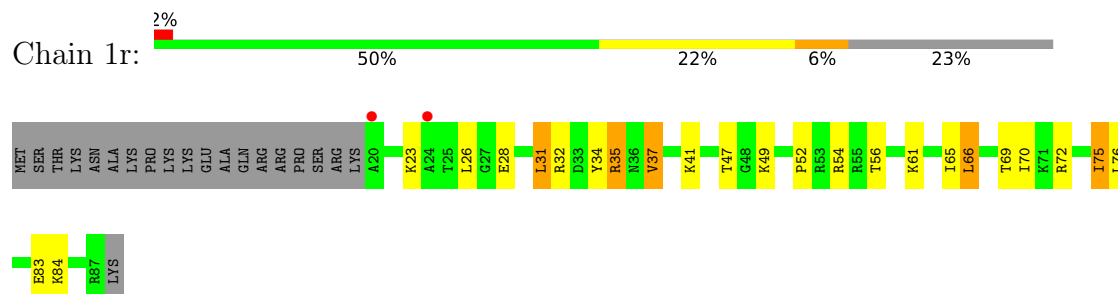
- Molecule 48: 30S ribosomal protein S17



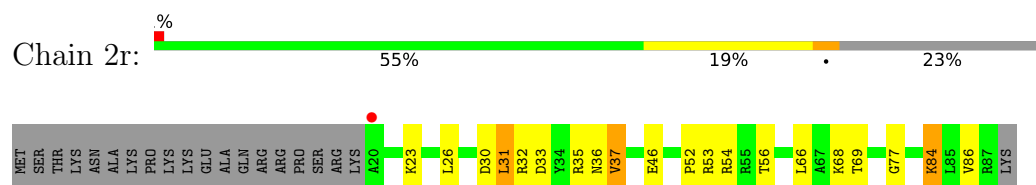
- Molecule 48: 30S ribosomal protein S17



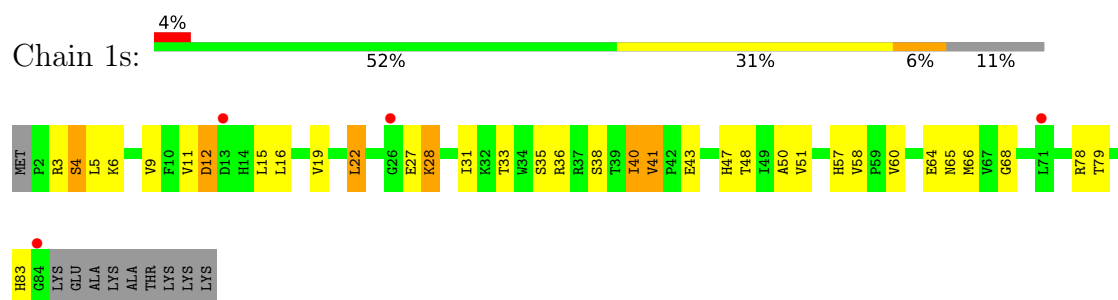
- Molecule 49: 30S ribosomal protein S18



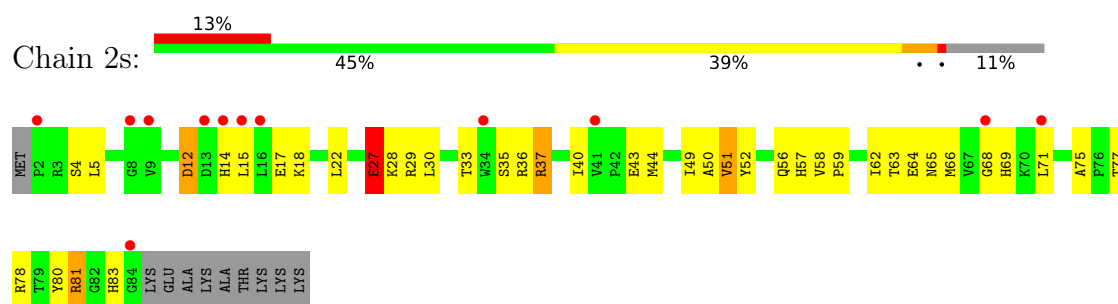
- Molecule 49: 30S ribosomal protein S18



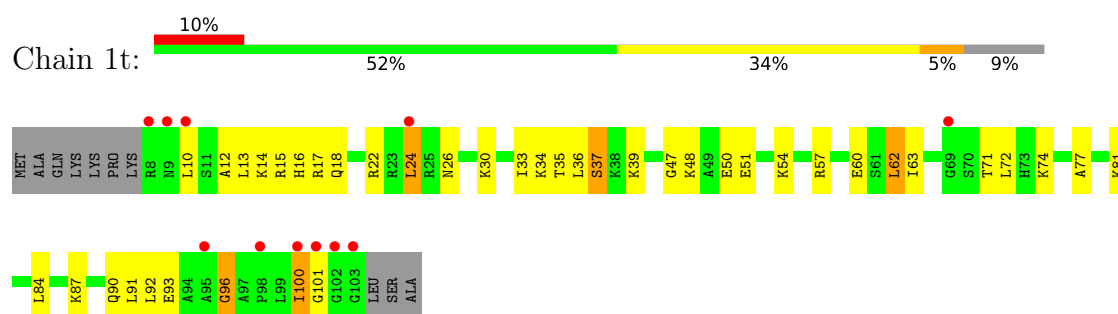
- Molecule 50: 30S ribosomal protein S19



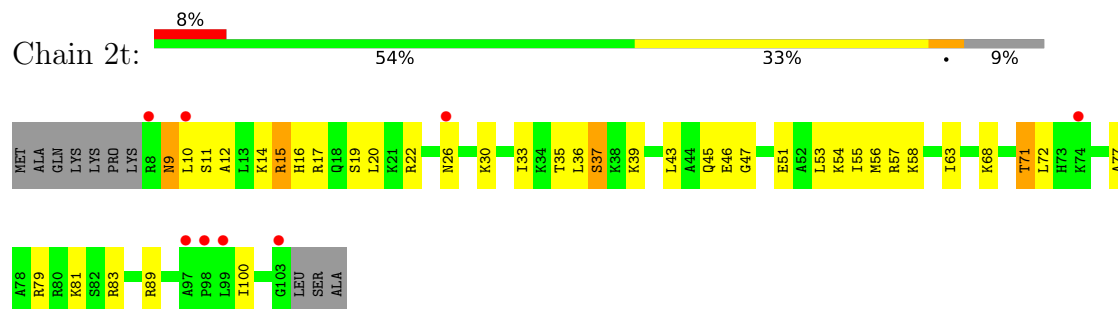
- Molecule 50: 30S ribosomal protein S19



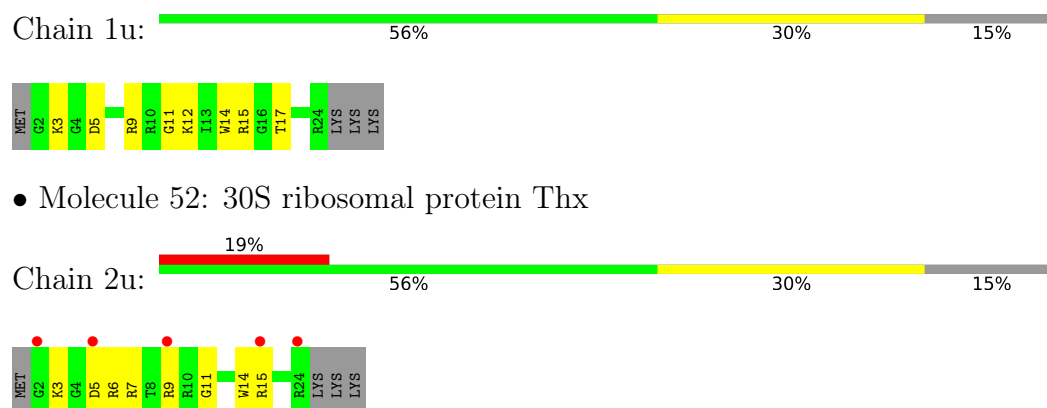
- Molecule 51: 30S ribosomal protein S20



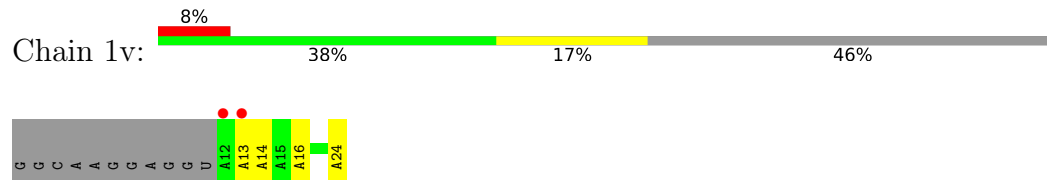
- Molecule 51: 30S ribosomal protein S20



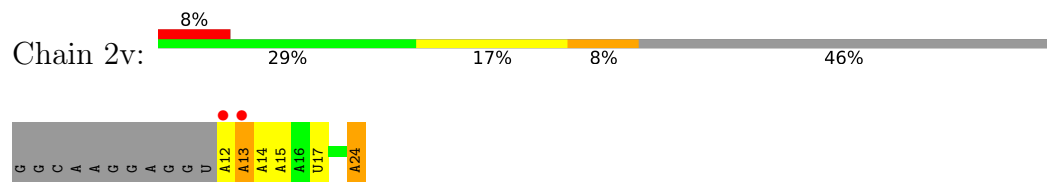
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: MET-PHE-mRNA



- Molecule 53: MET-PHE-mRNA



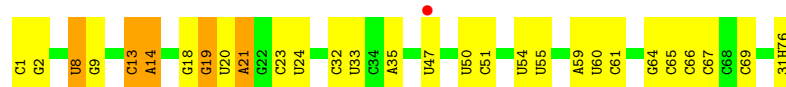
- Molecule 54: A-site Aminoacylated Phe-tRNAphe



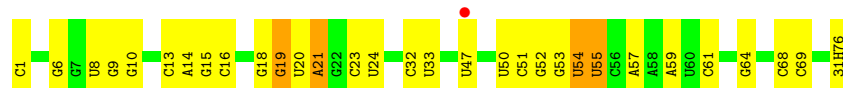
• Molecule 54: A-site Aminoacylated Phe-tRNAphe



• Molecule 55: P-site Aminoacylated fMet-tRNAmet



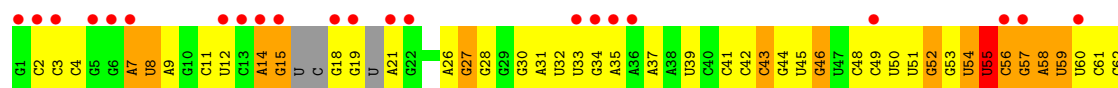
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

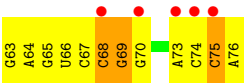


• Molecule 56: E-site Deacylated tRNAphe

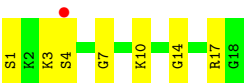


• Molecule 56: E-site Deacylated tRNAphe





● Molecule 57: Lasso peptide lariocidin



● Molecule 57: Lasso peptide lariocidin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.10Å 451.03Å 622.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 2.50 48.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.62-2.50) 100.0 (48.62-2.50)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.216 , 0.265 0.224 , 0.269	Depositor DCC
R_{free} test set	100652 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	300593	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 5MC, 31H, PSU, OMC, F3N, MIA, SF4, MA6, MG, UR3, 4OC, OMG, ZN, K, M2G, G7M, 4SU, 0TD, OMU, 2MA, 5MU, 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	0.72	7/107720 (0.0%)
1	2A	0.43	0/67295	0.62	9/105042 (0.0%)
2	1B	0.44	0/2882	0.65	0/4494
2	2B	0.37	0/2879	0.58	0/4487
3	1D	0.53	0/2186	0.75	2/2944 (0.1%)
3	2D	0.46	0/2186	0.68	0/2944
4	1E	0.52	0/1592	0.77	0/2149
4	2E	0.39	0/1592	0.64	0/2149
5	1F	0.52	0/1619	0.75	2/2193 (0.1%)
5	2F	0.41	0/1615	0.63	0/2188
6	1G	0.43	0/1448	0.66	0/1957
6	2G	0.37	0/1453	0.62	0/1963
7	1H	0.45	1/1356 (0.1%)	0.64	0/1834
7	2H	0.36	0/1356	0.51	0/1834
8	1I	0.39	0/1112	0.63	0/1514
8	2I	0.38	0/1079	0.66	0/1475
9	1N	0.52	0/1144	0.71	0/1543
9	2N	0.38	0/1144	0.59	0/1543
10	1O	0.46	0/943	0.66	0/1269
10	2O	0.39	0/943	0.61	0/1269
11	1P	0.49	0/1152	0.83	1/1533 (0.1%)
11	2P	0.41	0/1152	0.66	0/1533
12	1Q	0.50	0/1143	0.70	0/1527
12	2Q	0.41	0/1143	0.63	0/1527
13	1R	0.57	0/982	0.77	0/1312
13	2R	0.40	0/982	0.61	0/1312
14	1S	0.45	0/883	0.69	0/1176
14	2S	0.37	0/880	0.60	0/1172
15	1T	0.46	0/1105	0.68	0/1477
15	2T	0.41	0/1097	0.65	2/1468 (0.1%)
16	1U	0.56	0/977	0.76	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.40	0/977	0.58	0/1301
17	1V	0.52	0/782	0.76	0/1049
17	2V	0.38	0/782	0.56	0/1049
18	1W	0.57	0/897	0.73	0/1205
18	2W	0.45	0/897	0.61	0/1205
19	1X	0.55	0/764	0.75	2/1025 (0.2%)
19	2X	0.41	0/764	0.68	2/1025 (0.2%)
20	1Y	0.45	0/819	0.66	0/1095
20	2Y	0.41	0/819	0.66	0/1095
21	1Z	0.45	0/1267	0.69	1/1717 (0.1%)
21	2Z	0.41	0/1299	0.66	0/1763
22	10	0.53	0/662	0.75	0/881
22	20	0.39	0/662	0.57	0/881
23	11	0.49	0/762	0.66	0/1014
23	21	0.43	0/762	0.63	0/1014
24	12	0.50	0/590	0.62	0/781
24	22	0.36	0/590	0.56	0/781
25	13	0.53	0/474	0.73	0/635
25	23	0.36	0/469	0.62	0/630
26	14	0.47	0/565	0.84	0/761
26	24	0.42	0/545	0.70	0/737
27	15	0.52	0/469	0.72	0/635
27	25	0.46	0/469	0.64	0/635
28	16	0.47	0/460	0.70	0/613
28	26	0.38	0/456	0.64	0/608
29	17	0.61	0/426	0.79	0/561
29	27	0.49	0/426	0.68	0/561
30	18	0.51	0/525	0.75	0/691
30	28	0.43	0/525	0.64	0/691
31	19	0.48	0/310	0.81	0/407
31	29	0.32	0/310	0.60	0/407
32	1a	0.41	0/35795	0.61	4/55864 (0.0%)
32	2a	0.37	1/35886 (0.0%)	0.57	3/56005 (0.0%)
33	1b	0.40	0/1881	0.71	1/2542 (0.0%)
33	2b	0.41	0/1860	0.65	0/2518
34	1c	0.40	0/1572	0.59	0/2126
34	2c	0.39	0/1566	0.57	0/2119
35	1d	0.37	0/1685	0.60	0/2262
35	2d	0.37	0/1704	0.60	0/2284
36	1e	0.40	0/1145	0.65	0/1543
36	2e	0.39	0/1149	0.63	0/1548
37	1f	0.39	0/823	0.59	0/1115
37	2f	0.38	0/829	0.56	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.35	0/1250	0.53	0/1679
38	2g	0.38	0/1254	0.61	0/1683
39	1h	0.37	0/1108	0.56	0/1494
39	2h	0.34	0/1108	0.54	0/1494
40	1i	0.38	0/1002	0.66	0/1346
40	2i	0.39	0/997	0.65	0/1343
41	1j	0.39	0/722	0.60	0/982
41	2j	0.42	0/727	0.65	0/988
42	1k	0.40	0/844	0.62	0/1145
42	2k	0.37	0/848	0.56	0/1149
43	1l	0.43	0/937	0.65	2/1260 (0.2%)
43	2l	0.38	0/937	0.67	0/1260
44	1m	0.43	0/990	0.68	0/1327
44	2m	0.38	0/961	0.67	0/1291
45	1n	0.40	0/501	0.62	0/664
45	2n	0.38	0/501	0.64	0/664
46	1o	0.41	0/739	0.56	0/985
46	2o	0.36	0/739	0.54	0/985
47	1p	0.36	0/697	0.59	0/939
47	2p	0.38	0/693	0.65	0/935
48	1q	0.40	0/836	0.58	0/1117
48	2q	0.38	0/836	0.63	1/1117 (0.1%)
49	1r	0.39	0/560	0.64	0/746
49	2r	0.34	0/560	0.55	0/746
50	1s	0.37	0/667	0.72	0/900
50	2s	0.41	0/661	0.74	2/893 (0.2%)
51	1t	0.38	0/730	0.65	0/965
51	2t	0.44	0/729	0.66	0/965
52	1u	0.38	0/203	0.56	0/266
52	2u	0.40	0/203	0.65	0/266
53	1v	0.48	0/310	0.57	0/480
53	2v	0.43	0/310	0.51	0/480
54	1w	0.47	1/1603 (0.1%)	0.61	1/2492 (0.0%)
54	2w	0.45	1/1531 (0.1%)	0.61	0/2379
55	1x	0.47	0/1723	0.65	0/2684
55	2x	0.41	0/1723	0.58	0/2684
56	1y	0.56	2/1606 (0.1%)	0.55	0/2497
56	2y	0.60	2/1583 (0.1%)	0.57	0/2459
57	1z	0.40	0/133	0.99	0/168
57	2z	0.43	0/133	1.00	2/168 (1.2%)
All	All	0.45	8/316945 (0.0%)	0.65	44/474436 (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
3	2D	0	1
5	2F	0	2
6	1G	0	2
6	2G	0	1
21	1Z	0	1
21	2Z	0	2
23	11	0	1
23	21	0	1
26	14	0	1
26	24	0	1
33	1b	0	3
33	2b	0	1
41	1j	0	2
41	2j	0	1
44	2m	0	1
All	All	0	21

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	6.67	1.62	1.56
56	2y	8	4SU	O3'-P	6.19	1.62	1.56
7	1H	126	PRO	C-N	-5.50	1.17	1.33
56	1y	8	4SU	O3'-P	5.38	1.61	1.56
54	2w	46	G7M	O3'-P	5.29	1.61	1.56

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	2q	65	ILE	N-CA-C	-8.78	104.79	111.90
1	1A	2689	U	P-O3'-C3'	8.48	132.93	120.20
1	1A	1992	G	C2'-C3'-O3'	8.28	121.92	109.50
32	2a	1272	G	N1-C2-N2	-7.95	92.34	116.20
1	2A	1992	G	C2'-C3'-O3'	7.25	120.38	109.50

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	11	3	LYS	Peptide
26	14	61	ARG	Peptide
6	1G	50	ALA	Peptide
6	1G	95	ARG	Peptide
21	1Z	29	TYR	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	31196	678	0
1	2A	60322	0	30427	769	0
2	1B	2577	0	1305	34	0
2	2B	2575	0	1303	51	0
3	1D	2136	0	2218	49	0
3	2D	2136	0	2218	45	0
4	1E	1559	0	1618	41	0
4	2E	1559	0	1618	49	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	52	0
6	1G	1423	0	1436	42	0
6	2G	1428	0	1438	67	0
7	1H	1330	0	1407	44	0
7	2H	1330	0	1407	53	0
8	1I	1097	0	1140	48	1
8	2I	1064	0	1082	44	0
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	27	0
10	2O	933	0	996	24	0
11	1P	1135	0	1212	34	0
11	2P	1135	0	1212	30	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	32	0
13	1R	968	0	1033	18	0
13	2R	968	0	1033	22	0
14	1S	873	0	927	23	0
14	2S	870	0	923	44	0
15	1T	1091	0	1151	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	19	0
16	2U	959	0	1019	29	0
17	1V	771	0	830	14	0
17	2V	771	0	830	20	0
18	1W	886	0	940	10	0
18	2W	886	0	940	23	0
19	1X	750	0	814	21	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	21	0
21	1Z	1240	0	1240	42	0
21	2Z	1271	0	1273	69	0
22	10	653	0	674	14	0
22	20	653	0	674	25	0
23	11	755	0	826	19	0
23	21	755	0	826	22	0
24	12	588	0	643	7	0
24	22	588	0	643	11	0
25	13	469	0	518	9	0
25	23	464	0	514	19	0
26	14	552	0	533	32	0
26	24	532	0	503	34	0
27	15	455	0	465	4	0
27	25	455	0	465	9	0
28	16	453	0	473	12	0
28	26	449	0	469	13	0
29	17	418	0	467	6	0
29	27	418	0	467	6	0
30	18	517	0	582	17	0
30	28	517	0	582	12	0
31	19	307	0	335	5	0
31	29	307	0	335	5	0
32	1a	32246	0	16295	478	0
32	2a	32327	0	16337	553	1
33	1b	1846	0	1867	91	0
33	2b	1825	0	1828	80	0
34	1c	1548	0	1535	42	0
34	2c	1542	0	1517	63	0
35	1d	1655	0	1672	54	0
35	2d	1674	0	1714	70	0
36	1e	1129	0	1185	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	2e	1133	0	1191	50	0
37	1f	810	0	804	25	0
37	2f	816	0	808	25	0
38	1g	1231	0	1238	33	0
38	2g	1235	0	1249	42	0
39	1h	1088	0	1126	36	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	42	0
40	2i	978	0	966	50	0
41	1j	709	0	650	30	0
41	2j	714	0	672	41	0
42	1k	829	0	825	26	0
42	2k	833	0	836	24	0
43	1l	932	0	981	16	0
43	2l	932	0	980	24	0
44	1m	979	0	1028	34	0
44	2m	950	0	988	44	0
45	1n	492	0	529	12	0
45	2n	492	0	529	20	0
46	1o	728	0	760	23	0
46	2o	728	0	760	24	0
47	1p	681	0	697	19	0
47	2p	677	0	686	24	0
48	1q	823	0	891	19	0
48	2q	823	0	891	21	0
49	1r	555	0	618	22	0
49	2r	555	0	618	14	0
50	1s	652	0	662	28	0
50	2s	646	0	644	35	0
51	1t	728	0	798	27	0
51	2t	727	0	796	27	0
52	1u	199	0	208	8	0
52	2u	199	0	208	8	0
53	1v	277	0	140	1	0
53	2v	277	0	140	4	0
54	1w	1623	0	839	25	0
54	2w	1555	0	797	23	0
55	1x	1656	0	848	14	0
55	2x	1656	0	849	15	0
56	1y	1585	0	803	43	0
56	2y	1565	0	794	47	0
57	1z	132	0	145	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2z	132	0	145	3	0
58	10	10	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	14	1	0	0	0	0
58	15	7	0	0	0	0
58	16	2	0	0	0	0
58	17	4	0	0	0	0
58	18	3	0	0	0	0
58	19	1	0	0	0	0
58	1A	1108	0	0	0	0
58	1B	39	0	0	0	0
58	1D	13	0	0	0	0
58	1E	14	0	0	0	0
58	1F	12	0	0	0	0
58	1G	5	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	5	0	0	0	0
58	1P	4	0	0	0	0
58	1Q	6	0	0	0	0
58	1R	5	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	9	0	0	0	0
58	1W	6	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	216	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	1t	1	0	0	0	0
58	1v	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1w	9	0	0	0	0
58	1x	13	0	0	0	0
58	1y	1	0	0	0	0
58	1z	1	0	0	0	0
58	20	3	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
58	27	2	0	0	0	0
58	28	4	0	0	0	0
58	2A	882	0	0	0	0
58	2B	20	0	0	0	0
58	2D	7	0	0	0	0
58	2E	10	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	2	0	0	0	0
58	2T	4	0	0	0	0
58	2U	1	0	0	0	0
58	2V	2	0	0	0	0
58	2W	1	0	0	0	0
58	2X	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	240	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2j	1	0	0	0	0
58	2l	5	0	0	0	0
58	2n	1	0	0	0	0
58	2p	1	0	0	0	0
58	2q	3	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	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2y	6	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	11	0	0	0	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	9	0	0	0	0
62	18	8	0	0	1	0
62	1A	2017	0	0	76	0
62	1B	63	0	0	4	0
62	1D	28	0	0	1	0
62	1E	29	0	0	2	0
62	1F	14	0	0	2	0
62	1G	2	0	0	0	0
62	1H	2	0	0	0	0
62	1I	1	0	0	1	0
62	1N	6	0	0	0	0
62	1O	6	0	0	0	0
62	1P	20	0	0	0	0
62	1Q	7	0	0	0	0
62	1R	11	0	0	3	0
62	1S	5	0	0	0	0
62	1T	9	0	0	0	0
62	1U	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1V	8	0	0	1	0
62	1W	6	0	0	1	0
62	1X	6	0	0	0	0
62	1Y	2	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	386	0	0	30	0
62	1b	1	0	0	0	0
62	1g	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	9	0	0	1	0
62	1m	1	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	5	0	0	0	0
62	1w	21	0	0	0	0
62	1x	15	0	0	0	0
62	1y	1	0	0	0	0
62	1z	1	0	0	0	0
62	20	3	0	0	0	0
62	21	12	0	0	0	0
62	23	2	0	0	0	0
62	25	1	0	0	0	0
62	27	5	0	0	0	0
62	28	3	0	0	1	0
62	29	1	0	0	0	0
62	2A	1165	0	0	70	0
62	2B	22	0	0	2	0
62	2D	22	0	0	0	0
62	2E	14	0	0	0	0
62	2F	13	0	0	0	0
62	2I	2	0	0	1	0
62	2N	1	0	0	0	0
62	2O	3	0	0	0	0
62	2P	15	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	4	0	0	0	0
62	2T	4	0	0	0	0
62	2U	2	0	0	0	0
62	2V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2X	1	0	0	0	0
62	2Y	1	0	0	0	0
62	2Z	1	0	0	0	0
62	2a	283	0	0	27	0
62	2c	1	0	0	0	0
62	2d	2	0	0	0	0
62	2e	1	0	0	0	0
62	2g	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	3	0	0	1	0
62	2l	6	0	0	0	0
62	2p	1	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	1	0
62	2v	2	0	0	0	0
62	2w	7	0	0	0	0
62	2x	8	0	0	0	0
62	2y	6	0	0	1	0
All	All	300593	0	197076	4936	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 4936 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	1.34	1.23
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.43	1.01
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.43	1.00
1:2A:1604:C:OP2	62:2A:3903:HOH:O	1.77	0.98
1:1A:1082:U:O4	1:1A:1086:A:N1	1.97	0.98

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]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	19 (7%)	0	100	100
4	1E	202/206 (98%)	187 (93%)	15 (7%)	0	100	100
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	43
5	1F	201/210 (96%)	195 (97%)	6 (3%)	0	100	100
5	2F	201/210 (96%)	188 (94%)	13 (6%)	0	100	100
6	1G	179/182 (98%)	164 (92%)	14 (8%)	1 (1%)	21	38
6	2G	179/182 (98%)	154 (86%)	24 (13%)	1 (1%)	21	38
7	1H	172/180 (96%)	163 (95%)	9 (5%)	0	100	100
7	2H	172/180 (96%)	153 (89%)	18 (10%)	1 (1%)	21	38
8	1I	144/148 (97%)	122 (85%)	22 (15%)	0	100	100
8	2I	144/148 (97%)	125 (87%)	19 (13%)	0	100	100
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
11	2P	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	98 (91%)	10 (9%)	0	100	100
15	1T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
17	2V	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
21	1Z	148/206 (72%)	129 (87%)	18 (12%)	1 (1%)	18	34
21	2Z	156/206 (76%)	133 (85%)	21 (14%)	2 (1%)	9	18
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
22	20	81/85 (95%)	81 (100%)	0	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	22
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	22
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	51 (76%)	14 (21%)	2 (3%)	3	5
26	24	67/71 (94%)	50 (75%)	16 (24%)	1 (2%)	8	16
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	192 (84%)	34 (15%)	3 (1%)	9	18
33	2b	229/256 (90%)	190 (83%)	36 (16%)	3 (1%)	9	18
34	1c	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
34	2c	204/239 (85%)	175 (86%)	29 (14%)	0	100	100
35	1d	206/209 (99%)	185 (90%)	21 (10%)	0	100	100
35	2d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/162 (90%)	132 (90%)	14 (10%)	0	100	100
36	2e	146/162 (90%)	137 (94%)	9 (6%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
38	2g	153/156 (98%)	138 (90%)	15 (10%)	0	100	100
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
40	2i	125/128 (98%)	102 (82%)	23 (18%)	0	100	100
41	1j	95/105 (90%)	85 (90%)	9 (10%)	1 (1%)	11	22
41	2j	94/105 (90%)	84 (89%)	9 (10%)	1 (1%)	11	22
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	27
42	2k	112/129 (87%)	99 (88%)	13 (12%)	0	100	100
43	1l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	123/126 (98%)	107 (87%)	15 (12%)	1 (1%)	16	31
44	2m	120/126 (95%)	107 (89%)	13 (11%)	0	100	100
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
50	1s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10	20
51	1t	94/106 (89%)	80 (85%)	13 (14%)	1 (1%)	11	22
51	2t	94/106 (89%)	83 (88%)	11 (12%)	0	100	100
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
57	1z	16/18 (89%)	12 (75%)	3 (19%)	1 (6%)	1	1
57	2z	16/18 (89%)	11 (69%)	5 (31%)	0	100	100
All	All	11404/12164 (94%)	10474 (92%)	905 (8%)	25 (0%)	43	63

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
57	1z	4	SER
21	2Z	52	SER
33	2b	9	GLU
33	2b	17	PHE

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%)	197 (92%)	18 (8%)	10	22
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26	52
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	158 (96%)	6 (4%)	30	57
5	1F	160/166 (96%)	132 (82%)	28 (18%)	2	3
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	15
6	1G	143/156 (92%)	126 (88%)	17 (12%)	5	11
6	2G	143/156 (92%)	118 (82%)	25 (18%)	2	3
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	19
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5	11
8	1I	113/124 (91%)	89 (79%)	24 (21%)	1	2
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	3
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10	22
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	26
10	1O	100/100 (100%)	98 (98%)	2 (2%)	48	75
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	44
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	14
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	14
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	49
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	13	28
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22	44
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	44
14	1S	86/88 (98%)	78 (91%)	8 (9%)	8	18
14	2S	85/88 (97%)	66 (78%)	19 (22%)	1	2
15	1T	115/127 (91%)	103 (90%)	12 (10%)	7	14
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	29
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	21
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	26
17	1V	80/82 (98%)	69 (86%)	11 (14%)	3	7
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	15
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	31
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	20
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	82
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	72 (85%)	13 (15%)	3	5
20	2Y	85/91 (93%)	75 (88%)	10 (12%)	5	11
21	1Z	135/179 (75%)	115 (85%)	20 (15%)	3	6
21	2Z	137/179 (76%)	114 (83%)	23 (17%)	2	4
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	62
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	34
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	34
23	21	80/83 (96%)	72 (90%)	8 (10%)	7	15
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	19
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	11
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	24
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	2
26	24	53/63 (84%)	44 (83%)	9 (17%)	2	4
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	54
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	24
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	15
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	27
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	16
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	39
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	20
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4	8
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2	4
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	9
34	2c	140/188 (74%)	123 (88%)	17 (12%)	5	10
35	1d	169/181 (93%)	140 (83%)	29 (17%)	2	4
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4	9
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	97 (85%)	17 (15%)	3	6
37	1f	84/90 (93%)	72 (86%)	12 (14%)	3	6
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5	11
38	1g	119/127 (94%)	96 (81%)	23 (19%)	1	2
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7	15
39	1h	114/119 (96%)	108 (95%)	6 (5%)	20	42
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	10
40	1i	90/99 (91%)	79 (88%)	11 (12%)	5	10
40	2i	89/99 (90%)	72 (81%)	17 (19%)	1	3
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	26
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2	5
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	8
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	17
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	27
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	27
44	1m	95/101 (94%)	82 (86%)	13 (14%)	3	7
44	2m	92/101 (91%)	78 (85%)	14 (15%)	3	5
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	23
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	6
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	43
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	25
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	53 (78%)	15 (22%)	1	2
48	1q	94/97 (97%)	84 (89%)	10 (11%)	6	14
48	2q	94/97 (97%)	80 (85%)	14 (15%)	3	6
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	15
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	8
50	1s	69/80 (86%)	60 (87%)	9 (13%)	4	8
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	14
51	1t	70/82 (85%)	66 (94%)	4 (6%)	18	39
51	2t	70/82 (85%)	63 (90%)	7 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	39
52	2u	18/22 (82%)	18 (100%)	0	100	100
57	1z	13/13 (100%)	11 (85%)	2 (15%)	2	5
57	2z	13/13 (100%)	10 (77%)	3 (23%)	1	1
All	All	9331/10090 (92%)	8328 (89%)	1003 (11%)	6	13

5 of 1003 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	1q	89	LEU
40	2i	65	VAL
8	2I	82	ARG
39	2h	133	LEU
46	2o	60	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
42	2k	38	ASN
45	2n	49	HIS
40	1i	34	ASN
40	1i	31	GLN
47	2p	13	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	472 (16%)	37 (1%)
1	2A	2791/2915 (95%)	478 (17%)	32 (1%)
2	1B	119/121 (98%)	14 (11%)	0
2	2B	118/121 (97%)	22 (18%)	0
32	1a	1497/1521 (98%)	253 (16%)	0
32	2a	1501/1521 (98%)	279 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	72/76 (94%)	17 (23%)	0
54	2w	68/76 (89%)	23 (33%)	0
55	1x	75/77 (97%)	10 (13%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	75/77 (97%)	9 (12%)	0
56	1y	72/76 (94%)	28 (38%)	0
56	2y	70/76 (92%)	27 (38%)	0
All	All	9346/9620 (97%)	1638 (17%)	69 (0%)

5 of 1638 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
1	1A	61	G

5 of 69 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	1493	C
1	2A	1608	A
1	2A	2126	A
1	1A	1608	A
1	1A	1508	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	$\# Z > 2$
1	5MC	1A	1942	1	19,22,23	1.57	3 (15%)	26,32,35	1.48	4 (15%)
56	4SU	2y	8	56	18,21,22	1.72	5 (27%)	25,30,33	2.10	8 (32%)
1	5MU	1A	1939	1,58	19,22,23	1.62	6 (31%)	27,32,35	2.36	8 (29%)
56	MIA	1y	37	56	21,24,32	1.74	3 (14%)	30,35,47	2.05	9 (30%)
32	M2G	2a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	G7M	2a	527	58,32	23,26,27	1.37	4 (17%)	34,39,42	1.67	6 (17%)
32	5MC	1a	967	32	19,22,23	1.56	2 (10%)	26,32,35	1.17	1 (3%)
32	G7M	1a	527	32	23,26,27	1.59	4 (17%)	34,39,42	1.55	5 (14%)
1	2MA	2A	2503	1,58	22,25,26	1.52	4 (18%)	32,37,40	2.49	6 (18%)
54	G7M	1w	46	54	23,26,27	1.53	3 (13%)	34,39,42	1.77	4 (11%)
54	4SU	2w	8	54	18,21,22	1.83	3 (16%)	25,30,33	2.34	5 (20%)
1	5MU	1A	1915	1	19,22,23	1.32	4 (21%)	27,32,35	2.40	8 (29%)
54	5MU	1w	54	54	19,22,23	1.54	4 (21%)	27,32,35	1.88	6 (22%)
1	5MC	2A	1942	1	19,22,23	1.48	3 (15%)	26,32,35	1.23	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.85	0	25,31,34	1.09	2 (8%)
32	5MC	2a	1407	58,32	19,22,23	1.57	3 (15%)	26,32,35	1.33	4 (15%)
54	4SU	1w	8	54	18,21,22	2.02	4 (22%)	25,30,33	1.64	6 (24%)
32	MA6	1a	1518	32	23,26,27	0.50	0	33,38,41	2.12	11 (33%)
56	5MU	2y	54	56	19,22,23	1.59	5 (26%)	27,32,35	1.89	5 (18%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.84	0
1	PSU	2A	1917	1	18,21,22	1.44	2 (11%)	21,30,33	2.13	4 (19%)
54	PSU	2w	32	54	18,21,22	1.41	3 (16%)	21,30,33	2.09	5 (23%)
54	F3N	1w	76	1	33,36,37	1.53	4 (12%)	41,51,54	1.69	7 (17%)
56	PSU	2y	39	56	18,21,22	1.63	3 (16%)	21,30,33	1.45	2 (9%)
32	5MC	2a	967	58,32	19,22,23	1.60	2 (10%)	26,32,35	1.08	2 (7%)
32	MA6	2a	1519	32	23,26,27	0.50	0	33,38,41	2.09	8 (24%)
56	MIA	2y	37	56	21,24,32	1.70	3 (14%)	30,35,47	2.10	8 (26%)
54	PSU	1w	32	54	18,21,22	1.30	2 (11%)	21,30,33	1.99	4 (19%)
54	PSU	2w	39	54	18,21,22	1.42	3 (16%)	21,30,33	1.89	4 (19%)
1	OMU	2A	2552	1	19,22,23	1.06	2 (10%)	25,31,34	1.98	5 (20%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.14	4 (19%)
1	5MC	2A	1962	1,58	19,22,23	1.56	3 (15%)	26,32,35	1.16	2 (7%)
32	MA6	1a	1519	32	23,26,27	0.46	0	33,38,41	2.03	10 (30%)
56	PSU	1y	39	56	18,21,22	1.44	1 (5%)	21,30,33	1.88	4 (19%)
32	PSU	1a	516	32	18,21,22	1.42	3 (16%)	21,30,33	2.00	5 (23%)
43	0TD	1l	92	43	8,9,10	4.52	4 (50%)	6,11,13	6.34	3 (50%)
32	2MG	2a	1207	32	23,26,27	1.31	2 (8%)	33,38,41	2.25	9 (27%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	1.05	4 (16%)
55	PSU	1x	55	55	18,21,22	1.44	2 (11%)	21,30,33	1.93	5 (23%)
54	MIA	2w	37	54	24,27,32	1.94	5 (20%)	32,39,47	2.56	12 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.78	3 (11%)
55	31H	2x	76	55,58	31,34,35	1.19	3 (9%)	35,47,50	2.23	14 (40%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.07	9 (27%)
1	PSU	2A	2605	1	18,21,22	1.26	1 (5%)	21,30,33	2.14	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.86	0	25,32,35	0.89	1 (4%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.25	3 (11%)
1	OMG	2A	2251	55,1,58	23,26,27	1.29	3 (13%)	32,38,41	2.13	7 (21%)
1	PSU	1A	1911	1	18,21,22	1.46	2 (11%)	21,30,33	1.94	5 (23%)
54	5MU	2w	54	54	19,22,23	1.16	2 (10%)	27,32,35	1.90	6 (22%)
55	PSU	2x	55	55	18,21,22	1.45	3 (16%)	21,30,33	2.00	5 (23%)
54	MIA	1w	37	54	28,31,32	2.15	6 (21%)	38,44,47	2.88	13 (34%)
56	4SU	1y	8	56	18,21,22	1.55	4 (22%)	25,30,33	1.28	3 (12%)
1	OMG	1A	2251	55,1,58	23,26,27	1.38	3 (13%)	32,38,41	1.96	7 (21%)
1	PSU	2A	1911	1	18,21,22	1.44	2 (11%)	21,30,33	2.29	3 (14%)
32	UR3	2a	1498	32	19,22,23	1.15	2 (10%)	26,32,35	1.80	4 (15%)
56	PSU	2y	32	56	18,21,22	1.32	2 (11%)	21,30,33	2.05	4 (19%)
1	PSU	1A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	2.11	6 (28%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.11	3 (14%)
32	M2G	1a	966	32	24,27,28	1.33	3 (12%)	33,40,43	1.96	6 (18%)
56	5MU	1y	54	56	19,22,23	1.50	5 (26%)	27,32,35	2.02	8 (29%)
56	PSU	1y	55	56	18,21,22	1.40	2 (11%)	21,30,33	2.02	3 (14%)
56	PSU	1y	32	56	18,21,22	1.38	3 (16%)	21,30,33	1.84	4 (19%)
55	5MC	1x	32	55	19,22,23	1.56	3 (15%)	26,32,35	1.44	4 (15%)
32	2MG	1a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.15	7 (21%)
56	PSU	2y	55	56	18,21,22	1.46	2 (11%)	21,30,33	2.02	4 (19%)
55	4SU	1x	8	55	18,21,22	2.30	6 (33%)	25,30,33	2.44	6 (24%)
1	PSU	1A	2605	1,58	18,21,22	1.70	4 (22%)	21,30,33	2.08	4 (19%)
56	G7M	1y	46	56	23,26,27	1.42	3 (13%)	34,39,42	1.75	4 (11%)
55	5MU	1x	54	55,58	19,22,23	1.52	4 (21%)	27,32,35	2.08	6 (22%)
1	OMU	1A	2552	1,58	19,22,23	1.17	1 (5%)	25,31,34	1.73	4 (16%)
1	2MA	1A	2503	1,58	22,25,26	1.52	4 (18%)	32,37,40	2.22	7 (21%)
32	5MC	1a	1404	32	19,22,23	1.39	3 (15%)	26,32,35	1.30	4 (15%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	21,30,33	1.99	4 (19%)
32	5MC	2a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.36	3 (11%)
55	5MC	2x	32	55	19,22,23	1.76	3 (15%)	26,32,35	1.42	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	8,9,10	5.05	1 (12%)	6,11,13	5.38	2 (33%)
55	31H	1x	76	55,58	31,34,35	1.34	4 (12%)	35,47,50	2.36	15 (42%)
1	5MU	2A	1915	1	19,22,23	1.48	4 (21%)	27,32,35	2.50	9 (33%)
56	G7M	2y	46	56	23,26,27	1.72	5 (21%)	34,39,42	1.95	4 (11%)
54	PSU	2w	55	54	18,21,22	1.50	2 (11%)	21,30,33	2.23	5 (23%)
55	4SU	2x	8	55	18,21,22	2.06	5 (27%)	25,30,33	1.38	6 (24%)
1	5MC	1A	1962	1,58	19,22,23	1.82	3 (15%)	26,32,35	1.57	7 (26%)
32	5MC	1a	1407	32	19,22,23	1.53	2 (10%)	26,32,35	1.21	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.51	3 (15%)	26,32,35	1.30	3 (11%)
55	5MU	2x	54	55	19,22,23	1.45	5 (26%)	27,32,35	2.21	6 (22%)
54	F3N	2w	76	54,1	33,36,37	1.53	5 (15%)	41,51,54	1.77	9 (21%)
54	G7M	2w	46	54	23,26,27	1.42	4 (17%)	34,39,42	1.64	4 (11%)
1	5MU	2A	1939	1,58	19,22,23	1.31	3 (15%)	27,32,35	2.64	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	2/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	G7M	2a	527	58,32	-	3/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
1	2MA	2A	2503	1,58	-	2/7/25/26	0/3/3/3
54	G7M	1w	46	54	-	2/7/25/26	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1407	58,32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	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	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	1	-	2/19/37/38	0/4/4/4
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	58,32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
56	MIA	2y	37	56	-	1/7/25/34	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1	-	0/9/27/28	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,58	-	4/22/40/41	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1,58	-	0/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
56	4SU	1y	8	56	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,58	-	1/9/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	1/7/25/26	0/3/3/3
55	5MU	1x	54	55,58	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
1	2MA	1A	2503	1,58	-	1/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
55	31H	1x	76	55,58	-	4/22/40/41	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	2/19/37/38	0/4/4/4
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2

The worst 5 of 250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-13.85	1.68	1.82
43	1l	92	0TD	CB-SB	-11.51	1.70	1.82
1	1A	1962	5MC	C5-C4	6.95	1.49	1.44
54	1w	37	MIA	C13-C14	6.44	1.51	1.32
55	2x	32	5MC	C5-C4	6.41	1.49	1.44

The worst 5 of 474 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-14.82	75.72	102.36
43	2l	92	0TD	CSB-SB-CB	-12.88	79.21	102.36
54	1w	37	MIA	C12-C13-C14	-10.75	107.71	127.01
1	2A	2503	2MA	C5-C4-N3	-9.43	117.25	127.18
54	2w	37	MIA	C5-C4-N3	-8.66	118.06	127.18

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
54	1w	76	F3N	C3'-C4'-C5'-O5'

There are no ring outliers.

34 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2y	8	4SU	2	0
1	1A	1939	5MU	1	0
56	1y	37	MIA	2	0
32	2a	527	G7M	2	0
32	1a	967	5MC	1	0
54	1w	46	G7M	2	0
54	2w	8	4SU	2	0
54	1w	8	4SU	1	0
32	1a	1518	MA6	1	0
1	1A	1920	OMC	1	0
54	1w	76	F3N	3	0
32	2a	1519	MA6	2	0
54	2w	39	PSU	2	0
1	2A	2552	OMU	1	0
32	1a	1519	MA6	1	0
43	1l	92	0TD	1	0
32	2a	1207	2MG	2	0
32	1a	1402	4OC	1	0
32	1a	1498	UR3	1	0
32	2a	1518	MA6	3	0
32	2a	1402	4OC	2	0
32	2a	1404	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2251	OMG	1	0
55	2x	55	PSU	1	0
54	1w	37	MIA	1	0
56	1y	8	4SU	1	0
1	1A	2251	OMG	1	0
32	1a	966	M2G	3	0
56	2y	55	PSU	3	0
55	1x	8	4SU	1	0
43	2l	92	0TD	2	0
56	2y	46	G7M	3	0
55	2x	54	5MU	1	0
54	2w	76	F3N	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	2d	303	35	0,12,12	-	-	-		
61	SF4	1d	302	35	0,12,12	-	-	-		

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

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

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
54	1w	1
7	1H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1w	75:C	O3'	76:F3N	P	2.35
1	1H	126:PRO	C	127:GLU	N	1.17

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.72	131 (4%) 37 33	16, 32, 85, 95	0
1	2A	2789/2915 (95%)	-0.31	124 (4%) 39 34	28, 49, 84, 96	0
2	1B	120/121 (99%)	-0.61	0 100 100	26, 44, 58, 81	0
2	2B	120/121 (99%)	0.09	0 100 100	51, 63, 71, 83	0
3	1D	275/276 (99%)	-0.38	2 (0%) 84 81	16, 33, 47, 73	0
3	2D	275/276 (99%)	-0.05	3 (1%) 78 75	28, 44, 55, 76	0
4	1E	204/206 (99%)	-0.32	1 (0%) 87 85	15, 37, 56, 69	0
4	2E	204/206 (99%)	0.26	2 (0%) 79 76	30, 53, 65, 76	0
5	1F	203/210 (96%)	-0.21	0 100 100	17, 37, 61, 72	0
5	2F	203/210 (96%)	0.28	1 (0%) 87 85	31, 58, 68, 75	0
6	1G	181/182 (99%)	0.32	7 (3%) 43 38	36, 50, 65, 76	0
6	2G	181/182 (99%)	0.90	10 (5%) 30 27	53, 65, 73, 82	0
7	1H	174/180 (96%)	0.23	3 (1%) 69 65	36, 49, 62, 66	0
7	2H	174/180 (96%)	1.28	26 (14%) 5 4	61, 73, 80, 84	0
8	1I	146/148 (98%)	0.59	2 (1%) 73 70	43, 62, 73, 76	0
8	2I	146/148 (98%)	0.70	3 (2%) 63 59	48, 64, 72, 77	0
9	1N	140/140 (100%)	-0.25	2 (1%) 73 70	23, 35, 53, 64	0
9	2N	140/140 (100%)	0.49	2 (1%) 73 70	41, 56, 71, 78	0
10	1O	122/122 (100%)	-0.26	2 (1%) 70 67	24, 37, 54, 59	0
10	2O	122/122 (100%)	0.20	0 100 100	39, 52, 63, 67	0
11	1P	149/150 (99%)	-0.07	2 (1%) 75 71	18, 42, 62, 68	0
11	2P	149/150 (99%)	0.43	5 (3%) 48 43	33, 57, 71, 78	0
12	1Q	141/141 (100%)	-0.16	0 100 100	23, 36, 50, 63	0
12	2Q	141/141 (100%)	0.53	7 (4%) 34 30	40, 56, 66, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.37	0 100 100	22, 30, 46, 49	0
13	2R	118/118 (100%)	0.15	0 100 100	38, 47, 57, 64	0
14	1S	110/112 (98%)	-0.07	0 100 100	33, 44, 56, 60	0
14	2S	110/112 (98%)	0.66	1 (0%) 81 78	50, 60, 68, 73	0
15	1T	131/146 (89%)	-0.00	2 (1%) 72 68	31, 41, 61, 72	0
15	2T	131/146 (89%)	0.28	2 (1%) 72 68	45, 54, 65, 69	0
16	1U	116/118 (98%)	-0.59	0 100 100	16, 26, 40, 54	0
16	2U	116/118 (98%)	0.36	2 (1%) 69 65	34, 52, 65, 69	0
17	1V	101/101 (100%)	-0.50	0 100 100	18, 31, 50, 59	0
17	2V	101/101 (100%)	0.51	0 100 100	39, 60, 70, 78	0
18	1W	112/113 (99%)	-0.53	1 (0%) 81 78	17, 27, 45, 75	0
18	2W	112/113 (99%)	0.10	0 100 100	34, 44, 58, 83	0
19	1X	95/96 (98%)	-0.14	2 (2%) 63 59	22, 35, 56, 73	0
19	2X	95/96 (98%)	0.33	3 (3%) 50 46	41, 52, 66, 75	0
20	1Y	107/110 (97%)	0.04	0 100 100	30, 45, 58, 69	0
20	2Y	107/110 (97%)	0.89	8 (7%) 20 18	51, 61, 71, 79	0
21	1Z	154/206 (74%)	0.57	6 (3%) 43 38	32, 56, 71, 81	0
21	2Z	160/206 (77%)	1.16	19 (11%) 9 7	55, 70, 79, 81	0
22	10	83/85 (97%)	-0.30	0 100 100	18, 33, 44, 56	0
22	20	83/85 (97%)	0.38	1 (1%) 76 73	38, 51, 61, 66	0
23	11	97/98 (98%)	-0.00	0 100 100	24, 43, 63, 72	0
23	21	97/98 (98%)	0.27	2 (2%) 63 59	33, 50, 64, 69	0
24	12	70/72 (97%)	0.06	1 (1%) 73 70	29, 43, 56, 67	0
24	22	70/72 (97%)	0.52	1 (1%) 73 70	48, 59, 67, 74	0
25	13	59/60 (98%)	-0.35	0 100 100	21, 30, 54, 66	0
25	23	59/60 (98%)	0.38	1 (1%) 69 65	48, 55, 68, 76	0
26	14	69/71 (97%)	0.78	7 (10%) 12 10	46, 65, 76, 79	0
26	24	69/71 (97%)	1.23	13 (18%) 3 2	59, 73, 81, 82	0
27	15	59/60 (98%)	-0.59	0 100 100	17, 27, 45, 48	0
27	25	59/60 (98%)	-0.03	0 100 100	29, 43, 61, 69	0
28	16	53/54 (98%)	-0.28	0 100 100	32, 40, 54, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.24	1 (1%) 66 62	44, 52, 60, 64	0
29	17	48/49 (97%)	-0.55	1 (2%) 63 59	17, 24, 44, 55	0
29	27	48/49 (97%)	-0.05	3 (6%) 26 23	29, 35, 58, 63	0
30	18	64/65 (98%)	-0.35	0 100 100	24, 30, 36, 55	0
30	28	64/65 (98%)	0.15	0 100 100	41, 46, 52, 59	0
31	19	37/37 (100%)	-0.30	0 100 100	24, 33, 48, 56	0
31	29	37/37 (100%)	0.63	0 100 100	49, 57, 67, 73	0
32	1a	1488/1521 (97%)	-0.07	31 (2%) 63 59	31, 56, 82, 97	0
32	2a	1491/1521 (98%)	0.12	35 (2%) 61 57	42, 63, 82, 96	0
33	1b	231/256 (90%)	1.06	30 (12%) 7 6	53, 67, 76, 82	0
33	2b	231/256 (90%)	1.11	23 (9%) 12 10	59, 71, 78, 84	0
34	1c	206/239 (86%)	0.65	6 (2%) 53 49	50, 61, 72, 81	0
34	2c	206/239 (86%)	1.02	13 (6%) 26 23	61, 70, 77, 81	0
35	1d	208/209 (99%)	0.78	14 (6%) 24 21	48, 60, 69, 74	0
35	2d	208/209 (99%)	0.62	4 (1%) 66 62	51, 61, 68, 73	0
36	1e	148/162 (91%)	0.33	0 100 100	44, 56, 65, 70	0
36	2e	148/162 (91%)	0.68	5 (3%) 48 43	53, 64, 71, 79	0
37	1f	100/101 (99%)	0.51	1 (1%) 79 76	47, 58, 67, 69	0
37	2f	100/101 (99%)	0.40	0 100 100	51, 59, 66, 73	0
38	1g	155/156 (99%)	0.68	13 (8%) 17 15	51, 60, 74, 81	0
38	2g	155/156 (99%)	0.96	18 (11%) 9 8	58, 67, 75, 79	0
39	1h	137/138 (99%)	0.44	2 (1%) 72 68	46, 57, 65, 69	0
39	2h	137/138 (99%)	0.73	1 (0%) 84 81	56, 64, 70, 74	0
40	1i	127/128 (99%)	0.97	9 (7%) 22 19	41, 65, 72, 74	0
40	2i	127/128 (99%)	1.29	20 (15%) 5 4	57, 72, 77, 80	0
41	1j	97/105 (92%)	1.05	9 (9%) 14 12	49, 66, 75, 77	0
41	2j	96/105 (91%)	1.36	22 (22%) 2 1	59, 73, 79, 81	0
42	1k	114/129 (88%)	0.34	2 (1%) 67 64	37, 57, 67, 76	0
42	2k	114/129 (88%)	0.69	3 (2%) 57 52	48, 62, 71, 73	0
43	1l	121/132 (91%)	0.17	3 (2%) 58 54	39, 45, 56, 67	0
43	2l	121/132 (91%)	0.41	3 (2%) 58 54	47, 54, 64, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	125/126 (99%)	0.55	5 (4%) 42 38	44, 57, 64, 72	0
44	2m	122/126 (96%)	1.17	14 (11%) 9 8	55, 67, 72, 74	0
45	1n	60/61 (98%)	0.62	2 (3%) 49 45	50, 57, 63, 68	0
45	2n	60/61 (98%)	1.51	14 (23%) 2 1	62, 69, 72, 73	0
46	1o	88/89 (98%)	0.42	1 (1%) 78 75	41, 55, 64, 72	0
46	2o	88/89 (98%)	0.58	4 (4%) 38 33	49, 60, 70, 73	0
47	1p	82/88 (93%)	0.88	4 (4%) 35 31	47, 62, 68, 73	0
47	2p	82/88 (93%)	0.70	4 (4%) 35 31	51, 59, 68, 69	0
48	1q	99/105 (94%)	0.64	1 (1%) 79 76	48, 58, 66, 71	0
48	2q	99/105 (94%)	0.78	4 (4%) 42 38	50, 61, 71, 78	0
49	1r	68/88 (77%)	0.40	2 (2%) 53 49	47, 57, 68, 70	0
49	2r	68/88 (77%)	0.30	1 (1%) 72 68	53, 60, 68, 74	0
50	1s	83/93 (89%)	0.64	4 (4%) 35 31	48, 59, 66, 73	0
50	2s	83/93 (89%)	1.28	12 (14%) 6 5	60, 69, 75, 81	0
51	1t	96/106 (90%)	0.96	11 (11%) 9 8	53, 61, 69, 74	0
51	2t	96/106 (90%)	0.83	8 (8%) 17 15	51, 60, 70, 75	0
52	1u	23/27 (85%)	1.05	0 100 100	53, 57, 61, 62	0
52	2u	23/27 (85%)	1.59	5 (21%) 2 2	61, 67, 71, 74	0
53	1v	13/24 (54%)	0.41	2 (15%) 5 4	38, 45, 83, 90	0
53	2v	13/24 (54%)	0.76	2 (15%) 5 4	52, 58, 84, 93	0
54	1w	67/76 (88%)	0.20	3 (4%) 38 33	26, 66, 82, 86	0
54	2w	64/76 (84%)	0.53	4 (6%) 26 23	39, 76, 85, 89	0
55	1x	72/77 (93%)	-0.25	1 (1%) 73 70	21, 53, 69, 83	0
55	2x	72/77 (93%)	-0.07	1 (1%) 73 70	36, 63, 76, 90	0
56	1y	67/76 (88%)	1.69	19 (28%) 1 1	55, 87, 91, 92	0
56	2y	66/76 (86%)	1.76	27 (40%) 0 0	60, 89, 92, 94	0
57	1z	18/18 (100%)	0.70	1 (5%) 30 26	48, 54, 65, 65	0
57	2z	18/18 (100%)	1.15	2 (11%) 10 8	62, 65, 72, 86	0
All	All	20912/21784 (95%)	0.11	837 (4%) 42 38	15, 55, 77, 97	0

The worst 5 of 837 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2802	G	7.0
45	1n	2	ALA	6.5
1	2A	2113	U	6.3
38	1g	80	VAL	5.5
21	1Z	141	VAL	5.4

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(\AA^2)	Q<0.9
56	G7M	2y	46	24/25	0.48	0.17	80,89,94,111	0
56	4SU	2y	8	20/21	0.50	0.18	85,93,100,111	0
56	5MU	2y	54	21/22	0.55	0.16	70,84,93,107	0
56	4SU	1y	8	20/21	0.56	0.16	82,87,93,106	0
56	G7M	1y	46	24/25	0.57	0.17	77,89,95,101	0
56	PSU	1y	55	20/21	0.58	0.15	84,87,95,109	0
56	5MU	1y	54	21/22	0.64	0.14	79,84,91,101	0
56	PSU	2y	39	20/21	0.64	0.17	74,83,95,105	0
56	MIA	1y	37	22/30	0.67	0.17	77,84,91,100	0
56	PSU	2y	55	20/21	0.69	0.13	76,85,93,93	0
56	MIA	2y	37	22/30	0.73	0.17	71,86,101,112	0
54	G7M	1w	46	24/25	0.74	0.14	64,72,88,102	0
56	PSU	2y	32	20/21	0.77	0.13	75,84,91,98	0
56	PSU	1y	32	20/21	0.79	0.14	76,83,88,98	0
54	G7M	2w	46	24/25	0.80	0.12	73,78,90,103	0
56	PSU	1y	39	20/21	0.82	0.12	72,80,85,88	0
54	PSU	2w	55	20/21	0.88	0.12	68,73,80,81	0
54	4SU	2w	8	20/21	0.88	0.12	68,75,81,89	0
55	5MU	2x	54	21/22	0.91	0.12	64,68,71,72	0
55	5MU	1x	54	21/22	0.91	0.11	53,59,62,67	0
1	5MU	2A	1915	21/22	0.92	0.10	50,53,57,60	0
32	2MG	2a	1207	24/25	0.92	0.09	64,69,73,74	0
43	0TD	2l	92	10/11	0.92	0.13	52,55,63,64	0
55	4SU	2x	8	20/21	0.92	0.12	59,71,76,77	0
55	PSU	2x	55	20/21	0.93	0.09	60,65,70,72	0
43	0TD	1l	92	10/11	0.93	0.12	42,46,49,58	0
55	PSU	1x	55	20/21	0.93	0.08	46,52,63,65	0
54	5MU	2w	54	21/22	0.93	0.10	61,66,71,75	0
32	G7M	2a	527	24/25	0.94	0.10	52,57,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	4SU	1w	8	20/21	0.94	0.09	54,64,70,70	0
32	5MC	2a	1400	21/22	0.94	0.11	54,57,64,69	0
54	PSU	1w	55	20/21	0.94	0.09	43,59,67,68	0
55	5MC	2x	32	21/22	0.94	0.11	55,60,63,64	0
32	PSU	2a	516	20/21	0.94	0.09	54,59,64,65	0
54	PSU	2w	32	20/21	0.94	0.10	58,63,68,69	0
32	M2G	2a	966	25/26	0.95	0.11	50,59,66,74	0
32	5MC	2a	967	21/22	0.95	0.10	53,60,63,66	0
1	PSU	2A	1917	20/21	0.95	0.09	44,53,61,61	0
54	MIA	2w	37	25/30	0.95	0.09	46,57,61,63	0
1	5MC	2A	1942	21/22	0.95	0.09	43,49,57,62	0
32	4OC	2a	1402	22/23	0.95	0.10	44,50,53,56	0
32	2MG	1a	1207	24/25	0.96	0.07	48,54,57,58	0
1	5MU	1A	1915	21/22	0.96	0.09	39,47,49,51	0
1	PSU	1A	1917	20/21	0.96	0.08	36,43,48,50	0
54	PSU	1w	32	20/21	0.96	0.09	38,45,53,58	0
1	5MC	1A	1942	21/22	0.96	0.08	26,33,39,40	0
54	5MU	1w	54	21/22	0.96	0.07	35,47,51,53	0
32	G7M	1a	527	24/25	0.96	0.09	36,41,45,48	0
55	4SU	1x	8	20/21	0.96	0.08	44,51,57,59	0
32	MA6	2a	1519	24/25	0.96	0.09	45,50,53,56	0
1	PSU	2A	1911	20/21	0.96	0.07	41,50,54,61	0
55	5MC	1x	32	21/22	0.96	0.08	43,45,49,53	0
32	M2G	1a	966	25/26	0.96	0.09	40,45,48,51	0
1	OMC	2A	1920	21/22	0.96	0.08	44,49,53,55	0
54	PSU	2w	39	20/21	0.96	0.09	45,57,63,67	0
1	OMU	2A	2552	21/22	0.97	0.07	32,41,44,46	0
1	PSU	2A	2605	20/21	0.97	0.06	30,34,40,40	0
32	4OC	1a	1402	22/23	0.97	0.07	35,39,41,43	0
32	5MC	1a	1404	21/22	0.97	0.07	27,33,37,38	0
1	PSU	1A	1911	20/21	0.97	0.07	35,41,47,47	0
54	F3N	2w	76	33/34	0.97	0.08	27,34,37,38	0
1	5MC	1A	1962	21/22	0.97	0.06	24,31,35,39	0
32	5MC	1a	967	21/22	0.97	0.08	41,46,53,54	0
55	31H	1x	76	32/33	0.97	0.07	14,19,26,33	10
54	PSU	1w	39	20/21	0.97	0.07	34,43,50,53	0
55	31H	2x	76	32/33	0.97	0.08	28,36,42,43	0
32	5MC	2a	1407	21/22	0.97	0.07	40,45,49,52	0
32	UR3	2a	1498	21/22	0.97	0.09	38,47,51,55	0
32	MA6	2a	1518	24/25	0.97	0.07	45,48,51,52	0
32	PSU	1a	516	20/21	0.97	0.07	33,47,51,55	0
1	5MU	2A	1939	21/22	0.97	0.07	30,34,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	5MC	1a	1400	21/22	0.97	0.08	34,42,49,51	0
1	5MC	2A	1962	21/22	0.97	0.07	37,40,47,55	0
32	MA6	1a	1519	24/25	0.98	0.07	27,35,39,41	0
1	PSU	1A	2605	20/21	0.98	0.05	18,22,24,27	0
54	F3N	1w	76	33/34	0.98	0.07	14,19,23,24	0
1	OMC	1A	1920	21/22	0.98	0.06	33,40,44,46	0
1	5MU	1A	1939	21/22	0.98	0.06	20,26,30,32	0
54	MIA	1w	37	29/30	0.98	0.08	29,41,53,53	0
1	OMG	2A	2251	24/25	0.98	0.07	31,34,38,41	0
32	5MC	2a	1404	21/22	0.98	0.07	36,44,48,50	0
1	2MA	2A	2503	23/24	0.98	0.07	28,33,37,44	0
32	5MC	1a	1407	21/22	0.98	0.07	29,35,40,41	0
32	MA6	1a	1518	24/25	0.98	0.06	25,34,37,38	0
32	UR3	1a	1498	21/22	0.99	0.05	26,35,36,42	0
1	2MA	1A	2503	23/24	0.99	0.05	11,18,22,23	0
1	OMU	1A	2552	21/22	0.99	0.06	19,25,29,31	0
1	OMG	1A	2251	24/25	0.99	0.04	18,21,23,24	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	1634	1/1	0.23	0.51	93,93,93,93	0
58	MG	2A	3209	1/1	0.44	0.23	86,86,86,86	0
58	MG	10	108	1/1	0.54	0.32	60,60,60,60	0
58	MG	2a	1791	1/1	0.57	0.25	68,68,68,68	0
58	MG	2y	104	1/1	0.59	0.21	82,82,82,82	0
58	MG	2A	3756	1/1	0.60	0.24	61,61,61,61	0
58	MG	2A	3364	1/1	0.61	0.33	83,83,83,83	0
58	MG	1B	232	1/1	0.62	0.22	85,85,85,85	0
58	MG	2A	3272	1/1	0.63	0.21	74,74,74,74	0
58	MG	2a	1747	1/1	0.66	0.15	80,80,80,80	0
58	MG	20	102	1/1	0.66	0.33	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3571	1/1	0.66	0.25	73,73,73,73	0
58	MG	1A	3795	1/1	0.67	0.21	79,79,79,79	0
58	MG	1A	3480	1/1	0.67	0.23	64,64,64,64	0
58	MG	2B	214	1/1	0.68	0.17	72,72,72,72	0
58	MG	1A	4103	1/1	0.68	0.20	60,60,60,60	0
58	MG	2v	102	1/1	0.69	0.29	76,76,76,76	0
58	MG	1h	201	1/1	0.69	0.14	68,68,68,68	0
58	MG	2A	3345	1/1	0.70	0.24	71,71,71,71	0
58	MG	2A	3334	1/1	0.70	0.32	74,74,74,74	0
58	MG	1A	4100	1/1	0.71	0.18	66,66,66,66	0
58	MG	2A	3813	1/1	0.72	0.20	62,62,62,62	0
58	MG	2A	3253	1/1	0.72	0.18	70,70,70,70	0
58	MG	2A	3586	1/1	0.72	0.17	75,75,75,75	0
58	MG	2w	103	1/1	0.72	0.17	75,75,75,75	0
58	MG	1A	4090	1/1	0.72	0.26	46,46,46,46	0
58	MG	2A	3675	1/1	0.73	0.19	63,63,63,63	0
58	MG	2l	101	1/1	0.73	0.19	73,73,73,73	0
58	MG	1A	3418	1/1	0.73	0.41	82,82,82,82	0
58	MG	2B	220	1/1	0.73	0.26	69,69,69,69	0
58	MG	2A	3342	1/1	0.74	0.28	75,75,75,75	0
58	MG	2a	1802	1/1	0.74	0.33	76,76,76,76	0
58	MG	2a	1822	1/1	0.74	0.20	63,63,63,63	0
58	MG	2A	3705	1/1	0.74	0.14	64,64,64,64	0
58	MG	1B	231	1/1	0.74	0.17	70,70,70,70	0
58	MG	2E	301	1/1	0.74	0.21	62,62,62,62	0
58	MG	1A	4038	1/1	0.75	0.17	57,57,57,57	0
58	MG	2A	3625	1/1	0.75	0.18	66,66,66,66	0
58	MG	1a	1696	1/1	0.75	0.21	69,69,69,69	0
58	MG	2a	1820	1/1	0.75	0.19	57,57,57,57	0
58	MG	1A	3373	1/1	0.75	0.30	54,54,54,54	0
58	MG	2A	3749	1/1	0.75	0.14	49,49,49,49	0
58	MG	2A	3299	1/1	0.75	0.14	71,71,71,71	0
58	MG	2A	3803	1/1	0.75	0.14	60,60,60,60	0
58	MG	2a	1706	1/1	0.76	0.17	66,66,66,66	0
58	MG	1U	211	1/1	0.76	0.66	81,81,81,81	0
58	MG	1B	203	1/1	0.76	0.31	62,62,62,62	0
58	MG	1A	3885	1/1	0.76	0.20	73,73,73,73	0
58	MG	1A	3988	1/1	0.76	0.14	62,62,62,62	0
58	MG	2A	3370	1/1	0.76	0.15	78,78,78,78	0
58	MG	2A	3373	1/1	0.76	0.15	66,66,66,66	0
58	MG	2a	1633	1/1	0.76	0.20	83,83,83,83	0
58	MG	2A	3395	1/1	0.76	0.20	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	2a	1813	1/1	0.77	0.20	61,61,61,61	0
58	MG	1A	3520	1/1	0.77	0.15	55,55,55,55	0
58	MG	1A	3235	1/1	0.77	0.27	74,74,74,74	0
58	MG	2A	3064	1/1	0.77	0.15	65,65,65,65	0
58	MG	2A	3869	1/1	0.77	0.13	60,60,60,60	0
58	MG	2A	3193	1/1	0.77	0.17	71,71,71,71	0
58	MG	1A	4096	1/1	0.78	0.20	63,63,63,63	0
58	MG	2A	3469	1/1	0.78	0.24	70,70,70,70	0
58	MG	2A	3353	1/1	0.78	0.25	62,62,62,62	0
58	MG	2a	1628	1/1	0.78	0.30	76,76,76,76	0
58	MG	2A	3328	1/1	0.78	0.15	55,55,55,55	0
58	MG	2A	3096	1/1	0.78	0.23	65,65,65,65	0
58	MG	2A	3690	1/1	0.78	0.13	66,66,66,66	0
58	MG	1A	3852	1/1	0.78	0.14	61,61,61,61	0
58	MG	2A	3400	1/1	0.79	0.14	72,72,72,72	0
58	MG	1A	3807	1/1	0.79	0.13	49,49,49,49	0
58	MG	2A	3835	1/1	0.79	0.09	69,69,69,69	0
58	MG	2A	3473	1/1	0.79	0.15	68,68,68,68	0
58	MG	1A	4082	1/1	0.79	0.21	63,63,63,63	0
58	MG	2A	3291	1/1	0.79	0.13	68,68,68,68	0
58	MG	1a	1629	1/1	0.79	0.16	58,58,58,58	0
58	MG	1A	3540	1/1	0.79	0.14	66,66,66,66	0
58	MG	1a	1739	1/1	0.79	0.19	65,65,65,65	0
58	MG	2w	101	1/1	0.79	0.22	68,68,68,68	0
58	MG	2A	3337	1/1	0.79	0.16	71,71,71,71	0
58	MG	2w	105	1/1	0.79	0.20	79,79,79,79	0
58	MG	2A	3398	1/1	0.79	0.14	60,60,60,60	0
58	MG	2A	3477	1/1	0.80	0.13	75,75,75,75	0
58	MG	2A	3537	1/1	0.80	0.13	55,55,55,55	0
58	MG	1A	3959	1/1	0.80	0.26	76,76,76,76	0
58	MG	2a	1742	1/1	0.80	0.15	63,63,63,63	0
58	MG	1A	3714	1/1	0.80	0.16	43,43,43,43	0
58	MG	2A	3881	1/1	0.80	0.19	65,65,65,65	0
58	MG	1A	3998	1/1	0.80	0.14	59,59,59,59	0
58	MG	1A	4023	1/1	0.80	0.12	60,60,60,60	0
58	MG	1A	4032	1/1	0.80	0.17	47,47,47,47	0
58	MG	1A	3753	1/1	0.80	0.16	63,63,63,63	0
58	MG	1A	3572	1/1	0.80	0.18	61,61,61,61	0
58	MG	2a	1604	1/1	0.80	0.13	62,62,62,62	0
58	MG	2a	1606	1/1	0.80	0.27	66,66,66,66	0
58	MG	2a	1607	1/1	0.80	0.29	67,67,67,67	0
58	MG	2A	3797	1/1	0.80	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4097	1/1	0.81	0.14	75,75,75,75	0
58	MG	2a	1679	1/1	0.81	0.31	64,64,64,64	0
58	MG	2A	3630	1/1	0.81	0.18	60,60,60,60	0
58	MG	2A	3397	1/1	0.81	0.26	69,69,69,69	0
58	MG	2A	3685	1/1	0.81	0.18	57,57,57,57	0
58	MG	1a	1780	1/1	0.81	0.13	49,49,49,49	0
58	MG	2A	3704	1/1	0.81	0.19	58,58,58,58	0
58	MG	1a	1808	1/1	0.81	0.19	71,71,71,71	0
58	MG	2A	3728	1/1	0.81	0.13	64,64,64,64	0
58	MG	2A	3268	1/1	0.81	0.31	65,65,65,65	0
58	MG	1A	3850	1/1	0.81	0.17	45,45,45,45	0
58	MG	1a	1724	1/1	0.81	0.17	60,60,60,60	0
58	MG	2a	1623	1/1	0.81	0.13	55,55,55,55	0
58	MG	1a	1733	1/1	0.81	0.13	53,53,53,53	0
58	MG	2A	3101	1/1	0.81	0.21	72,72,72,72	0
58	MG	2A	3699	1/1	0.82	0.12	73,73,73,73	0
58	MG	2A	3314	1/1	0.82	0.13	60,60,60,60	0
58	MG	2a	1609	1/1	0.82	0.19	59,59,59,59	0
58	MG	1A	3793	1/1	0.82	0.08	41,41,41,41	0
58	MG	2A	3721	1/1	0.82	0.23	64,64,64,64	0
58	MG	2A	3404	1/1	0.82	0.18	67,67,67,67	0
58	MG	2A	3411	1/1	0.82	0.14	63,63,63,63	0
58	MG	2A	3455	1/1	0.82	0.23	68,68,68,68	0
58	MG	1A	3429	1/1	0.82	0.11	54,54,54,54	0
58	MG	1A	3589	1/1	0.82	0.12	68,68,68,68	0
58	MG	2A	3255	1/1	0.82	0.22	73,73,73,73	0
58	MG	2A	3257	1/1	0.82	0.16	58,58,58,58	0
58	MG	2A	3560	1/1	0.82	0.14	61,61,61,61	0
58	MG	2A	3871	1/1	0.82	0.13	65,65,65,65	0
58	MG	1a	1671	1/1	0.82	0.21	63,63,63,63	0
58	MG	2A	3601	1/1	0.82	0.14	66,66,66,66	0
58	MG	1a	1690	1/1	0.82	0.31	59,59,59,59	0
58	MG	2A	3274	1/1	0.82	0.19	64,64,64,64	0
58	MG	2A	3289	1/1	0.82	0.12	67,67,67,67	0
58	MG	2A	3175	1/1	0.82	0.31	70,70,70,70	0
58	MG	2A	3192	1/1	0.82	0.28	67,67,67,67	0
58	MG	1a	1749	1/1	0.83	0.12	55,55,55,55	0
58	MG	2a	1610	1/1	0.83	0.17	66,66,66,66	0
58	MG	2A	3741	1/1	0.83	0.14	54,54,54,54	0
58	MG	1A	4099	1/1	0.83	0.17	59,59,59,59	0
58	MG	1A	3028	1/1	0.83	0.11	70,70,70,70	0
58	MG	1a	1719	1/1	0.83	0.33	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1668	1/1	0.83	0.19	55,55,55,55	0
58	MG	2A	3607	1/1	0.83	0.13	72,72,72,72	0
58	MG	2A	3612	1/1	0.83	0.20	68,68,68,68	0
58	MG	2a	1727	1/1	0.83	0.14	54,54,54,54	0
58	MG	1l	202	1/1	0.83	0.10	56,56,56,56	0
58	MG	1x	113	1/1	0.83	0.17	58,58,58,58	0
58	MG	2A	3652	1/1	0.83	0.21	56,56,56,56	0
58	MG	2A	3668	1/1	0.83	0.13	59,59,59,59	0
58	MG	1A	3991	1/1	0.83	0.09	26,26,26,26	0
58	MG	2A	3406	1/1	0.83	0.11	62,62,62,62	0
58	MG	1a	1668	1/1	0.83	0.26	62,62,62,62	0
58	MG	1E	311	1/1	0.83	0.14	55,55,55,55	0
58	MG	2A	3110	1/1	0.83	0.27	60,60,60,60	0
58	MG	2A	3361	1/1	0.83	0.15	62,62,62,62	0
58	MG	2A	3713	1/1	0.83	0.22	64,64,64,64	0
58	MG	2x	101	1/1	0.83	0.22	52,52,52,52	0
58	MG	2A	3281	1/1	0.83	0.17	54,54,54,54	0
58	MG	2A	3380	1/1	0.84	0.10	49,49,49,49	0
58	MG	2A	3393	1/1	0.84	0.20	63,63,63,63	0
58	MG	2A	3745	1/1	0.84	0.11	59,59,59,59	0
58	MG	1A	3615	1/1	0.84	0.12	59,59,59,59	0
58	MG	2a	1627	1/1	0.84	0.17	68,68,68,68	0
58	MG	2A	3330	1/1	0.84	0.25	62,62,62,62	0
58	MG	2A	3759	1/1	0.84	0.14	37,37,37,37	0
58	MG	1a	1788	1/1	0.84	0.11	74,74,74,74	0
58	MG	2a	1658	1/1	0.84	0.33	71,71,71,71	0
58	MG	2a	1664	1/1	0.84	0.25	62,62,62,62	0
58	MG	2A	3798	1/1	0.84	0.09	45,45,45,45	0
58	MG	1A	3485	1/1	0.84	0.17	47,47,47,47	0
58	MG	2A	3338	1/1	0.84	0.14	72,72,72,72	0
58	MG	2a	1710	1/1	0.84	0.21	64,64,64,64	0
58	MG	2A	3405	1/1	0.84	0.15	61,61,61,61	0
58	MG	2A	3849	1/1	0.84	0.12	64,64,64,64	0
58	MG	2A	3136	1/1	0.84	0.35	68,68,68,68	0
58	MG	2a	1778	1/1	0.84	0.12	69,69,69,69	0
58	MG	1a	1657	1/1	0.84	0.20	62,62,62,62	0
58	MG	2A	3874	1/1	0.84	0.17	65,65,65,65	0
58	MG	2a	1808	1/1	0.84	0.18	66,66,66,66	0
58	MG	2a	1811	1/1	0.84	0.20	49,49,49,49	0
58	MG	2A	3448	1/1	0.84	0.34	60,60,60,60	0
58	MG	1A	3479	1/1	0.84	0.31	62,62,62,62	0
58	MG	1A	3942	1/1	0.84	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2v	101	1/1	0.84	0.17	62,62,62,62	0
58	MG	1A	4003	1/1	0.84	0.14	37,37,37,37	0
58	MG	2E	304	1/1	0.84	0.31	58,58,58,58	0
58	MG	2A	3250	1/1	0.84	0.16	64,64,64,64	0
58	MG	2A	3707	1/1	0.84	0.13	66,66,66,66	0
58	MG	2A	3499	1/1	0.84	0.17	59,59,59,59	0
58	MG	2A	3090	1/1	0.84	0.14	70,70,70,70	0
58	MG	2y	105	1/1	0.84	0.31	70,70,70,70	0
58	MG	2A	3190	1/1	0.85	0.17	64,64,64,64	0
58	MG	2A	3191	1/1	0.85	0.14	61,61,61,61	0
58	MG	1A	3344	1/1	0.85	0.21	51,51,51,51	0
58	MG	2a	1645	1/1	0.85	0.36	69,69,69,69	0
58	MG	2A	3347	1/1	0.85	0.14	71,71,71,71	0
58	MG	1A	3211	1/1	0.85	0.12	62,62,62,62	0
58	MG	1A	3261	1/1	0.85	0.08	64,64,64,64	0
58	MG	2A	3220	1/1	0.85	0.10	54,54,54,54	0
58	MG	2a	1704	1/1	0.85	0.28	56,56,56,56	0
58	MG	1A	3504	1/1	0.85	0.22	74,74,74,74	0
58	MG	1A	3844	1/1	0.85	0.15	56,56,56,56	0
58	MG	1v	101	1/1	0.85	0.22	69,69,69,69	0
58	MG	2A	3391	1/1	0.85	0.20	63,63,63,63	0
58	MG	1A	3515	1/1	0.85	0.22	62,62,62,62	0
58	MG	2a	1777	1/1	0.85	0.13	58,58,58,58	0
58	MG	2B	204	1/1	0.85	0.20	71,71,71,71	0
58	MG	2A	3041	1/1	0.85	0.25	55,55,55,55	0
58	MG	2a	1795	1/1	0.85	0.16	65,65,65,65	0
58	MG	2A	3057	1/1	0.85	0.17	61,61,61,61	0
58	MG	2A	3058	1/1	0.85	0.31	71,71,71,71	0
58	MG	1A	4009	1/1	0.85	0.09	61,61,61,61	0
58	MG	2A	3073	1/1	0.85	0.11	46,46,46,46	0
58	MG	2a	1818	1/1	0.85	0.16	61,61,61,61	0
58	MG	1A	3648	1/1	0.85	0.14	55,55,55,55	0
58	MG	2a	1603	1/1	0.85	0.14	64,64,64,64	0
58	MG	2j	201	1/1	0.85	0.14	63,63,63,63	0
58	MG	1A	3299	1/1	0.85	0.31	69,69,69,69	0
58	MG	1a	1732	1/1	0.85	0.11	60,60,60,60	0
58	MG	2A	3445	1/1	0.85	0.26	61,61,61,61	0
58	MG	1A	3913	1/1	0.85	0.09	40,40,40,40	0
58	MG	1A	4043	1/1	0.85	0.17	46,46,46,46	0
58	MG	2a	1616	1/1	0.85	0.27	65,65,65,65	0
58	MG	2A	3165	1/1	0.85	0.36	70,70,70,70	0
58	MG	1A	4073	1/1	0.85	0.14	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	2A	3358	1/1	0.86	0.23	56,56,56,56	0
58	MG	2E	309	1/1	0.86	0.12	45,45,45,45	0
58	MG	2F	306	1/1	0.86	0.10	49,49,49,49	0
58	MG	1d	301	1/1	0.86	0.25	55,55,55,55	0
58	MG	2A	3223	1/1	0.86	0.29	63,63,63,63	0
58	MG	2A	3249	1/1	0.86	0.13	68,68,68,68	0
58	MG	1A	3858	1/1	0.86	0.19	74,74,74,74	0
58	MG	2A	3653	1/1	0.86	0.10	50,50,50,50	0
58	MG	1a	1661	1/1	0.86	0.13	60,60,60,60	0
58	MG	2A	3390	1/1	0.86	0.17	67,67,67,67	0
58	MG	2A	3679	1/1	0.86	0.17	56,56,56,56	0
58	MG	2a	1615	1/1	0.86	0.29	64,64,64,64	0
58	MG	1A	3417	1/1	0.86	0.16	55,55,55,55	0
58	MG	1A	3687	1/1	0.86	0.19	60,60,60,60	0
58	MG	1a	1673	1/1	0.86	0.29	65,65,65,65	0
58	MG	1A	3838	1/1	0.86	0.11	62,62,62,62	0
58	MG	1A	3953	1/1	0.86	0.12	69,69,69,69	0
58	MG	1A	3440	1/1	0.86	0.12	40,40,40,40	0
58	MG	1A	4042	1/1	0.86	0.16	47,47,47,47	0
58	MG	1a	1731	1/1	0.86	0.15	47,47,47,47	0
58	MG	1B	217	1/1	0.86	0.13	58,58,58,58	0
58	MG	2A	3739	1/1	0.86	0.18	64,64,64,64	0
58	MG	2A	3409	1/1	0.86	0.10	62,62,62,62	0
58	MG	2A	3306	1/1	0.86	0.11	56,56,56,56	0
58	MG	2A	3746	1/1	0.86	0.12	40,40,40,40	0
58	MG	2A	3433	1/1	0.86	0.28	55,55,55,55	0
58	MG	2A	3754	1/1	0.86	0.17	71,71,71,71	0
58	MG	2a	1728	1/1	0.86	0.11	50,50,50,50	0
58	MG	1A	3986	1/1	0.86	0.16	60,60,60,60	0
58	MG	2A	3318	1/1	0.86	0.12	53,53,53,53	0
58	MG	2A	3779	1/1	0.86	0.16	67,67,67,67	0
58	MG	2A	3794	1/1	0.86	0.09	35,35,35,35	0
58	MG	2a	1781	1/1	0.86	0.14	59,59,59,59	0
58	MG	1A	4046	1/1	0.86	0.09	50,50,50,50	0
58	MG	1A	4047	1/1	0.86	0.10	41,41,41,41	0
58	MG	1a	1750	1/1	0.86	0.22	62,62,62,62	0
58	MG	1a	1777	1/1	0.86	0.10	56,56,56,56	0
58	MG	2A	3815	1/1	0.86	0.11	68,68,68,68	0
58	MG	2A	3480	1/1	0.86	0.18	56,56,56,56	0
58	MG	2A	3842	1/1	0.86	0.11	58,58,58,58	0
58	MG	2A	3481	1/1	0.86	0.33	65,65,65,65	0
58	MG	2A	3497	1/1	0.86	0.20	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4063	1/1	0.86	0.13	38,38,38,38	0
58	MG	1A	3269	1/1	0.86	0.09	43,43,43,43	0
58	MG	2A	3553	1/1	0.86	0.13	39,39,39,39	0
58	MG	1a	1795	1/1	0.86	0.10	59,59,59,59	0
58	MG	2A	3563	1/1	0.86	0.22	48,48,48,48	0
58	MG	2w	104	1/1	0.86	0.11	68,68,68,68	0
58	MG	2B	218	1/1	0.86	0.19	74,74,74,74	0
58	MG	1a	1805	1/1	0.86	0.22	59,59,59,59	0
58	MG	2y	103	1/1	0.86	0.18	70,70,70,70	0
58	MG	1A	3547	1/1	0.86	0.28	57,57,57,57	0
58	MG	2E	303	1/1	0.86	0.12	52,52,52,52	0
58	MG	17	104	1/1	0.87	0.11	54,54,54,54	0
58	MG	1A	3404	1/1	0.87	0.12	68,68,68,68	0
58	MG	2A	3626	1/1	0.87	0.17	49,49,49,49	0
58	MG	2A	3195	1/1	0.87	0.19	49,49,49,49	0
58	MG	2A	3651	1/1	0.87	0.12	58,58,58,58	0
58	MG	1A	3929	1/1	0.87	0.14	59,59,59,59	0
58	MG	2A	3215	1/1	0.87	0.15	71,71,71,71	0
58	MG	1A	4034	1/1	0.87	0.14	44,44,44,44	0
58	MG	2A	3374	1/1	0.87	0.18	70,70,70,70	0
58	MG	2A	3678	1/1	0.87	0.16	53,53,53,53	0
58	MG	1A	3805	1/1	0.87	0.11	52,52,52,52	0
58	MG	2A	3228	1/1	0.87	0.22	59,59,59,59	0
58	MG	2A	3243	1/1	0.87	0.13	55,55,55,55	0
58	MG	2a	1620	1/1	0.87	0.13	59,59,59,59	0
58	MG	1a	1670	1/1	0.87	0.13	49,49,49,49	0
58	MG	2A	3394	1/1	0.87	0.09	59,59,59,59	0
58	MG	1A	3546	1/1	0.87	0.26	60,60,60,60	0
58	MG	2A	3396	1/1	0.87	0.24	50,50,50,50	0
58	MG	2A	3709	1/1	0.87	0.18	64,64,64,64	0
58	MG	2a	1636	1/1	0.87	0.12	63,63,63,63	0
58	MG	2A	3251	1/1	0.87	0.29	66,66,66,66	0
58	MG	2a	1651	1/1	0.87	0.19	69,69,69,69	0
58	MG	2a	1652	1/1	0.87	0.26	65,65,65,65	0
58	MG	2a	1654	1/1	0.87	0.22	59,59,59,59	0
58	MG	2a	1657	1/1	0.87	0.33	72,72,72,72	0
58	MG	1A	3662	1/1	0.87	0.12	39,39,39,39	0
58	MG	2A	3725	1/1	0.87	0.10	53,53,53,53	0
58	MG	1a	1674	1/1	0.87	0.10	50,50,50,50	0
58	MG	1a	1675	1/1	0.87	0.21	60,60,60,60	0
58	MG	2a	1698	1/1	0.87	0.17	56,56,56,56	0
58	MG	1y	101	1/1	0.87	0.10	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	2A	3023	1/1	0.87	0.25	57,57,57,57	0
58	MG	2A	3273	1/1	0.87	0.19	63,63,63,63	0
58	MG	2a	1721	1/1	0.87	0.12	62,62,62,62	0
58	MG	1a	1681	1/1	0.87	0.23	62,62,62,62	0
58	MG	1a	1686	1/1	0.87	0.20	57,57,57,57	0
58	MG	2A	3435	1/1	0.87	0.20	52,52,52,52	0
58	MG	1B	208	1/1	0.87	0.10	55,55,55,55	0
58	MG	1B	209	1/1	0.87	0.10	52,52,52,52	0
58	MG	2A	3449	1/1	0.87	0.14	57,57,57,57	0
58	MG	1B	215	1/1	0.87	0.19	65,65,65,65	0
58	MG	2a	1786	1/1	0.87	0.21	54,54,54,54	0
58	MG	1A	3671	1/1	0.87	0.09	32,32,32,32	0
58	MG	1B	225	1/1	0.87	0.13	46,46,46,46	0
58	MG	2A	3811	1/1	0.87	0.16	63,63,63,63	0
58	MG	2A	3812	1/1	0.87	0.10	72,72,72,72	0
58	MG	2a	1810	1/1	0.87	0.13	63,63,63,63	0
58	MG	1A	3416	1/1	0.87	0.21	46,46,46,46	0
58	MG	2A	3325	1/1	0.87	0.14	66,66,66,66	0
58	MG	1A	3275	1/1	0.87	0.11	51,51,51,51	0
58	MG	2A	3841	1/1	0.87	0.11	29,29,29,29	0
58	MG	2A	3494	1/1	0.87	0.16	58,58,58,58	0
58	MG	2a	1825	1/1	0.87	0.31	70,70,70,70	0
58	MG	2A	3112	1/1	0.87	0.16	49,49,49,49	0
58	MG	1a	1735	1/1	0.87	0.17	67,67,67,67	0
58	MG	2A	3528	1/1	0.87	0.15	63,63,63,63	0
58	MG	1A	3249	1/1	0.87	0.17	52,52,52,52	0
58	MG	1G	203	1/1	0.87	0.13	60,60,60,60	0
58	MG	2A	3340	1/1	0.87	0.13	58,58,58,58	0
58	MG	2A	3185	1/1	0.87	0.28	63,63,63,63	0
58	MG	2A	3579	1/1	0.87	0.15	62,62,62,62	0
58	MG	1A	3529	1/1	0.87	0.24	65,65,65,65	0
58	MG	1A	3908	1/1	0.87	0.17	54,54,54,54	0
58	MG	2A	3350	1/1	0.87	0.12	63,63,63,63	0
58	MG	2A	3661	1/1	0.88	0.15	65,65,65,65	0
58	MG	1A	3696	1/1	0.88	0.10	24,24,24,24	0
58	MG	2A	3672	1/1	0.88	0.13	54,54,54,54	0
58	MG	2A	3050	1/1	0.88	0.12	57,57,57,57	0
58	MG	1A	4027	1/1	0.88	0.08	57,57,57,57	0
58	MG	1A	3106	1/1	0.88	0.16	50,50,50,50	0
58	MG	1A	3907	1/1	0.88	0.13	42,42,42,42	0
58	MG	2A	3279	1/1	0.88	0.13	61,61,61,61	0
58	MG	2A	3698	1/1	0.88	0.16	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	1692	1/1	0.88	0.23	47,47,47,47	0
58	MG	1A	3728	1/1	0.88	0.13	54,54,54,54	0
58	MG	1A	3729	1/1	0.88	0.10	40,40,40,40	0
58	MG	1A	3255	1/1	0.88	0.07	53,53,53,53	0
58	MG	2A	3413	1/1	0.88	0.20	54,54,54,54	0
58	MG	2A	3302	1/1	0.88	0.22	49,49,49,49	0
58	MG	2A	3104	1/1	0.88	0.17	59,59,59,59	0
58	MG	1A	3931	1/1	0.88	0.07	24,24,24,24	0
58	MG	2a	1644	1/1	0.88	0.29	58,58,58,58	0
58	MG	1E	308	1/1	0.88	0.16	63,63,63,63	0
58	MG	2a	1647	1/1	0.88	0.16	61,61,61,61	0
58	MG	2A	3113	1/1	0.88	0.23	63,63,63,63	0
58	MG	1A	3183	1/1	0.88	0.22	49,49,49,49	0
58	MG	2A	3743	1/1	0.88	0.09	57,57,57,57	0
58	MG	2a	1655	1/1	0.88	0.12	68,68,68,68	0
58	MG	2a	1656	1/1	0.88	0.33	62,62,62,62	0
58	MG	2A	3153	1/1	0.88	0.10	62,62,62,62	0
58	MG	1A	3507	1/1	0.88	0.11	51,51,51,51	0
58	MG	2A	3747	1/1	0.88	0.10	53,53,53,53	0
58	MG	1Q	203	1/1	0.88	0.08	56,56,56,56	0
58	MG	1a	1740	1/1	0.88	0.15	52,52,52,52	0
58	MG	1A	4067	1/1	0.88	0.10	41,41,41,41	0
58	MG	2A	3482	1/1	0.88	0.12	55,55,55,55	0
58	MG	2A	3760	1/1	0.88	0.12	61,61,61,61	0
58	MG	2a	1708	1/1	0.88	0.16	60,60,60,60	0
58	MG	2A	3767	1/1	0.88	0.12	59,59,59,59	0
58	MG	2A	3773	1/1	0.88	0.15	54,54,54,54	0
58	MG	2a	1722	1/1	0.88	0.34	65,65,65,65	0
58	MG	2A	3774	1/1	0.88	0.12	45,45,45,45	0
58	MG	1A	3410	1/1	0.88	0.16	55,55,55,55	0
58	MG	2a	1735	1/1	0.88	0.15	58,58,58,58	0
58	MG	2a	1737	1/1	0.88	0.23	52,52,52,52	0
58	MG	2A	3496	1/1	0.88	0.16	63,63,63,63	0
58	MG	2a	1746	1/1	0.88	0.32	63,63,63,63	0
58	MG	2A	3344	1/1	0.88	0.12	78,78,78,78	0
58	MG	2a	1751	1/1	0.88	0.14	85,85,85,85	0
58	MG	2a	1760	1/1	0.88	0.08	81,81,81,81	0
58	MG	1a	1761	1/1	0.88	0.11	73,73,73,73	0
58	MG	16	102	1/1	0.88	0.14	41,41,41,41	0
58	MG	1A	4074	1/1	0.88	0.09	38,38,38,38	0
58	MG	2A	3543	1/1	0.88	0.12	52,52,52,52	0
58	MG	1a	1609	1/1	0.88	0.25	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2a	1793	1/1	0.88	0.21	61,61,61,61	0
58	MG	2a	1794	1/1	0.88	0.14	67,67,67,67	0
58	MG	1A	3616	1/1	0.88	0.10	27,27,27,27	0
58	MG	2A	3820	1/1	0.88	0.10	51,51,51,51	0
58	MG	1a	1634	1/1	0.88	0.21	65,65,65,65	0
58	MG	1A	3441	1/1	0.88	0.14	61,61,61,61	0
58	MG	2A	3580	1/1	0.88	0.13	46,46,46,46	0
58	MG	1a	1660	1/1	0.88	0.20	55,55,55,55	0
58	MG	2a	1814	1/1	0.88	0.29	58,58,58,58	0
58	MG	2A	3596	1/1	0.88	0.15	65,65,65,65	0
58	MG	1A	4093	1/1	0.88	0.21	57,57,57,57	0
58	MG	1A	3841	1/1	0.88	0.10	42,42,42,42	0
58	MG	2A	3877	1/1	0.88	0.19	76,76,76,76	0
58	MG	2a	1835	1/1	0.88	0.20	45,45,45,45	0
58	MG	2A	3608	1/1	0.88	0.12	45,45,45,45	0
58	MG	2l	205	1/1	0.88	0.11	66,66,66,66	0
58	MG	2A	3376	1/1	0.88	0.18	56,56,56,56	0
58	MG	2B	211	1/1	0.88	0.22	73,73,73,73	0
58	MG	1A	3995	1/1	0.88	0.09	34,34,34,34	0
58	MG	2A	3383	1/1	0.88	0.19	56,56,56,56	0
58	MG	1A	3447	1/1	0.88	0.12	62,62,62,62	0
58	MG	2A	3640	1/1	0.88	0.12	35,35,35,35	0
58	MG	2w	112	1/1	0.88	0.15	65,65,65,65	0
58	MG	2A	3649	1/1	0.88	0.12	45,45,45,45	0
58	MG	2A	3252	1/1	0.88	0.16	65,65,65,65	0
58	MG	1A	3448	1/1	0.88	0.11	48,48,48,48	0
58	MG	1A	3333	1/1	0.88	0.15	47,47,47,47	0
58	MG	1A	3468	1/1	0.89	0.23	40,40,40,40	0
58	MG	2A	3619	1/1	0.89	0.11	30,30,30,30	0
58	MG	1A	3478	1/1	0.89	0.20	69,69,69,69	0
58	MG	2A	3169	1/1	0.89	0.12	68,68,68,68	0
58	MG	2F	309	1/1	0.89	0.11	54,54,54,54	0
58	MG	2N	201	1/1	0.89	0.07	54,54,54,54	0
58	MG	2T	202	1/1	0.89	0.14	66,66,66,66	0
58	MG	2A	3173	1/1	0.89	0.24	75,75,75,75	0
58	MG	2A	3351	1/1	0.89	0.29	64,64,64,64	0
58	MG	2A	3647	1/1	0.89	0.12	35,35,35,35	0
58	MG	2A	3352	1/1	0.89	0.10	50,50,50,50	0
58	MG	1A	3744	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	3552	1/1	0.89	0.20	51,51,51,51	0
58	MG	1A	4068	1/1	0.89	0.11	45,45,45,45	0
58	MG	2A	3656	1/1	0.89	0.10	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	1Y	202	1/1	0.89	0.08	62,62,62,62	0
58	MG	1A	3415	1/1	0.89	0.12	52,52,52,52	0
58	MG	2a	1618	1/1	0.89	0.22	61,61,61,61	0
58	MG	15	102	1/1	0.89	0.17	35,35,35,35	0
58	MG	2a	1621	1/1	0.89	0.21	72,72,72,72	0
58	MG	2A	3194	1/1	0.89	0.28	63,63,63,63	0
58	MG	1A	3174	1/1	0.89	0.15	42,42,42,42	0
58	MG	2A	3199	1/1	0.89	0.20	64,64,64,64	0
58	MG	2A	3204	1/1	0.89	0.12	62,62,62,62	0
58	MG	2A	3686	1/1	0.89	0.18	60,60,60,60	0
58	MG	2A	3207	1/1	0.89	0.10	53,53,53,53	0
58	MG	1a	1775	1/1	0.89	0.11	64,64,64,64	0
58	MG	2A	3211	1/1	0.89	0.14	62,62,62,62	0
58	MG	2A	3703	1/1	0.89	0.14	50,50,50,50	0
58	MG	2a	1650	1/1	0.89	0.19	58,58,58,58	0
58	MG	2A	3212	1/1	0.89	0.26	54,54,54,54	0
58	MG	1A	3349	1/1	0.89	0.12	54,54,54,54	0
58	MG	1a	1603	1/1	0.89	0.12	64,64,64,64	0
58	MG	1a	1606	1/1	0.89	0.24	59,59,59,59	0
58	MG	1A	3806	1/1	0.89	0.06	38,38,38,38	0
58	MG	2A	3715	1/1	0.89	0.19	54,54,54,54	0
58	MG	2A	3237	1/1	0.89	0.15	66,66,66,66	0
58	MG	2A	3724	1/1	0.89	0.09	47,47,47,47	0
58	MG	2A	3238	1/1	0.89	0.15	55,55,55,55	0
58	MG	1A	4091	1/1	0.89	0.13	43,43,43,43	0
58	MG	2a	1688	1/1	0.89	0.20	53,53,53,53	0
58	MG	2a	1697	1/1	0.89	0.13	66,66,66,66	0
58	MG	2A	3245	1/1	0.89	0.10	60,60,60,60	0
58	MG	2A	3407	1/1	0.89	0.09	66,66,66,66	0
58	MG	1A	3350	1/1	0.89	0.16	64,64,64,64	0
58	MG	1A	3833	1/1	0.89	0.19	43,43,43,43	0
58	MG	2a	1709	1/1	0.89	0.19	59,59,59,59	0
58	MG	1A	3131	1/1	0.89	0.10	58,58,58,58	0
58	MG	2a	1718	1/1	0.89	0.28	62,62,62,62	0
58	MG	2A	3426	1/1	0.89	0.17	57,57,57,57	0
58	MG	2A	3431	1/1	0.89	0.20	60,60,60,60	0
58	MG	1A	4098	1/1	0.89	0.13	60,60,60,60	0
58	MG	2A	3434	1/1	0.89	0.19	58,58,58,58	0
58	MG	1a	1667	1/1	0.89	0.16	45,45,45,45	0
58	MG	1w	109	1/1	0.89	0.15	65,65,65,65	0
58	MG	1x	105	1/1	0.89	0.10	59,59,59,59	0
58	MG	2a	1745	1/1	0.89	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3770	1/1	0.89	0.16	68,68,68,68	0
58	MG	2A	3771	1/1	0.89	0.13	53,53,53,53	0
58	MG	2A	3260	1/1	0.89	0.12	50,50,50,50	0
58	MG	1A	3511	1/1	0.89	0.08	67,67,67,67	0
58	MG	1A	3843	1/1	0.89	0.15	53,53,53,53	0
58	MG	2A	3017	1/1	0.89	0.13	38,38,38,38	0
58	MG	1A	3390	1/1	0.89	0.11	63,63,63,63	0
58	MG	1A	3314	1/1	0.89	0.14	60,60,60,60	0
58	MG	1A	3273	1/1	0.89	0.08	52,52,52,52	0
58	MG	2a	1792	1/1	0.89	0.12	60,60,60,60	0
58	MG	2A	3288	1/1	0.89	0.09	57,57,57,57	0
58	MG	1A	3691	1/1	0.89	0.13	53,53,53,53	0
58	MG	1a	1677	1/1	0.89	0.19	47,47,47,47	0
58	MG	2A	3294	1/1	0.89	0.26	62,62,62,62	0
58	MG	2A	3059	1/1	0.89	0.18	51,51,51,51	0
58	MG	2A	3520	1/1	0.89	0.17	47,47,47,47	0
58	MG	1A	3870	1/1	0.89	0.12	56,56,56,56	0
58	MG	2A	3071	1/1	0.89	0.19	48,48,48,48	0
58	MG	2A	3847	1/1	0.89	0.12	67,67,67,67	0
58	MG	2A	3542	1/1	0.89	0.11	46,46,46,46	0
58	MG	2A	3853	1/1	0.89	0.16	67,67,67,67	0
58	MG	2A	3856	1/1	0.89	0.11	52,52,52,52	0
58	MG	2a	1824	1/1	0.89	0.21	67,67,67,67	0
58	MG	1a	1682	1/1	0.89	0.09	64,64,64,64	0
58	MG	2a	1833	1/1	0.89	0.18	54,54,54,54	0
58	MG	2A	3315	1/1	0.89	0.11	59,59,59,59	0
58	MG	2A	3085	1/1	0.89	0.13	45,45,45,45	0
58	MG	1A	3873	1/1	0.89	0.11	42,42,42,42	0
58	MG	2p	101	1/1	0.89	0.15	64,64,64,64	0
58	MG	2A	3879	1/1	0.89	0.12	39,39,39,39	0
58	MG	1a	1688	1/1	0.89	0.27	47,47,47,47	0
58	MG	2A	3882	1/1	0.89	0.27	55,55,55,55	0
58	MG	2B	202	1/1	0.89	0.11	62,62,62,62	0
58	MG	1B	223	1/1	0.89	0.09	53,53,53,53	0
58	MG	2B	205	1/1	0.89	0.18	59,59,59,59	0
58	MG	2w	109	1/1	0.89	0.33	72,72,72,72	0
58	MG	1A	3530	1/1	0.89	0.11	68,68,68,68	0
58	MG	1A	3412	1/1	0.89	0.10	44,44,44,44	0
58	MG	2y	101	1/1	0.89	0.14	73,73,73,73	0
58	MG	2y	102	1/1	0.89	0.16	69,69,69,69	0
58	MG	1a	1703	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	4045	1/1	0.89	0.11	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	1D	312	1/1	0.89	0.13	59,59,59,59	0
58	MG	26	101	1/1	0.90	0.22	58,58,58,58	0
58	MG	1A	3270	1/1	0.90	0.10	62,62,62,62	0
58	MG	1A	3921	1/1	0.90	0.08	21,21,21,21	0
58	MG	2A	3385	1/1	0.90	0.09	59,59,59,59	0
58	MG	1A	3926	1/1	0.90	0.12	70,70,70,70	0
58	MG	2a	1608	1/1	0.90	0.38	66,66,66,66	0
58	MG	2A	3682	1/1	0.90	0.10	41,41,41,41	0
58	MG	2A	3683	1/1	0.90	0.10	51,51,51,51	0
58	MG	1A	3598	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3392	1/1	0.90	0.19	50,50,50,50	0
58	MG	1A	3804	1/1	0.90	0.11	34,34,34,34	0
58	MG	2A	3694	1/1	0.90	0.14	47,47,47,47	0
58	MG	1a	1815	1/1	0.90	0.20	65,65,65,65	0
58	MG	2A	3213	1/1	0.90	0.14	60,60,60,60	0
58	MG	2a	1626	1/1	0.90	0.12	56,56,56,56	0
58	MG	1A	3510	1/1	0.90	0.10	47,47,47,47	0
58	MG	2A	3219	1/1	0.90	0.17	61,61,61,61	0
58	MG	2a	1630	1/1	0.90	0.10	58,58,58,58	0
58	MG	1A	3253	1/1	0.90	0.16	47,47,47,47	0
58	MG	1l	201	1/1	0.90	0.12	68,68,68,68	0
58	MG	1A	3074	1/1	0.90	0.20	53,53,53,53	0
58	MG	2a	1639	1/1	0.90	0.25	53,53,53,53	0
58	MG	1t	201	1/1	0.90	0.13	55,55,55,55	0
58	MG	1A	3983	1/1	0.90	0.09	68,68,68,68	0
58	MG	1w	102	1/1	0.90	0.13	49,49,49,49	0
58	MG	2a	1648	1/1	0.90	0.20	59,59,59,59	0
58	MG	2A	3723	1/1	0.90	0.10	43,43,43,43	0
58	MG	1w	108	1/1	0.90	0.19	52,52,52,52	0
58	MG	1A	3354	1/1	0.90	0.10	48,48,48,48	0
58	MG	1A	3668	1/1	0.90	0.11	53,53,53,53	0
58	MG	2A	3738	1/1	0.90	0.14	53,53,53,53	0
58	MG	1A	3458	1/1	0.90	0.13	61,61,61,61	0
58	MG	1A	3842	1/1	0.90	0.11	54,54,54,54	0
58	MG	2A	3432	1/1	0.90	0.10	55,55,55,55	0
58	MG	1A	3360	1/1	0.90	0.17	55,55,55,55	0
58	MG	1A	3338	1/1	0.90	0.10	45,45,45,45	0
58	MG	2A	3024	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3441	1/1	0.90	0.16	54,54,54,54	0
58	MG	2A	3029	1/1	0.90	0.22	60,60,60,60	0
58	MG	1A	3382	1/1	0.90	0.19	46,46,46,46	0
58	MG	2a	1700	1/1	0.90	0.15	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	1703	1/1	0.90	0.23	59,59,59,59	0
58	MG	1A	4010	1/1	0.90	0.07	72,72,72,72	0
58	MG	1A	4018	1/1	0.90	0.07	35,35,35,35	0
58	MG	2A	3765	1/1	0.90	0.10	38,38,38,38	0
58	MG	2A	3462	1/1	0.90	0.27	62,62,62,62	0
58	MG	1a	1678	1/1	0.90	0.18	62,62,62,62	0
58	MG	2A	3277	1/1	0.90	0.14	64,64,64,64	0
58	MG	2A	3772	1/1	0.90	0.09	51,51,51,51	0
58	MG	1B	214	1/1	0.90	0.20	56,56,56,56	0
58	MG	2a	1724	1/1	0.90	0.24	59,59,59,59	0
58	MG	1A	3386	1/1	0.90	0.10	39,39,39,39	0
58	MG	2A	3070	1/1	0.90	0.16	51,51,51,51	0
58	MG	1a	1685	1/1	0.90	0.20	57,57,57,57	0
58	MG	2A	3487	1/1	0.90	0.18	48,48,48,48	0
58	MG	1A	4024	1/1	0.90	0.09	55,55,55,55	0
58	MG	2A	3293	1/1	0.90	0.22	55,55,55,55	0
58	MG	2A	3807	1/1	0.90	0.09	41,41,41,41	0
58	MG	2A	3074	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	4026	1/1	0.90	0.12	48,48,48,48	0
58	MG	2a	1755	1/1	0.90	0.14	63,63,63,63	0
58	MG	2A	3514	1/1	0.90	0.13	29,29,29,29	0
58	MG	1A	3482	1/1	0.90	0.14	61,61,61,61	0
58	MG	2A	3093	1/1	0.90	0.21	54,54,54,54	0
58	MG	2A	3825	1/1	0.90	0.10	39,39,39,39	0
58	MG	2A	3309	1/1	0.90	0.22	63,63,63,63	0
58	MG	1B	229	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3100	1/1	0.90	0.24	58,58,58,58	0
58	MG	2A	3845	1/1	0.90	0.10	35,35,35,35	0
58	MG	2A	3546	1/1	0.90	0.16	48,48,48,48	0
58	MG	1A	4030	1/1	0.90	0.09	65,65,65,65	0
58	MG	2a	1796	1/1	0.90	0.16	42,42,42,42	0
58	MG	2A	3102	1/1	0.90	0.15	50,50,50,50	0
58	MG	2a	1803	1/1	0.90	0.10	59,59,59,59	0
58	MG	1A	4031	1/1	0.90	0.08	46,46,46,46	0
58	MG	2A	3567	1/1	0.90	0.11	61,61,61,61	0
58	MG	1A	3859	1/1	0.90	0.11	57,57,57,57	0
58	MG	2a	1812	1/1	0.90	0.14	67,67,67,67	0
58	MG	2A	3333	1/1	0.90	0.13	62,62,62,62	0
58	MG	1A	3554	1/1	0.90	0.13	54,54,54,54	0
58	MG	2a	1815	1/1	0.90	0.23	64,64,64,64	0
58	MG	2a	1816	1/1	0.90	0.16	66,66,66,66	0
58	MG	1a	1726	1/1	0.90	0.09	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	2A	3131	1/1	0.90	0.10	58,58,58,58	0
58	MG	1A	4035	1/1	0.90	0.10	44,44,44,44	0
58	MG	2a	1823	1/1	0.90	0.11	59,59,59,59	0
58	MG	2A	3883	1/1	0.90	0.21	74,74,74,74	0
58	MG	1A	3731	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3609	1/1	0.90	0.26	48,48,48,48	0
58	MG	2A	3162	1/1	0.90	0.18	49,49,49,49	0
58	MG	2a	1837	1/1	0.90	0.25	56,56,56,56	0
58	MG	2d	301	1/1	0.90	0.27	50,50,50,50	0
58	MG	1O	205	1/1	0.90	0.16	60,60,60,60	0
58	MG	2l	201	1/1	0.90	0.15	60,60,60,60	0
58	MG	1A	3738	1/1	0.90	0.15	72,72,72,72	0
58	MG	2B	217	1/1	0.90	0.12	46,46,46,46	0
58	MG	1A	3901	1/1	0.90	0.19	64,64,64,64	0
58	MG	2A	3627	1/1	0.90	0.12	63,63,63,63	0
58	MG	1A	3903	1/1	0.90	0.15	33,33,33,33	0
58	MG	2A	3178	1/1	0.90	0.13	47,47,47,47	0
58	MG	10	106	1/1	0.90	0.12	57,57,57,57	0
58	MG	1A	3419	1/1	0.90	0.14	57,57,57,57	0
58	MG	10	110	1/1	0.90	0.07	43,43,43,43	0
58	MG	1a	1767	1/1	0.90	0.10	66,66,66,66	0
58	MG	1a	1772	1/1	0.90	0.12	64,64,64,64	0
58	MG	2x	105	1/1	0.90	0.07	50,50,50,50	0
58	MG	2Q	202	1/1	0.90	0.14	45,45,45,45	0
58	MG	14	101	1/1	0.90	0.20	62,62,62,62	0
58	MG	2U	201	1/1	0.90	0.19	42,42,42,42	0
58	MG	1A	3387	1/1	0.90	0.08	53,53,53,53	0
58	MG	2A	3196	1/1	0.90	0.21	60,60,60,60	0
58	MG	2A	3324	1/1	0.91	0.18	55,55,55,55	0
58	MG	1A	3413	1/1	0.91	0.11	47,47,47,47	0
58	MG	2a	1602	1/1	0.91	0.10	53,53,53,53	0
58	MG	2A	3326	1/1	0.91	0.10	57,57,57,57	0
58	MG	1A	3950	1/1	0.91	0.10	55,55,55,55	0
58	MG	2A	3633	1/1	0.91	0.14	46,46,46,46	0
58	MG	2A	3329	1/1	0.91	0.17	51,51,51,51	0
58	MG	1A	4095	1/1	0.91	0.11	53,53,53,53	0
58	MG	1A	3617	1/1	0.91	0.11	49,49,49,49	0
58	MG	1A	3955	1/1	0.91	0.07	59,59,59,59	0
58	MG	2a	1612	1/1	0.91	0.11	60,60,60,60	0
58	MG	1A	3456	1/1	0.91	0.09	48,48,48,48	0
58	MG	1a	1676	1/1	0.91	0.16	56,56,56,56	0
58	MG	2a	1617	1/1	0.91	0.27	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	3979	1/1	0.91	0.11	71,71,71,71	0
58	MG	1A	3982	1/1	0.91	0.08	55,55,55,55	0
58	MG	2A	3343	1/1	0.91	0.20	52,52,52,52	0
58	MG	1a	1679	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3649	1/1	0.91	0.09	65,65,65,65	0
58	MG	1A	3985	1/1	0.91	0.08	60,60,60,60	0
58	MG	1A	3655	1/1	0.91	0.10	59,59,59,59	0
58	MG	1A	3660	1/1	0.91	0.07	34,34,34,34	0
58	MG	2a	1632	1/1	0.91	0.26	56,56,56,56	0
58	MG	1B	212	1/1	0.91	0.08	46,46,46,46	0
58	MG	1A	3814	1/1	0.91	0.14	51,51,51,51	0
58	MG	2A	3354	1/1	0.91	0.20	65,65,65,65	0
58	MG	2a	1637	1/1	0.91	0.20	48,48,48,48	0
58	MG	2A	3124	1/1	0.91	0.14	50,50,50,50	0
58	MG	2A	3693	1/1	0.91	0.12	61,61,61,61	0
58	MG	1A	3993	1/1	0.91	0.06	20,20,20,20	0
58	MG	1a	1695	1/1	0.91	0.24	54,54,54,54	0
58	MG	2A	3365	1/1	0.91	0.13	66,66,66,66	0
58	MG	2A	3146	1/1	0.91	0.19	50,50,50,50	0
58	MG	1A	3819	1/1	0.91	0.15	63,63,63,63	0
58	MG	2A	3161	1/1	0.91	0.23	67,67,67,67	0
58	MG	2A	3706	1/1	0.91	0.08	51,51,51,51	0
58	MG	1A	3830	1/1	0.91	0.09	34,34,34,34	0
58	MG	1a	1707	1/1	0.91	0.10	50,50,50,50	0
58	MG	1a	1711	1/1	0.91	0.13	42,42,42,42	0
58	MG	2A	3171	1/1	0.91	0.15	56,56,56,56	0
58	MG	2a	1660	1/1	0.91	0.10	61,61,61,61	0
58	MG	1B	224	1/1	0.91	0.10	49,49,49,49	0
58	MG	1a	1720	1/1	0.91	0.25	54,54,54,54	0
58	MG	2a	1670	1/1	0.91	0.14	70,70,70,70	0
58	MG	2a	1672	1/1	0.91	0.16	57,57,57,57	0
58	MG	1A	3999	1/1	0.91	0.08	46,46,46,46	0
58	MG	2a	1686	1/1	0.91	0.15	51,51,51,51	0
58	MG	1A	3494	1/1	0.91	0.18	49,49,49,49	0
58	MG	1A	3837	1/1	0.91	0.12	52,52,52,52	0
58	MG	1A	3496	1/1	0.91	0.17	52,52,52,52	0
58	MG	1B	233	1/1	0.91	0.10	62,62,62,62	0
58	MG	1B	235	1/1	0.91	0.14	47,47,47,47	0
58	MG	1A	3839	1/1	0.91	0.11	35,35,35,35	0
58	MG	1A	3669	1/1	0.91	0.07	41,41,41,41	0
58	MG	2A	3401	1/1	0.91	0.07	64,64,64,64	0
58	MG	2A	3403	1/1	0.91	0.10	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	1a	1741	1/1	0.91	0.14	51,51,51,51	0
58	MG	2a	1715	1/1	0.91	0.29	60,60,60,60	0
58	MG	1A	3498	1/1	0.91	0.18	51,51,51,51	0
58	MG	1A	3684	1/1	0.91	0.16	49,49,49,49	0
58	MG	1a	1756	1/1	0.91	0.11	42,42,42,42	0
58	MG	2A	3208	1/1	0.91	0.16	51,51,51,51	0
58	MG	1G	205	1/1	0.91	0.11	41,41,41,41	0
58	MG	1A	3502	1/1	0.91	0.10	44,44,44,44	0
58	MG	2a	1734	1/1	0.91	0.25	52,52,52,52	0
58	MG	1A	3689	1/1	0.91	0.09	39,39,39,39	0
58	MG	1A	3050	1/1	0.91	0.13	47,47,47,47	0
58	MG	1V	209	1/1	0.91	0.09	49,49,49,49	0
58	MG	2a	1744	1/1	0.91	0.29	58,58,58,58	0
58	MG	1W	202	1/1	0.91	0.18	41,41,41,41	0
58	MG	1a	1781	1/1	0.91	0.08	58,58,58,58	0
58	MG	2A	3777	1/1	0.91	0.12	36,36,36,36	0
58	MG	1a	1786	1/1	0.91	0.07	56,56,56,56	0
58	MG	2A	3785	1/1	0.91	0.09	73,73,73,73	0
58	MG	2A	3440	1/1	0.91	0.12	59,59,59,59	0
58	MG	1X	106	1/1	0.91	0.09	48,48,48,48	0
58	MG	1A	3853	1/1	0.91	0.10	37,37,37,37	0
58	MG	2A	3800	1/1	0.91	0.10	61,61,61,61	0
58	MG	1A	3555	1/1	0.91	0.18	53,53,53,53	0
58	MG	2a	1788	1/1	0.91	0.10	50,50,50,50	0
58	MG	1A	3709	1/1	0.91	0.11	44,44,44,44	0
58	MG	1a	1813	1/1	0.91	0.16	53,53,53,53	0
58	MG	2A	3247	1/1	0.91	0.17	55,55,55,55	0
58	MG	2A	3248	1/1	0.91	0.14	71,71,71,71	0
58	MG	1A	3557	1/1	0.91	0.11	53,53,53,53	0
58	MG	11	102	1/1	0.91	0.11	60,60,60,60	0
58	MG	1A	3716	1/1	0.91	0.13	66,66,66,66	0
58	MG	1A	3432	1/1	0.91	0.19	54,54,54,54	0
58	MG	2a	1807	1/1	0.91	0.20	59,59,59,59	0
58	MG	16	101	1/1	0.91	0.15	51,51,51,51	0
58	MG	1A	3476	1/1	0.91	0.10	45,45,45,45	0
58	MG	2A	3491	1/1	0.91	0.10	55,55,55,55	0
58	MG	1A	3303	1/1	0.91	0.20	44,44,44,44	0
58	MG	19	101	1/1	0.91	0.16	46,46,46,46	0
58	MG	2A	3851	1/1	0.91	0.08	53,53,53,53	0
58	MG	1a	1602	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3592	1/1	0.91	0.14	52,52,52,52	0
58	MG	2A	3512	1/1	0.91	0.08	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	1x	101	1/1	0.91	0.18	57,57,57,57	0
58	MG	1x	104	1/1	0.91	0.10	50,50,50,50	0
58	MG	1A	3739	1/1	0.91	0.13	52,52,52,52	0
58	MG	1A	3342	1/1	0.91	0.08	49,49,49,49	0
58	MG	2A	3541	1/1	0.91	0.14	46,46,46,46	0
58	MG	2a	1827	1/1	0.91	0.20	51,51,51,51	0
58	MG	1A	3745	1/1	0.91	0.10	56,56,56,56	0
58	MG	2A	3283	1/1	0.91	0.19	60,60,60,60	0
58	MG	2A	3006	1/1	0.91	0.22	58,58,58,58	0
58	MG	2a	1838	1/1	0.91	0.09	73,73,73,73	0
58	MG	2A	3548	1/1	0.91	0.10	32,32,32,32	0
58	MG	1A	3925	1/1	0.91	0.07	27,27,27,27	0
58	MG	2B	206	1/1	0.91	0.19	54,54,54,54	0
58	MG	2l	204	1/1	0.91	0.11	59,59,59,59	0
58	MG	1a	1638	1/1	0.91	0.23	56,56,56,56	0
58	MG	1a	1647	1/1	0.91	0.12	49,49,49,49	0
58	MG	1a	1656	1/1	0.91	0.26	55,55,55,55	0
58	MG	2A	3295	1/1	0.91	0.09	65,65,65,65	0
58	MG	2A	3039	1/1	0.91	0.16	62,62,62,62	0
58	MG	2A	3585	1/1	0.91	0.09	55,55,55,55	0
58	MG	2A	3300	1/1	0.91	0.11	69,69,69,69	0
58	MG	1A	3080	1/1	0.91	0.11	53,53,53,53	0
58	MG	2w	106	1/1	0.91	0.14	46,46,46,46	0
58	MG	2E	306	1/1	0.91	0.15	54,54,54,54	0
58	MG	2w	110	1/1	0.91	0.17	57,57,57,57	0
58	MG	2A	3045	1/1	0.91	0.15	58,58,58,58	0
58	MG	2A	3605	1/1	0.91	0.14	47,47,47,47	0
58	MG	2x	103	1/1	0.91	0.15	55,55,55,55	0
58	MG	2A	3606	1/1	0.91	0.08	31,31,31,31	0
58	MG	1A	4081	1/1	0.91	0.08	47,47,47,47	0
58	MG	1A	3763	1/1	0.91	0.11	38,38,38,38	0
58	MG	1a	1663	1/1	0.91	0.12	51,51,51,51	0
58	MG	1A	3767	1/1	0.91	0.10	27,27,27,27	0
58	MG	2A	3320	1/1	0.91	0.09	64,64,64,64	0
58	MG	2B	207	1/1	0.92	0.10	66,66,66,66	0
58	MG	1a	1797	1/1	0.92	0.07	69,69,69,69	0
58	MG	1A	3145	1/1	0.92	0.10	40,40,40,40	0
58	MG	2B	216	1/1	0.92	0.21	58,58,58,58	0
58	MG	1a	1807	1/1	0.92	0.17	57,57,57,57	0
58	MG	2A	3503	1/1	0.92	0.13	46,46,46,46	0
58	MG	2A	3509	1/1	0.92	0.12	61,61,61,61	0
58	MG	1A	3661	1/1	0.92	0.12	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	1810	1/1	0.92	0.11	58,58,58,58	0
58	MG	1A	3503	1/1	0.92	0.19	60,60,60,60	0
58	MG	2A	3256	1/1	0.92	0.16	51,51,51,51	0
58	MG	1A	3267	1/1	0.92	0.11	59,59,59,59	0
58	MG	2F	302	1/1	0.92	0.12	51,51,51,51	0
58	MG	2F	303	1/1	0.92	0.16	56,56,56,56	0
58	MG	2F	304	1/1	0.92	0.10	58,58,58,58	0
58	MG	2A	3540	1/1	0.92	0.19	58,58,58,58	0
58	MG	1A	3425	1/1	0.92	0.09	55,55,55,55	0
58	MG	2A	3267	1/1	0.92	0.11	52,52,52,52	0
58	MG	1f	202	1/1	0.92	0.21	50,50,50,50	0
58	MG	1A	3165	1/1	0.92	0.17	48,48,48,48	0
58	MG	1A	3062	1/1	0.92	0.09	52,52,52,52	0
58	MG	2V	202	1/1	0.92	0.09	58,58,58,58	0
58	MG	2Z	301	1/1	0.92	0.15	64,64,64,64	0
58	MG	1A	3854	1/1	0.92	0.08	43,43,43,43	0
58	MG	1A	3365	1/1	0.92	0.20	60,60,60,60	0
58	MG	1A	3519	1/1	0.92	0.14	56,56,56,56	0
58	MG	28	101	1/1	0.92	0.20	61,61,61,61	0
58	MG	2A	3280	1/1	0.92	0.14	59,59,59,59	0
58	MG	2A	3577	1/1	0.92	0.10	60,60,60,60	0
58	MG	1A	4052	1/1	0.92	0.06	42,42,42,42	0
58	MG	2a	1605	1/1	0.92	0.21	50,50,50,50	0
58	MG	1a	1618	1/1	0.92	0.07	44,44,44,44	0
58	MG	1a	1626	1/1	0.92	0.18	50,50,50,50	0
58	MG	1a	1627	1/1	0.92	0.17	36,36,36,36	0
58	MG	1A	4054	1/1	0.92	0.07	45,45,45,45	0
58	MG	2A	3597	1/1	0.92	0.08	61,61,61,61	0
58	MG	2A	3598	1/1	0.92	0.16	65,65,65,65	0
58	MG	2a	1613	1/1	0.92	0.24	59,59,59,59	0
58	MG	1A	3865	1/1	0.92	0.10	46,46,46,46	0
58	MG	2A	3604	1/1	0.92	0.16	54,54,54,54	0
58	MG	1x	107	1/1	0.92	0.12	56,56,56,56	0
58	MG	1x	109	1/1	0.92	0.07	63,63,63,63	0
58	MG	1a	1635	1/1	0.92	0.12	49,49,49,49	0
58	MG	1A	3868	1/1	0.92	0.13	46,46,46,46	0
58	MG	1a	1643	1/1	0.92	0.12	63,63,63,63	0
58	MG	2a	1624	1/1	0.92	0.16	66,66,66,66	0
58	MG	2A	3610	1/1	0.92	0.10	49,49,49,49	0
58	MG	2A	3305	1/1	0.92	0.08	48,48,48,48	0
58	MG	2A	3012	1/1	0.92	0.07	40,40,40,40	0
58	MG	2A	3620	1/1	0.92	0.09	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	3624	1/1	0.92	0.11	39,39,39,39	0
58	MG	1A	3367	1/1	0.92	0.17	58,58,58,58	0
58	MG	2A	3311	1/1	0.92	0.10	54,54,54,54	0
58	MG	2a	1635	1/1	0.92	0.24	70,70,70,70	0
58	MG	2A	3019	1/1	0.92	0.08	43,43,43,43	0
58	MG	1a	1654	1/1	0.92	0.07	44,44,44,44	0
58	MG	2A	3316	1/1	0.92	0.11	61,61,61,61	0
58	MG	2a	1642	1/1	0.92	0.23	62,62,62,62	0
58	MG	2A	3317	1/1	0.92	0.11	51,51,51,51	0
58	MG	1a	1655	1/1	0.92	0.20	50,50,50,50	0
58	MG	1A	3370	1/1	0.92	0.14	54,54,54,54	0
58	MG	2A	3322	1/1	0.92	0.09	53,53,53,53	0
58	MG	2a	1649	1/1	0.92	0.19	61,61,61,61	0
58	MG	2A	3036	1/1	0.92	0.14	61,61,61,61	0
58	MG	1A	3707	1/1	0.92	0.06	22,22,22,22	0
58	MG	2A	3654	1/1	0.92	0.22	57,57,57,57	0
58	MG	1A	4076	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3890	1/1	0.92	0.05	18,18,18,18	0
58	MG	2A	3662	1/1	0.92	0.15	55,55,55,55	0
58	MG	2A	3664	1/1	0.92	0.14	61,61,61,61	0
58	MG	2A	3666	1/1	0.92	0.10	49,49,49,49	0
58	MG	1a	1662	1/1	0.92	0.12	59,59,59,59	0
58	MG	2a	1661	1/1	0.92	0.13	60,60,60,60	0
58	MG	1A	3892	1/1	0.92	0.14	29,29,29,29	0
58	MG	2a	1665	1/1	0.92	0.15	61,61,61,61	0
58	MG	2a	1666	1/1	0.92	0.12	59,59,59,59	0
58	MG	2A	3332	1/1	0.92	0.15	61,61,61,61	0
58	MG	1A	3893	1/1	0.92	0.08	32,32,32,32	0
58	MG	1A	3092	1/1	0.92	0.08	37,37,37,37	0
58	MG	2A	3336	1/1	0.92	0.10	56,56,56,56	0
58	MG	2a	1683	1/1	0.92	0.09	47,47,47,47	0
58	MG	1A	3902	1/1	0.92	0.07	30,30,30,30	0
58	MG	2A	3066	1/1	0.92	0.21	52,52,52,52	0
58	MG	2a	1696	1/1	0.92	0.29	51,51,51,51	0
58	MG	1A	3531	1/1	0.92	0.12	72,72,72,72	0
58	MG	1A	3532	1/1	0.92	0.08	54,54,54,54	0
58	MG	1A	3717	1/1	0.92	0.09	40,40,40,40	0
58	MG	2a	1702	1/1	0.92	0.19	68,68,68,68	0
58	MG	1A	3912	1/1	0.92	0.09	54,54,54,54	0
58	MG	2A	3080	1/1	0.92	0.09	41,41,41,41	0
58	MG	2A	3082	1/1	0.92	0.15	51,51,51,51	0
58	MG	1A	3723	1/1	0.92	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3726	1/1	0.92	0.14	38,38,38,38	0
58	MG	1A	4101	1/1	0.92	0.10	48,48,48,48	0
58	MG	1A	3536	1/1	0.92	0.12	44,44,44,44	0
58	MG	2a	1717	1/1	0.92	0.13	54,54,54,54	0
58	MG	1A	3455	1/1	0.92	0.13	38,38,38,38	0
58	MG	2a	1720	1/1	0.92	0.15	56,56,56,56	0
58	MG	1A	3544	1/1	0.92	0.11	36,36,36,36	0
58	MG	1A	3735	1/1	0.92	0.07	44,44,44,44	0
58	MG	2a	1723	1/1	0.92	0.21	57,57,57,57	0
58	MG	1A	3184	1/1	0.92	0.16	43,43,43,43	0
58	MG	2A	3716	1/1	0.92	0.10	43,43,43,43	0
58	MG	1A	3945	1/1	0.92	0.09	52,52,52,52	0
58	MG	2A	3366	1/1	0.92	0.09	57,57,57,57	0
58	MG	2A	3367	1/1	0.92	0.29	46,46,46,46	0
58	MG	2A	3369	1/1	0.92	0.09	57,57,57,57	0
58	MG	2a	1740	1/1	0.92	0.16	52,52,52,52	0
58	MG	2A	3727	1/1	0.92	0.09	42,42,42,42	0
58	MG	2a	1743	1/1	0.92	0.30	60,60,60,60	0
58	MG	1A	3208	1/1	0.92	0.20	45,45,45,45	0
58	MG	2A	3734	1/1	0.92	0.08	61,61,61,61	0
58	MG	2A	3372	1/1	0.92	0.11	53,53,53,53	0
58	MG	1B	216	1/1	0.92	0.09	57,57,57,57	0
58	MG	2A	3740	1/1	0.92	0.10	42,42,42,42	0
58	MG	2a	1754	1/1	0.92	0.09	62,62,62,62	0
58	MG	2A	3121	1/1	0.92	0.09	58,58,58,58	0
58	MG	1A	3461	1/1	0.92	0.12	54,54,54,54	0
58	MG	2A	3378	1/1	0.92	0.12	45,45,45,45	0
58	MG	1B	220	1/1	0.92	0.08	45,45,45,45	0
58	MG	1a	1698	1/1	0.92	0.14	51,51,51,51	0
58	MG	2A	3384	1/1	0.92	0.12	52,52,52,52	0
58	MG	2A	3139	1/1	0.92	0.16	48,48,48,48	0
58	MG	1A	3464	1/1	0.92	0.08	51,51,51,51	0
58	MG	1a	1705	1/1	0.92	0.12	49,49,49,49	0
58	MG	1A	3300	1/1	0.92	0.13	57,57,57,57	0
58	MG	1a	1710	1/1	0.92	0.24	60,60,60,60	0
58	MG	1A	3977	1/1	0.92	0.10	62,62,62,62	0
58	MG	1a	1712	1/1	0.92	0.19	50,50,50,50	0
58	MG	1a	1713	1/1	0.92	0.26	50,50,50,50	0
58	MG	1a	1718	1/1	0.92	0.18	65,65,65,65	0
58	MG	2a	1806	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3758	1/1	0.92	0.11	31,31,31,31	0
58	MG	1A	3762	1/1	0.92	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	1A	3473	1/1	0.92	0.09	60,60,60,60	0
58	MG	2A	3187	1/1	0.92	0.24	63,63,63,63	0
58	MG	2A	3189	1/1	0.92	0.09	62,62,62,62	0
58	MG	1A	3765	1/1	0.92	0.13	40,40,40,40	0
58	MG	1A	3093	1/1	0.92	0.07	50,50,50,50	0
58	MG	1B	239	1/1	0.92	0.07	38,38,38,38	0
58	MG	1A	3477	1/1	0.92	0.08	42,42,42,42	0
58	MG	1A	3402	1/1	0.92	0.11	52,52,52,52	0
58	MG	2A	3806	1/1	0.92	0.11	47,47,47,47	0
58	MG	1A	3226	1/1	0.92	0.12	38,38,38,38	0
58	MG	2A	3809	1/1	0.92	0.10	66,66,66,66	0
58	MG	2A	3420	1/1	0.92	0.15	52,52,52,52	0
58	MG	1F	304	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3597	1/1	0.92	0.11	35,35,35,35	0
58	MG	2a	1828	1/1	0.92	0.12	54,54,54,54	0
58	MG	2A	3814	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3315	1/1	0.92	0.10	53,53,53,53	0
58	MG	2A	3816	1/1	0.92	0.09	44,44,44,44	0
58	MG	2A	3817	1/1	0.92	0.10	54,54,54,54	0
58	MG	1A	3603	1/1	0.92	0.17	53,53,53,53	0
58	MG	1a	1755	1/1	0.92	0.10	62,62,62,62	0
58	MG	1A	3318	1/1	0.92	0.14	47,47,47,47	0
58	MG	1a	1758	1/1	0.92	0.16	57,57,57,57	0
58	MG	1R	202	1/1	0.92	0.14	47,47,47,47	0
58	MG	2A	3444	1/1	0.92	0.07	52,52,52,52	0
58	MG	2r	101	1/1	0.92	0.14	64,64,64,64	0
58	MG	2t	201	1/1	0.92	0.15	47,47,47,47	0
58	MG	1a	1764	1/1	0.92	0.14	55,55,55,55	0
58	MG	1A	3095	1/1	0.92	0.08	47,47,47,47	0
58	MG	1a	1770	1/1	0.92	0.07	71,71,71,71	0
58	MG	1A	3821	1/1	0.92	0.10	55,55,55,55	0
58	MG	2A	3458	1/1	0.92	0.18	52,52,52,52	0
58	MG	1A	3067	1/1	0.92	0.08	39,39,39,39	0
58	MG	2A	3224	1/1	0.92	0.09	57,57,57,57	0
58	MG	2A	3872	1/1	0.92	0.11	64,64,64,64	0
58	MG	2A	3227	1/1	0.92	0.10	51,51,51,51	0
58	MG	1A	3832	1/1	0.92	0.13	46,46,46,46	0
58	MG	1a	1779	1/1	0.92	0.10	61,61,61,61	0
58	MG	1A	3640	1/1	0.92	0.11	44,44,44,44	0
58	MG	1Z	3700	1/1	0.92	0.17	55,55,55,55	0
58	MG	2x	106	1/1	0.92	0.26	64,64,64,64	0
58	MG	2A	3485	1/1	0.92	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3125	1/1	0.92	0.21	50,50,50,50	0
58	MG	1A	3497	1/1	0.92	0.13	56,56,56,56	0
58	MG	2A	3493	1/1	0.92	0.09	55,55,55,55	0
58	MG	1A	3027	1/1	0.92	0.12	51,51,51,51	0
58	MG	2A	3533	1/1	0.93	0.09	32,32,32,32	0
58	MG	1A	4106	1/1	0.93	0.20	55,55,55,55	0
58	MG	1A	4107	1/1	0.93	0.19	55,55,55,55	0
58	MG	2B	219	1/1	0.93	0.24	65,65,65,65	0
58	MG	2A	3003	1/1	0.93	0.20	47,47,47,47	0
58	MG	2D	304	1/1	0.93	0.26	57,57,57,57	0
58	MG	1A	3835	1/1	0.93	0.21	59,59,59,59	0
58	MG	1B	204	1/1	0.93	0.10	44,44,44,44	0
58	MG	1A	3548	1/1	0.93	0.18	41,41,41,41	0
58	MG	2A	3286	1/1	0.93	0.19	56,56,56,56	0
58	MG	1A	3066	1/1	0.93	0.08	35,35,35,35	0
58	MG	1A	3711	1/1	0.93	0.07	21,21,21,21	0
58	MG	1A	3713	1/1	0.93	0.12	40,40,40,40	0
58	MG	2A	3292	1/1	0.93	0.19	49,49,49,49	0
58	MG	1A	3987	1/1	0.93	0.13	53,53,53,53	0
58	MG	2A	3031	1/1	0.93	0.09	57,57,57,57	0
58	MG	2G	201	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3553	1/1	0.93	0.27	54,54,54,54	0
58	MG	2A	3581	1/1	0.93	0.12	40,40,40,40	0
58	MG	2R	202	1/1	0.93	0.08	45,45,45,45	0
58	MG	2A	3584	1/1	0.93	0.10	48,48,48,48	0
58	MG	2A	3296	1/1	0.93	0.07	52,52,52,52	0
58	MG	2A	3298	1/1	0.93	0.24	56,56,56,56	0
58	MG	2W	201	1/1	0.93	0.09	50,50,50,50	0
58	MG	2A	3037	1/1	0.93	0.13	48,48,48,48	0
58	MG	1A	3493	1/1	0.93	0.07	39,39,39,39	0
58	MG	1A	3096	1/1	0.93	0.10	48,48,48,48	0
58	MG	25	104	1/1	0.93	0.08	48,48,48,48	0
58	MG	2A	3042	1/1	0.93	0.18	50,50,50,50	0
58	MG	2A	3043	1/1	0.93	0.08	60,60,60,60	0
58	MG	28	104	1/1	0.93	0.23	53,53,53,53	0
58	MG	2A	3308	1/1	0.93	0.12	61,61,61,61	0
58	MG	1A	3719	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3305	1/1	0.93	0.09	45,45,45,45	0
58	MG	2A	3052	1/1	0.93	0.13	64,64,64,64	0
58	MG	1A	3101	1/1	0.93	0.10	59,59,59,59	0
58	MG	1B	227	1/1	0.93	0.07	47,47,47,47	0
58	MG	2A	3611	1/1	0.93	0.16	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	1684	1/1	0.93	0.20	50,50,50,50	0
58	MG	2A	3617	1/1	0.93	0.10	64,64,64,64	0
58	MG	2A	3062	1/1	0.93	0.20	50,50,50,50	0
58	MG	2A	3319	1/1	0.93	0.11	62,62,62,62	0
58	MG	1A	3256	1/1	0.93	0.09	57,57,57,57	0
58	MG	2A	3321	1/1	0.93	0.08	62,62,62,62	0
58	MG	1A	3501	1/1	0.93	0.10	50,50,50,50	0
58	MG	1a	1687	1/1	0.93	0.07	55,55,55,55	0
58	MG	1A	3257	1/1	0.93	0.08	53,53,53,53	0
58	MG	2A	3631	1/1	0.93	0.15	51,51,51,51	0
58	MG	2a	1622	1/1	0.93	0.11	71,71,71,71	0
58	MG	1A	4017	1/1	0.93	0.08	41,41,41,41	0
58	MG	1B	234	1/1	0.93	0.09	58,58,58,58	0
58	MG	2A	3645	1/1	0.93	0.09	37,37,37,37	0
58	MG	1a	1693	1/1	0.93	0.27	46,46,46,46	0
58	MG	1a	1694	1/1	0.93	0.21	53,53,53,53	0
58	MG	1A	3863	1/1	0.93	0.08	50,50,50,50	0
58	MG	2A	3088	1/1	0.93	0.13	50,50,50,50	0
58	MG	1A	4019	1/1	0.93	0.07	33,33,33,33	0
58	MG	1D	302	1/1	0.93	0.17	51,51,51,51	0
58	MG	2A	3094	1/1	0.93	0.16	40,40,40,40	0
58	MG	2A	3657	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3658	1/1	0.93	0.13	48,48,48,48	0
58	MG	2a	1638	1/1	0.93	0.25	46,46,46,46	0
58	MG	1A	3732	1/1	0.93	0.14	44,44,44,44	0
58	MG	1D	313	1/1	0.93	0.16	31,31,31,31	0
58	MG	2A	3663	1/1	0.93	0.09	54,54,54,54	0
58	MG	2A	3341	1/1	0.93	0.27	68,68,68,68	0
58	MG	1A	3451	1/1	0.93	0.12	35,35,35,35	0
58	MG	1E	309	1/1	0.93	0.06	24,24,24,24	0
58	MG	1A	3320	1/1	0.93	0.06	32,32,32,32	0
58	MG	2A	3673	1/1	0.93	0.08	48,48,48,48	0
58	MG	2A	3674	1/1	0.93	0.11	49,49,49,49	0
58	MG	2A	3109	1/1	0.93	0.06	63,63,63,63	0
58	MG	2A	3677	1/1	0.93	0.16	56,56,56,56	0
58	MG	1E	313	1/1	0.93	0.10	42,42,42,42	0
58	MG	2A	3349	1/1	0.93	0.29	56,56,56,56	0
58	MG	2A	3680	1/1	0.93	0.07	56,56,56,56	0
58	MG	1A	3260	1/1	0.93	0.07	50,50,50,50	0
58	MG	2a	1659	1/1	0.93	0.12	74,74,74,74	0
58	MG	1F	311	1/1	0.93	0.17	29,29,29,29	0
58	MG	2A	3114	1/1	0.93	0.20	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	2a	1662	1/1	0.93	0.21	69,69,69,69	0
58	MG	1A	4029	1/1	0.93	0.06	39,39,39,39	0
58	MG	2A	3687	1/1	0.93	0.08	54,54,54,54	0
58	MG	1G	204	1/1	0.93	0.06	53,53,53,53	0
58	MG	2a	1667	1/1	0.93	0.11	64,64,64,64	0
58	MG	1A	3605	1/1	0.93	0.15	35,35,35,35	0
58	MG	1N	205	1/1	0.93	0.12	45,45,45,45	0
58	MG	2A	3697	1/1	0.93	0.12	44,44,44,44	0
58	MG	2a	1673	1/1	0.93	0.20	57,57,57,57	0
58	MG	1O	201	1/1	0.93	0.15	63,63,63,63	0
58	MG	2a	1680	1/1	0.93	0.19	54,54,54,54	0
58	MG	2a	1682	1/1	0.93	0.19	55,55,55,55	0
58	MG	2A	3141	1/1	0.93	0.21	48,48,48,48	0
58	MG	2a	1685	1/1	0.93	0.08	49,49,49,49	0
58	MG	1A	3886	1/1	0.93	0.09	34,34,34,34	0
58	MG	2A	3151	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3368	1/1	0.93	0.28	62,62,62,62	0
58	MG	1A	3889	1/1	0.93	0.08	18,18,18,18	0
58	MG	2A	3156	1/1	0.93	0.20	51,51,51,51	0
58	MG	2A	3708	1/1	0.93	0.08	60,60,60,60	0
58	MG	2A	3160	1/1	0.93	0.07	51,51,51,51	0
58	MG	2A	3712	1/1	0.93	0.06	27,27,27,27	0
58	MG	1A	3335	1/1	0.93	0.05	49,49,49,49	0
58	MG	2a	1705	1/1	0.93	0.16	48,48,48,48	0
58	MG	1A	3751	1/1	0.93	0.18	52,52,52,52	0
58	MG	1A	3194	1/1	0.93	0.11	47,47,47,47	0
58	MG	2A	3166	1/1	0.93	0.22	52,52,52,52	0
58	MG	2A	3379	1/1	0.93	0.08	48,48,48,48	0
58	MG	2a	1711	1/1	0.93	0.09	51,51,51,51	0
58	MG	2A	3167	1/1	0.93	0.14	41,41,41,41	0
58	MG	1A	3899	1/1	0.93	0.07	23,23,23,23	0
58	MG	1a	1744	1/1	0.93	0.07	51,51,51,51	0
58	MG	1a	1745	1/1	0.93	0.14	63,63,63,63	0
58	MG	1A	3755	1/1	0.93	0.06	30,30,30,30	0
58	MG	1A	3756	1/1	0.93	0.09	55,55,55,55	0
58	MG	2A	3180	1/1	0.93	0.13	53,53,53,53	0
58	MG	2A	3183	1/1	0.93	0.10	45,45,45,45	0
58	MG	1a	1754	1/1	0.93	0.17	49,49,49,49	0
58	MG	2A	3742	1/1	0.93	0.15	66,66,66,66	0
58	MG	2a	1729	1/1	0.93	0.13	50,50,50,50	0
58	MG	2a	1730	1/1	0.93	0.16	61,61,61,61	0
58	MG	1A	3512	1/1	0.93	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1Z	3701	1/1	0.93	0.05	56,56,56,56	0
58	MG	2a	1736	1/1	0.93	0.24	47,47,47,47	0
58	MG	1A	3462	1/1	0.93	0.18	39,39,39,39	0
58	MG	1a	1759	1/1	0.93	0.09	56,56,56,56	0
58	MG	2A	3748	1/1	0.93	0.15	50,50,50,50	0
58	MG	1A	4050	1/1	0.93	0.08	18,18,18,18	0
58	MG	1A	3266	1/1	0.93	0.07	47,47,47,47	0
58	MG	1A	3198	1/1	0.93	0.21	44,44,44,44	0
58	MG	2A	3757	1/1	0.93	0.09	64,64,64,64	0
58	MG	2A	3758	1/1	0.93	0.13	59,59,59,59	0
58	MG	1a	1768	1/1	0.93	0.07	50,50,50,50	0
58	MG	1l	106	1/1	0.93	0.10	49,49,49,49	0
58	MG	2A	3764	1/1	0.93	0.31	43,43,43,43	0
58	MG	1a	1771	1/1	0.93	0.11	58,58,58,58	0
58	MG	2a	1764	1/1	0.93	0.13	53,53,53,53	0
58	MG	2a	1770	1/1	0.93	0.07	50,50,50,50	0
58	MG	2a	1773	1/1	0.93	0.08	63,63,63,63	0
58	MG	2a	1775	1/1	0.93	0.08	59,59,59,59	0
58	MG	12	101	1/1	0.93	0.11	48,48,48,48	0
58	MG	2A	3206	1/1	0.93	0.19	61,61,61,61	0
58	MG	2a	1779	1/1	0.93	0.14	62,62,62,62	0
58	MG	1A	4057	1/1	0.93	0.10	59,59,59,59	0
58	MG	2a	1782	1/1	0.93	0.12	56,56,56,56	0
58	MG	2a	1785	1/1	0.93	0.15	40,40,40,40	0
58	MG	1A	4058	1/1	0.93	0.07	12,12,12,12	0
58	MG	2a	1787	1/1	0.93	0.15	57,57,57,57	0
58	MG	2A	3417	1/1	0.93	0.23	44,44,44,44	0
58	MG	1A	3522	1/1	0.93	0.21	35,35,35,35	0
58	MG	2A	3421	1/1	0.93	0.15	39,39,39,39	0
58	MG	1A	3527	1/1	0.93	0.09	55,55,55,55	0
58	MG	2A	3781	1/1	0.93	0.12	67,67,67,67	0
58	MG	2A	3427	1/1	0.93	0.23	46,46,46,46	0
58	MG	2A	3429	1/1	0.93	0.24	59,59,59,59	0
58	MG	2a	1798	1/1	0.93	0.08	58,58,58,58	0
58	MG	2A	3796	1/1	0.93	0.11	56,56,56,56	0
58	MG	2A	3430	1/1	0.93	0.21	53,53,53,53	0
58	MG	1A	3923	1/1	0.93	0.11	41,41,41,41	0
58	MG	2A	3799	1/1	0.93	0.07	55,55,55,55	0
58	MG	1A	3471	1/1	0.93	0.13	63,63,63,63	0
58	MG	2a	1809	1/1	0.93	0.20	60,60,60,60	0
58	MG	2A	3801	1/1	0.93	0.12	45,45,45,45	0
58	MG	1A	3153	1/1	0.93	0.15	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	3928	1/1	0.93	0.08	41,41,41,41	0
58	MG	1a	1796	1/1	0.93	0.10	54,54,54,54	0
58	MG	2A	3221	1/1	0.93	0.20	49,49,49,49	0
58	MG	1A	4079	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	4080	1/1	0.93	0.10	49,49,49,49	0
58	MG	2A	3226	1/1	0.93	0.11	58,58,58,58	0
58	MG	1a	1614	1/1	0.93	0.10	48,48,48,48	0
58	MG	1A	3087	1/1	0.93	0.20	38,38,38,38	0
58	MG	2A	3230	1/1	0.93	0.19	46,46,46,46	0
58	MG	1a	1619	1/1	0.93	0.08	46,46,46,46	0
58	MG	2A	3819	1/1	0.93	0.05	44,44,44,44	0
58	MG	2A	3460	1/1	0.93	0.10	51,51,51,51	0
58	MG	1a	1812	1/1	0.93	0.09	58,58,58,58	0
58	MG	2a	1829	1/1	0.93	0.12	55,55,55,55	0
58	MG	2A	3466	1/1	0.93	0.10	68,68,68,68	0
58	MG	2A	3838	1/1	0.93	0.07	53,53,53,53	0
58	MG	1a	1621	1/1	0.93	0.25	55,55,55,55	0
58	MG	1A	3169	1/1	0.93	0.19	35,35,35,35	0
58	MG	2A	3246	1/1	0.93	0.08	49,49,49,49	0
58	MG	2e	201	1/1	0.93	0.05	69,69,69,69	0
58	MG	2f	202	1/1	0.93	0.12	65,65,65,65	0
58	MG	1A	4086	1/1	0.93	0.10	21,21,21,21	0
58	MG	1A	3935	1/1	0.93	0.07	42,42,42,42	0
58	MG	1a	1631	1/1	0.93	0.27	53,53,53,53	0
58	MG	1A	3173	1/1	0.93	0.22	50,50,50,50	0
58	MG	1A	3674	1/1	0.93	0.08	27,27,27,27	0
58	MG	2q	201	1/1	0.93	0.32	71,71,71,71	0
58	MG	2q	203	1/1	0.93	0.12	67,67,67,67	0
58	MG	2A	3489	1/1	0.93	0.19	54,54,54,54	0
58	MG	2A	3870	1/1	0.93	0.11	59,59,59,59	0
58	MG	1A	3364	1/1	0.93	0.09	53,53,53,53	0
58	MG	1a	1639	1/1	0.93	0.13	45,45,45,45	0
58	MG	2A	3254	1/1	0.93	0.09	58,58,58,58	0
58	MG	2A	3876	1/1	0.93	0.10	35,35,35,35	0
58	MG	1A	3542	1/1	0.93	0.19	45,45,45,45	0
58	MG	1A	3421	1/1	0.93	0.16	34,34,34,34	0
58	MG	1a	1648	1/1	0.93	0.17	66,66,66,66	0
58	MG	1A	3957	1/1	0.93	0.06	51,51,51,51	0
58	MG	2A	3506	1/1	0.93	0.11	42,42,42,42	0
58	MG	2B	201	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	3248	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3511	1/1	0.93	0.10	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	3967	1/1	0.93	0.08	48,48,48,48	0
58	MG	2A	3271	1/1	0.93	0.06	56,56,56,56	0
58	MG	1A	3971	1/1	0.93	0.10	40,40,40,40	0
58	MG	2B	208	1/1	0.93	0.13	50,50,50,50	0
58	MG	1A	3483	1/1	0.93	0.18	41,41,41,41	0
58	MG	2B	212	1/1	0.93	0.14	62,62,62,62	0
58	MG	2A	3532	1/1	0.93	0.08	50,50,50,50	0
58	MG	2A	3508	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3443	1/1	0.94	0.15	38,38,38,38	0
58	MG	2B	213	1/1	0.94	0.16	48,48,48,48	0
58	MG	2A	3240	1/1	0.94	0.12	55,55,55,55	0
58	MG	1A	3653	1/1	0.94	0.08	19,19,19,19	0
58	MG	2A	3513	1/1	0.94	0.06	44,44,44,44	0
58	MG	1A	3361	1/1	0.94	0.14	63,63,63,63	0
58	MG	2A	3515	1/1	0.94	0.20	47,47,47,47	0
58	MG	2A	3516	1/1	0.94	0.13	57,57,57,57	0
58	MG	1a	1787	1/1	0.94	0.07	42,42,42,42	0
58	MG	2D	307	1/1	0.94	0.21	49,49,49,49	0
58	MG	2A	3526	1/1	0.94	0.09	55,55,55,55	0
58	MG	1A	3298	1/1	0.94	0.14	41,41,41,41	0
58	MG	1a	1791	1/1	0.94	0.12	59,59,59,59	0
58	MG	1A	3041	1/1	0.94	0.14	55,55,55,55	0
58	MG	2E	308	1/1	0.94	0.11	61,61,61,61	0
58	MG	1A	3366	1/1	0.94	0.13	42,42,42,42	0
58	MG	2A	3539	1/1	0.94	0.10	63,63,63,63	0
58	MG	1A	3665	1/1	0.94	0.05	22,22,22,22	0
58	MG	1A	3251	1/1	0.94	0.11	44,44,44,44	0
58	MG	1I	101	1/1	0.94	0.30	34,34,34,34	0
58	MG	1A	3368	1/1	0.94	0.13	44,44,44,44	0
58	MG	2A	3544	1/1	0.94	0.10	40,40,40,40	0
58	MG	1a	1809	1/1	0.94	0.17	48,48,48,48	0
58	MG	1A	3845	1/1	0.94	0.07	35,35,35,35	0
58	MG	2A	3551	1/1	0.94	0.09	40,40,40,40	0
58	MG	1A	4033	1/1	0.94	0.07	35,35,35,35	0
58	MG	2T	203	1/1	0.94	0.18	55,55,55,55	0
58	MG	1A	3524	1/1	0.94	0.14	39,39,39,39	0
58	MG	2A	3561	1/1	0.94	0.09	33,33,33,33	0
58	MG	2A	3262	1/1	0.94	0.09	53,53,53,53	0
58	MG	2X	101	1/1	0.94	0.10	56,56,56,56	0
58	MG	2A	3264	1/1	0.94	0.39	64,64,64,64	0
58	MG	2A	3575	1/1	0.94	0.06	30,30,30,30	0
58	MG	2A	3266	1/1	0.94	0.10	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	25	101	1/1	0.94	0.09	46,46,46,46	0
58	MG	25	102	1/1	0.94	0.19	47,47,47,47	0
58	MG	1A	3672	1/1	0.94	0.06	31,31,31,31	0
58	MG	1b	301	1/1	0.94	0.08	53,53,53,53	0
58	MG	2A	3270	1/1	0.94	0.09	56,56,56,56	0
58	MG	1A	3526	1/1	0.94	0.06	41,41,41,41	0
58	MG	1A	3459	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3686	1/1	0.94	0.06	30,30,30,30	0
58	MG	2A	3590	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	4044	1/1	0.94	0.06	24,24,24,24	0
58	MG	2A	3276	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3460	1/1	0.94	0.20	48,48,48,48	0
58	MG	1A	3103	1/1	0.94	0.23	57,57,57,57	0
58	MG	2A	3603	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3186	1/1	0.94	0.19	64,64,64,64	0
58	MG	1A	4049	1/1	0.94	0.09	26,26,26,26	0
58	MG	1a	1611	1/1	0.94	0.09	51,51,51,51	0
58	MG	2A	3285	1/1	0.94	0.10	42,42,42,42	0
58	MG	1a	1613	1/1	0.94	0.18	52,52,52,52	0
58	MG	1A	3867	1/1	0.94	0.07	48,48,48,48	0
58	MG	1A	3381	1/1	0.94	0.17	57,57,57,57	0
58	MG	2a	1619	1/1	0.94	0.14	58,58,58,58	0
58	MG	1A	3702	1/1	0.94	0.07	29,29,29,29	0
58	MG	1x	106	1/1	0.94	0.15	51,51,51,51	0
58	MG	2A	3615	1/1	0.94	0.11	58,58,58,58	0
58	MG	1A	3309	1/1	0.94	0.30	48,48,48,48	0
58	MG	1a	1622	1/1	0.94	0.07	47,47,47,47	0
58	MG	1a	1624	1/1	0.94	0.20	51,51,51,51	0
58	MG	2A	3621	1/1	0.94	0.07	41,41,41,41	0
58	MG	1A	3878	1/1	0.94	0.09	29,29,29,29	0
58	MG	1A	4062	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3537	1/1	0.94	0.16	45,45,45,45	0
58	MG	2A	3007	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3011	1/1	0.94	0.16	47,47,47,47	0
58	MG	1A	4064	1/1	0.94	0.16	51,51,51,51	0
58	MG	2A	3013	1/1	0.94	0.07	40,40,40,40	0
58	MG	2A	3634	1/1	0.94	0.11	38,38,38,38	0
58	MG	1A	3470	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3888	1/1	0.94	0.08	44,44,44,44	0
58	MG	1a	1637	1/1	0.94	0.17	54,54,54,54	0
58	MG	2A	3312	1/1	0.94	0.12	59,59,59,59	0
58	MG	2A	3650	1/1	0.94	0.10	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	2a	1646	1/1	0.94	0.13	57,57,57,57	0
58	MG	1A	3190	1/1	0.94	0.15	46,46,46,46	0
58	MG	1A	3159	1/1	0.94	0.06	48,48,48,48	0
58	MG	1a	1640	1/1	0.94	0.14	53,53,53,53	0
58	MG	2A	3032	1/1	0.94	0.09	33,33,33,33	0
58	MG	1a	1641	1/1	0.94	0.22	54,54,54,54	0
58	MG	1A	3316	1/1	0.94	0.15	47,47,47,47	0
58	MG	2a	1653	1/1	0.94	0.16	57,57,57,57	0
58	MG	1a	1644	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3164	1/1	0.94	0.25	49,49,49,49	0
58	MG	1A	3898	1/1	0.94	0.09	24,24,24,24	0
58	MG	1A	3016	1/1	0.94	0.17	56,56,56,56	0
58	MG	1A	3900	1/1	0.94	0.08	15,15,15,15	0
58	MG	2A	3665	1/1	0.94	0.06	48,48,48,48	0
58	MG	1A	3550	1/1	0.94	0.18	43,43,43,43	0
58	MG	1A	3551	1/1	0.94	0.19	49,49,49,49	0
58	MG	2A	3053	1/1	0.94	0.09	50,50,50,50	0
58	MG	1a	1659	1/1	0.94	0.09	49,49,49,49	0
58	MG	1A	3322	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	3329	1/1	0.94	0.15	45,45,45,45	0
58	MG	1A	3264	1/1	0.94	0.07	31,31,31,31	0
58	MG	1A	3265	1/1	0.94	0.10	45,45,45,45	0
58	MG	1a	1665	1/1	0.94	0.13	50,50,50,50	0
58	MG	1A	3733	1/1	0.94	0.10	57,57,57,57	0
58	MG	1A	3916	1/1	0.94	0.08	35,35,35,35	0
58	MG	1A	3484	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3558	1/1	0.94	0.07	69,69,69,69	0
58	MG	2a	1681	1/1	0.94	0.12	53,53,53,53	0
58	MG	2A	3079	1/1	0.94	0.07	39,39,39,39	0
58	MG	1A	3568	1/1	0.94	0.15	37,37,37,37	0
58	MG	2A	3081	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3346	1/1	0.94	0.11	66,66,66,66	0
58	MG	1A	3743	1/1	0.94	0.06	50,50,50,50	0
58	MG	2a	1690	1/1	0.94	0.13	55,55,55,55	0
58	MG	2a	1692	1/1	0.94	0.19	40,40,40,40	0
58	MG	2A	3696	1/1	0.94	0.08	40,40,40,40	0
58	MG	2A	3083	1/1	0.94	0.09	51,51,51,51	0
58	MG	1A	3927	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3569	1/1	0.94	0.19	45,45,45,45	0
58	MG	1A	3210	1/1	0.94	0.06	43,43,43,43	0
58	MG	2A	3091	1/1	0.94	0.11	53,53,53,53	0
58	MG	1A	3747	1/1	0.94	0.07	17,17,17,17	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	0.94	0.09	56,56,56,56	0
58	MG	2A	3357	1/1	0.94	0.12	51,51,51,51	0
58	MG	1B	207	1/1	0.94	0.21	46,46,46,46	0
58	MG	1A	3486	1/1	0.94	0.06	34,34,34,34	0
58	MG	2A	3711	1/1	0.94	0.10	58,58,58,58	0
58	MG	2A	3363	1/1	0.94	0.16	63,63,63,63	0
58	MG	2A	3097	1/1	0.94	0.14	58,58,58,58	0
58	MG	2a	1716	1/1	0.94	0.12	58,58,58,58	0
58	MG	1A	3940	1/1	0.94	0.05	34,34,34,34	0
58	MG	1A	3491	1/1	0.94	0.09	41,41,41,41	0
58	MG	2a	1719	1/1	0.94	0.13	59,59,59,59	0
58	MG	1A	3019	1/1	0.94	0.08	44,44,44,44	0
58	MG	2A	3722	1/1	0.94	0.09	44,44,44,44	0
58	MG	1A	3268	1/1	0.94	0.11	46,46,46,46	0
58	MG	1A	3952	1/1	0.94	0.06	42,42,42,42	0
58	MG	1A	3345	1/1	0.94	0.13	53,53,53,53	0
58	MG	1B	218	1/1	0.94	0.08	51,51,51,51	0
58	MG	1A	3761	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3956	1/1	0.94	0.12	57,57,57,57	0
58	MG	1A	3602	1/1	0.94	0.21	58,58,58,58	0
58	MG	2a	1733	1/1	0.94	0.16	58,58,58,58	0
58	MG	2A	3122	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3123	1/1	0.94	0.15	47,47,47,47	0
58	MG	1A	3170	1/1	0.94	0.13	50,50,50,50	0
58	MG	2A	3126	1/1	0.94	0.10	58,58,58,58	0
58	MG	2a	1739	1/1	0.94	0.17	58,58,58,58	0
58	MG	2A	3127	1/1	0.94	0.14	50,50,50,50	0
58	MG	2a	1741	1/1	0.94	0.27	36,36,36,36	0
58	MG	2A	3744	1/1	0.94	0.09	48,48,48,48	0
58	MG	2A	3129	1/1	0.94	0.11	45,45,45,45	0
58	MG	2A	3387	1/1	0.94	0.07	61,61,61,61	0
58	MG	2A	3389	1/1	0.94	0.11	47,47,47,47	0
58	MG	1B	226	1/1	0.94	0.09	53,53,53,53	0
58	MG	1A	3962	1/1	0.94	0.08	46,46,46,46	0
58	MG	2A	3750	1/1	0.94	0.09	64,64,64,64	0
58	MG	2a	1753	1/1	0.94	0.07	75,75,75,75	0
58	MG	2A	3752	1/1	0.94	0.10	60,60,60,60	0
58	MG	1a	1700	1/1	0.94	0.27	57,57,57,57	0
58	MG	2a	1757	1/1	0.94	0.10	56,56,56,56	0
58	MG	1a	1702	1/1	0.94	0.09	47,47,47,47	0
58	MG	2a	1762	1/1	0.94	0.08	63,63,63,63	0
58	MG	2A	3142	1/1	0.94	0.14	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	1B	228	1/1	0.94	0.09	42,42,42,42	0
58	MG	2a	1771	1/1	0.94	0.06	78,78,78,78	0
58	MG	2A	3147	1/1	0.94	0.10	44,44,44,44	0
58	MG	1a	1704	1/1	0.94	0.14	55,55,55,55	0
58	MG	2A	3762	1/1	0.94	0.07	34,34,34,34	0
58	MG	2A	3763	1/1	0.94	0.15	55,55,55,55	0
58	MG	2A	3152	1/1	0.94	0.20	51,51,51,51	0
58	MG	2A	3399	1/1	0.94	0.10	51,51,51,51	0
58	MG	1A	3966	1/1	0.94	0.07	24,24,24,24	0
58	MG	2A	3154	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	3604	1/1	0.94	0.10	54,54,54,54	0
58	MG	1a	1708	1/1	0.94	0.19	45,45,45,45	0
58	MG	1A	3422	1/1	0.94	0.15	53,53,53,53	0
58	MG	2a	1790	1/1	0.94	0.12	48,48,48,48	0
58	MG	1A	3772	1/1	0.94	0.11	27,27,27,27	0
58	MG	1A	3978	1/1	0.94	0.09	57,57,57,57	0
58	MG	2A	3778	1/1	0.94	0.06	54,54,54,54	0
58	MG	1A	3777	1/1	0.94	0.07	53,53,53,53	0
58	MG	1B	236	1/1	0.94	0.12	72,72,72,72	0
58	MG	1A	3981	1/1	0.94	0.09	40,40,40,40	0
58	MG	2A	3789	1/1	0.94	0.07	61,61,61,61	0
58	MG	2a	1799	1/1	0.94	0.14	57,57,57,57	0
58	MG	2a	1801	1/1	0.94	0.12	52,52,52,52	0
58	MG	2A	3791	1/1	0.94	0.11	50,50,50,50	0
58	MG	2A	3792	1/1	0.94	0.09	59,59,59,59	0
58	MG	2a	1804	1/1	0.94	0.09	51,51,51,51	0
58	MG	2A	3416	1/1	0.94	0.20	51,51,51,51	0
58	MG	2A	3795	1/1	0.94	0.09	45,45,45,45	0
58	MG	1A	3607	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3419	1/1	0.94	0.18	28,28,28,28	0
58	MG	1a	1721	1/1	0.94	0.12	48,48,48,48	0
58	MG	2A	3174	1/1	0.94	0.18	52,52,52,52	0
58	MG	2A	3423	1/1	0.94	0.23	50,50,50,50	0
58	MG	1A	3611	1/1	0.94	0.10	49,49,49,49	0
58	MG	1a	1725	1/1	0.94	0.07	47,47,47,47	0
58	MG	2A	3804	1/1	0.94	0.12	48,48,48,48	0
58	MG	1A	3801	1/1	0.94	0.10	26,26,26,26	0
58	MG	2A	3181	1/1	0.94	0.13	51,51,51,51	0
58	MG	1E	307	1/1	0.94	0.11	50,50,50,50	0
58	MG	1A	3233	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3351	1/1	0.94	0.10	37,37,37,37	0
58	MG	1A	3129	1/1	0.94	0.12	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	1736	1/1	0.94	0.12	46,46,46,46	0
58	MG	2A	3437	1/1	0.94	0.27	53,53,53,53	0
58	MG	1A	3626	1/1	0.94	0.09	54,54,54,54	0
58	MG	1A	3813	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3630	1/1	0.94	0.11	32,32,32,32	0
58	MG	1A	3996	1/1	0.94	0.15	52,52,52,52	0
58	MG	2A	3447	1/1	0.94	0.12	57,57,57,57	0
58	MG	2A	3831	1/1	0.94	0.12	48,48,48,48	0
58	MG	2a	1839	1/1	0.94	0.19	52,52,52,52	0
58	MG	1A	3632	1/1	0.94	0.08	47,47,47,47	0
58	MG	1a	1748	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3840	1/1	0.94	0.10	55,55,55,55	0
58	MG	1A	3358	1/1	0.94	0.09	54,54,54,54	0
58	MG	1A	4000	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3844	1/1	0.94	0.06	45,45,45,45	0
58	MG	1a	1751	1/1	0.94	0.06	54,54,54,54	0
58	MG	2n	101	1/1	0.94	0.34	61,61,61,61	0
58	MG	1A	4002	1/1	0.94	0.08	49,49,49,49	0
58	MG	2A	3463	1/1	0.94	0.06	52,52,52,52	0
58	MG	1O	204	1/1	0.94	0.06	44,44,44,44	0
58	MG	1A	3827	1/1	0.94	0.07	22,22,22,22	0
58	MG	1a	1757	1/1	0.94	0.08	52,52,52,52	0
58	MG	2A	3860	1/1	0.94	0.09	36,36,36,36	0
58	MG	2A	3476	1/1	0.94	0.08	60,60,60,60	0
58	MG	2v	103	1/1	0.94	0.25	54,54,54,54	0
58	MG	1P	202	1/1	0.94	0.08	23,23,23,23	0
58	MG	2w	102	1/1	0.94	0.07	82,82,82,82	0
58	MG	2A	3478	1/1	0.94	0.17	41,41,41,41	0
58	MG	1A	4008	1/1	0.94	0.10	54,54,54,54	0
58	MG	1Q	205	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3645	1/1	0.94	0.13	42,42,42,42	0
58	MG	1a	1766	1/1	0.94	0.07	49,49,49,49	0
58	MG	1R	205	1/1	0.94	0.13	29,29,29,29	0
58	MG	1S	203	1/1	0.94	0.07	61,61,61,61	0
58	MG	1T	201	1/1	0.94	0.12	54,54,54,54	0
58	MG	1U	205	1/1	0.94	0.05	33,33,33,33	0
58	MG	2x	104	1/1	0.94	0.18	71,71,71,71	0
58	MG	1A	3831	1/1	0.94	0.06	32,32,32,32	0
58	MG	2A	3495	1/1	0.94	0.06	47,47,47,47	0
58	MG	1V	202	1/1	0.94	0.11	38,38,38,38	0
58	MG	1V	208	1/1	0.94	0.12	58,58,58,58	0
58	MG	2A	3234	1/1	0.94	0.10	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	2A	3235	1/1	0.94	0.11	49,49,49,49	0
58	MG	1A	3100	1/1	0.94	0.08	39,39,39,39	0
60	ZN	24	501	1/1	0.94	0.10	111,111,111,111	0
58	MG	2A	3200	1/1	0.95	0.11	46,46,46,46	0
58	MG	2A	3201	1/1	0.95	0.11	43,43,43,43	0
58	MG	2A	3483	1/1	0.95	0.28	58,58,58,58	0
58	MG	2A	3202	1/1	0.95	0.15	62,62,62,62	0
58	MG	1A	3803	1/1	0.95	0.07	32,32,32,32	0
58	MG	2A	3488	1/1	0.95	0.18	41,41,41,41	0
58	MG	2A	3205	1/1	0.95	0.17	54,54,54,54	0
58	MG	1Q	204	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3989	1/1	0.95	0.13	55,55,55,55	0
58	MG	1a	1762	1/1	0.95	0.15	45,45,45,45	0
58	MG	1R	201	1/1	0.95	0.10	28,28,28,28	0
58	MG	1A	3990	1/1	0.95	0.07	16,16,16,16	0
58	MG	1A	3122	1/1	0.95	0.07	33,33,33,33	0
58	MG	1A	3172	1/1	0.95	0.13	39,39,39,39	0
58	MG	2A	3214	1/1	0.95	0.20	65,65,65,65	0
58	MG	1a	1769	1/1	0.95	0.07	59,59,59,59	0
58	MG	2A	3217	1/1	0.95	0.12	40,40,40,40	0
58	MG	1A	3319	1/1	0.95	0.08	45,45,45,45	0
58	MG	1T	202	1/1	0.95	0.09	45,45,45,45	0
58	MG	2D	301	1/1	0.95	0.07	40,40,40,40	0
58	MG	1T	203	1/1	0.95	0.14	48,48,48,48	0
58	MG	1A	3057	1/1	0.95	0.10	37,37,37,37	0
58	MG	1A	3811	1/1	0.95	0.05	18,18,18,18	0
58	MG	1A	3127	1/1	0.95	0.11	32,32,32,32	0
58	MG	1A	3635	1/1	0.95	0.04	26,26,26,26	0
58	MG	2A	3519	1/1	0.95	0.10	17,17,17,17	0
58	MG	2E	307	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3817	1/1	0.95	0.06	52,52,52,52	0
58	MG	1A	3818	1/1	0.95	0.16	62,62,62,62	0
58	MG	2E	310	1/1	0.95	0.10	32,32,32,32	0
58	MG	2A	3232	1/1	0.95	0.19	44,44,44,44	0
58	MG	2A	3529	1/1	0.95	0.06	36,36,36,36	0
58	MG	1A	3637	1/1	0.95	0.06	18,18,18,18	0
58	MG	1A	3182	1/1	0.95	0.08	34,34,34,34	0
58	MG	2A	3236	1/1	0.95	0.23	60,60,60,60	0
58	MG	1A	3644	1/1	0.95	0.08	33,33,33,33	0
58	MG	1a	1794	1/1	0.95	0.09	69,69,69,69	0
58	MG	1A	4011	1/1	0.95	0.07	30,30,30,30	0
58	MG	2A	3242	1/1	0.95	0.08	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	1Z	3702	1/1	0.95	0.13	43,43,43,43	0
58	MG	10	102	1/1	0.95	0.16	41,41,41,41	0
58	MG	1a	1800	1/1	0.95	0.05	50,50,50,50	0
58	MG	1a	1802	1/1	0.95	0.06	58,58,58,58	0
58	MG	1A	3828	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3331	1/1	0.95	0.22	48,48,48,48	0
58	MG	1A	3646	1/1	0.95	0.05	12,12,12,12	0
58	MG	1A	4021	1/1	0.95	0.12	41,41,41,41	0
58	MG	20	103	1/1	0.95	0.13	58,58,58,58	0
58	MG	2A	3562	1/1	0.95	0.11	27,27,27,27	0
58	MG	1A	3508	1/1	0.95	0.08	32,32,32,32	0
58	MG	1A	3509	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3420	1/1	0.95	0.07	41,41,41,41	0
58	MG	2A	3576	1/1	0.95	0.13	49,49,49,49	0
58	MG	1a	1814	1/1	0.95	0.06	47,47,47,47	0
58	MG	28	102	1/1	0.95	0.22	49,49,49,49	0
58	MG	28	103	1/1	0.95	0.08	42,42,42,42	0
58	MG	1A	3332	1/1	0.95	0.27	56,56,56,56	0
58	MG	1A	3656	1/1	0.95	0.09	44,44,44,44	0
58	MG	2A	3258	1/1	0.95	0.12	41,41,41,41	0
58	MG	2A	3259	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3015	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3261	1/1	0.95	0.17	54,54,54,54	0
58	MG	2A	3587	1/1	0.95	0.05	22,22,22,22	0
58	MG	2A	3588	1/1	0.95	0.11	44,44,44,44	0
58	MG	1e	201	1/1	0.95	0.08	55,55,55,55	0
58	MG	2A	3591	1/1	0.95	0.10	50,50,50,50	0
58	MG	2a	1611	1/1	0.95	0.20	56,56,56,56	0
58	MG	1A	3513	1/1	0.95	0.08	34,34,34,34	0
58	MG	2A	3265	1/1	0.95	0.18	53,53,53,53	0
58	MG	2a	1614	1/1	0.95	0.20	53,53,53,53	0
58	MG	17	103	1/1	0.95	0.12	30,30,30,30	0
58	MG	1A	3004	1/1	0.95	0.07	23,23,23,23	0
58	MG	18	101	1/1	0.95	0.39	46,46,46,46	0
58	MG	1A	3664	1/1	0.95	0.05	25,25,25,25	0
58	MG	1a	1601	1/1	0.95	0.08	55,55,55,55	0
58	MG	1A	3517	1/1	0.95	0.07	48,48,48,48	0
58	MG	1w	104	1/1	0.95	0.24	53,53,53,53	0
58	MG	1w	105	1/1	0.95	0.08	54,54,54,54	0
58	MG	1A	3666	1/1	0.95	0.05	18,18,18,18	0
58	MG	1A	3846	1/1	0.95	0.14	46,46,46,46	0
58	MG	2A	3278	1/1	0.95	0.07	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	3848	1/1	0.95	0.07	55,55,55,55	0
58	MG	2A	3613	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3614	1/1	0.95	0.10	37,37,37,37	0
58	MG	1A	3144	1/1	0.95	0.08	39,39,39,39	0
58	MG	1A	3851	1/1	0.95	0.09	48,48,48,48	0
58	MG	1A	3431	1/1	0.95	0.07	42,42,42,42	0
58	MG	2A	3284	1/1	0.95	0.05	38,38,38,38	0
58	MG	1a	1616	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3622	1/1	0.95	0.13	38,38,38,38	0
58	MG	1A	3339	1/1	0.95	0.13	42,42,42,42	0
58	MG	1A	3523	1/1	0.95	0.23	32,32,32,32	0
58	MG	2a	1640	1/1	0.95	0.16	51,51,51,51	0
58	MG	1A	3438	1/1	0.95	0.09	58,58,58,58	0
58	MG	2a	1643	1/1	0.95	0.19	55,55,55,55	0
58	MG	1A	3675	1/1	0.95	0.06	34,34,34,34	0
58	MG	2A	3005	1/1	0.95	0.17	52,52,52,52	0
58	MG	1a	1623	1/1	0.95	0.09	43,43,43,43	0
58	MG	1A	3439	1/1	0.95	0.06	44,44,44,44	0
58	MG	2A	3008	1/1	0.95	0.08	54,54,54,54	0
58	MG	2A	3637	1/1	0.95	0.06	36,36,36,36	0
58	MG	1a	1625	1/1	0.95	0.14	54,54,54,54	0
58	MG	2A	3643	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3263	1/1	0.95	0.05	20,20,20,20	0
58	MG	2A	3646	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3036	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3648	1/1	0.95	0.10	41,41,41,41	0
58	MG	1a	1628	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3301	1/1	0.95	0.14	56,56,56,56	0
58	MG	1A	3191	1/1	0.95	0.12	40,40,40,40	0
58	MG	2A	3304	1/1	0.95	0.14	55,55,55,55	0
58	MG	2A	3020	1/1	0.95	0.09	52,52,52,52	0
58	MG	2A	3022	1/1	0.95	0.11	42,42,42,42	0
58	MG	1A	4059	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	4061	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3869	1/1	0.95	0.09	44,44,44,44	0
58	MG	2A	3660	1/1	0.95	0.10	47,47,47,47	0
58	MG	1A	3444	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3871	1/1	0.95	0.06	19,19,19,19	0
58	MG	2A	3033	1/1	0.95	0.16	42,42,42,42	0
58	MG	1A	3695	1/1	0.95	0.11	22,22,22,22	0
58	MG	1A	3875	1/1	0.95	0.12	36,36,36,36	0
58	MG	1A	3877	1/1	0.95	0.04	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1642	1/1	0.95	0.12	53,53,53,53	0
58	MG	2A	3669	1/1	0.95	0.14	54,54,54,54	0
58	MG	1A	3346	1/1	0.95	0.07	41,41,41,41	0
58	MG	1A	3697	1/1	0.95	0.07	27,27,27,27	0
58	MG	2a	1684	1/1	0.95	0.13	54,54,54,54	0
58	MG	1a	1645	1/1	0.95	0.14	43,43,43,43	0
58	MG	2A	3323	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3048	1/1	0.95	0.12	43,43,43,43	0
58	MG	1A	3534	1/1	0.95	0.09	43,43,43,43	0
58	MG	2A	3051	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3705	1/1	0.95	0.11	47,47,47,47	0
58	MG	1a	1653	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3054	1/1	0.95	0.07	57,57,57,57	0
58	MG	2A	3684	1/1	0.95	0.11	48,48,48,48	0
58	MG	1A	3348	1/1	0.95	0.09	36,36,36,36	0
58	MG	1A	3149	1/1	0.95	0.24	36,36,36,36	0
58	MG	1A	4083	1/1	0.95	0.12	46,46,46,46	0
58	MG	2A	3060	1/1	0.95	0.18	54,54,54,54	0
58	MG	2A	3692	1/1	0.95	0.10	51,51,51,51	0
58	MG	2a	1707	1/1	0.95	0.15	51,51,51,51	0
58	MG	1A	4085	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3891	1/1	0.95	0.07	28,28,28,28	0
58	MG	2A	3065	1/1	0.95	0.22	53,53,53,53	0
58	MG	1A	3151	1/1	0.95	0.10	30,30,30,30	0
58	MG	2A	3067	1/1	0.95	0.16	49,49,49,49	0
58	MG	2A	3068	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3701	1/1	0.95	0.07	56,56,56,56	0
58	MG	1A	3204	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3895	1/1	0.95	0.05	34,34,34,34	0
58	MG	1A	3205	1/1	0.95	0.09	44,44,44,44	0
58	MG	1a	1664	1/1	0.95	0.08	60,60,60,60	0
58	MG	2A	3348	1/1	0.95	0.09	55,55,55,55	0
58	MG	2A	3077	1/1	0.95	0.07	49,49,49,49	0
58	MG	1A	3097	1/1	0.95	0.16	31,31,31,31	0
58	MG	1a	1666	1/1	0.95	0.19	50,50,50,50	0
58	MG	1A	3156	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3718	1/1	0.95	0.08	65,65,65,65	0
58	MG	1A	3005	1/1	0.95	0.08	40,40,40,40	0
58	MG	2A	3355	1/1	0.95	0.13	62,62,62,62	0
58	MG	2A	3719	1/1	0.95	0.08	26,26,26,26	0
58	MG	2A	3720	1/1	0.95	0.06	31,31,31,31	0
58	MG	1A	3276	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	3905	1/1	0.95	0.09	26,26,26,26	0
58	MG	1A	3294	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3297	1/1	0.95	0.06	31,31,31,31	0
58	MG	1A	3910	1/1	0.95	0.09	40,40,40,40	0
58	MG	1A	3469	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3213	1/1	0.95	0.12	39,39,39,39	0
58	MG	1B	205	1/1	0.95	0.27	55,55,55,55	0
58	MG	2A	3737	1/1	0.95	0.10	60,60,60,60	0
58	MG	1a	1680	1/1	0.95	0.07	55,55,55,55	0
58	MG	1A	3915	1/1	0.95	0.18	37,37,37,37	0
58	MG	2a	1748	1/1	0.95	0.07	55,55,55,55	0
58	MG	2a	1750	1/1	0.95	0.06	59,59,59,59	0
58	MG	1A	3221	1/1	0.95	0.11	35,35,35,35	0
58	MG	1A	3918	1/1	0.95	0.12	23,23,23,23	0
58	MG	2A	3371	1/1	0.95	0.14	60,60,60,60	0
58	MG	2A	3105	1/1	0.95	0.17	60,60,60,60	0
58	MG	2a	1756	1/1	0.95	0.08	58,58,58,58	0
58	MG	1B	210	1/1	0.95	0.06	37,37,37,37	0
58	MG	1A	3920	1/1	0.95	0.04	28,28,28,28	0
58	MG	2A	3375	1/1	0.95	0.32	61,61,61,61	0
58	MG	1A	3222	1/1	0.95	0.14	43,43,43,43	0
58	MG	2a	1765	1/1	0.95	0.07	42,42,42,42	0
58	MG	2a	1769	1/1	0.95	0.09	62,62,62,62	0
58	MG	1A	3922	1/1	0.95	0.08	28,28,28,28	0
58	MG	1A	3475	1/1	0.95	0.10	33,33,33,33	0
58	MG	2A	3117	1/1	0.95	0.07	41,41,41,41	0
58	MG	2A	3751	1/1	0.95	0.09	45,45,45,45	0
58	MG	2A	3381	1/1	0.95	0.21	40,40,40,40	0
58	MG	2A	3118	1/1	0.95	0.13	63,63,63,63	0
58	MG	2A	3755	1/1	0.95	0.22	50,50,50,50	0
58	MG	2a	1780	1/1	0.95	0.12	54,54,54,54	0
58	MG	1a	1691	1/1	0.95	0.20	37,37,37,37	0
58	MG	1A	3559	1/1	0.95	0.07	47,47,47,47	0
58	MG	2a	1784	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3566	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	3301	1/1	0.95	0.06	41,41,41,41	0
58	MG	2A	3125	1/1	0.95	0.08	49,49,49,49	0
58	MG	1A	3376	1/1	0.95	0.09	52,52,52,52	0
58	MG	1A	3049	1/1	0.95	0.06	15,15,15,15	0
58	MG	1A	3304	1/1	0.95	0.29	58,58,58,58	0
58	MG	1A	3932	1/1	0.95	0.06	39,39,39,39	0
58	MG	2A	3132	1/1	0.95	0.07	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1a	1701	1/1	0.95	0.18	48,48,48,48	0
58	MG	2A	3137	1/1	0.95	0.14	39,39,39,39	0
58	MG	1A	3578	1/1	0.95	0.10	44,44,44,44	0
58	MG	1A	3752	1/1	0.95	0.09	55,55,55,55	0
58	MG	1A	3025	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3144	1/1	0.95	0.11	42,42,42,42	0
58	MG	2A	3145	1/1	0.95	0.25	68,68,68,68	0
58	MG	1B	230	1/1	0.95	0.06	32,32,32,32	0
58	MG	1A	3308	1/1	0.95	0.16	39,39,39,39	0
58	MG	2a	1805	1/1	0.95	0.12	53,53,53,53	0
58	MG	2A	3782	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3784	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3948	1/1	0.95	0.07	18,18,18,18	0
58	MG	1A	3594	1/1	0.95	0.23	32,32,32,32	0
58	MG	1A	3167	1/1	0.95	0.13	29,29,29,29	0
58	MG	1A	3400	1/1	0.95	0.22	36,36,36,36	0
58	MG	2A	3793	1/1	0.95	0.08	53,53,53,53	0
58	MG	2A	3155	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3414	1/1	0.95	0.12	31,31,31,31	0
58	MG	1A	3599	1/1	0.95	0.09	48,48,48,48	0
58	MG	2A	3159	1/1	0.95	0.11	52,52,52,52	0
58	MG	2A	3418	1/1	0.95	0.17	41,41,41,41	0
58	MG	2a	1819	1/1	0.95	0.05	52,52,52,52	0
58	MG	1A	3310	1/1	0.95	0.14	38,38,38,38	0
58	MG	1A	3246	1/1	0.95	0.12	38,38,38,38	0
58	MG	1D	304	1/1	0.95	0.18	32,32,32,32	0
58	MG	2A	3802	1/1	0.95	0.09	73,73,73,73	0
58	MG	2A	3422	1/1	0.95	0.18	39,39,39,39	0
58	MG	2a	1826	1/1	0.95	0.14	47,47,47,47	0
58	MG	2A	3163	1/1	0.95	0.13	48,48,48,48	0
58	MG	1A	3489	1/1	0.95	0.18	34,34,34,34	0
58	MG	1A	3405	1/1	0.95	0.18	31,31,31,31	0
58	MG	2a	1831	1/1	0.95	0.09	47,47,47,47	0
58	MG	2a	1832	1/1	0.95	0.22	67,67,67,67	0
58	MG	1E	305	1/1	0.95	0.12	45,45,45,45	0
58	MG	2a	1834	1/1	0.95	0.08	63,63,63,63	0
58	MG	1E	306	1/1	0.95	0.08	35,35,35,35	0
58	MG	2A	3170	1/1	0.95	0.06	58,58,58,58	0
58	MG	1A	3965	1/1	0.95	0.06	40,40,40,40	0
58	MG	2A	3172	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3773	1/1	0.95	0.08	35,35,35,35	0
58	MG	1A	3775	1/1	0.95	0.05	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	3606	1/1	0.95	0.12	48,48,48,48	0
58	MG	2A	3176	1/1	0.95	0.09	56,56,56,56	0
58	MG	1A	3972	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3823	1/1	0.95	0.11	35,35,35,35	0
58	MG	2A	3443	1/1	0.95	0.20	47,47,47,47	0
58	MG	2A	3179	1/1	0.95	0.21	59,59,59,59	0
58	MG	1A	3973	1/1	0.95	0.11	48,48,48,48	0
58	MG	1F	310	1/1	0.95	0.10	55,55,55,55	0
58	MG	2q	202	1/1	0.95	0.06	63,63,63,63	0
58	MG	2A	3182	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3779	1/1	0.95	0.06	22,22,22,22	0
58	MG	2A	3451	1/1	0.95	0.24	52,52,52,52	0
58	MG	2A	3452	1/1	0.95	0.09	50,50,50,50	0
58	MG	1a	1742	1/1	0.95	0.07	49,49,49,49	0
58	MG	2A	3186	1/1	0.95	0.07	45,45,45,45	0
58	MG	1G	202	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3850	1/1	0.95	0.07	64,64,64,64	0
58	MG	2A	3461	1/1	0.95	0.18	38,38,38,38	0
58	MG	2A	3852	1/1	0.95	0.06	23,23,23,23	0
58	MG	1A	3786	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3855	1/1	0.95	0.10	31,31,31,31	0
58	MG	2w	108	1/1	0.95	0.09	46,46,46,46	0
58	MG	1A	3787	1/1	0.95	0.11	48,48,48,48	0
58	MG	2A	3465	1/1	0.95	0.20	50,50,50,50	0
58	MG	2A	3864	1/1	0.95	0.07	56,56,56,56	0
58	MG	2A	3865	1/1	0.95	0.07	54,54,54,54	0
58	MG	2x	102	1/1	0.95	0.15	43,43,43,43	0
58	MG	2A	3868	1/1	0.95	0.08	47,47,47,47	0
58	MG	1A	3790	1/1	0.95	0.07	42,42,42,42	0
58	MG	1N	202	1/1	0.95	0.12	41,41,41,41	0
58	MG	2A	3471	1/1	0.95	0.05	42,42,42,42	0
58	MG	2x	107	1/1	0.95	0.05	31,31,31,31	0
58	MG	1A	3407	1/1	0.95	0.15	29,29,29,29	0
58	MG	2A	3873	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3408	1/1	0.95	0.13	46,46,46,46	0
58	MG	1A	3797	1/1	0.95	0.09	46,46,46,46	0
58	MG	1A	3090	1/1	0.95	0.11	41,41,41,41	0
58	MG	2y	106	1/1	0.95	0.10	66,66,66,66	0
59	K	2A	3467	1/1	0.95	0.08	50,50,50,50	0
58	MG	1A	3802	1/1	0.95	0.09	16,16,16,16	0
58	MG	1A	4013	1/1	0.96	0.06	11,11,11,11	0
58	MG	1A	3006	1/1	0.96	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	3547	1/1	0.96	0.06	40,40,40,40	0
58	MG	13	102	1/1	0.96	0.10	38,38,38,38	0
58	MG	2A	3550	1/1	0.96	0.07	36,36,36,36	0
58	MG	1A	3185	1/1	0.96	0.10	56,56,56,56	0
58	MG	2A	3552	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3409	1/1	0.96	0.11	39,39,39,39	0
58	MG	1w	107	1/1	0.96	0.10	47,47,47,47	0
58	MG	15	107	1/1	0.96	0.08	50,50,50,50	0
58	MG	1A	3321	1/1	0.96	0.13	49,49,49,49	0
58	MG	1A	3411	1/1	0.96	0.07	45,45,45,45	0
58	MG	1x	103	1/1	0.96	0.04	45,45,45,45	0
58	MG	2A	3574	1/1	0.96	0.10	40,40,40,40	0
58	MG	2F	301	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3652	1/1	0.96	0.06	23,23,23,23	0
58	MG	1A	3834	1/1	0.96	0.16	39,39,39,39	0
58	MG	1A	3133	1/1	0.96	0.11	32,32,32,32	0
58	MG	2F	305	1/1	0.96	0.06	41,41,41,41	0
58	MG	2A	3578	1/1	0.96	0.05	33,33,33,33	0
58	MG	2F	308	1/1	0.96	0.15	44,44,44,44	0
58	MG	1A	3324	1/1	0.96	0.17	31,31,31,31	0
58	MG	1A	3325	1/1	0.96	0.06	48,48,48,48	0
58	MG	1x	110	1/1	0.96	0.05	48,48,48,48	0
58	MG	2Q	201	1/1	0.96	0.09	48,48,48,48	0
58	MG	1A	3658	1/1	0.96	0.07	35,35,35,35	0
58	MG	2Q	203	1/1	0.96	0.15	47,47,47,47	0
58	MG	2R	201	1/1	0.96	0.15	58,58,58,58	0
58	MG	1A	3840	1/1	0.96	0.04	30,30,30,30	0
58	MG	2A	3001	1/1	0.96	0.19	43,43,43,43	0
58	MG	1a	1604	1/1	0.96	0.10	55,55,55,55	0
58	MG	2T	204	1/1	0.96	0.06	58,58,58,58	0
58	MG	1A	3259	1/1	0.96	0.07	26,26,26,26	0
58	MG	2V	201	1/1	0.96	0.15	46,46,46,46	0
58	MG	1A	3136	1/1	0.96	0.09	48,48,48,48	0
58	MG	1A	3138	1/1	0.96	0.26	35,35,35,35	0
58	MG	2A	3594	1/1	0.96	0.09	52,52,52,52	0
58	MG	1a	1612	1/1	0.96	0.07	63,63,63,63	0
58	MG	2A	3287	1/1	0.96	0.08	55,55,55,55	0
58	MG	1A	3262	1/1	0.96	0.09	21,21,21,21	0
58	MG	1A	4040	1/1	0.96	0.05	38,38,38,38	0
58	MG	1a	1615	1/1	0.96	0.06	50,50,50,50	0
58	MG	2A	3015	1/1	0.96	0.09	41,41,41,41	0
58	MG	1A	4041	1/1	0.96	0.06	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	3018	1/1	0.96	0.12	49,49,49,49	0
58	MG	1A	3063	1/1	0.96	0.14	42,42,42,42	0
58	MG	1A	3336	1/1	0.96	0.20	46,46,46,46	0
58	MG	1A	3022	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3521	1/1	0.96	0.17	29,29,29,29	0
58	MG	1A	3201	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3428	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3011	1/1	0.96	0.09	38,38,38,38	0
58	MG	1A	3430	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3676	1/1	0.96	0.08	38,38,38,38	0
58	MG	2A	3616	1/1	0.96	0.14	53,53,53,53	0
58	MG	1A	3069	1/1	0.96	0.05	40,40,40,40	0
58	MG	2A	3618	1/1	0.96	0.07	23,23,23,23	0
58	MG	2A	3307	1/1	0.96	0.06	54,54,54,54	0
58	MG	1A	3860	1/1	0.96	0.08	15,15,15,15	0
58	MG	1A	3862	1/1	0.96	0.07	33,33,33,33	0
58	MG	2A	3310	1/1	0.96	0.19	42,42,42,42	0
58	MG	1A	3207	1/1	0.96	0.09	26,26,26,26	0
58	MG	1A	3864	1/1	0.96	0.28	39,39,39,39	0
58	MG	2A	3313	1/1	0.96	0.07	55,55,55,55	0
58	MG	1a	1636	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3434	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	3152	1/1	0.96	0.10	28,28,28,28	0
58	MG	1A	3001	1/1	0.96	0.06	32,32,32,32	0
58	MG	1A	3694	1/1	0.96	0.10	33,33,33,33	0
58	MG	1A	3533	1/1	0.96	0.07	56,56,56,56	0
58	MG	2A	3639	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3272	1/1	0.96	0.10	40,40,40,40	0
58	MG	2A	3641	1/1	0.96	0.06	30,30,30,30	0
58	MG	1A	3102	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3056	1/1	0.96	0.17	52,52,52,52	0
58	MG	2a	1629	1/1	0.96	0.18	62,62,62,62	0
58	MG	1A	4075	1/1	0.96	0.07	14,14,14,14	0
58	MG	1A	3874	1/1	0.96	0.10	32,32,32,32	0
58	MG	1a	1646	1/1	0.96	0.12	49,49,49,49	0
58	MG	1A	4077	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3327	1/1	0.96	0.16	47,47,47,47	0
58	MG	2A	3061	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3698	1/1	0.96	0.09	55,55,55,55	0
58	MG	1a	1650	1/1	0.96	0.06	42,42,42,42	0
58	MG	1A	3876	1/1	0.96	0.18	29,29,29,29	0
58	MG	1A	3699	1/1	0.96	0.10	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	3053	1/1	0.96	0.09	32,32,32,32	0
58	MG	2A	3335	1/1	0.96	0.12	51,51,51,51	0
58	MG	2A	3659	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3879	1/1	0.96	0.12	28,28,28,28	0
58	MG	1A	3880	1/1	0.96	0.21	28,28,28,28	0
58	MG	1a	1658	1/1	0.96	0.06	46,46,46,46	0
58	MG	2A	3072	1/1	0.96	0.05	46,46,46,46	0
58	MG	1A	3882	1/1	0.96	0.10	38,38,38,38	0
58	MG	1A	4087	1/1	0.96	0.05	17,17,17,17	0
58	MG	2A	3076	1/1	0.96	0.16	42,42,42,42	0
58	MG	2A	3667	1/1	0.96	0.09	51,51,51,51	0
58	MG	1A	3883	1/1	0.96	0.09	24,24,24,24	0
58	MG	1A	3217	1/1	0.96	0.05	44,44,44,44	0
58	MG	2A	3670	1/1	0.96	0.10	60,60,60,60	0
58	MG	2A	3671	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3541	1/1	0.96	0.17	38,38,38,38	0
58	MG	1A	3446	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3543	1/1	0.96	0.14	50,50,50,50	0
58	MG	1A	3281	1/1	0.96	0.06	36,36,36,36	0
58	MG	1A	3359	1/1	0.96	0.09	48,48,48,48	0
58	MG	2A	3086	1/1	0.96	0.05	44,44,44,44	0
58	MG	2a	1663	1/1	0.96	0.05	57,57,57,57	0
58	MG	2A	3087	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3449	1/1	0.96	0.12	33,33,33,33	0
58	MG	2A	3089	1/1	0.96	0.07	48,48,48,48	0
58	MG	1a	1669	1/1	0.96	0.17	53,53,53,53	0
58	MG	1A	3450	1/1	0.96	0.22	49,49,49,49	0
58	MG	1A	3293	1/1	0.96	0.07	37,37,37,37	0
58	MG	2a	1671	1/1	0.96	0.06	51,51,51,51	0
58	MG	1a	1672	1/1	0.96	0.18	48,48,48,48	0
58	MG	1A	4102	1/1	0.96	0.09	38,38,38,38	0
58	MG	2a	1674	1/1	0.96	0.13	39,39,39,39	0
58	MG	2a	1677	1/1	0.96	0.20	52,52,52,52	0
58	MG	2A	3689	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3896	1/1	0.96	0.07	12,12,12,12	0
58	MG	1A	3220	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3721	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	4108	1/1	0.96	0.14	43,43,43,43	0
58	MG	1A	3722	1/1	0.96	0.06	23,23,23,23	0
58	MG	1A	3362	1/1	0.96	0.14	33,33,33,33	0
58	MG	1A	3457	1/1	0.96	0.09	33,33,33,33	0
58	MG	2a	1687	1/1	0.96	0.16	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	1A	3083	1/1	0.96	0.11	44,44,44,44	0
58	MG	2a	1689	1/1	0.96	0.12	51,51,51,51	0
58	MG	2A	3700	1/1	0.96	0.09	30,30,30,30	0
58	MG	2a	1691	1/1	0.96	0.18	51,51,51,51	0
58	MG	1A	3109	1/1	0.96	0.18	39,39,39,39	0
58	MG	2a	1693	1/1	0.96	0.22	53,53,53,53	0
58	MG	1A	3906	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3223	1/1	0.96	0.09	38,38,38,38	0
58	MG	2A	3115	1/1	0.96	0.18	54,54,54,54	0
58	MG	1A	3224	1/1	0.96	0.08	31,31,31,31	0
58	MG	2a	1701	1/1	0.96	0.22	51,51,51,51	0
58	MG	1A	3114	1/1	0.96	0.12	32,32,32,32	0
58	MG	1A	3561	1/1	0.96	0.10	33,33,33,33	0
58	MG	1A	3369	1/1	0.96	0.07	52,52,52,52	0
58	MG	1A	3465	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3741	1/1	0.96	0.04	42,42,42,42	0
58	MG	2A	3382	1/1	0.96	0.33	52,52,52,52	0
58	MG	1B	219	1/1	0.96	0.09	41,41,41,41	0
58	MG	1A	3917	1/1	0.96	0.08	28,28,28,28	0
58	MG	1A	3742	1/1	0.96	0.07	26,26,26,26	0
58	MG	2A	3386	1/1	0.96	0.08	60,60,60,60	0
58	MG	2a	1713	1/1	0.96	0.07	64,64,64,64	0
58	MG	2a	1714	1/1	0.96	0.17	57,57,57,57	0
58	MG	1A	3115	1/1	0.96	0.12	37,37,37,37	0
58	MG	2A	3130	1/1	0.96	0.15	46,46,46,46	0
58	MG	1a	1697	1/1	0.96	0.32	54,54,54,54	0
58	MG	1A	3371	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3134	1/1	0.96	0.19	48,48,48,48	0
58	MG	1A	3119	1/1	0.96	0.15	27,27,27,27	0
58	MG	1A	3573	1/1	0.96	0.24	45,45,45,45	0
58	MG	2A	3731	1/1	0.96	0.09	55,55,55,55	0
58	MG	1A	3749	1/1	0.96	0.06	14,14,14,14	0
58	MG	2A	3736	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	3750	1/1	0.96	0.04	9,9,9,9	0
58	MG	1A	3374	1/1	0.96	0.09	45,45,45,45	0
58	MG	1A	3580	1/1	0.96	0.10	40,40,40,40	0
58	MG	1a	1706	1/1	0.96	0.15	44,44,44,44	0
58	MG	2a	1732	1/1	0.96	0.15	48,48,48,48	0
58	MG	1A	3582	1/1	0.96	0.16	44,44,44,44	0
58	MG	1A	3754	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3585	1/1	0.96	0.05	27,27,27,27	0
58	MG	1A	3236	1/1	0.96	0.07	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	3937	1/1	0.96	0.04	32,32,32,32	0
58	MG	1A	3591	1/1	0.96	0.11	40,40,40,40	0
58	MG	1a	1714	1/1	0.96	0.24	52,52,52,52	0
58	MG	1A	3941	1/1	0.96	0.07	26,26,26,26	0
58	MG	1D	303	1/1	0.96	0.21	44,44,44,44	0
58	MG	1A	3379	1/1	0.96	0.08	47,47,47,47	0
58	MG	1D	310	1/1	0.96	0.07	37,37,37,37	0
58	MG	2A	3415	1/1	0.96	0.23	42,42,42,42	0
58	MG	1a	1723	1/1	0.96	0.07	52,52,52,52	0
58	MG	1A	3380	1/1	0.96	0.23	46,46,46,46	0
58	MG	1A	3947	1/1	0.96	0.04	15,15,15,15	0
58	MG	1A	3595	1/1	0.96	0.09	46,46,46,46	0
58	MG	1a	1727	1/1	0.96	0.04	39,39,39,39	0
58	MG	2a	1752	1/1	0.96	0.06	55,55,55,55	0
58	MG	1A	3596	1/1	0.96	0.27	42,42,42,42	0
58	MG	1A	3306	1/1	0.96	0.08	25,25,25,25	0
58	MG	1A	3768	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3954	1/1	0.96	0.08	64,64,64,64	0
58	MG	1E	310	1/1	0.96	0.07	21,21,21,21	0
58	MG	1A	3769	1/1	0.96	0.05	20,20,20,20	0
58	MG	2A	3766	1/1	0.96	0.08	57,57,57,57	0
58	MG	1A	3771	1/1	0.96	0.07	23,23,23,23	0
58	MG	1E	314	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3055	1/1	0.96	0.08	40,40,40,40	0
58	MG	1F	307	1/1	0.96	0.08	20,20,20,20	0
58	MG	1F	309	1/1	0.96	0.06	41,41,41,41	0
58	MG	2a	1772	1/1	0.96	0.09	41,41,41,41	0
58	MG	1A	3958	1/1	0.96	0.06	44,44,44,44	0
58	MG	2a	1774	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3384	1/1	0.96	0.07	49,49,49,49	0
58	MG	2a	1776	1/1	0.96	0.09	57,57,57,57	0
58	MG	2A	3438	1/1	0.96	0.12	47,47,47,47	0
58	MG	2A	3439	1/1	0.96	0.18	55,55,55,55	0
58	MG	1A	3774	1/1	0.96	0.08	19,19,19,19	0
58	MG	1A	3385	1/1	0.96	0.15	31,31,31,31	0
58	MG	2A	3783	1/1	0.96	0.06	56,56,56,56	0
58	MG	2A	3442	1/1	0.96	0.18	42,42,42,42	0
58	MG	2a	1783	1/1	0.96	0.09	41,41,41,41	0
58	MG	1a	1753	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3776	1/1	0.96	0.06	14,14,14,14	0
58	MG	1A	3247	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	3088	1/1	0.96	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3388	1/1	0.96	0.05	33,33,33,33	0
58	MG	1A	3389	1/1	0.96	0.19	22,22,22,22	0
58	MG	1O	202	1/1	0.96	0.24	44,44,44,44	0
58	MG	1O	203	1/1	0.96	0.11	42,42,42,42	0
58	MG	2A	3453	1/1	0.96	0.20	41,41,41,41	0
58	MG	1A	3975	1/1	0.96	0.08	47,47,47,47	0
58	MG	2A	3456	1/1	0.96	0.22	42,42,42,42	0
58	MG	2A	3457	1/1	0.96	0.28	54,54,54,54	0
58	MG	1A	3976	1/1	0.96	0.12	41,41,41,41	0
58	MG	2A	3459	1/1	0.96	0.08	34,34,34,34	0
58	MG	2a	1800	1/1	0.96	0.07	52,52,52,52	0
58	MG	1a	1765	1/1	0.96	0.06	68,68,68,68	0
58	MG	1A	3788	1/1	0.96	0.05	22,22,22,22	0
58	MG	1A	3789	1/1	0.96	0.06	66,66,66,66	0
58	MG	1A	3002	1/1	0.96	0.07	46,46,46,46	0
58	MG	2A	3808	1/1	0.96	0.07	57,57,57,57	0
58	MG	2A	3203	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3980	1/1	0.96	0.11	59,59,59,59	0
58	MG	1Q	206	1/1	0.96	0.10	33,33,33,33	0
58	MG	2A	3470	1/1	0.96	0.12	45,45,45,45	0
58	MG	1A	3608	1/1	0.96	0.07	39,39,39,39	0
58	MG	1A	3610	1/1	0.96	0.05	27,27,27,27	0
58	MG	2A	3475	1/1	0.96	0.09	53,53,53,53	0
58	MG	1A	3391	1/1	0.96	0.06	37,37,37,37	0
58	MG	1a	1776	1/1	0.96	0.07	40,40,40,40	0
58	MG	1S	202	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3822	1/1	0.96	0.06	60,60,60,60	0
58	MG	2A	3479	1/1	0.96	0.20	45,45,45,45	0
58	MG	2A	3824	1/1	0.96	0.07	26,26,26,26	0
58	MG	1a	1778	1/1	0.96	0.07	53,53,53,53	0
58	MG	2a	1821	1/1	0.96	0.09	57,57,57,57	0
58	MG	2A	3828	1/1	0.96	0.05	38,38,38,38	0
58	MG	2A	3829	1/1	0.96	0.08	30,30,30,30	0
58	MG	2A	3830	1/1	0.96	0.07	33,33,33,33	0
58	MG	1A	3800	1/1	0.96	0.05	16,16,16,16	0
58	MG	1A	3490	1/1	0.96	0.10	34,34,34,34	0
58	MG	2A	3837	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	3393	1/1	0.96	0.13	58,58,58,58	0
58	MG	1a	1785	1/1	0.96	0.07	53,53,53,53	0
58	MG	2a	1830	1/1	0.96	0.13	42,42,42,42	0
58	MG	1A	3492	1/1	0.96	0.12	50,50,50,50	0
58	MG	1U	203	1/1	0.96	0.10	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	1U	204	1/1	0.96	0.13	28,28,28,28	0
58	MG	1A	3620	1/1	0.96	0.08	38,38,38,38	0
58	MG	2A	3492	1/1	0.96	0.06	35,35,35,35	0
58	MG	2a	1836	1/1	0.96	0.08	55,55,55,55	0
58	MG	2A	3848	1/1	0.96	0.06	51,51,51,51	0
58	MG	1a	1793	1/1	0.96	0.06	71,71,71,71	0
58	MG	1A	3623	1/1	0.96	0.11	10,10,10,10	0
58	MG	2a	1840	1/1	0.96	0.07	71,71,71,71	0
58	MG	1A	3059	1/1	0.96	0.05	29,29,29,29	0
58	MG	1V	203	1/1	0.96	0.18	27,27,27,27	0
58	MG	1A	3628	1/1	0.96	0.06	31,31,31,31	0
58	MG	2g	201	1/1	0.96	0.12	56,56,56,56	0
58	MG	2A	3854	1/1	0.96	0.05	49,49,49,49	0
58	MG	2A	3231	1/1	0.96	0.12	42,42,42,42	0
58	MG	2l	203	1/1	0.96	0.08	52,52,52,52	0
58	MG	1A	3401	1/1	0.96	0.08	53,53,53,53	0
58	MG	2A	3857	1/1	0.96	0.07	33,33,33,33	0
58	MG	2A	3858	1/1	0.96	0.07	52,52,52,52	0
58	MG	2A	3504	1/1	0.96	0.06	43,43,43,43	0
58	MG	2A	3862	1/1	0.96	0.07	42,42,42,42	0
58	MG	2A	3863	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3812	1/1	0.96	0.21	16,16,16,16	0
58	MG	1a	1803	1/1	0.96	0.06	53,53,53,53	0
58	MG	1W	205	1/1	0.96	0.14	38,38,38,38	0
58	MG	1a	1806	1/1	0.96	0.18	41,41,41,41	0
58	MG	1W	206	1/1	0.96	0.15	24,24,24,24	0
58	MG	1A	3495	1/1	0.96	0.07	42,42,42,42	0
58	MG	1Y	201	1/1	0.96	0.12	41,41,41,41	0
58	MG	1A	3130	1/1	0.96	0.07	44,44,44,44	0
58	MG	1a	1811	1/1	0.96	0.12	50,50,50,50	0
58	MG	2A	3875	1/1	0.96	0.11	50,50,50,50	0
58	MG	2A	3518	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3317	1/1	0.96	0.17	53,53,53,53	0
58	MG	2A	3878	1/1	0.96	0.13	50,50,50,50	0
58	MG	1A	3254	1/1	0.96	0.17	34,34,34,34	0
58	MG	2A	3523	1/1	0.96	0.11	52,52,52,52	0
58	MG	2w	111	1/1	0.96	0.07	53,53,53,53	0
58	MG	2A	3524	1/1	0.96	0.11	50,50,50,50	0
58	MG	2A	3525	1/1	0.96	0.11	44,44,44,44	0
58	MG	1A	3642	1/1	0.96	0.04	15,15,15,15	0
58	MG	10	101	1/1	0.96	0.13	39,39,39,39	0
58	MG	1A	4004	1/1	0.96	0.07	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	10	105	1/1	0.96	0.17	53,53,53,53	0
58	MG	1A	3643	1/1	0.96	0.07	42,42,42,42	0
58	MG	2A	3535	1/1	0.96	0.06	29,29,29,29	0
58	MG	1e	202	1/1	0.96	0.19	56,56,56,56	0
58	MG	2B	209	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3538	1/1	0.96	0.04	26,26,26,26	0
58	MG	1A	3822	1/1	0.96	0.18	25,25,25,25	0
58	MG	1A	3823	1/1	0.96	0.08	34,34,34,34	0
58	MG	1A	3824	1/1	0.96	0.07	23,23,23,23	0
58	MG	1A	4012	1/1	0.96	0.04	24,24,24,24	0
58	MG	1n	101	1/1	0.96	0.06	33,33,33,33	0
58	MG	2A	3880	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3227	1/1	0.97	0.11	41,41,41,41	0
58	MG	1A	3636	1/1	0.97	0.04	31,31,31,31	0
58	MG	2A	3216	1/1	0.97	0.09	38,38,38,38	0
58	MG	1A	3228	1/1	0.97	0.06	34,34,34,34	0
58	MG	2A	3517	1/1	0.97	0.11	32,32,32,32	0
58	MG	2B	203	1/1	0.97	0.08	56,56,56,56	0
58	MG	2A	3218	1/1	0.97	0.09	38,38,38,38	0
58	MG	1a	1783	1/1	0.97	0.06	45,45,45,45	0
58	MG	1U	206	1/1	0.97	0.12	39,39,39,39	0
58	MG	2A	3521	1/1	0.97	0.08	33,33,33,33	0
58	MG	1U	207	1/1	0.97	0.16	30,30,30,30	0
58	MG	2A	3222	1/1	0.97	0.16	41,41,41,41	0
58	MG	1A	3394	1/1	0.97	0.17	49,49,49,49	0
58	MG	1A	3815	1/1	0.97	0.05	28,28,28,28	0
58	MG	1A	3997	1/1	0.97	0.06	41,41,41,41	0
58	MG	1a	1792	1/1	0.97	0.04	56,56,56,56	0
58	MG	2B	215	1/1	0.97	0.14	49,49,49,49	0
58	MG	2A	3530	1/1	0.97	0.06	49,49,49,49	0
58	MG	2A	3531	1/1	0.97	0.06	26,26,26,26	0
58	MG	1V	204	1/1	0.97	0.30	37,37,37,37	0
58	MG	2A	3229	1/1	0.97	0.11	44,44,44,44	0
58	MG	1V	207	1/1	0.97	0.07	33,33,33,33	0
58	MG	1A	3641	1/1	0.97	0.07	29,29,29,29	0
58	MG	1A	3396	1/1	0.97	0.22	35,35,35,35	0
58	MG	2A	3233	1/1	0.97	0.13	36,36,36,36	0
58	MG	1A	3397	1/1	0.97	0.07	21,21,21,21	0
58	MG	1a	1799	1/1	0.97	0.04	63,63,63,63	0
58	MG	1A	3398	1/1	0.97	0.06	42,42,42,42	0
58	MG	1a	1801	1/1	0.97	0.05	57,57,57,57	0
58	MG	1A	3229	1/1	0.97	0.11	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	2A	3545	1/1	0.97	0.04	38,38,38,38	0
58	MG	2A	3239	1/1	0.97	0.05	37,37,37,37	0
58	MG	1X	104	1/1	0.97	0.14	35,35,35,35	0
58	MG	2A	3241	1/1	0.97	0.17	42,42,42,42	0
58	MG	2A	3549	1/1	0.97	0.04	46,46,46,46	0
58	MG	1X	105	1/1	0.97	0.05	36,36,36,36	0
58	MG	1A	3499	1/1	0.97	0.13	44,44,44,44	0
58	MG	1A	3312	1/1	0.97	0.10	46,46,46,46	0
58	MG	1A	3825	1/1	0.97	0.04	18,18,18,18	0
58	MG	2F	307	1/1	0.97	0.14	39,39,39,39	0
58	MG	2A	3556	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3826	1/1	0.97	0.04	27,27,27,27	0
58	MG	1A	3231	1/1	0.97	0.13	25,25,25,25	0
58	MG	1A	3651	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3829	1/1	0.97	0.04	29,29,29,29	0
58	MG	2A	3565	1/1	0.97	0.07	26,26,26,26	0
58	MG	2A	3566	1/1	0.97	0.11	35,35,35,35	0
58	MG	1A	4016	1/1	0.97	0.06	16,16,16,16	0
58	MG	2A	3571	1/1	0.97	0.04	34,34,34,34	0
58	MG	2A	3573	1/1	0.97	0.08	30,30,30,30	0
58	MG	10	103	1/1	0.97	0.05	33,33,33,33	0
58	MG	10	104	1/1	0.97	0.14	28,28,28,28	0
58	MG	1a	1816	1/1	0.97	0.14	38,38,38,38	0
58	MG	1A	3403	1/1	0.97	0.20	52,52,52,52	0
58	MG	1A	3033	1/1	0.97	0.18	23,23,23,23	0
58	MG	10	107	1/1	0.97	0.05	35,35,35,35	0
58	MG	1A	3654	1/1	0.97	0.04	26,26,26,26	0
58	MG	1f	201	1/1	0.97	0.13	46,46,46,46	0
58	MG	2A	3583	1/1	0.97	0.08	32,32,32,32	0
58	MG	1A	3505	1/1	0.97	0.11	26,26,26,26	0
58	MG	1A	3024	1/1	0.97	0.11	36,36,36,36	0
58	MG	1A	3118	1/1	0.97	0.20	42,42,42,42	0
58	MG	2A	3263	1/1	0.97	0.06	53,53,53,53	0
58	MG	25	103	1/1	0.97	0.05	41,41,41,41	0
58	MG	11	103	1/1	0.97	0.04	28,28,28,28	0
58	MG	1A	3836	1/1	0.97	0.07	49,49,49,49	0
58	MG	1A	3659	1/1	0.97	0.04	30,30,30,30	0
58	MG	2A	3592	1/1	0.97	0.08	52,52,52,52	0
58	MG	1A	4028	1/1	0.97	0.08	56,56,56,56	0
58	MG	2A	3595	1/1	0.97	0.06	53,53,53,53	0
58	MG	2a	1601	1/1	0.97	0.05	47,47,47,47	0
58	MG	1v	102	1/1	0.97	0.06	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	2A	3269	1/1	0.97	0.07	47,47,47,47	0
58	MG	1A	3237	1/1	0.97	0.11	33,33,33,33	0
58	MG	1w	103	1/1	0.97	0.10	37,37,37,37	0
58	MG	2A	3602	1/1	0.97	0.07	52,52,52,52	0
58	MG	1A	3238	1/1	0.97	0.05	51,51,51,51	0
58	MG	15	103	1/1	0.97	0.14	33,33,33,33	0
58	MG	15	104	1/1	0.97	0.14	28,28,28,28	0
58	MG	2A	3275	1/1	0.97	0.05	51,51,51,51	0
58	MG	1A	3239	1/1	0.97	0.20	25,25,25,25	0
58	MG	1A	3240	1/1	0.97	0.09	23,23,23,23	0
58	MG	1A	3241	1/1	0.97	0.07	37,37,37,37	0
58	MG	1x	102	1/1	0.97	0.11	48,48,48,48	0
58	MG	1A	3323	1/1	0.97	0.12	29,29,29,29	0
58	MG	1A	3667	1/1	0.97	0.03	14,14,14,14	0
58	MG	2A	3282	1/1	0.97	0.12	52,52,52,52	0
58	MG	1A	3516	1/1	0.97	0.11	16,16,16,16	0
58	MG	1A	3414	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3242	1/1	0.97	0.10	26,26,26,26	0
58	MG	1A	3061	1/1	0.97	0.06	28,28,28,28	0
58	MG	1A	3673	1/1	0.97	0.05	19,19,19,19	0
58	MG	1x	111	1/1	0.97	0.10	49,49,49,49	0
58	MG	1x	112	1/1	0.97	0.12	49,49,49,49	0
58	MG	2a	1625	1/1	0.97	0.06	46,46,46,46	0
58	MG	2A	3290	1/1	0.97	0.09	45,45,45,45	0
58	MG	1A	3327	1/1	0.97	0.08	41,41,41,41	0
58	MG	2A	3623	1/1	0.97	0.10	33,33,33,33	0
58	MG	1a	1605	1/1	0.97	0.08	43,43,43,43	0
58	MG	1z	101	1/1	0.97	0.06	59,59,59,59	0
58	MG	2a	1631	1/1	0.97	0.09	66,66,66,66	0
58	MG	1A	3328	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3002	1/1	0.97	0.22	44,44,44,44	0
58	MG	2A	3628	1/1	0.97	0.06	30,30,30,30	0
58	MG	1a	1608	1/1	0.97	0.14	40,40,40,40	0
58	MG	2A	3297	1/1	0.97	0.09	45,45,45,45	0
58	MG	2A	3004	1/1	0.97	0.20	48,48,48,48	0
58	MG	1A	3121	1/1	0.97	0.14	41,41,41,41	0
58	MG	2A	3635	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3856	1/1	0.97	0.09	18,18,18,18	0
58	MG	2a	1641	1/1	0.97	0.10	50,50,50,50	0
58	MG	2A	3638	1/1	0.97	0.11	49,49,49,49	0
58	MG	1A	3857	1/1	0.97	0.10	46,46,46,46	0
58	MG	1A	3678	1/1	0.97	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	4051	1/1	0.97	0.04	29,29,29,29	0
58	MG	2A	3642	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3680	1/1	0.97	0.04	15,15,15,15	0
58	MG	1A	4053	1/1	0.97	0.04	34,34,34,34	0
58	MG	1a	1617	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3681	1/1	0.97	0.03	22,22,22,22	0
58	MG	1A	3861	1/1	0.97	0.08	20,20,20,20	0
58	MG	1a	1620	1/1	0.97	0.04	36,36,36,36	0
58	MG	1A	3330	1/1	0.97	0.09	30,30,30,30	0
58	MG	1A	3525	1/1	0.97	0.13	26,26,26,26	0
58	MG	1A	3091	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	3688	1/1	0.97	0.06	15,15,15,15	0
58	MG	2A	3028	1/1	0.97	0.28	46,46,46,46	0
58	MG	2A	3655	1/1	0.97	0.10	40,40,40,40	0
58	MG	1A	3123	1/1	0.97	0.12	44,44,44,44	0
58	MG	1A	3528	1/1	0.97	0.05	39,39,39,39	0
58	MG	1A	3423	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3424	1/1	0.97	0.07	48,48,48,48	0
58	MG	2A	3035	1/1	0.97	0.08	30,30,30,30	0
58	MG	1A	4071	1/1	0.97	0.04	14,14,14,14	0
58	MG	1a	1630	1/1	0.97	0.13	53,53,53,53	0
58	MG	1A	3040	1/1	0.97	0.11	28,28,28,28	0
58	MG	2A	3040	1/1	0.97	0.05	44,44,44,44	0
58	MG	1a	1632	1/1	0.97	0.19	55,55,55,55	0
58	MG	2a	1669	1/1	0.97	0.12	38,38,38,38	0
58	MG	1a	1633	1/1	0.97	0.15	29,29,29,29	0
58	MG	1A	3872	1/1	0.97	0.07	37,37,37,37	0
58	MG	2A	3044	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3426	1/1	0.97	0.14	49,49,49,49	0
58	MG	2A	3046	1/1	0.97	0.10	42,42,42,42	0
58	MG	2A	3047	1/1	0.97	0.26	54,54,54,54	0
58	MG	2a	1678	1/1	0.97	0.05	41,41,41,41	0
58	MG	1A	3427	1/1	0.97	0.16	43,43,43,43	0
58	MG	2A	3049	1/1	0.97	0.13	21,21,21,21	0
58	MG	1A	3020	1/1	0.97	0.15	49,49,49,49	0
58	MG	1A	3700	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3676	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3535	1/1	0.97	0.07	49,49,49,49	0
58	MG	1A	3704	1/1	0.97	0.05	12,12,12,12	0
58	MG	2A	3339	1/1	0.97	0.11	55,55,55,55	0
58	MG	1A	3064	1/1	0.97	0.12	39,39,39,39	0
58	MG	2A	3055	1/1	0.97	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3706	1/1	0.97	0.07	25,25,25,25	0
58	MG	1A	4084	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3881	1/1	0.97	0.25	36,36,36,36	0
58	MG	1A	3337	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3538	1/1	0.97	0.13	32,32,32,32	0
58	MG	2a	1694	1/1	0.97	0.19	52,52,52,52	0
58	MG	2a	1695	1/1	0.97	0.12	42,42,42,42	0
58	MG	2A	3688	1/1	0.97	0.09	36,36,36,36	0
58	MG	1A	3884	1/1	0.97	0.10	24,24,24,24	0
58	MG	1A	3048	1/1	0.97	0.10	34,34,34,34	0
58	MG	2a	1699	1/1	0.97	0.13	31,31,31,31	0
58	MG	2A	3691	1/1	0.97	0.10	42,42,42,42	0
58	MG	2A	3063	1/1	0.97	0.06	58,58,58,58	0
58	MG	1a	1649	1/1	0.97	0.18	53,53,53,53	0
58	MG	1A	4092	1/1	0.97	0.10	43,43,43,43	0
58	MG	2A	3695	1/1	0.97	0.13	51,51,51,51	0
58	MG	1a	1652	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3026	1/1	0.97	0.12	31,31,31,31	0
58	MG	1A	3433	1/1	0.97	0.15	42,42,42,42	0
58	MG	1A	3341	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3435	1/1	0.97	0.09	38,38,38,38	0
58	MG	1A	3545	1/1	0.97	0.23	45,45,45,45	0
58	MG	2A	3702	1/1	0.97	0.06	55,55,55,55	0
58	MG	2a	1712	1/1	0.97	0.05	45,45,45,45	0
58	MG	1A	3436	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3437	1/1	0.97	0.07	41,41,41,41	0
58	MG	2A	3362	1/1	0.97	0.08	57,57,57,57	0
58	MG	2A	3075	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3187	1/1	0.97	0.07	32,32,32,32	0
58	MG	1A	3343	1/1	0.97	0.07	48,48,48,48	0
58	MG	1A	3725	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	4105	1/1	0.97	0.07	48,48,48,48	0
58	MG	1A	3188	1/1	0.97	0.10	32,32,32,32	0
58	MG	1A	3021	1/1	0.97	0.07	20,20,20,20	0
58	MG	2A	3714	1/1	0.97	0.09	45,45,45,45	0
58	MG	1A	3051	1/1	0.97	0.09	24,24,24,24	0
58	MG	2a	1726	1/1	0.97	0.16	43,43,43,43	0
58	MG	1B	202	1/1	0.97	0.16	48,48,48,48	0
58	MG	2A	3717	1/1	0.97	0.12	44,44,44,44	0
58	MG	1A	3730	1/1	0.97	0.05	38,38,38,38	0
58	MG	1A	3192	1/1	0.97	0.11	28,28,28,28	0
58	MG	2a	1731	1/1	0.97	0.12	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	1A	3904	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3445	1/1	0.97	0.17	40,40,40,40	0
58	MG	1A	3075	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	3195	1/1	0.97	0.23	38,38,38,38	0
58	MG	1A	3736	1/1	0.97	0.07	21,21,21,21	0
58	MG	1B	211	1/1	0.97	0.09	40,40,40,40	0
58	MG	2A	3095	1/1	0.97	0.07	39,39,39,39	0
58	MG	2A	3729	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3909	1/1	0.97	0.07	41,41,41,41	0
58	MG	2A	3733	1/1	0.97	0.06	31,31,31,31	0
58	MG	1A	3139	1/1	0.97	0.06	34,34,34,34	0
58	MG	2A	3099	1/1	0.97	0.06	42,42,42,42	0
58	MG	1A	3911	1/1	0.97	0.23	15,15,15,15	0
58	MG	1A	3353	1/1	0.97	0.19	28,28,28,28	0
58	MG	1A	3740	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3388	1/1	0.97	0.29	60,60,60,60	0
58	MG	1A	3563	1/1	0.97	0.07	47,47,47,47	0
58	MG	1A	3199	1/1	0.97	0.05	32,32,32,32	0
58	MG	2A	3108	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3567	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3357	1/1	0.97	0.17	48,48,48,48	0
58	MG	2A	3111	1/1	0.97	0.16	39,39,39,39	0
58	MG	1A	3452	1/1	0.97	0.13	29,29,29,29	0
58	MG	1A	3454	1/1	0.97	0.15	35,35,35,35	0
58	MG	2a	1758	1/1	0.97	0.04	61,61,61,61	0
58	MG	2a	1759	1/1	0.97	0.08	62,62,62,62	0
58	MG	1A	3200	1/1	0.97	0.09	31,31,31,31	0
58	MG	1a	1689	1/1	0.97	0.20	44,44,44,44	0
58	MG	2a	1763	1/1	0.97	0.06	60,60,60,60	0
58	MG	2A	3116	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	3140	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3202	1/1	0.97	0.11	18,18,18,18	0
58	MG	2A	3402	1/1	0.97	0.06	54,54,54,54	0
58	MG	2A	3120	1/1	0.97	0.08	33,33,33,33	0
58	MG	1A	3203	1/1	0.97	0.08	37,37,37,37	0
58	MG	1A	3143	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3363	1/1	0.97	0.05	39,39,39,39	0
58	MG	1A	3587	1/1	0.97	0.12	35,35,35,35	0
58	MG	2A	3761	1/1	0.97	0.06	45,45,45,45	0
58	MG	2A	3408	1/1	0.97	0.15	41,41,41,41	0
58	MG	1A	3077	1/1	0.97	0.17	41,41,41,41	0
58	MG	1A	3274	1/1	0.97	0.21	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	3412	1/1	0.97	0.09	34,34,34,34	0
58	MG	1A	3934	1/1	0.97	0.05	29,29,29,29	0
58	MG	2A	3128	1/1	0.97	0.05	45,45,45,45	0
58	MG	2A	3768	1/1	0.97	0.05	47,47,47,47	0
58	MG	1a	1699	1/1	0.97	0.16	41,41,41,41	0
58	MG	1A	3759	1/1	0.97	0.05	17,17,17,17	0
58	MG	1B	237	1/1	0.97	0.08	44,44,44,44	0
58	MG	1A	3760	1/1	0.97	0.05	23,23,23,23	0
58	MG	1A	3938	1/1	0.97	0.06	57,57,57,57	0
58	MG	2a	1789	1/1	0.97	0.20	51,51,51,51	0
58	MG	2A	3776	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3463	1/1	0.97	0.17	39,39,39,39	0
58	MG	1A	3104	1/1	0.97	0.09	27,27,27,27	0
58	MG	1D	306	1/1	0.97	0.06	31,31,31,31	0
58	MG	2A	3780	1/1	0.97	0.05	54,54,54,54	0
58	MG	1D	307	1/1	0.97	0.06	28,28,28,28	0
58	MG	2A	3425	1/1	0.97	0.09	40,40,40,40	0
58	MG	2a	1797	1/1	0.97	0.14	43,43,43,43	0
58	MG	1D	308	1/1	0.97	0.12	30,30,30,30	0
58	MG	1A	3148	1/1	0.97	0.04	27,27,27,27	0
58	MG	2A	3428	1/1	0.97	0.29	54,54,54,54	0
58	MG	2A	3787	1/1	0.97	0.05	65,65,65,65	0
58	MG	1A	3944	1/1	0.97	0.04	53,53,53,53	0
58	MG	2A	3790	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3764	1/1	0.97	0.09	14,14,14,14	0
58	MG	1A	3946	1/1	0.97	0.06	38,38,38,38	0
58	MG	2A	3148	1/1	0.97	0.13	28,28,28,28	0
58	MG	2A	3150	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3012	1/1	0.97	0.05	21,21,21,21	0
58	MG	1a	1715	1/1	0.97	0.16	40,40,40,40	0
58	MG	2A	3436	1/1	0.97	0.22	53,53,53,53	0
58	MG	1A	3287	1/1	0.97	0.20	27,27,27,27	0
58	MG	1A	3289	1/1	0.97	0.11	34,34,34,34	0
58	MG	1A	3951	1/1	0.97	0.05	49,49,49,49	0
58	MG	1A	3291	1/1	0.97	0.14	31,31,31,31	0
58	MG	2A	3158	1/1	0.97	0.05	42,42,42,42	0
58	MG	1a	1722	1/1	0.97	0.06	45,45,45,45	0
58	MG	1A	3472	1/1	0.97	0.07	28,28,28,28	0
58	MG	2A	3805	1/1	0.97	0.10	35,35,35,35	0
58	MG	1A	3372	1/1	0.97	0.26	33,33,33,33	0
58	MG	1A	3474	1/1	0.97	0.18	37,37,37,37	0
58	MG	2A	3446	1/1	0.97	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	1F	302	1/1	0.97	0.15	24,24,24,24	0
58	MG	2A	3164	1/1	0.97	0.04	33,33,33,33	0
58	MG	1F	303	1/1	0.97	0.11	25,25,25,25	0
58	MG	1a	1729	1/1	0.97	0.10	27,27,27,27	0
58	MG	1a	1730	1/1	0.97	0.09	32,32,32,32	0
58	MG	1A	3292	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3454	1/1	0.97	0.22	44,44,44,44	0
58	MG	1A	3108	1/1	0.97	0.04	24,24,24,24	0
58	MG	2A	3818	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3030	1/1	0.97	0.05	27,27,27,27	0
58	MG	1a	1734	1/1	0.97	0.05	53,53,53,53	0
58	MG	2A	3821	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3295	1/1	0.97	0.07	53,53,53,53	0
58	MG	1A	3960	1/1	0.97	0.10	51,51,51,51	0
58	MG	1F	312	1/1	0.97	0.09	42,42,42,42	0
58	MG	1G	201	1/1	0.97	0.10	34,34,34,34	0
58	MG	2A	3827	1/1	0.97	0.06	25,25,25,25	0
58	MG	1A	3778	1/1	0.97	0.04	14,14,14,14	0
58	MG	1A	3963	1/1	0.97	0.04	44,44,44,44	0
58	MG	2d	302	1/1	0.97	0.07	65,65,65,65	0
58	MG	2A	3464	1/1	0.97	0.13	43,43,43,43	0
58	MG	2f	201	1/1	0.97	0.11	42,42,42,42	0
58	MG	1A	3296	1/1	0.97	0.17	22,22,22,22	0
58	MG	2A	3833	1/1	0.97	0.10	33,33,33,33	0
58	MG	1A	3781	1/1	0.97	0.05	54,54,54,54	0
58	MG	1I	201	1/1	0.97	0.05	62,62,62,62	0
58	MG	1A	3782	1/1	0.97	0.07	39,39,39,39	0
58	MG	2A	3839	1/1	0.97	0.06	58,58,58,58	0
58	MG	2A	3184	1/1	0.97	0.13	35,35,35,35	0
58	MG	1N	203	1/1	0.97	0.04	36,36,36,36	0
58	MG	1A	3969	1/1	0.97	0.05	30,30,30,30	0
58	MG	1A	3970	1/1	0.97	0.09	20,20,20,20	0
58	MG	2A	3188	1/1	0.97	0.05	43,43,43,43	0
58	MG	1A	3215	1/1	0.97	0.03	34,34,34,34	0
58	MG	1A	3612	1/1	0.97	0.06	22,22,22,22	0
58	MG	1A	3481	1/1	0.97	0.10	58,58,58,58	0
58	MG	1A	3216	1/1	0.97	0.13	34,34,34,34	0
58	MG	1A	3110	1/1	0.97	0.20	32,32,32,32	0
58	MG	1P	204	1/1	0.97	0.08	38,38,38,38	0
58	MG	1A	3618	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3794	1/1	0.97	0.05	16,16,16,16	0
58	MG	2A	3197	1/1	0.97	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	2A	3198	1/1	0.97	0.14	50,50,50,50	0
58	MG	2A	3490	1/1	0.97	0.09	49,49,49,49	0
58	MG	1A	3619	1/1	0.97	0.06	35,35,35,35	0
58	MG	2w	107	1/1	0.97	0.13	57,57,57,57	0
58	MG	1A	3154	1/1	0.97	0.09	28,28,28,28	0
58	MG	2A	3861	1/1	0.97	0.10	49,49,49,49	0
58	MG	1A	3622	1/1	0.97	0.05	29,29,29,29	0
58	MG	1A	3111	1/1	0.97	0.15	27,27,27,27	0
58	MG	1R	203	1/1	0.97	0.12	27,27,27,27	0
58	MG	1A	3157	1/1	0.97	0.19	28,28,28,28	0
58	MG	2A	3866	1/1	0.97	0.08	39,39,39,39	0
58	MG	2A	3867	1/1	0.97	0.05	53,53,53,53	0
58	MG	1S	201	1/1	0.97	0.22	40,40,40,40	0
58	MG	1A	3112	1/1	0.97	0.04	37,37,37,37	0
58	MG	2A	3501	1/1	0.97	0.10	33,33,33,33	0
58	MG	2A	3502	1/1	0.97	0.13	36,36,36,36	0
58	MG	2x	108	1/1	0.97	0.08	51,51,51,51	0
58	MG	1A	3163	1/1	0.97	0.25	28,28,28,28	0
58	MG	1a	1774	1/1	0.97	0.06	56,56,56,56	0
58	MG	1A	3631	1/1	0.97	0.07	44,44,44,44	0
58	MG	2A	3210	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3113	1/1	0.97	0.08	26,26,26,26	0
58	MG	2A	3510	1/1	0.97	0.05	28,28,28,28	0
58	MG	1A	3634	1/1	0.97	0.05	48,48,48,48	0
58	MG	1U	202	1/1	0.97	0.13	42,42,42,42	0
58	MG	23	101	1/1	0.98	0.07	43,43,43,43	0
58	MG	1A	4025	1/1	0.98	0.07	40,40,40,40	0
58	MG	1A	3117	1/1	0.98	0.16	31,31,31,31	0
58	MG	1U	201	1/1	0.98	0.13	23,23,23,23	0
58	MG	1a	1743	1/1	0.98	0.07	44,44,44,44	0
58	MG	2A	3133	1/1	0.98	0.04	35,35,35,35	0
58	MG	27	101	1/1	0.98	0.17	40,40,40,40	0
58	MG	27	102	1/1	0.98	0.07	40,40,40,40	0
58	MG	1A	3724	1/1	0.98	0.06	34,34,34,34	0
58	MG	2A	3135	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3206	1/1	0.98	0.03	12,12,12,12	0
58	MG	1a	1746	1/1	0.98	0.12	40,40,40,40	0
58	MG	2A	3138	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3032	1/1	0.98	0.06	28,28,28,28	0
58	MG	2A	3140	1/1	0.98	0.12	33,33,33,33	0
58	MG	1A	3727	1/1	0.98	0.06	19,19,19,19	0
58	MG	1A	3017	1/1	0.98	0.05	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	2A	3143	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3334	1/1	0.98	0.05	33,33,33,33	0
58	MG	1a	1752	1/1	0.98	0.05	49,49,49,49	0
58	MG	1U	209	1/1	0.98	0.15	26,26,26,26	0
58	MG	1U	210	1/1	0.98	0.16	22,22,22,22	0
58	MG	1A	3600	1/1	0.98	0.14	27,27,27,27	0
58	MG	2A	3149	1/1	0.98	0.03	26,26,26,26	0
58	MG	1V	201	1/1	0.98	0.09	25,25,25,25	0
58	MG	1A	3209	1/1	0.98	0.09	39,39,39,39	0
58	MG	1A	3158	1/1	0.98	0.07	36,36,36,36	0
58	MG	1A	4037	1/1	0.98	0.04	44,44,44,44	0
58	MG	1a	1760	1/1	0.98	0.04	49,49,49,49	0
58	MG	2A	3681	1/1	0.98	0.11	40,40,40,40	0
58	MG	1V	206	1/1	0.98	0.12	40,40,40,40	0
58	MG	1A	3018	1/1	0.98	0.08	24,24,24,24	0
58	MG	2A	3157	1/1	0.98	0.11	37,37,37,37	0
58	MG	1a	1763	1/1	0.98	0.06	45,45,45,45	0
58	MG	1A	4039	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3212	1/1	0.98	0.11	36,36,36,36	0
58	MG	1A	3161	1/1	0.98	0.07	25,25,25,25	0
58	MG	1W	203	1/1	0.98	0.06	46,46,46,46	0
58	MG	1A	3737	1/1	0.98	0.04	22,22,22,22	0
58	MG	2A	3410	1/1	0.98	0.12	44,44,44,44	0
58	MG	1A	3500	1/1	0.98	0.09	35,35,35,35	0
58	MG	1X	101	1/1	0.98	0.10	31,31,31,31	0
58	MG	1X	103	1/1	0.98	0.15	32,32,32,32	0
58	MG	1A	3340	1/1	0.98	0.04	36,36,36,36	0
58	MG	2A	3168	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3271	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3052	1/1	0.98	0.13	26,26,26,26	0
58	MG	1A	3070	1/1	0.98	0.10	16,16,16,16	0
58	MG	1A	4048	1/1	0.98	0.06	26,26,26,26	0
58	MG	1Y	203	1/1	0.98	0.14	45,45,45,45	0
58	MG	1A	3614	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3124	1/1	0.98	0.05	30,30,30,30	0
58	MG	1A	3506	1/1	0.98	0.11	25,25,25,25	0
58	MG	1A	3887	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	3218	1/1	0.98	0.12	35,35,35,35	0
58	MG	1A	3748	1/1	0.98	0.07	26,26,26,26	0
58	MG	1A	4055	1/1	0.98	0.05	23,23,23,23	0
58	MG	1A	4056	1/1	0.98	0.07	47,47,47,47	0
58	MG	2A	3710	1/1	0.98	0.06	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	3219	1/1	0.98	0.17	32,32,32,32	0
58	MG	1A	3347	1/1	0.98	0.16	41,41,41,41	0
58	MG	1A	3277	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	4060	1/1	0.98	0.09	50,50,50,50	0
58	MG	1A	3621	1/1	0.98	0.06	20,20,20,20	0
58	MG	1A	3894	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3279	1/1	0.98	0.04	31,31,31,31	0
58	MG	11	104	1/1	0.98	0.04	33,33,33,33	0
58	MG	11	105	1/1	0.98	0.04	46,46,46,46	0
58	MG	1A	3280	1/1	0.98	0.10	34,34,34,34	0
58	MG	1A	3897	1/1	0.98	0.06	25,25,25,25	0
58	MG	12	102	1/1	0.98	0.09	36,36,36,36	0
58	MG	1a	1804	1/1	0.98	0.16	40,40,40,40	0
58	MG	1A	3624	1/1	0.98	0.04	27,27,27,27	0
58	MG	13	103	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	4069	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	4070	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3166	1/1	0.98	0.11	30,30,30,30	0
58	MG	2A	3732	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	4072	1/1	0.98	0.07	20,20,20,20	0
58	MG	15	105	1/1	0.98	0.04	23,23,23,23	0
58	MG	2A	3450	1/1	0.98	0.20	42,42,42,42	0
58	MG	15	106	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	3757	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3627	1/1	0.98	0.10	25,25,25,25	0
58	MG	1A	3514	1/1	0.98	0.05	39,39,39,39	0
58	MG	17	101	1/1	0.98	0.07	24,24,24,24	0
58	MG	2a	1675	1/1	0.98	0.14	42,42,42,42	0
58	MG	2a	1676	1/1	0.98	0.08	34,34,34,34	0
58	MG	1A	3352	1/1	0.98	0.21	28,28,28,28	0
58	MG	1A	3284	1/1	0.98	0.07	22,22,22,22	0
58	MG	1A	3285	1/1	0.98	0.19	36,36,36,36	0
58	MG	18	102	1/1	0.98	0.14	32,32,32,32	0
58	MG	18	103	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3633	1/1	0.98	0.06	18,18,18,18	0
58	MG	1A	3518	1/1	0.98	0.08	43,43,43,43	0
58	MG	1A	3355	1/1	0.98	0.16	25,25,25,25	0
58	MG	1A	3356	1/1	0.98	0.13	31,31,31,31	0
58	MG	1m	3001	1/1	0.98	0.04	51,51,51,51	0
58	MG	1A	3286	1/1	0.98	0.13	30,30,30,30	0
58	MG	1A	3638	1/1	0.98	0.05	20,20,20,20	0
58	MG	1A	3770	1/1	0.98	0.04	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	3639	1/1	0.98	0.05	11,11,11,11	0
58	MG	2A	3472	1/1	0.98	0.17	40,40,40,40	0
58	MG	1w	101	1/1	0.98	0.06	40,40,40,40	0
58	MG	2A	3474	1/1	0.98	0.12	40,40,40,40	0
58	MG	1A	4088	1/1	0.98	0.03	26,26,26,26	0
58	MG	1a	1610	1/1	0.98	0.08	23,23,23,23	0
58	MG	2A	3225	1/1	0.98	0.18	30,30,30,30	0
58	MG	1A	3072	1/1	0.98	0.15	27,27,27,27	0
58	MG	1A	3288	1/1	0.98	0.31	26,26,26,26	0
58	MG	1A	3168	1/1	0.98	0.05	28,28,28,28	0
58	MG	1A	3290	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	4094	1/1	0.98	0.06	42,42,42,42	0
58	MG	1A	3126	1/1	0.98	0.16	24,24,24,24	0
58	MG	2A	3769	1/1	0.98	0.04	49,49,49,49	0
58	MG	2A	3484	1/1	0.98	0.03	19,19,19,19	0
58	MG	1A	3098	1/1	0.98	0.10	35,35,35,35	0
58	MG	2A	3486	1/1	0.98	0.09	34,34,34,34	0
58	MG	1A	3442	1/1	0.98	0.08	35,35,35,35	0
58	MG	1A	3647	1/1	0.98	0.05	11,11,11,11	0
58	MG	2A	3775	1/1	0.98	0.05	27,27,27,27	0
58	MG	1A	3924	1/1	0.98	0.06	39,39,39,39	0
58	MG	1A	3225	1/1	0.98	0.10	34,34,34,34	0
58	MG	1A	3128	1/1	0.98	0.20	29,29,29,29	0
58	MG	1x	108	1/1	0.98	0.05	18,18,18,18	0
58	MG	1A	3783	1/1	0.98	0.05	25,25,25,25	0
58	MG	1A	3785	1/1	0.98	0.07	20,20,20,20	0
58	MG	1A	4104	1/1	0.98	0.05	48,48,48,48	0
58	MG	1A	3650	1/1	0.98	0.06	13,13,13,13	0
58	MG	1A	3930	1/1	0.98	0.04	42,42,42,42	0
58	MG	2A	3498	1/1	0.98	0.18	46,46,46,46	0
58	MG	2A	3786	1/1	0.98	0.09	41,41,41,41	0
58	MG	2A	3244	1/1	0.98	0.06	36,36,36,36	0
58	MG	2A	3500	1/1	0.98	0.12	51,51,51,51	0
58	MG	1A	3037	1/1	0.98	0.07	31,31,31,31	0
58	MG	1A	3039	1/1	0.98	0.16	27,27,27,27	0
58	MG	2a	1725	1/1	0.98	0.12	42,42,42,42	0
58	MG	1A	3933	1/1	0.98	0.07	35,35,35,35	0
58	MG	1A	3175	1/1	0.98	0.05	32,32,32,32	0
58	MG	2A	3505	1/1	0.98	0.07	56,56,56,56	0
58	MG	1A	3230	1/1	0.98	0.12	27,27,27,27	0
58	MG	1A	3791	1/1	0.98	0.04	31,31,31,31	0
58	MG	1B	206	1/1	0.98	0.04	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	3792	1/1	0.98	0.03	26,26,26,26	0
58	MG	1A	3939	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3179	1/1	0.98	0.07	23,23,23,23	0
58	MG	2A	3009	1/1	0.98	0.04	34,34,34,34	0
58	MG	2A	3010	1/1	0.98	0.11	43,43,43,43	0
58	MG	1A	3180	1/1	0.98	0.10	18,18,18,18	0
58	MG	2a	1738	1/1	0.98	0.16	52,52,52,52	0
58	MG	1A	3657	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3943	1/1	0.98	0.05	26,26,26,26	0
58	MG	1B	213	1/1	0.98	0.06	30,30,30,30	0
58	MG	2A	3016	1/1	0.98	0.11	55,55,55,55	0
58	MG	1A	3796	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3234	1/1	0.98	0.14	33,33,33,33	0
58	MG	2A	3810	1/1	0.98	0.10	55,55,55,55	0
58	MG	1A	3798	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	3799	1/1	0.98	0.04	10,10,10,10	0
58	MG	1A	3302	1/1	0.98	0.04	24,24,24,24	0
58	MG	2a	1749	1/1	0.98	0.05	58,58,58,58	0
58	MG	1A	3949	1/1	0.98	0.10	44,44,44,44	0
58	MG	2A	3527	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3539	1/1	0.98	0.17	37,37,37,37	0
58	MG	2A	3025	1/1	0.98	0.06	48,48,48,48	0
58	MG	2A	3026	1/1	0.98	0.06	36,36,36,36	0
58	MG	2A	3027	1/1	0.98	0.06	32,32,32,32	0
58	MG	1B	221	1/1	0.98	0.10	31,31,31,31	0
58	MG	1B	222	1/1	0.98	0.05	29,29,29,29	0
58	MG	1a	1651	1/1	0.98	0.10	37,37,37,37	0
58	MG	2A	3536	1/1	0.98	0.06	51,51,51,51	0
58	MG	1A	3453	1/1	0.98	0.10	40,40,40,40	0
58	MG	2a	1761	1/1	0.98	0.07	56,56,56,56	0
58	MG	1A	3181	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3826	1/1	0.98	0.09	37,37,37,37	0
58	MG	2A	3034	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3663	1/1	0.98	0.04	25,25,25,25	0
58	MG	2a	1766	1/1	0.98	0.14	48,48,48,48	0
58	MG	2a	1767	1/1	0.98	0.03	54,54,54,54	0
58	MG	1A	3375	1/1	0.98	0.11	33,33,33,33	0
58	MG	1A	3076	1/1	0.98	0.03	20,20,20,20	0
58	MG	2A	3038	1/1	0.98	0.09	22,22,22,22	0
58	MG	2A	3832	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3377	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3834	1/1	0.98	0.04	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	1A	3809	1/1	0.98	0.05	13,13,13,13	0
58	MG	1A	3378	1/1	0.98	0.10	27,27,27,27	0
58	MG	1A	3132	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3056	1/1	0.98	0.05	29,29,29,29	0
58	MG	1A	3961	1/1	0.98	0.04	35,35,35,35	0
58	MG	1A	3134	1/1	0.98	0.04	35,35,35,35	0
58	MG	1A	3549	1/1	0.98	0.05	19,19,19,19	0
58	MG	2A	3843	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3964	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3816	1/1	0.98	0.05	39,39,39,39	0
58	MG	2A	3555	1/1	0.98	0.06	31,31,31,31	0
58	MG	1A	3078	1/1	0.98	0.07	24,24,24,24	0
58	MG	2A	3557	1/1	0.98	0.12	28,28,28,28	0
58	MG	1D	301	1/1	0.98	0.12	23,23,23,23	0
58	MG	1A	3383	1/1	0.98	0.14	41,41,41,41	0
58	MG	1A	3968	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3137	1/1	0.98	0.10	24,24,24,24	0
58	MG	2A	3564	1/1	0.98	0.08	42,42,42,42	0
58	MG	1A	3820	1/1	0.98	0.07	22,22,22,22	0
58	MG	1A	3311	1/1	0.98	0.03	29,29,29,29	0
58	MG	1A	3677	1/1	0.98	0.05	19,19,19,19	0
58	MG	2A	3568	1/1	0.98	0.04	44,44,44,44	0
58	MG	2A	3859	1/1	0.98	0.07	29,29,29,29	0
58	MG	2A	3569	1/1	0.98	0.07	29,29,29,29	0
58	MG	2A	3570	1/1	0.98	0.05	53,53,53,53	0
58	MG	1A	3466	1/1	0.98	0.07	42,42,42,42	0
58	MG	1D	311	1/1	0.98	0.14	29,29,29,29	0
58	MG	1A	3974	1/1	0.98	0.07	36,36,36,36	0
58	MG	2A	3303	1/1	0.98	0.06	44,44,44,44	0
58	MG	1A	3467	1/1	0.98	0.12	43,43,43,43	0
58	MG	1E	301	1/1	0.98	0.07	32,32,32,32	0
58	MG	1E	303	1/1	0.98	0.14	28,28,28,28	0
58	MG	1A	3556	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3079	1/1	0.98	0.04	24,24,24,24	0
58	MG	1a	1683	1/1	0.98	0.05	51,51,51,51	0
58	MG	2A	3582	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3685	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3313	1/1	0.98	0.20	41,41,41,41	0
58	MG	1A	3244	1/1	0.98	0.12	25,25,25,25	0
58	MG	1A	3560	1/1	0.98	0.06	47,47,47,47	0
58	MG	1A	3107	1/1	0.98	0.06	34,34,34,34	0
58	MG	1E	312	1/1	0.98	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	2a	1817	1/1	0.98	0.18	48,48,48,48	0
58	MG	2A	3589	1/1	0.98	0.16	46,46,46,46	0
58	MG	1A	3007	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3984	1/1	0.98	0.03	34,34,34,34	0
58	MG	1F	301	1/1	0.98	0.07	19,19,19,19	0
58	MG	1A	3693	1/1	0.98	0.05	23,23,23,23	0
58	MG	1A	3564	1/1	0.98	0.11	26,26,26,26	0
58	MG	2A	3078	1/1	0.98	0.08	27,27,27,27	0
58	MG	1A	3565	1/1	0.98	0.13	24,24,24,24	0
58	MG	1F	305	1/1	0.98	0.03	25,25,25,25	0
58	MG	2A	3600	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3141	1/1	0.98	0.07	31,31,31,31	0
58	MG	1A	3392	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3029	1/1	0.98	0.17	25,25,25,25	0
58	MG	2A	3084	1/1	0.98	0.06	38,38,38,38	0
58	MG	2B	210	1/1	0.98	0.04	50,50,50,50	0
58	MG	1A	3084	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	3992	1/1	0.98	0.11	32,32,32,32	0
58	MG	1A	3570	1/1	0.98	0.15	30,30,30,30	0
58	MG	2A	3331	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3196	1/1	0.98	0.25	29,29,29,29	0
58	MG	1A	3703	1/1	0.98	0.07	20,20,20,20	0
58	MG	1A	3085	1/1	0.98	0.12	33,33,33,33	0
58	MG	1A	3042	1/1	0.98	0.04	34,34,34,34	0
58	MG	2A	3092	1/1	0.98	0.17	38,38,38,38	0
58	MG	1A	3577	1/1	0.98	0.17	29,29,29,29	0
58	MG	1N	201	1/1	0.98	0.09	28,28,28,28	0
58	MG	2D	302	1/1	0.98	0.16	46,46,46,46	0
58	MG	2D	303	1/1	0.98	0.16	40,40,40,40	0
58	MG	1a	1709	1/1	0.98	0.08	33,33,33,33	0
58	MG	2D	305	1/1	0.98	0.03	22,22,22,22	0
58	MG	2D	306	1/1	0.98	0.24	35,35,35,35	0
58	MG	2l	202	1/1	0.98	0.11	55,55,55,55	0
58	MG	1A	3399	1/1	0.98	0.28	39,39,39,39	0
58	MG	1A	4001	1/1	0.98	0.04	43,43,43,43	0
58	MG	2E	302	1/1	0.98	0.05	50,50,50,50	0
58	MG	1N	204	1/1	0.98	0.14	37,37,37,37	0
58	MG	1A	3847	1/1	0.98	0.08	28,28,28,28	0
58	MG	2E	305	1/1	0.98	0.08	41,41,41,41	0
58	MG	1A	3708	1/1	0.98	0.04	8,8,8,8	0
58	MG	1A	3579	1/1	0.98	0.13	33,33,33,33	0
58	MG	2A	3103	1/1	0.98	0.06	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	1717	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	4005	1/1	0.98	0.18	23,23,23,23	0
58	MG	2A	3106	1/1	0.98	0.07	42,42,42,42	0
58	MG	2A	3107	1/1	0.98	0.20	41,41,41,41	0
58	MG	1A	3710	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3046	1/1	0.98	0.03	22,22,22,22	0
58	MG	1P	201	1/1	0.98	0.15	29,29,29,29	0
58	MG	2A	3632	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3712	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3150	1/1	0.98	0.14	29,29,29,29	0
58	MG	1Q	201	1/1	0.98	0.10	32,32,32,32	0
58	MG	2A	3636	1/1	0.98	0.07	30,30,30,30	0
58	MG	1A	3855	1/1	0.98	0.06	35,35,35,35	0
58	MG	2O	201	1/1	0.98	0.12	50,50,50,50	0
58	MG	1A	3258	1/1	0.98	0.08	43,43,43,43	0
58	MG	2A	3359	1/1	0.98	0.16	48,48,48,48	0
58	MG	2A	3360	1/1	0.98	0.12	55,55,55,55	0
58	MG	1A	4014	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	4015	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	3715	1/1	0.98	0.04	44,44,44,44	0
58	MG	2A	3644	1/1	0.98	0.05	34,34,34,34	0
58	MG	2A	3119	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3326	1/1	0.98	0.08	30,30,30,30	0
58	MG	1A	3089	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3590	1/1	0.98	0.13	39,39,39,39	0
58	MG	1A	4020	1/1	0.98	0.08	33,33,33,33	0
58	MG	1A	3013	1/1	0.98	0.09	18,18,18,18	0
58	MG	1A	3487	1/1	0.98	0.05	33,33,33,33	0
58	MG	20	101	1/1	0.98	0.04	55,55,55,55	0
58	MG	1a	1737	1/1	0.98	0.03	29,29,29,29	0
58	MG	1a	1738	1/1	0.98	0.08	34,34,34,34	0
60	ZN	14	102	1/1	0.98	0.05	96,96,96,96	0
60	ZN	2Y	501	1/1	0.98	0.04	79,79,79,79	0
58	MG	1A	3116	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3038	1/1	0.99	0.08	14,14,14,14	0
58	MG	2A	3788	1/1	0.99	0.04	45,45,45,45	0
58	MG	1A	3780	1/1	0.99	0.04	36,36,36,36	0
58	MG	1A	3701	1/1	0.99	0.06	31,31,31,31	0
58	MG	1A	3866	1/1	0.99	0.07	36,36,36,36	0
58	MG	1B	238	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3245	1/1	0.99	0.19	25,25,25,25	0
58	MG	1A	3073	1/1	0.99	0.03	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3784	1/1	0.99	0.04	16,16,16,16	0
58	MG	1A	3629	1/1	0.99	0.06	22,22,22,22	0
58	MG	1A	3160	1/1	0.99	0.06	26,26,26,26	0
58	MG	1D	305	1/1	0.99	0.03	11,11,11,11	0
58	MG	1A	3562	1/1	0.99	0.12	24,24,24,24	0
58	MG	1A	3099	1/1	0.99	0.10	13,13,13,13	0
58	MG	1A	3162	1/1	0.99	0.13	22,22,22,22	0
58	MG	10	109	1/1	0.99	0.05	44,44,44,44	0
58	MG	1D	309	1/1	0.99	0.04	41,41,41,41	0
58	MG	2A	3098	1/1	0.99	0.09	36,36,36,36	0
58	MG	1A	3250	1/1	0.99	0.06	45,45,45,45	0
58	MG	1A	3023	1/1	0.99	0.04	10,10,10,10	0
58	MG	2A	3507	1/1	0.99	0.05	56,56,56,56	0
58	MG	1A	3252	1/1	0.99	0.16	31,31,31,31	0
58	MG	1A	3406	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	3054	1/1	0.99	0.05	40,40,40,40	0
58	MG	1E	302	1/1	0.99	0.06	23,23,23,23	0
58	MG	1A	3009	1/1	0.99	0.03	17,17,17,17	0
58	MG	1E	304	1/1	0.99	0.10	26,26,26,26	0
58	MG	13	101	1/1	0.99	0.06	21,21,21,21	0
58	MG	1A	3031	1/1	0.99	0.14	22,22,22,22	0
58	MG	2A	3377	1/1	0.99	0.02	30,30,30,30	0
58	MG	1A	3014	1/1	0.99	0.04	17,17,17,17	0
58	MG	1A	3307	1/1	0.99	0.04	19,19,19,19	0
58	MG	2a	1768	1/1	0.99	0.04	53,53,53,53	0
58	MG	15	101	1/1	0.99	0.14	20,20,20,20	0
58	MG	1A	4065	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	4066	1/1	0.99	0.04	13,13,13,13	0
58	MG	2A	3522	1/1	0.99	0.06	34,34,34,34	0
58	MG	1A	3575	1/1	0.99	0.12	27,27,27,27	0
58	MG	1A	3576	1/1	0.99	0.03	15,15,15,15	0
58	MG	1w	106	1/1	0.99	0.05	51,51,51,51	0
58	MG	1A	3720	1/1	0.99	0.02	10,10,10,10	0
58	MG	1A	3105	1/1	0.99	0.07	33,33,33,33	0
58	MG	1A	3058	1/1	0.99	0.05	15,15,15,15	0
58	MG	1A	3135	1/1	0.99	0.07	29,29,29,29	0
58	MG	1A	3171	1/1	0.99	0.04	13,13,13,13	0
58	MG	17	102	1/1	0.99	0.15	28,28,28,28	0
58	MG	1A	3581	1/1	0.99	0.19	30,30,30,30	0
58	MG	1A	3214	1/1	0.99	0.17	26,26,26,26	0
58	MG	2A	3534	1/1	0.99	0.04	36,36,36,36	0
58	MG	1a	1716	1/1	0.99	0.11	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	2A	3836	1/1	0.99	0.04	48,48,48,48	0
58	MG	1A	3808	1/1	0.99	0.03	18,18,18,18	0
58	MG	1F	306	1/1	0.99	0.03	30,30,30,30	0
58	MG	1A	3583	1/1	0.99	0.06	30,30,30,30	0
58	MG	1F	308	1/1	0.99	0.10	26,26,26,26	0
58	MG	1A	4078	1/1	0.99	0.03	28,28,28,28	0
58	MG	1A	3810	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3584	1/1	0.99	0.09	25,25,25,25	0
58	MG	1A	3043	1/1	0.99	0.12	17,17,17,17	0
58	MG	1A	3586	1/1	0.99	0.12	24,24,24,24	0
58	MG	2A	3846	1/1	0.99	0.06	29,29,29,29	0
58	MG	1A	3081	1/1	0.99	0.07	24,24,24,24	0
58	MG	1a	1607	1/1	0.99	0.03	40,40,40,40	0
58	MG	1a	1728	1/1	0.99	0.04	31,31,31,31	0
58	MG	1A	3588	1/1	0.99	0.18	32,32,32,32	0
58	MG	1A	3082	1/1	0.99	0.08	29,29,29,29	0
58	MG	1A	3734	1/1	0.99	0.04	30,30,30,30	0
58	MG	1A	3060	1/1	0.99	0.09	40,40,40,40	0
58	MG	1A	3176	1/1	0.99	0.20	28,28,28,28	0
58	MG	1A	4089	1/1	0.99	0.04	30,30,30,30	0
58	MG	2A	3554	1/1	0.99	0.09	39,39,39,39	0
58	MG	1A	3177	1/1	0.99	0.18	20,20,20,20	0
58	MG	1A	3994	1/1	0.99	0.05	21,21,21,21	0
58	MG	1A	3593	1/1	0.99	0.04	34,34,34,34	0
58	MG	2A	3558	1/1	0.99	0.05	30,30,30,30	0
58	MG	2A	3559	1/1	0.99	0.05	45,45,45,45	0
58	MG	1A	3044	1/1	0.99	0.15	26,26,26,26	0
58	MG	2A	3014	1/1	0.99	0.07	36,36,36,36	0
58	MG	1A	3045	1/1	0.99	0.03	26,26,26,26	0
58	MG	1A	3142	1/1	0.99	0.04	9,9,9,9	0
58	MG	1A	3086	1/1	0.99	0.19	28,28,28,28	0
58	MG	1A	3010	1/1	0.99	0.04	22,22,22,22	0
58	MG	1A	3047	1/1	0.99	0.08	32,32,32,32	0
58	MG	1A	3146	1/1	0.99	0.15	24,24,24,24	0
58	MG	2A	3424	1/1	0.99	0.07	30,30,30,30	0
58	MG	1P	203	1/1	0.99	0.10	23,23,23,23	0
58	MG	1A	3914	1/1	0.99	0.04	32,32,32,32	0
58	MG	2A	3718	1/1	0.99	0.03	25,25,25,25	0
58	MG	1a	1747	1/1	0.99	0.04	40,40,40,40	0
58	MG	2A	3572	1/1	0.99	0.05	33,33,33,33	0
58	MG	1A	3746	1/1	0.99	0.06	41,41,41,41	0
58	MG	1Q	202	1/1	0.99	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MG	1A	3601	1/1	0.99	0.20	30,30,30,30	0
58	MG	1A	4006	1/1	0.99	0.04	14,14,14,14	0
58	MG	1A	4007	1/1	0.99	0.02	25,25,25,25	0
58	MG	2A	3726	1/1	0.99	0.03	42,42,42,42	0
58	MG	2A	3030	1/1	0.99	0.10	36,36,36,36	0
58	MG	1A	3670	1/1	0.99	0.07	26,26,26,26	0
58	MG	1A	3147	1/1	0.99	0.15	25,25,25,25	0
58	MG	2A	3730	1/1	0.99	0.09	39,39,39,39	0
58	MG	1A	3919	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	3065	1/1	0.99	0.12	33,33,33,33	0
58	MG	1R	204	1/1	0.99	0.05	22,22,22,22	0
58	MG	1A	4109	1/1	0.99	0.03	45,45,45,45	0
58	MG	2A	3735	1/1	0.99	0.04	30,30,30,30	0
58	MG	1B	201	1/1	0.99	0.06	37,37,37,37	0
58	MG	1A	3034	1/1	0.99	0.18	23,23,23,23	0
58	MG	1A	3278	1/1	0.99	0.07	21,21,21,21	0
58	MG	1A	3189	1/1	0.99	0.09	30,30,30,30	0
58	MG	1A	3488	1/1	0.99	0.09	34,34,34,34	0
58	MG	1A	3232	1/1	0.99	0.10	19,19,19,19	0
58	MG	1A	3609	1/1	0.99	0.04	17,17,17,17	0
58	MG	2A	3177	1/1	0.99	0.05	24,24,24,24	0
58	MG	2A	3593	1/1	0.99	0.05	32,32,32,32	0
58	MG	1A	3679	1/1	0.99	0.03	15,15,15,15	0
58	MG	1A	3035	1/1	0.99	0.26	30,30,30,30	0
58	MG	1A	3282	1/1	0.99	0.08	34,34,34,34	0
58	MG	1A	3682	1/1	0.99	0.03	21,21,21,21	0
58	MG	1A	4022	1/1	0.99	0.03	51,51,51,51	0
58	MG	2A	3599	1/1	0.99	0.08	31,31,31,31	0
58	MG	1A	3683	1/1	0.99	0.05	29,29,29,29	0
58	MG	1U	208	1/1	0.99	0.19	29,29,29,29	0
58	MG	2A	3753	1/1	0.99	0.10	33,33,33,33	0
58	MG	1a	1773	1/1	0.99	0.03	45,45,45,45	0
58	MG	1A	3283	1/1	0.99	0.09	21,21,21,21	0
58	MG	1A	3613	1/1	0.99	0.07	34,34,34,34	0
58	MG	1A	3068	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3120	1/1	0.99	0.13	29,29,29,29	0
58	MG	1A	3936	1/1	0.99	0.05	8,8,8,8	0
58	MG	1A	3849	1/1	0.99	0.03	48,48,48,48	0
58	MG	1A	3766	1/1	0.99	0.06	31,31,31,31	0
58	MG	1V	205	1/1	0.99	0.04	17,17,17,17	0
58	MG	1a	1782	1/1	0.99	0.04	59,59,59,59	0
58	MG	1A	3193	1/1	0.99	0.14	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	1784	1/1	0.99	0.02	41,41,41,41	0
58	MG	2A	3468	1/1	0.99	0.09	24,24,24,24	0
58	MG	1A	3003	1/1	0.99	0.06	23,23,23,23	0
58	MG	1A	3690	1/1	0.99	0.04	24,24,24,24	0
58	MG	1A	3094	1/1	0.99	0.04	23,23,23,23	0
58	MG	1W	201	1/1	0.99	0.07	38,38,38,38	0
58	MG	1a	1789	1/1	0.99	0.03	49,49,49,49	0
58	MG	1a	1790	1/1	0.99	0.02	33,33,33,33	0
58	MG	2A	3069	1/1	0.99	0.02	23,23,23,23	0
58	MG	1A	3692	1/1	0.99	0.06	17,17,17,17	0
58	MG	1A	4036	1/1	0.99	0.02	16,16,16,16	0
58	MG	1W	204	1/1	0.99	0.13	23,23,23,23	0
58	MG	1A	3155	1/1	0.99	0.05	27,27,27,27	0
58	MG	1A	3197	1/1	0.99	0.18	26,26,26,26	0
58	MG	1A	3008	1/1	0.99	0.04	16,16,16,16	0
58	MG	1X	102	1/1	0.99	0.05	39,39,39,39	0
58	MG	2A	3629	1/1	0.99	0.05	30,30,30,30	0
58	MG	1a	1798	1/1	0.99	0.04	59,59,59,59	0
58	MG	2T	201	1/1	0.99	0.03	47,47,47,47	0
59	K	1A	3574	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3071	1/1	0.99	0.05	10,10,10,10	0
60	ZN	1Y	204	1/1	0.99	0.03	52,52,52,52	0
58	MG	1A	3395	1/1	0.99	0.17	24,24,24,24	0
60	ZN	16	103	1/1	0.99	0.02	39,39,39,39	0
60	ZN	19	102	1/1	0.99	0.04	37,37,37,37	0
60	ZN	1n	102	1/1	0.99	0.03	55,55,55,55	0
58	MG	1A	3243	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3625	1/1	0.99	0.05	28,28,28,28	0
60	ZN	25	105	1/1	0.99	0.04	55,55,55,55	0
60	ZN	29	501	1/1	0.99	0.03	71,71,71,71	0
60	ZN	2n	102	1/1	0.99	0.02	77,77,77,77	0
61	SF4	1d	302	8/8	0.99	0.05	52,55,58,66	0
61	SF4	2d	303	8/8	0.99	0.04	60,65,68,76	0
58	MG	2A	3021	1/1	1.00	0.05	19,19,19,19	0
58	MG	1A	3178	1/1	1.00	0.03	31,31,31,31	0
60	ZN	15	108	1/1	1.00	0.02	36,36,36,36	0
60	ZN	26	102	1/1	1.00	0.03	54,54,54,54	0

6.5 Other polymers ⓘ

There are no such residues in this entry.