



# wwPDB X-ray Structure Validation Summary Report

Jan 3, 2024 – 06:33 am GMT

PDB ID : 5FDU  
Title : Crystal structure of the Metalnikowin I antimicrobial peptide bound to the *Thermus thermophilus* 70S ribosome  
Authors : Seefeldt, A.C.; Graf, M.; Perebaskine, N.; Nguyen, F.; Arenz, S.; Mardirossian, M.; Scocchi, M.; Wilson, D.N.; Innis, C.A.  
Deposited on : 2015-12-16  
Resolution : 2.90 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

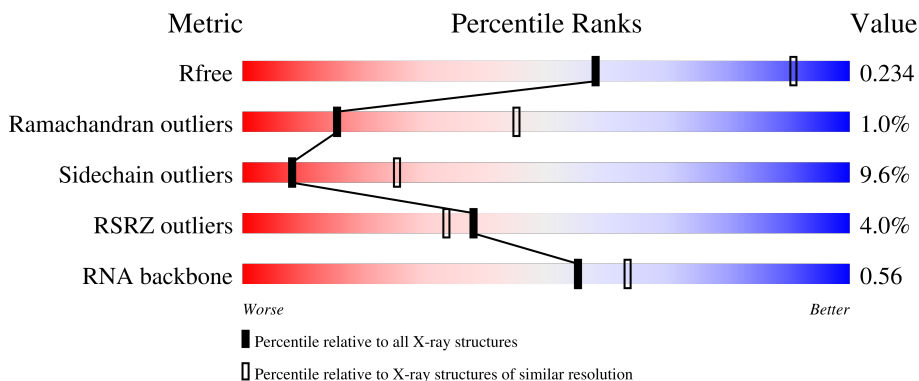
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	
1	2A	2915	
2	1B	120	
2	2B	120	
3	1D	275	


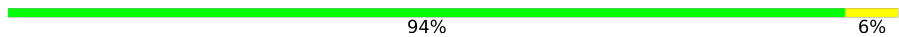



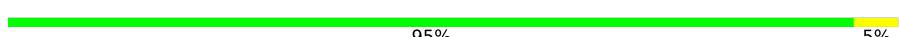




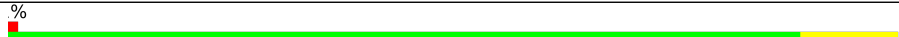


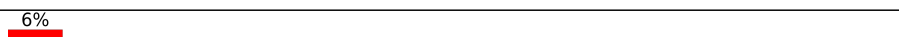
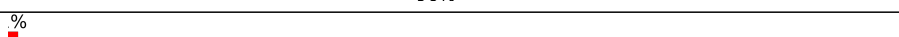
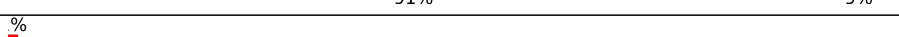

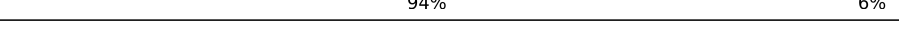
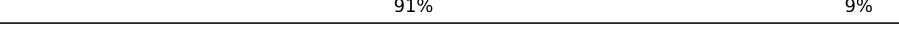
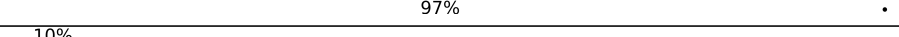
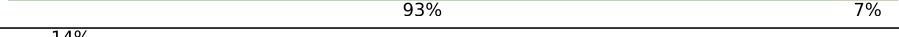




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Mol	Chain	Length	Quality of chain
3	2D	275	92% 7% .
4	1E	204	89% 10% .
4	2E	204	89% 11%
5	1F	203	85% 14%
5	2F	203	91% 9%
6	1G	181	88% 10% .
6	2G	181	7% 93% 6% .
7	1H	174	93% 7%
7	2H	174	16% 87% 13% .
8	1I	147	88% 12% .
8	2I	147	5% 88% 10% ..
9	1N	140	89% 11%
9	2N	140	91% 9%
10	1O	122	90% 9% .
10	2O	122	94% 6%
11	1P	149	93% 7%
11	2P	149	2% 93% 7%
12	1Q	141	93% 5% ..
12	2Q	141	92% 7% .
13	1R	118	86% 14% .
13	2R	118	86% 13% .
14	1S	110	90% 8% ..
14	2S	110	5% 90% 10%
15	1T	131	92% 8%
15	2T	131	95% 5%

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Mol	Chain	Length	Quality of chain
16	1U	116	 84% 14%
16	2U	116	 94% 6%
17	1V	101	 85% 15%
17	2V	101	 89% 10%
18	1W	112	 90% 10%
18	2W	112	 95% 5%
19	1X	95	 92% 8%
19	2X	95	 97%
20	1Y	107	 91% 9%
20	2Y	107	 15% 91% 8%
21	1Z	203	 89% 11%
21	2Z	203	 3% 91% 8%
22	10	77	 92% 8%
22	20	77	 6% 96%
23	11	97	 91% 9%
23	21	97	 90% 9%
24	12	70	 94% 6%
24	22	70	 91% 9%
25	13	59	 97%
25	23	59	 10% 93% 7%
26	14	69	 14% 83% 16%
26	24	69	 25% 78% 22%
27	15	59	 83% 14%
27	25	59	 90% 10%
28	16	53	 89% 11%

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Mol	Chain	Length	Quality of chain
28	26	53	89% 11%
29	17	48	2% 83% 17%
29	27	48	90% 10%
30	18	64	88% 12%
30	28	64	89% 11%
31	19	37	92% 8%
31	29	37	5% 95% 5%
32	1a	1521	3% 55% 36% 7% .
32	2a	1521	4% 58% 35% 6% .
33	1b	231	7% 87% 11% .
33	2b	231	8% 84% 15% .
34	1c	206	6% 95% 5%
34	2c	206	3% 92% 8%
35	1d	208	2% 88% 12%
35	2d	208	92% 8%
36	1e	148	% 93% 7%
36	2e	148	% 95% 5%
37	1f	100	% 94% 6%
37	2f	100	96% .
38	1g	155	4% 93% 7%
38	2g	155	8% 94% 6%
39	1h	137	% 91% 8% .
39	2h	137	% 94% 6%
40	1i	127	9% 90% 10%
40	2i	127	17% 89% 9% ..

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Mol	Chain	Length	Quality of chain
41	1j	97	22% 90% 10%
41	2j	97	21% 90% 9%
42	1k	114	% 96% .
42	2k	114	% 92% 8%
43	1l	122	2% 94% 6%
43	2l	122	% 93% 7%
44	1m	116	6% 90% 10%
44	2m	116	7% 88% 10%
45	1n	60	2% 90% 8%
45	2n	60	18% 93% 5%
46	1o	88	3% 93% 6%
46	2o	88	% 92% 8%
47	1p	82	7% 85% 13%
47	2p	82	4% 90% 10%
48	1q	99	% 92% 7%
48	2q	99	% 93% 7%
49	1r	68	4% 91% 9%
49	2r	68	4% 87% 13%
50	1s	83	12% 90% 10%
50	2s	83	42% 93% 7%
51	1t	98	3% 91% 7%
51	2t	98	% 94% 5%
52	1u	23	22% 87% 13%
52	2u	23	43% 87% 9%
53	1x	97	2% 95% 5%

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Mol	Chain	Length	Quality of chain
53	2x	97	
54	1y	10	
54	2y	10	

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
55	MG	18	3301	-	-	-	X
55	MG	1A	3071	-	-	-	X
55	MG	1A	3077	-	-	-	X
55	MG	1A	3084	-	-	-	X
55	MG	1A	3095	-	-	-	X
55	MG	1A	3106	-	-	-	X
55	MG	1A	3143	-	-	-	X
55	MG	1A	3173	-	-	-	X
55	MG	1A	3183	-	-	-	X
55	MG	1A	3193	-	-	-	X
55	MG	1A	3204	-	-	-	X
55	MG	1A	3220	-	-	-	X
55	MG	1A	3244	-	-	-	X
55	MG	1A	3396	-	-	-	X
55	MG	1A	3516	-	-	-	X
55	MG	1A	3611	-	-	-	X
55	MG	1A	3702	-	-	-	X
55	MG	1A	3725	-	-	-	X
55	MG	1A	3734	-	-	-	X
55	MG	1A	3758	-	-	-	X
55	MG	1A	3848	-	-	-	X
55	MG	1A	3895	-	-	-	X
55	MG	1A	3905	-	-	-	X
55	MG	1A	3913	-	-	-	X
55	MG	1A	3914	-	-	-	X
55	MG	1Q	204	-	-	-	X
55	MG	1V	201	-	-	-	X
55	MG	1a	3022	-	-	-	X
55	MG	1a	3038	-	-	-	X
55	MG	1a	3058	-	-	-	X
55	MG	1a	3063	-	-	-	X
55	MG	1a	3161	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1h	3001	-	-	-	X
55	MG	27	103	-	-	-	X
55	MG	28	101	-	-	-	X
55	MG	28	102	-	-	-	X
55	MG	2A	3047	-	-	-	X
55	MG	2A	3058	-	-	-	X
55	MG	2A	3074	-	-	-	X
55	MG	2A	3080	-	-	-	X
55	MG	2A	3090	-	-	-	X
55	MG	2A	3091	-	-	-	X
55	MG	2A	3109	-	-	-	X
55	MG	2A	3129	-	-	-	X
55	MG	2A	3136	-	-	-	X
55	MG	2A	3138	-	-	-	X
55	MG	2A	3142	-	-	-	X
55	MG	2A	3150	-	-	-	X
55	MG	2A	3154	-	-	-	X
55	MG	2A	3155	-	-	-	X
55	MG	2A	3163	-	-	-	X
55	MG	2A	3192	-	-	-	X
55	MG	2A	3257	-	-	-	X
55	MG	2A	3375	-	-	-	X
55	MG	2A	3455	-	-	-	X
55	MG	2A	3476	-	-	-	X
55	MG	2A	3485	-	-	-	X
55	MG	2A	3507	-	-	-	X
55	MG	2A	3553	-	-	-	X
55	MG	2A	3555	-	-	-	X
55	MG	2A	3563	-	-	-	X
55	MG	2A	3582	-	-	-	X
55	MG	2A	3643	-	-	-	X
55	MG	2A	3762	-	-	-	X
55	MG	2A	3765	-	-	-	X
55	MG	2A	3792	-	-	-	X
55	MG	2A	3813	-	-	-	X
55	MG	2D	302	-	-	-	X
55	MG	2H	201	-	-	-	X
55	MG	2P	202	-	-	-	X
55	MG	2Q	8004	-	-	-	X
55	MG	2X	102	-	-	-	X
55	MG	2a	1609	-	-	-	X
55	MG	2a	1614	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
55	MG	2a	1631	-	-	-	X
55	MG	2a	1636	-	-	-	X
55	MG	2a	1637	-	-	-	X
55	MG	2a	1653	-	-	-	X
55	MG	2a	1656	-	-	-	X
55	MG	2a	1710	-	-	-	X
55	MG	2a	1734	-	-	-	X
55	MG	2a	1742	-	-	-	X
55	MG	2n	502	-	-	-	X

## 2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 293484 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
			Total	C	N	O	P			
1	1A	2872	Total	C	N	O	P	0	0	0
			61862	27535	11569	19886	2872			
1	2A	2867	Total	C	N	O	P	0	0	0
			61751	27486	11547	19852	2866			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1B	120	Total	C	N	O	P	0	0	0
			2575	1145	476	834	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2571	1146	476	831	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	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
			Total	C	N	O	S			
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
			1574	1004	294	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			Total	C	N	O	S			
10	2O	122	933	588	171	170	4	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	1S	110	877	553	175	149	0	0	0
14	2S	110	870	549	173	148	0	0	0

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

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

- 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
			775	498	141	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
			880	554	171	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			877	553	171	151	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	155	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	1m	116	914	564	189	159	2	0	0	0
44	2m	114	895	550	186	157	2	0	0	0

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

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

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

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

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

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

- 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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1x	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2x	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is a protein called Metalnikowin I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	1y	10	Total	C	N	O	0	0	0
			87	55	17	15			
54	2y	10	Total	C	N	O	0	0	0
			87	55	17	15			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1A	917	Total	Mg	0	0
			917	917		
55	1B	24	Total	Mg	0	0
			24	24		
55	1D	18	Total	Mg	0	0
			18	18		
55	1E	8	Total	Mg	0	0
			8	8		
55	1F	16	Total	Mg	0	0
			16	16		
55	1G	3	Total	Mg	0	0
			3	3		
55	1H	2	Total	Mg	0	0
			2	2		
55	1N	3	Total	Mg	0	0
			3	3		
55	1P	4	Total	Mg	0	0
			4	4		
55	1Q	5	Total	Mg	0	0
			5	5		
55	1R	5	Total	Mg	0	0
			5	5		
55	1S	1	Total	Mg	0	0
			1	1		
55	1T	1	Total	Mg	0	0
			1	1		
55	1U	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1V	3	Total Mg 3 3	0	0
55	1W	3	Total Mg 3 3	0	0
55	1X	1	Total Mg 1 1	0	0
55	1Y	1	Total Mg 1 1	0	0
55	10	8	Total Mg 8 8	0	0
55	11	3	Total Mg 3 3	0	0
55	13	2	Total Mg 2 2	0	0
55	15	6	Total Mg 6 6	0	0
55	17	5	Total Mg 5 5	0	0
55	18	3	Total Mg 3 3	0	0
55	19	2	Total Mg 2 2	0	0
55	1a	223	Total Mg 223 223	0	0
55	1b	1	Total Mg 1 1	0	0
55	1d	5	Total Mg 5 5	0	0
55	1e	2	Total Mg 2 2	0	0
55	1f	1	Total Mg 1 1	0	0
55	1g	1	Total Mg 1 1	0	0
55	1h	2	Total Mg 2 2	0	0
55	1k	1	Total Mg 1 1	0	0
55	1l	1	Total Mg 1 1	0	0
55	1m	1	Total Mg 1 1	0	0

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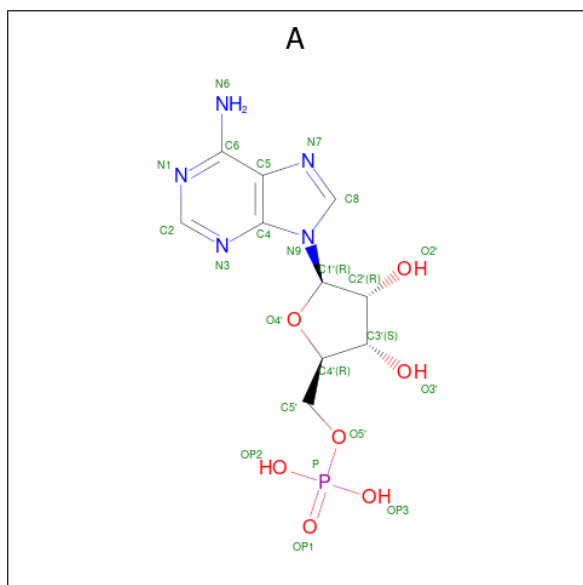
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1n	1	Total Mg 1 1	0	0
55	1o	1	Total Mg 1 1	0	0
55	1t	1	Total Mg 1 1	0	0
55	2A	821	Total Mg 821 821	0	0
55	2B	18	Total Mg 18 18	0	0
55	2D	11	Total Mg 11 11	0	0
55	2E	7	Total Mg 7 7	0	0
55	2F	10	Total Mg 10 10	0	0
55	2G	3	Total Mg 3 3	0	0
55	2H	1	Total Mg 1 1	0	0
55	2N	1	Total Mg 1 1	0	0
55	2P	2	Total Mg 2 2	0	0
55	2Q	5	Total Mg 5 5	0	0
55	2R	3	Total Mg 3 3	0	0
55	2S	1	Total Mg 1 1	0	0
55	2T	1	Total Mg 1 1	0	0
55	2U	4	Total Mg 4 4	0	0
55	2V	5	Total Mg 5 5	0	0
55	2W	1	Total Mg 1 1	0	0
55	2X	3	Total Mg 3 3	0	0
55	20	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	21	2	Total 2	Mg 2	0	0
55	23	1	Total 1	Mg 1	0	0
55	25	3	Total 3	Mg 3	0	0
55	27	4	Total 4	Mg 4	0	0
55	28	3	Total 3	Mg 3	0	0
55	2a	196	Total 196	Mg 196	0	0
55	2b	1	Total 1	Mg 1	0	0
55	2d	4	Total 4	Mg 4	0	0
55	2e	2	Total 2	Mg 2	0	0
55	2f	1	Total 1	Mg 1	0	0
55	2g	1	Total 1	Mg 1	0	0
55	2h	1	Total 1	Mg 1	0	0
55	2l	1	Total 1	Mg 1	0	0
55	2m	1	Total 1	Mg 1	0	0
55	2n	2	Total 2	Mg 2	0	0
55	2o	1	Total 1	Mg 1	0	0

- Molecule 56 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1B	1	Total C 1 1	0	0
56	2A	1	Total P 1 1	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	16	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	2Y	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0

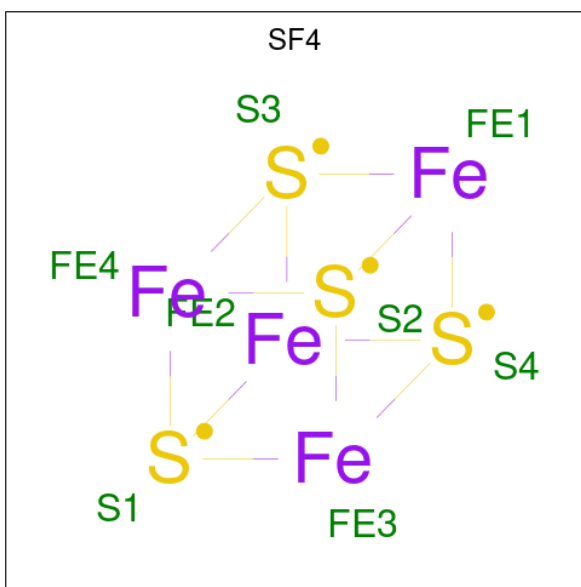
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	29	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1d	1	Total Fe S 8 4 4	0	0
58	2d	1	Total Fe S 8 4 4	0	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1740	Total O 1740 1740	0	0
59	1B	42	Total O 42 42	0	0
59	1D	14	Total O 14 14	0	0
59	1E	18	Total O 18 18	0	0
59	1F	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1G	2	Total 2	O 2	0	0
59	1H	3	Total 3	O 3	0	0
59	1N	9	Total 9	O 9	0	0
59	1P	13	Total 13	O 13	0	0
59	1Q	5	Total 5	O 5	0	0
59	1R	3	Total 3	O 3	0	0
59	1T	5	Total 5	O 5	0	0
59	1U	6	Total 6	O 6	0	0
59	1V	4	Total 4	O 4	0	0
59	1W	2	Total 2	O 2	0	0
59	1X	1	Total 1	O 1	0	0
59	1Y	5	Total 5	O 5	0	0
59	10	4	Total 4	O 4	0	0
59	11	2	Total 2	O 2	0	0
59	13	1	Total 1	O 1	0	0
59	15	2	Total 2	O 2	0	0
59	16	3	Total 3	O 3	0	0
59	17	1	Total 1	O 1	0	0
59	18	7	Total 7	O 7	0	0
59	19	2	Total 2	O 2	0	0
59	1a	393	Total 393	O 393	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1d	10	Total O 10 10	0	0
59	1e	3	Total O 3 3	0	0
59	1f	1	Total O 1 1	0	0
59	1h	1	Total O 1 1	0	0
59	1j	1	Total O 1 1	0	0
59	1l	3	Total O 3 3	0	0
59	1m	2	Total O 2 2	0	0
59	1n	1	Total O 1 1	0	0
59	1o	1	Total O 1 1	0	0
59	1t	2	Total O 2 2	0	0
59	2A	1666	Total O 1666 1666	0	0
59	2B	35	Total O 35 35	0	0
59	2D	12	Total O 12 12	0	0
59	2E	17	Total O 17 17	0	0
59	2F	11	Total O 11 11	0	0
59	2G	2	Total O 2 2	0	0
59	2H	3	Total O 3 3	0	0
59	2N	1	Total O 1 1	0	0
59	2P	9	Total O 9 9	0	0
59	2Q	5	Total O 5 5	0	0
59	2R	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2T	3	Total O 3 3	0	0
59	2U	2	Total O 2 2	0	0
59	2V	2	Total O 2 2	0	0
59	2W	2	Total O 2 2	0	0
59	2X	6	Total O 6 6	0	0
59	2Y	3	Total O 3 3	0	0
59	20	6	Total O 6 6	0	0
59	21	3	Total O 3 3	0	0
59	23	1	Total O 1 1	0	0
59	25	2	Total O 2 2	0	0
59	26	2	Total O 2 2	0	0
59	27	1	Total O 1 1	0	0
59	28	5	Total O 5 5	0	0
59	29	1	Total O 1 1	0	0
59	2a	384	Total O 384 384	0	0
59	2c	1	Total O 1 1	0	0
59	2d	7	Total O 7 7	0	0
59	2e	4	Total O 4 4	0	0
59	2f	1	Total O 1 1	0	0
59	2h	1	Total O 1 1	0	0
59	2j	1	Total O 1 1	0	0

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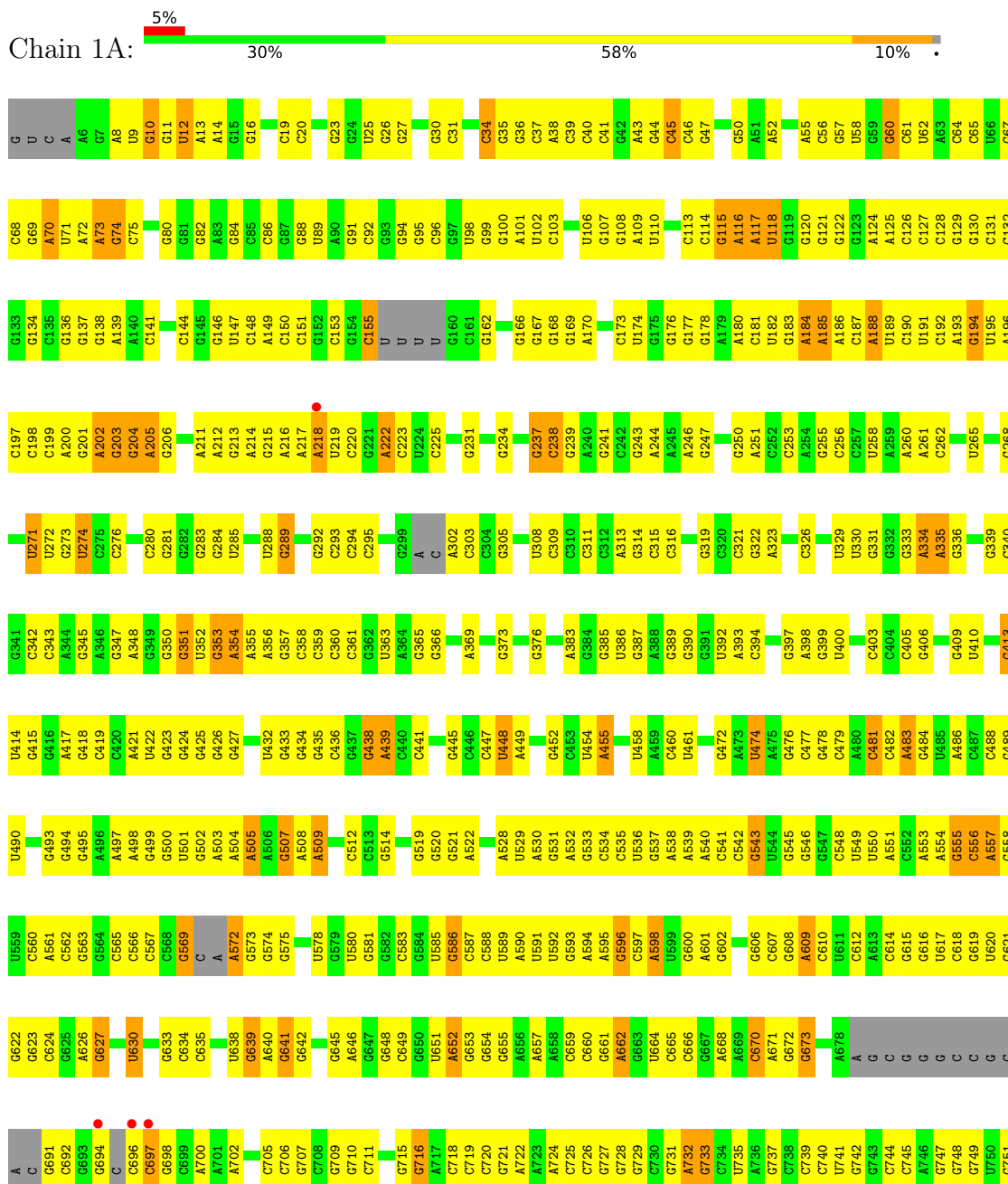
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
59	2l	3	Total O 3 3	0	0
59	2m	3	Total O 3 3	0	0
59	2o	1	Total O 1 1	0	0
59	2p	1	Total O 1 1	0	0
59	2t	1	Total O 1 1	0	0

### 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



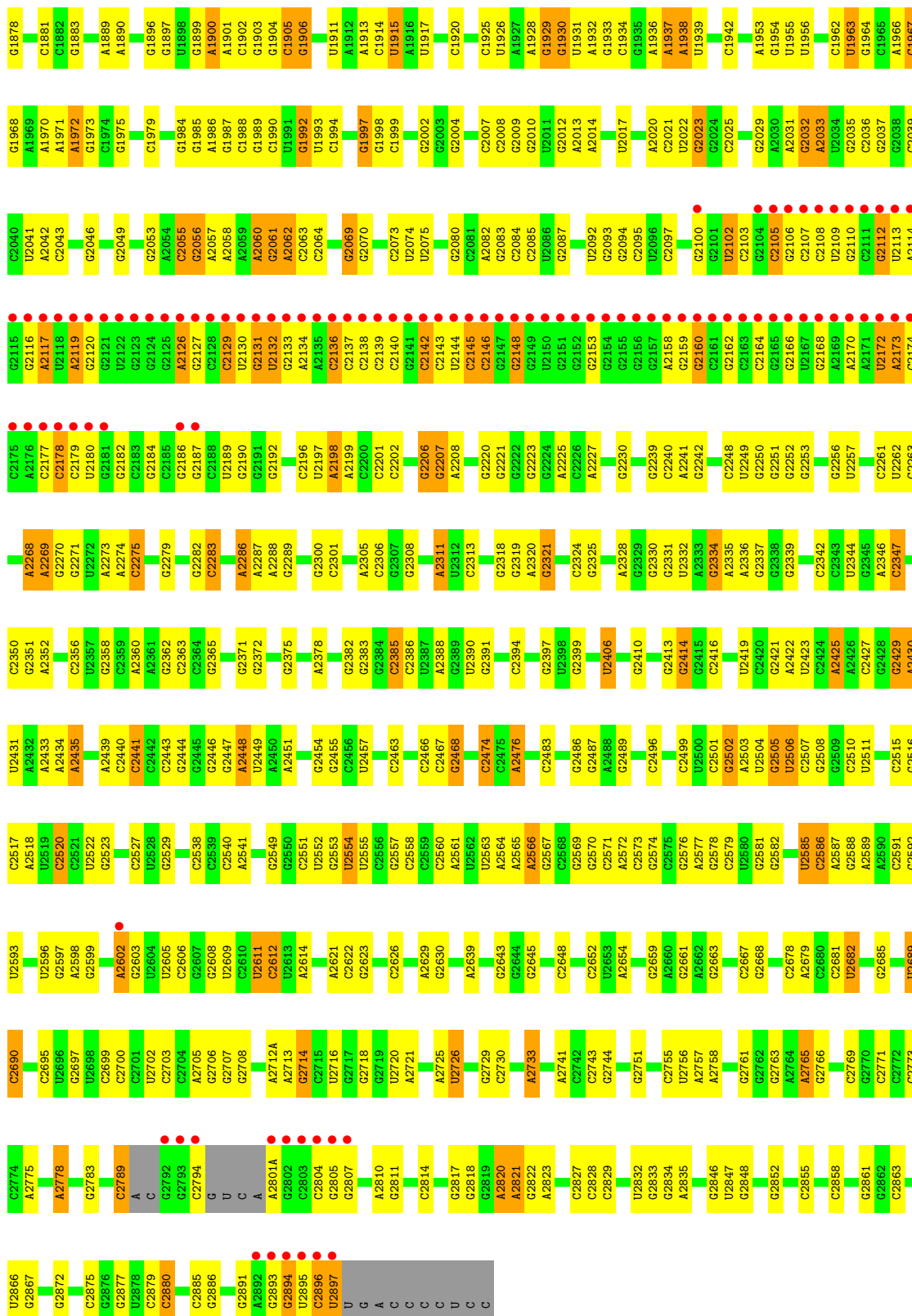


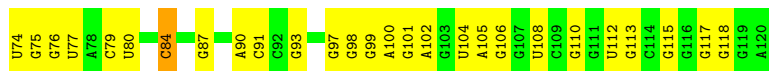
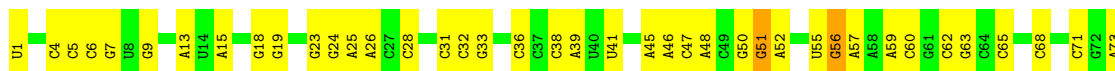
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A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530
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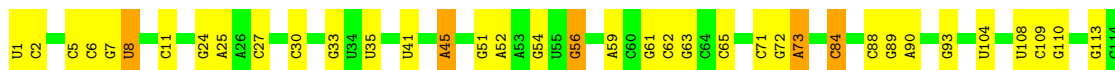








- Molecule 2: 5S ribosomal RNA



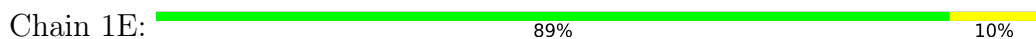
- Molecule 3: 50S ribosomal protein L2



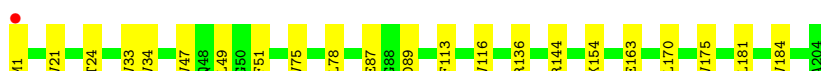
- Molecule 3: 50S ribosomal protein L2



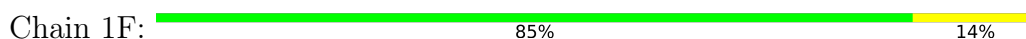
- Molecule 4: 50S ribosomal protein L3

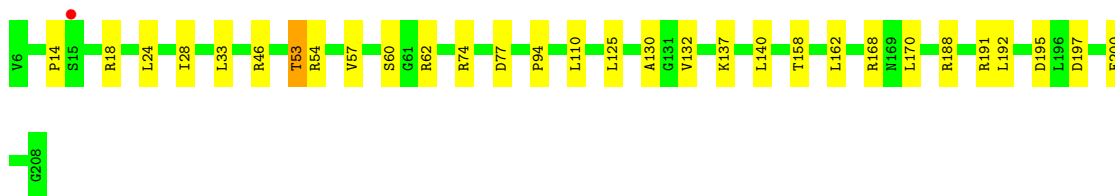


- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4





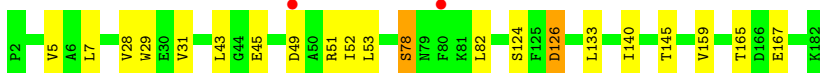
- Molecule 5: 50S ribosomal protein L4

Chain 2F: 91% 9%



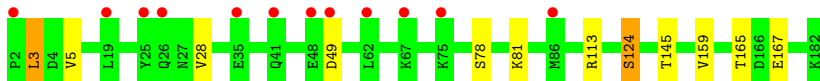
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 88% 10% 2%



- Molecule 6: 50S ribosomal protein L5

Chain 2G: 93% 6% 7%



- Molecule 7: 50S ribosomal protein L6

Chain 1H: 93% 7%



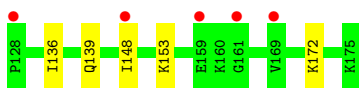
- Molecule 7: 50S ribosomal protein L6

Chain 2H: 87% 13% 16%



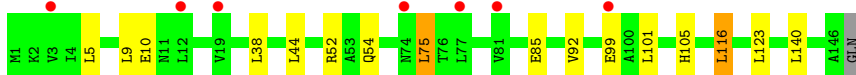
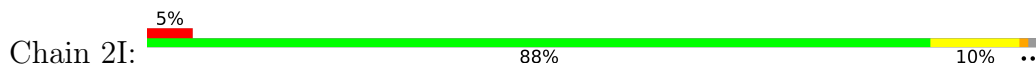
- Molecule 8: 50S ribosomal protein L9

Chain 1I: 88% 12%





- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13

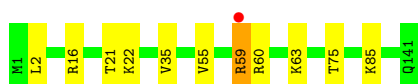
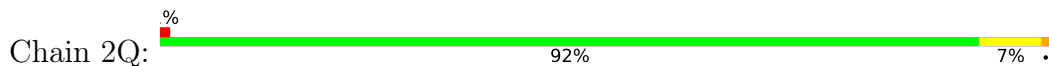




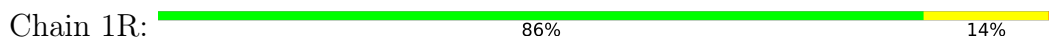
- Molecule 12: 50S ribosomal protein L16



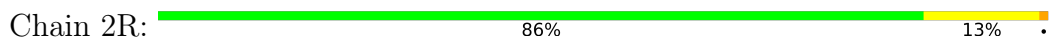
- Molecule 12: 50S ribosomal protein L16



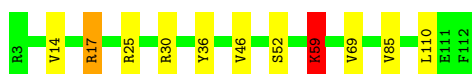
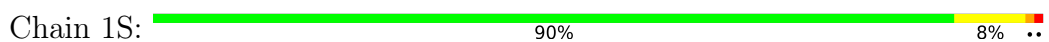
- Molecule 13: 50S ribosomal protein L17



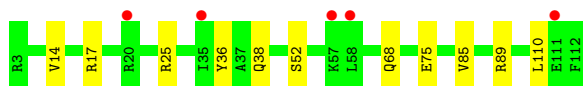
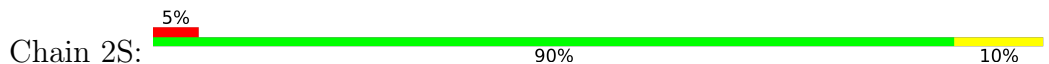
- Molecule 13: 50S ribosomal protein L17



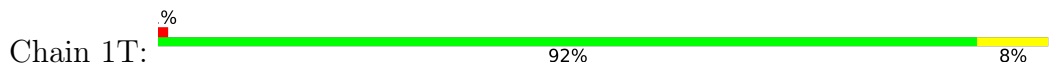
- Molecule 14: 50S ribosomal protein L18

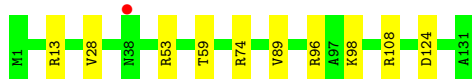


- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

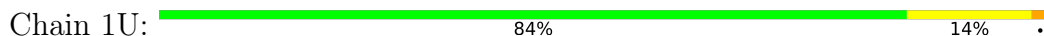




- Molecule 15: 50S ribosomal protein L19



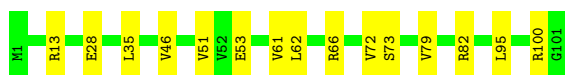
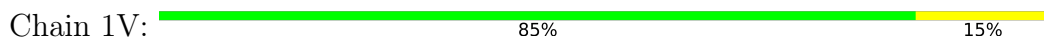
- Molecule 16: 50S ribosomal protein L20



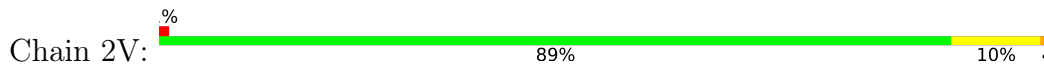
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21



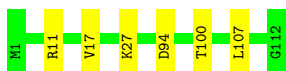
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22







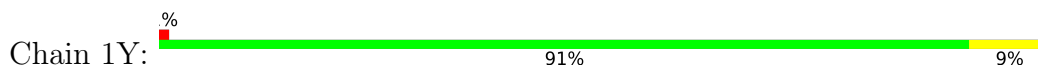
- Molecule 19: 50S ribosomal protein L23



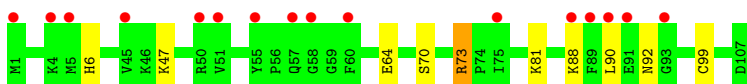
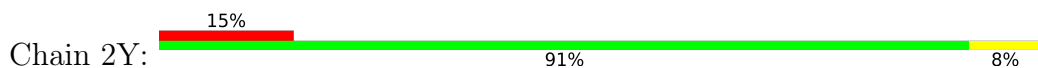
- Molecule 19: 50S ribosomal protein L23



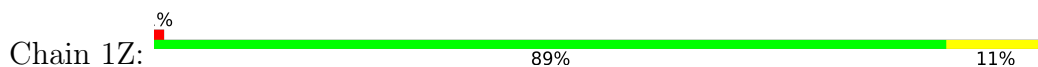
- Molecule 20: 50S ribosomal protein L24



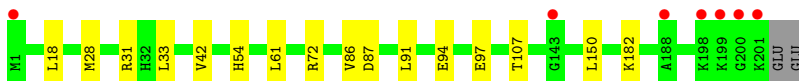
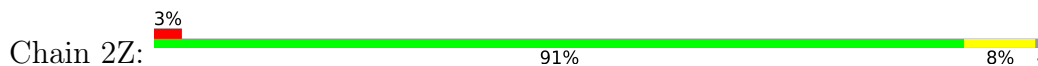
- Molecule 20: 50S ribosomal protein L24



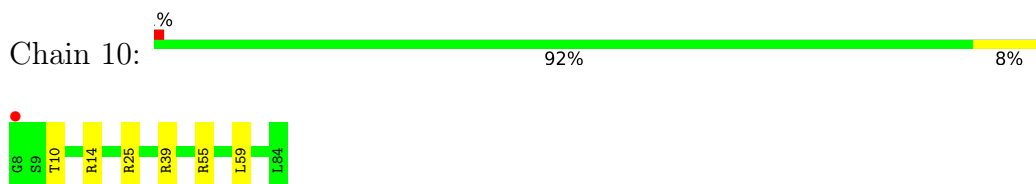
- Molecule 21: 50S ribosomal protein L25



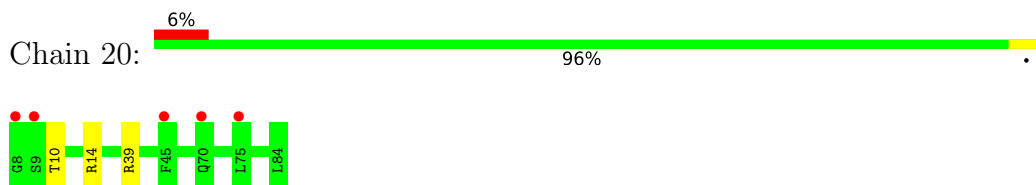
- Molecule 21: 50S ribosomal protein L25



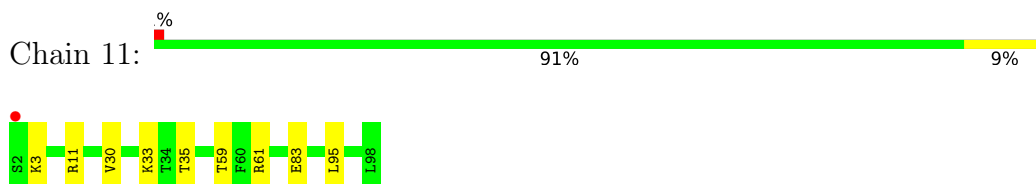
- Molecule 22: 50S ribosomal protein L27



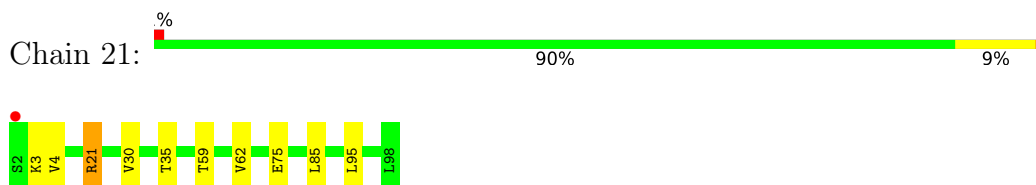
- Molecule 22: 50S ribosomal protein L27



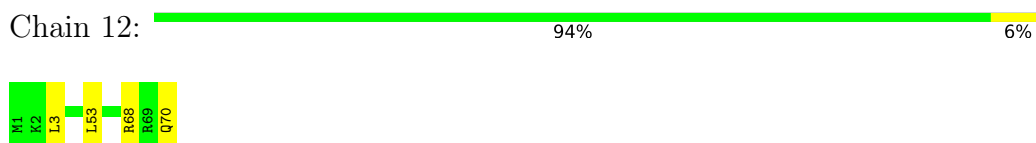
- Molecule 23: 50S ribosomal protein L28



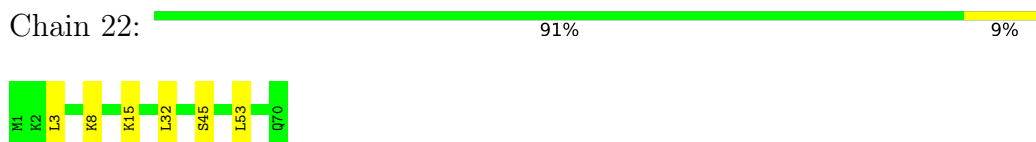
- Molecule 23: 50S ribosomal protein L28



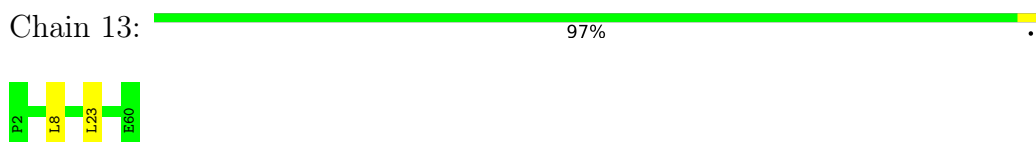
- Molecule 24: 50S ribosomal protein L29



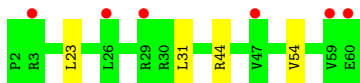
- Molecule 24: 50S ribosomal protein L29



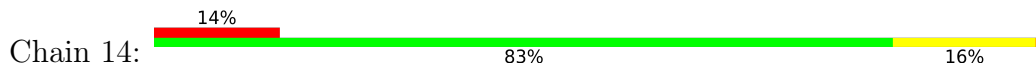
- Molecule 25: 50S ribosomal protein L30



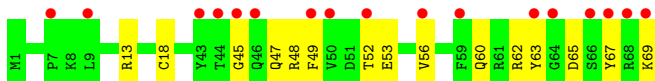
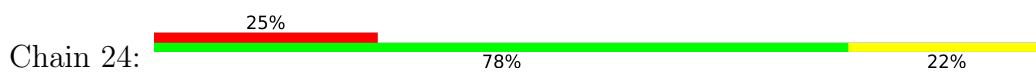
- Molecule 25: 50S ribosomal protein L30



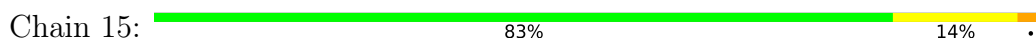
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



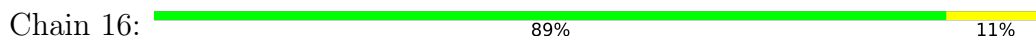
- Molecule 27: 50S ribosomal protein L32



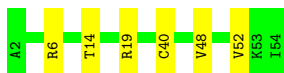
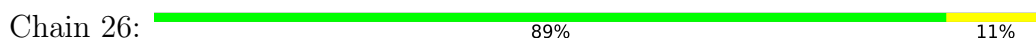
- Molecule 27: 50S ribosomal protein L32



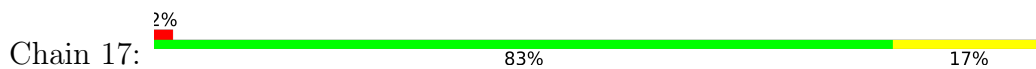
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



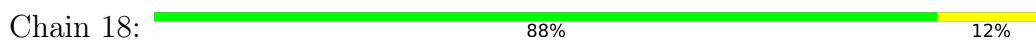
- Molecule 29: 50S ribosomal protein L34



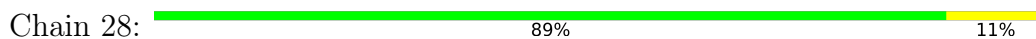
- Molecule 29: 50S ribosomal protein L34



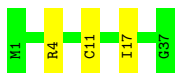
- Molecule 30: 50S ribosomal protein L35



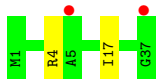
- Molecule 30: 50S ribosomal protein L35



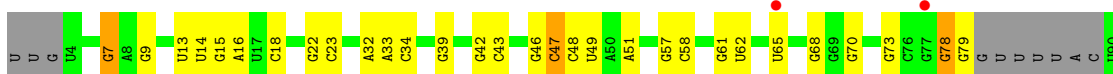
- Molecule 31: 50S ribosomal protein L36

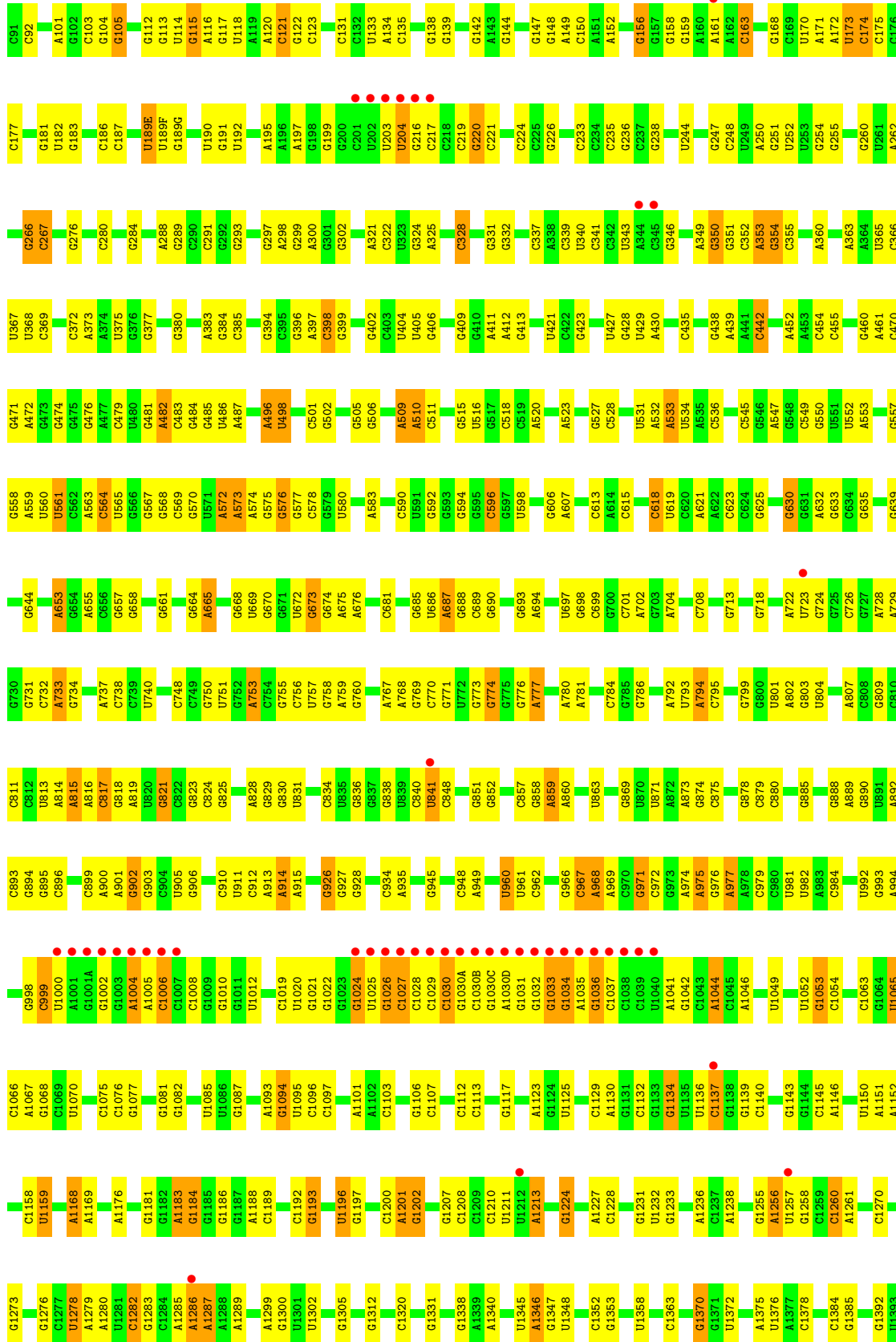


- Molecule 31: 50S ribosomal protein L36



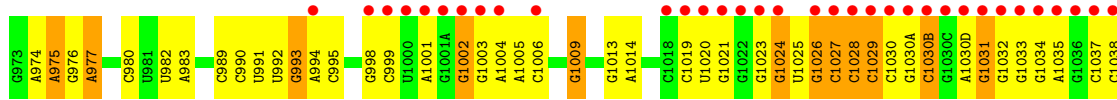
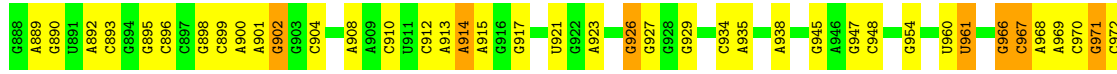
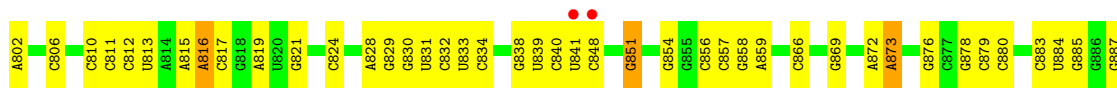
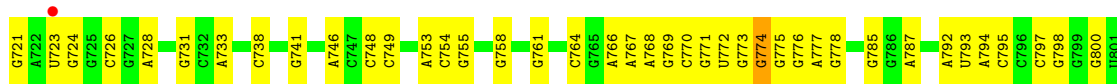
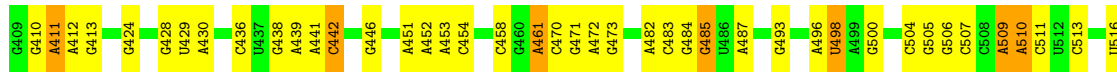
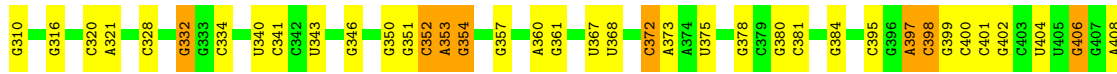
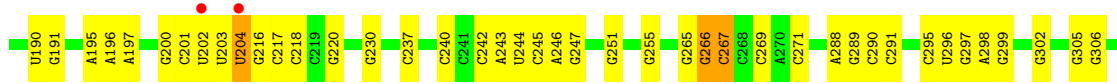
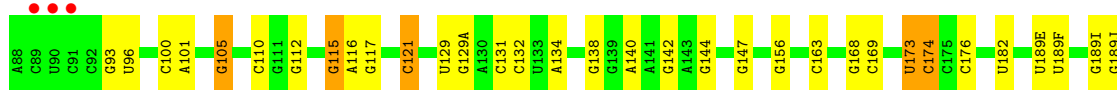
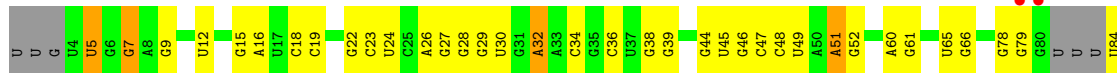
- Molecule 32: 16S ribosomal RNA

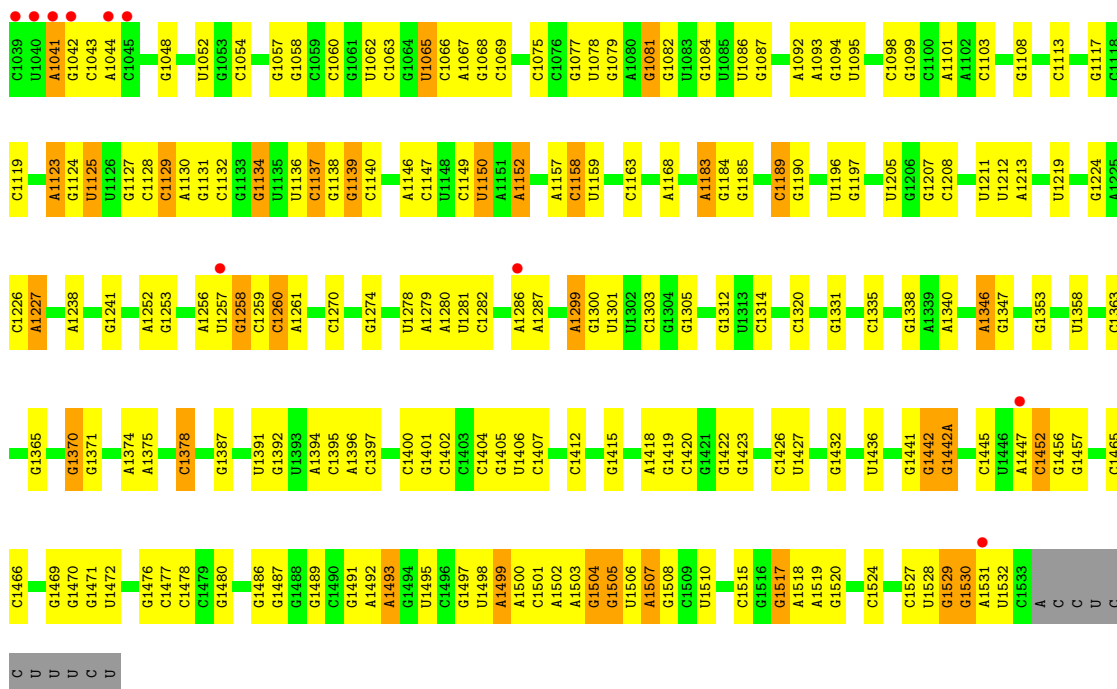




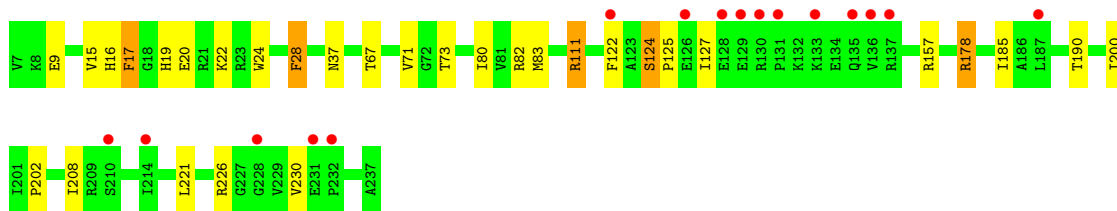
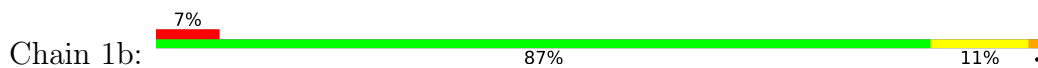


• Molecule 32: 16S ribosomal RNA

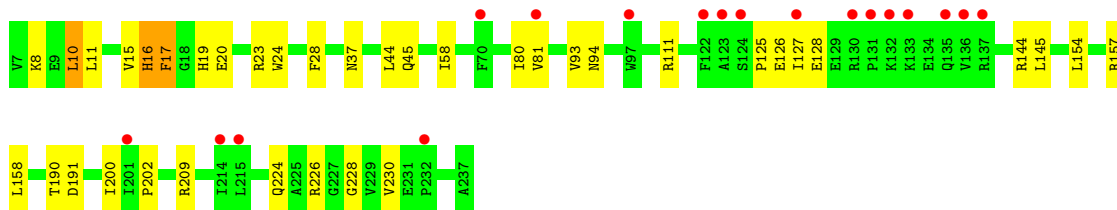
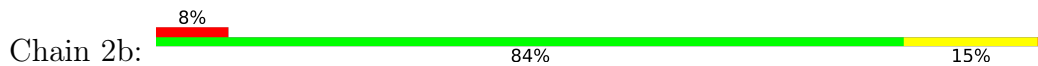




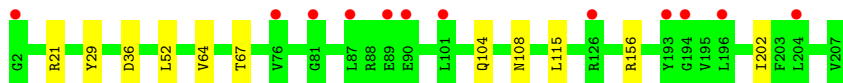
• Molecule 33: 30S ribosomal protein S2



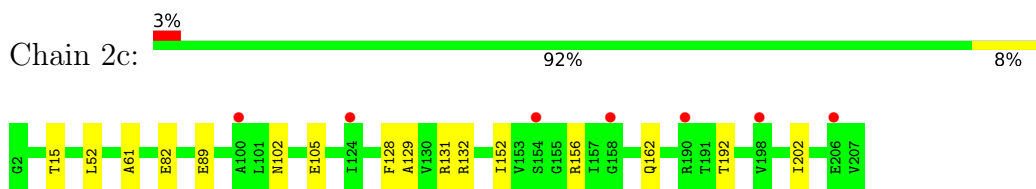
• Molecule 33: 30S ribosomal protein S2



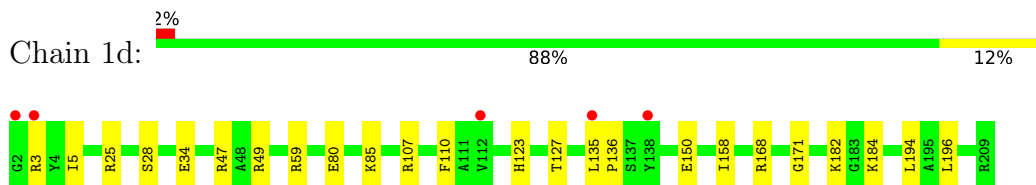
• Molecule 34: 30S ribosomal protein S3



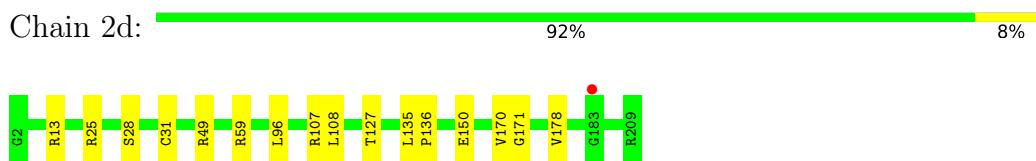
- Molecule 34: 30S ribosomal protein S3



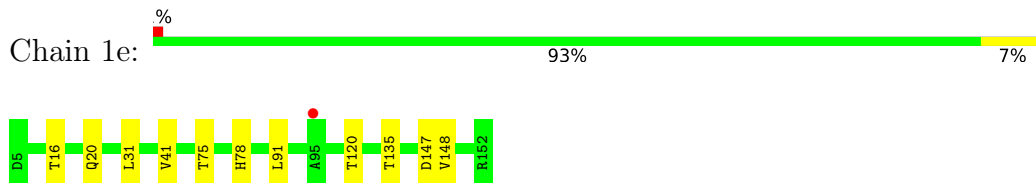
- Molecule 35: 30S ribosomal protein S4



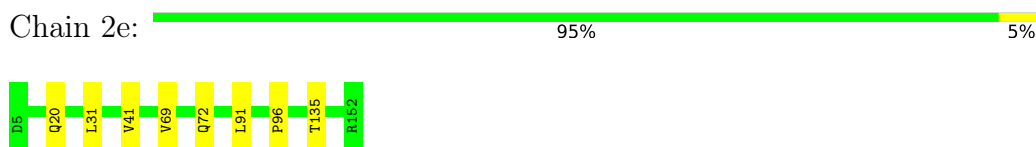
- Molecule 35: 30S ribosomal protein S4



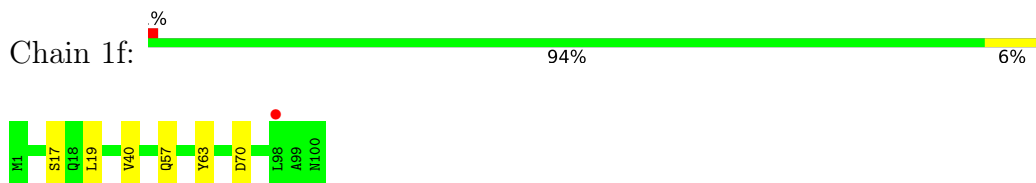
- Molecule 36: 30S ribosomal protein S5



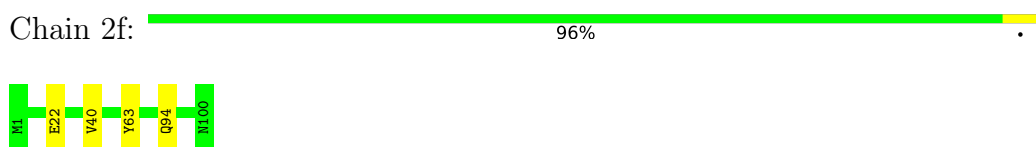
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

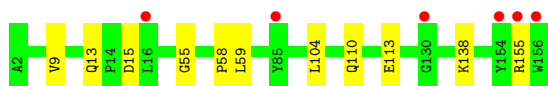
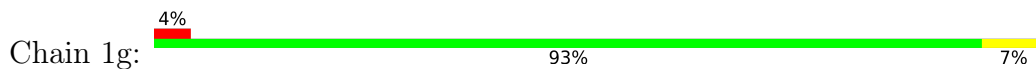


- Molecule 37: 30S ribosomal protein S6

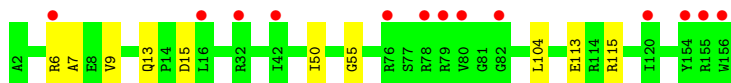




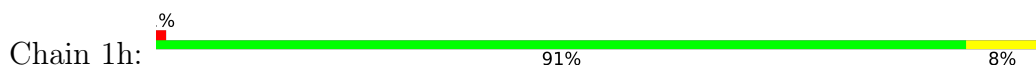
- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7



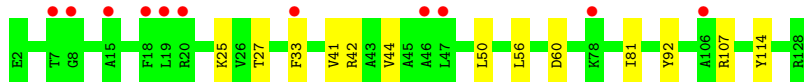
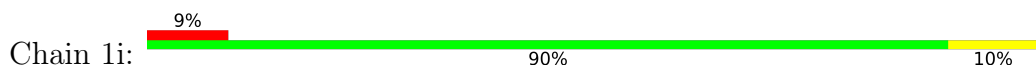
- Molecule 39: 30S ribosomal protein S8



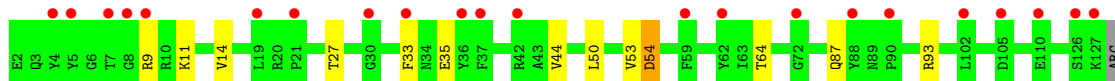
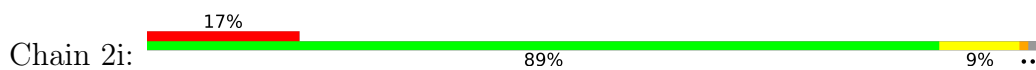
- Molecule 39: 30S ribosomal protein S8



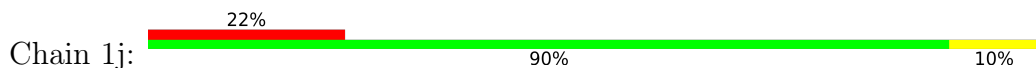
- Molecule 40: 30S ribosomal protein S9

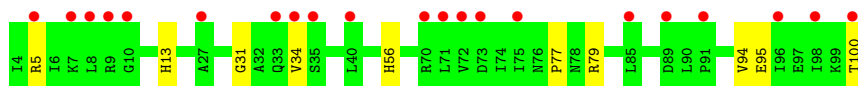


- Molecule 40: 30S ribosomal protein S9

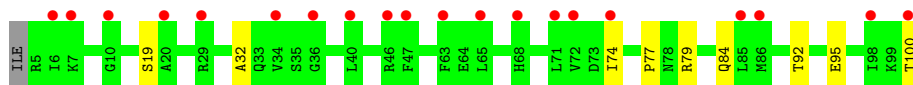
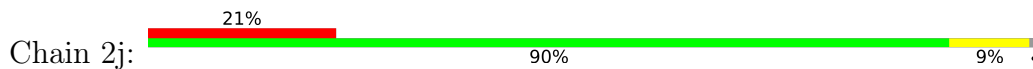


- Molecule 41: 30S ribosomal protein S10





- Molecule 41: 30S ribosomal protein S10



- Molecule 42: 30S ribosomal protein S11



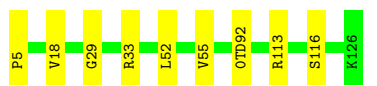
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



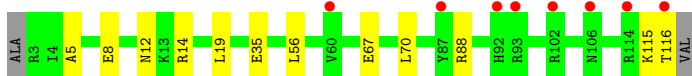
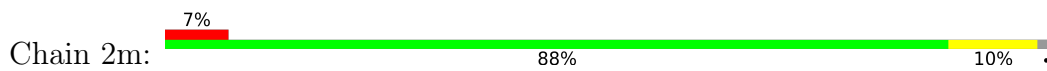
- Molecule 43: 30S ribosomal protein S12



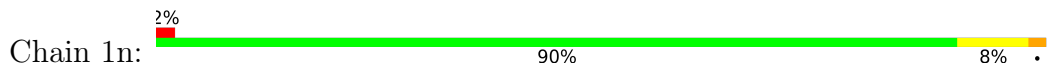
- Molecule 44: 30S ribosomal protein S13



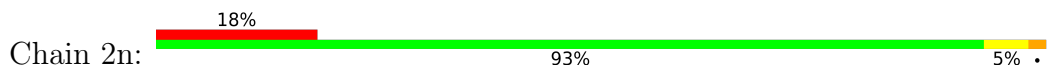
- Molecule 44: 30S ribosomal protein S13



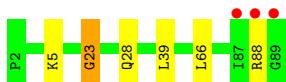
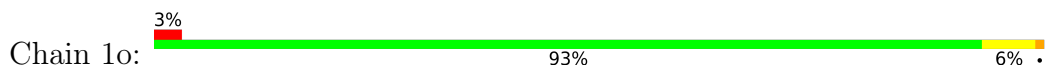
- Molecule 45: 30S ribosomal protein S14 type Z



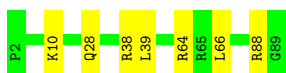
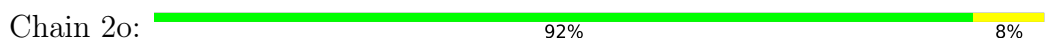
- Molecule 45: 30S ribosomal protein S14 type Z



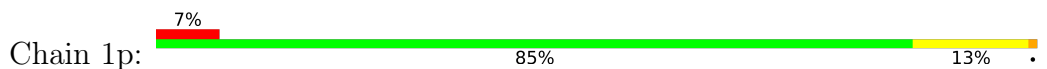
- Molecule 46: 30S ribosomal protein S15



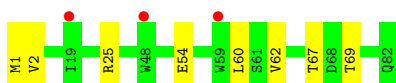
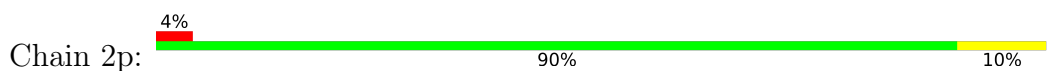
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



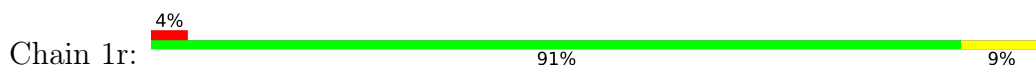
- Molecule 48: 30S ribosomal protein S17



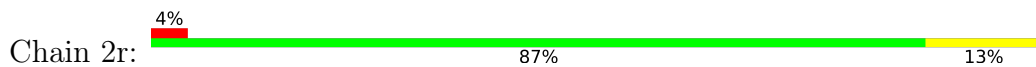
- Molecule 48: 30S ribosomal protein S17



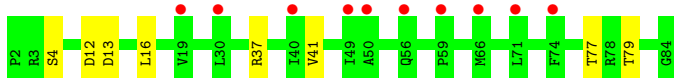
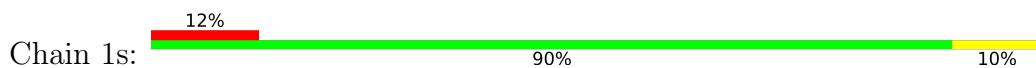
- Molecule 49: 30S ribosomal protein S18



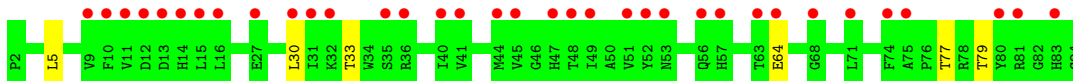
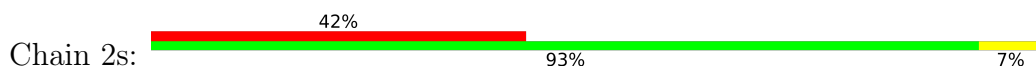
- Molecule 49: 30S ribosomal protein S18



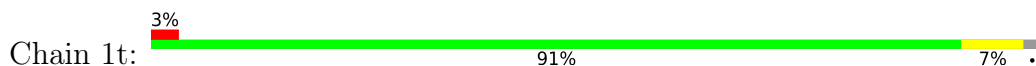
- Molecule 50: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S19

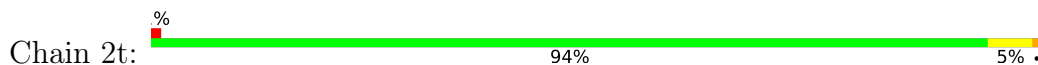


- Molecule 51: 30S ribosomal protein S20

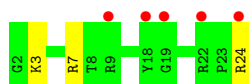
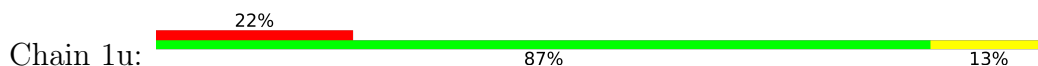




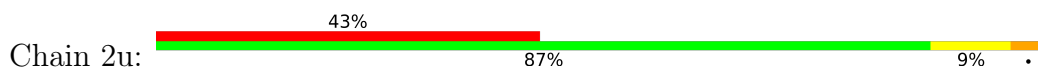
- Molecule 51: 30S ribosomal protein S20



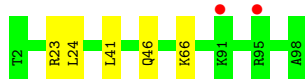
- Molecule 52: 30S ribosomal protein Thx



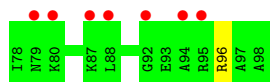
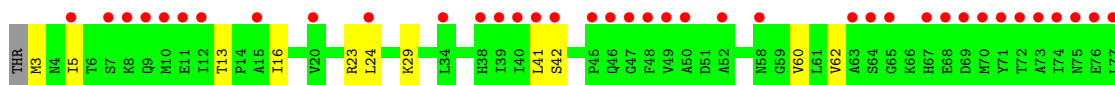
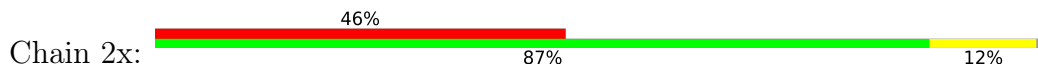
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A




- Molecule 53: Ribosome-associated inhibitor A

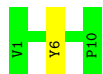


- Molecule 54: Metalnikowin I



- Molecule 54: Metalnikowin I

Chain 2y:  90% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.65Å 448.09Å 623.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.90 49.72 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.72-2.90) 99.1 (49.72-2.79)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 2.77Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.183 , 0.234 0.185 , 0.234	Depositor DCC
$R_{free}$ test set	69999 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	293484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, SF4, 0TD, 5MC, UR3, 7MG, M2G, 2MA, ZN, PSU, OMG, 4OC, 2MG, 5MU, OMU, MG

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	1.58	593/69021 (0.9%)	2.13	4360/107735 (4.0%)
1	2A	1.20	117/68892 (0.2%)	1.77	2077/107529 (1.9%)
2	1B	1.24	7/2879 (0.2%)	2.02	149/4490 (3.3%)
2	2B	1.00	1/2874 (0.0%)	1.65	63/4482 (1.4%)
3	1D	0.99	2/2181 (0.1%)	1.03	6/2940 (0.2%)
3	2D	0.81	0/2186	0.95	3/2944 (0.1%)
4	1E	1.01	1/1592 (0.1%)	1.09	8/2149 (0.4%)
4	2E	0.78	0/1592	0.93	1/2149 (0.0%)
5	1F	0.99	0/1619	1.06	6/2193 (0.3%)
5	2F	0.73	0/1609	0.86	0/2181
6	1G	0.72	1/1451 (0.1%)	0.89	1/1961 (0.1%)
6	2G	0.69	1/1449 (0.1%)	0.83	1/1957 (0.1%)
7	1H	0.83	0/1356	0.95	1/1834 (0.1%)
7	2H	0.70	0/1350	0.82	0/1826
8	1I	0.75	2/1109 (0.2%)	0.87	1/1512 (0.1%)
8	2I	0.68	0/1091	0.87	2/1490 (0.1%)
9	1N	0.98	0/1148	0.97	2/1547 (0.1%)
9	2N	0.64	0/1144	0.82	0/1543
10	1O	1.08	1/943 (0.1%)	1.04	2/1269 (0.2%)
10	2O	0.79	0/943	0.87	0/1269
11	1P	0.88	0/1152	1.01	4/1533 (0.3%)
11	2P	0.69	0/1152	0.86	1/1533 (0.1%)
12	1Q	0.98	2/1143 (0.2%)	0.99	3/1527 (0.2%)
12	2Q	0.68	0/1143	0.83	0/1527
13	1R	0.96	0/982	1.10	5/1312 (0.4%)
13	2R	0.73	0/982	0.94	3/1312 (0.2%)
14	1S	0.80	0/887	0.99	3/1180 (0.3%)
14	2S	0.66	0/880	0.85	0/1172
15	1T	0.91	1/1105 (0.1%)	1.08	4/1477 (0.3%)
15	2T	0.73	0/1097	0.93	1/1468 (0.1%)
16	1U	1.10	5/977 (0.5%)	1.07	4/1301 (0.3%)
16	2U	0.76	0/977	0.83	0/1301



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.98	1/786 (0.1%)	1.01	2/1053 (0.2%)
17	2V	0.67	0/782	0.85	0/1049
18	1W	1.09	1/891 (0.1%)	1.06	2/1198 (0.2%)
18	2W	0.84	0/888	0.92	1/1194 (0.1%)
19	1X	0.95	0/764	0.98	1/1025 (0.1%)
19	2X	0.76	0/764	0.84	1/1025 (0.1%)
20	1Y	0.95	1/823 (0.1%)	1.07	3/1099 (0.3%)
20	2Y	0.77	0/823	0.95	1/1100 (0.1%)
21	1Z	0.77	0/1620	0.86	1/2200 (0.0%)
21	2Z	0.66	0/1590	0.84	0/2162
22	10	0.91	0/616	0.97	1/821 (0.1%)
22	20	0.67	0/616	0.88	0/821
23	11	0.98	0/761	0.99	1/1013 (0.1%)
23	21	0.82	0/766	1.03	2/1018 (0.2%)
24	12	0.88	0/590	0.92	0/781
24	22	0.81	0/594	0.86	0/785
25	13	0.94	0/474	1.02	0/635
25	23	0.66	0/469	0.82	0/630
26	14	0.85	0/559	0.86	0/754
26	24	0.92	0/549	0.91	1/741 (0.1%)
27	15	1.11	2/473 (0.4%)	1.19	4/639 (0.6%)
27	25	0.81	1/469 (0.2%)	0.96	2/635 (0.3%)
28	16	0.94	1/460 (0.2%)	0.97	0/613
28	26	0.76	1/456 (0.2%)	0.81	0/608
29	17	1.08	1/426 (0.2%)	1.14	3/561 (0.5%)
29	27	0.81	0/426	0.97	2/561 (0.4%)
30	18	1.00	1/525 (0.2%)	0.96	1/691 (0.1%)
30	28	0.72	0/525	0.83	0/691
31	19	0.90	1/310 (0.3%)	0.96	0/407
31	29	0.60	0/310	0.78	0/407
32	1a	1.09	48/35795 (0.1%)	1.70	858/55864 (1.5%)
32	2a	1.04	35/35890 (0.1%)	1.67	813/56012 (1.5%)
33	1b	0.71	0/1876	0.92	3/2533 (0.1%)
33	2b	0.73	0/1860	0.89	0/2518
34	1c	0.67	0/1582	0.80	0/2137
34	2c	0.73	0/1566	0.83	0/2119
35	1d	0.68	0/1695	0.84	0/2274
35	2d	0.70	0/1698	0.86	0/2277
36	1e	0.66	0/1149	0.84	0/1548
36	2e	0.66	0/1149	0.87	0/1548
37	1f	0.68	0/827	0.82	1/1120 (0.1%)
37	2f	0.69	0/829	0.82	0/1123
38	1g	0.67	0/1254	0.80	1/1683 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.68	0/1248	0.79	0/1676
39	1h	0.66	0/1118	0.86	1/1506 (0.1%)
39	2h	0.62	0/1108	0.84	0/1494
40	1i	0.69	0/1005	0.82	0/1351
40	2i	0.75	0/985	0.87	1/1329 (0.1%)
41	1j	0.74	0/732	0.86	0/993
41	2j	0.73	0/723	0.81	0/984
42	1k	0.70	0/849	0.82	0/1150
42	2k	0.67	0/848	0.86	1/1149 (0.1%)
43	1l	0.69	0/937	0.84	0/1260
43	2l	0.68	0/937	0.89	1/1260 (0.1%)
44	1m	0.66	0/924	0.79	0/1242
44	2m	0.70	0/905	0.80	0/1217
45	1n	0.64	0/501	0.87	1/664 (0.2%)
45	2n	0.65	0/501	0.81	1/664 (0.2%)
46	1o	0.72	0/739	0.87	1/985 (0.1%)
46	2o	0.64	0/739	0.79	0/985
47	1p	0.63	0/697	0.86	0/939
47	2p	0.68	0/693	0.91	1/935 (0.1%)
48	1q	0.74	0/836	0.94	3/1117 (0.3%)
48	2q	0.68	0/836	0.92	1/1117 (0.1%)
49	1r	0.69	0/560	0.87	0/746
49	2r	0.70	0/560	0.81	0/746
50	1s	0.61	0/663	0.79	0/895
50	2s	0.72	0/660	0.81	1/893 (0.1%)
51	1t	0.67	0/734	0.88	0/969
51	2t	0.63	0/736	0.86	0/976
52	1u	0.57	0/203	0.73	0/266
52	2u	0.64	0/203	0.79	0/266
53	1x	0.67	0/776	0.78	0/1048
53	2x	0.67	0/761	0.77	0/1030
54	1y	1.01	0/90	1.06	0/122
54	2y	0.88	0/90	0.97	0/122
All	All	1.16	828/310078 (0.3%)	1.66	8429/463412 (1.8%)

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
19	1X	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	2X	0	1
33	1b	0	1
All	All	0	3

The worst 5 of 828 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	354	A	N9-C4	-12.86	1.30	1.37
1	1A	2633	A	N7-C5	-9.63	1.33	1.39
1	1A	2026	G	N7-C5	-9.47	1.33	1.39
1	2A	1046	A	N9-C4	9.45	1.43	1.37
1	1A	2037	A	N3-C4	-9.27	1.29	1.34

The worst 5 of 8429 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1208	C	O5'-P-OP1	-35.12	68.56	110.70
32	1a	1520	G	O5'-P-OP1	-30.95	73.56	110.70
32	1a	1520	G	O5'-P-OP2	27.90	144.18	110.70
32	2a	1208	C	OP1-P-OP2	-24.71	82.53	119.60
32	1a	1520	G	OP1-P-OP2	-23.77	83.94	119.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	124	SER	Peptide
19	2X	93	GLU	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/275 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/275 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	61
4	2E	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	29	61
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	29	61
5	2F	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	15	45
6	1G	179/181 (99%)	163 (91%)	12 (7%)	4 (2%)	6	24
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	9	31
7	1H	172/174 (99%)	163 (95%)	9 (5%)	0	100	100
7	2H	171/174 (98%)	164 (96%)	7 (4%)	0	100	100
8	1I	145/147 (99%)	127 (88%)	15 (10%)	3 (2%)	7	26
8	2I	144/147 (98%)	125 (87%)	16 (11%)	3 (2%)	7	26
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	51
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	19	51
11	1P	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	22	54
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	54
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	54
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	48
14	2S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	48
15	1T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
15	2T	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/116 (98%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	45
18	1W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
20	1Y	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
21	2Z	199/203 (98%)	189 (95%)	10 (5%)	0	100	100
22	10	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
22	20	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
23	11	95/97 (98%)	94 (99%)	0	1 (1%)	14	42
23	21	95/97 (98%)	93 (98%)	1 (1%)	1 (1%)	14	42
24	12	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
24	22	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
25	13	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
25	23	57/59 (97%)	54 (95%)	3 (5%)	0	100	100
26	14	67/69 (97%)	52 (78%)	11 (16%)	4 (6%)	1	4
26	24	67/69 (97%)	52 (78%)	10 (15%)	5 (8%)	1	2
27	15	57/59 (97%)	57 (100%)	0	0	100	100
27	25	57/59 (97%)	57 (100%)	0	0	100	100
28	16	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
28	26	51/53 (96%)	50 (98%)	1 (2%)	0	100	100
29	17	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
29	27	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
30	18	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
30	28	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/231 (99%)	190 (83%)	27 (12%)	12 (5%)	2	6
33	2b	229/231 (99%)	192 (84%)	27 (12%)	10 (4%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	1c	204/206 (99%)	171 (84%)	31 (15%)	2 (1%)	15	45
34	2c	204/206 (99%)	176 (86%)	25 (12%)	3 (2%)	10	34
35	1d	206/208 (99%)	183 (89%)	19 (9%)	4 (2%)	8	28
35	2d	206/208 (99%)	186 (90%)	17 (8%)	3 (2%)	10	34
36	1e	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	22	54
36	2e	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	22	54
37	1f	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/155 (99%)	143 (94%)	9 (6%)	1 (1%)	22	54
38	2g	153/155 (99%)	142 (93%)	8 (5%)	3 (2%)	7	27
39	1h	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
39	2h	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	6	22
40	2i	124/127 (98%)	105 (85%)	15 (12%)	4 (3%)	4	16
41	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	4	16
41	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	4	16
42	1k	112/114 (98%)	100 (89%)	11 (10%)	1 (1%)	17	48
42	2k	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
43	1l	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/116 (98%)	104 (91%)	5 (4%)	5 (4%)	2	10
44	2m	112/116 (97%)	103 (92%)	7 (6%)	2 (2%)	8	29
45	1n	58/60 (97%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	40
46	2o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	13	40
47	1p	80/82 (98%)	67 (84%)	12 (15%)	1 (1%)	12	37
47	2p	80/82 (98%)	65 (81%)	15 (19%)	0	100	100
48	1q	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/68 (97%)	61 (92%)	4 (6%)	1 (2%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	2r	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	10	34
50	1s	81/83 (98%)	73 (90%)	6 (7%)	2 (2%)	5	21
50	2s	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
51	1t	94/98 (96%)	87 (93%)	6 (6%)	1 (1%)	14	42
51	2t	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	4	16
52	1u	21/23 (91%)	19 (90%)	0	2 (10%)	0	1
52	2u	21/23 (91%)	17 (81%)	3 (14%)	1 (5%)	2	8
53	1x	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
53	2x	94/97 (97%)	90 (96%)	4 (4%)	0	100	100
54	1y	8/10 (80%)	8 (100%)	0	0	100	100
54	2y	8/10 (80%)	8 (100%)	0	0	100	100
All	All	11645/11862 (98%)	10762 (92%)	770 (7%)	113 (1%)	15	45

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	52	LEU
6	1G	49	ASP
6	1G	51	ARG
6	1G	78	SER
8	1I	73	GLU

### 5.3.2 Protein sidechains [i](#)

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	214/217 (99%)	190 (89%)	24 (11%)	6	18
3	2D	215/217 (99%)	195 (91%)	20 (9%)	9	27
4	1E	164/165 (99%)	147 (90%)	17 (10%)	7	21
4	2E	164/165 (99%)	144 (88%)	20 (12%)	5	15
5	1F	160/161 (99%)	136 (85%)	24 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	158/161 (98%)	142 (90%)	16 (10%)	7	23
6	1G	144/155 (93%)	127 (88%)	17 (12%)	5	16
6	2G	142/155 (92%)	133 (94%)	9 (6%)	18	46
7	1H	144/145 (99%)	132 (92%)	12 (8%)	11	32
7	2H	143/145 (99%)	121 (85%)	22 (15%)	2	8
8	1I	111/123 (90%)	97 (87%)	14 (13%)	4	13
8	2I	108/123 (88%)	95 (88%)	13 (12%)	5	15
9	1N	119/119 (100%)	105 (88%)	14 (12%)	5	16
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	19
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9	29
10	2O	100/100 (100%)	94 (94%)	6 (6%)	19	49
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	41
11	2P	115/116 (99%)	106 (92%)	9 (8%)	12	34
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	39
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	8	24
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4	13
13	2R	101/101 (100%)	87 (86%)	14 (14%)	3	10
14	1S	87/87 (100%)	77 (88%)	10 (12%)	5	17
14	2S	85/87 (98%)	75 (88%)	10 (12%)	5	16
15	1T	115/115 (100%)	109 (95%)	6 (5%)	23	55
15	2T	113/115 (98%)	108 (96%)	5 (4%)	28	61
16	1U	93/93 (100%)	82 (88%)	11 (12%)	5	16
16	2U	93/93 (100%)	86 (92%)	7 (8%)	13	37
17	1V	81/82 (99%)	70 (86%)	11 (14%)	3	11
17	2V	80/82 (98%)	69 (86%)	11 (14%)	3	10
18	1W	89/91 (98%)	81 (91%)	8 (9%)	9	29
18	2W	88/91 (97%)	83 (94%)	5 (6%)	20	51
19	1X	77/77 (100%)	71 (92%)	6 (8%)	12	34
19	2X	77/77 (100%)	75 (97%)	2 (3%)	46	77
20	1Y	86/88 (98%)	79 (92%)	7 (8%)	11	33
20	2Y	86/88 (98%)	76 (88%)	10 (12%)	5	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	169/176 (96%)	147 (87%)	22 (13%)	4	12
21	2Z	165/176 (94%)	149 (90%)	16 (10%)	8	25
22	10	61/62 (98%)	56 (92%)	5 (8%)	11	32
22	20	61/62 (98%)	58 (95%)	3 (5%)	25	57
23	11	79/82 (96%)	72 (91%)	7 (9%)	9	29
23	21	81/82 (99%)	72 (89%)	9 (11%)	6	19
24	12	65/66 (98%)	61 (94%)	4 (6%)	18	47
24	22	66/66 (100%)	60 (91%)	6 (9%)	9	28
25	13	51/51 (100%)	49 (96%)	2 (4%)	32	66
25	23	50/51 (98%)	46 (92%)	4 (8%)	12	33
26	14	58/62 (94%)	49 (84%)	9 (16%)	2	8
26	24	54/62 (87%)	45 (83%)	9 (17%)	2	6
27	15	51/51 (100%)	45 (88%)	6 (12%)	5	16
27	25	50/51 (98%)	47 (94%)	3 (6%)	19	49
28	16	51/51 (100%)	46 (90%)	5 (10%)	8	24
28	26	50/51 (98%)	45 (90%)	5 (10%)	7	23
29	17	41/41 (100%)	36 (88%)	5 (12%)	5	15
29	27	41/41 (100%)	38 (93%)	3 (7%)	14	38
30	18	54/54 (100%)	48 (89%)	6 (11%)	6	19
30	28	54/54 (100%)	47 (87%)	7 (13%)	4	12
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	49
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	49
33	1b	191/199 (96%)	170 (89%)	21 (11%)	6	19
33	2b	187/199 (94%)	156 (83%)	31 (17%)	2	7
34	1c	144/160 (90%)	135 (94%)	9 (6%)	18	46
34	2c	140/160 (88%)	127 (91%)	13 (9%)	9	27
35	1d	171/180 (95%)	151 (88%)	20 (12%)	5	16
35	2d	172/180 (96%)	159 (92%)	13 (8%)	13	36
36	1e	114/114 (100%)	104 (91%)	10 (9%)	10	30
36	2e	114/114 (100%)	107 (94%)	7 (6%)	18	48
37	1f	85/90 (94%)	80 (94%)	5 (6%)	19	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	59
38	1g	120/126 (95%)	111 (92%)	9 (8%)	13	37
38	2g	119/126 (94%)	112 (94%)	7 (6%)	19	49
39	1h	116/118 (98%)	104 (90%)	12 (10%)	7	22
39	2h	114/118 (97%)	106 (93%)	8 (7%)	15	41
40	1i	91/98 (93%)	81 (89%)	10 (11%)	6	19
40	2i	88/98 (90%)	79 (90%)	9 (10%)	7	22
41	1j	68/87 (78%)	61 (90%)	7 (10%)	7	22
41	2j	68/87 (78%)	62 (91%)	6 (9%)	10	30
42	1k	83/86 (96%)	79 (95%)	4 (5%)	25	58
42	2k	83/86 (96%)	75 (90%)	8 (10%)	8	25
43	1l	96/102 (94%)	90 (94%)	6 (6%)	18	46
43	2l	96/102 (94%)	89 (93%)	7 (7%)	14	38
44	1m	90/94 (96%)	83 (92%)	7 (8%)	12	34
44	2m	87/94 (93%)	77 (88%)	10 (12%)	5	17
45	1n	49/49 (100%)	43 (88%)	6 (12%)	5	15
45	2n	49/49 (100%)	45 (92%)	4 (8%)	11	32
46	1o	78/79 (99%)	73 (94%)	5 (6%)	17	45
46	2o	78/79 (99%)	72 (92%)	6 (8%)	13	35
47	1p	69/71 (97%)	57 (83%)	12 (17%)	2	6
47	2p	68/71 (96%)	61 (90%)	7 (10%)	7	22
48	1q	94/94 (100%)	88 (94%)	6 (6%)	17	45
48	2q	94/94 (100%)	88 (94%)	6 (6%)	17	45
49	1r	59/59 (100%)	54 (92%)	5 (8%)	10	31
49	2r	59/59 (100%)	51 (86%)	8 (14%)	3	11
50	1s	68/72 (94%)	62 (91%)	6 (9%)	10	30
50	2s	67/72 (93%)	62 (92%)	5 (8%)	13	37
51	1t	71/76 (93%)	65 (92%)	6 (8%)	10	31
51	2t	70/76 (92%)	66 (94%)	4 (6%)	20	51
52	1u	18/18 (100%)	17 (94%)	1 (6%)	21	52
52	2u	18/18 (100%)	15 (83%)	3 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	1x	82/83 (99%)	77 (94%)	5 (6%)	18	48
53	2x	79/83 (95%)	67 (85%)	12 (15%)	3	8
54	1y	10/10 (100%)	9 (90%)	1 (10%)	7	23
54	2y	10/10 (100%)	9 (90%)	1 (10%)	7	23
All	All	9540/9882 (96%)	8626 (90%)	914 (10%)	8	25

5 of 914 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	1x	66	LYS
49	2r	76	LEU
9	2N	73	THR
48	2q	63	ARG
37	2f	22	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
9	2N	8	GLN
33	2b	19	HIS
15	2T	58	ASN
21	2Z	73	GLN
34	2c	6	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	403 (14%)	58 (2%)
1	2A	2855/2915 (97%)	418 (14%)	51 (1%)
2	1B	119/120 (99%)	6 (5%)	0
2	2B	118/120 (98%)	8 (6%)	0
32	1a	1494/1521 (98%)	250 (16%)	0
32	2a	1498/1521 (98%)	249 (16%)	0
All	All	8948/9112 (98%)	1334 (14%)	109 (1%)

5 of 1334 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	60	G

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2902	G
1	2A	764	A
1	2A	2288	A
1	2A	196	A
1	2A	310	A

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

48 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	2MA	1A	2515	55,1	17,25,26	1.60	3 (17%)	17,37,40	2.04	4 (23%)
1	5MU	2A	1939	55,1	19,22,23	1.02	1 (5%)	28,32,35	1.52	4 (14%)
32	MA6	1a	1519	32	19,26,27	1.14	2 (10%)	18,38,41	4.49	3 (16%)
32	5MC	2a	1407	32	18,22,23	1.03	1 (5%)	26,32,35	1.29	3 (11%)
32	2MG	2a	1207	32	18,26,27	1.90	4 (22%)	16,38,41	1.16	2 (12%)
32	5MC	1a	967	32	18,22,23	0.99	2 (11%)	26,32,35	1.30	4 (15%)
1	5MC	2A	1942	1	18,22,23	0.79	0	26,32,35	1.16	2 (7%)
1	PSU	1A	2617	1	18,21,22	1.45	4 (22%)	22,30,33	1.51	5 (22%)
1	PSU	1A	1939	55,1	18,21,22	1.22	1 (5%)	22,30,33	1.77	4 (18%)
1	PSU	1A	1933	1	18,21,22	1.19	3 (16%)	22,30,33	1.55	6 (27%)
32	UR3	2a	1498	32	19,22,23	1.74	3 (15%)	26,32,35	1.88	6 (23%)
32	M2G	2a	966	32	20,27,28	3.04	7 (35%)	22,40,43	1.88	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	1A	1984	55,1	18,22,23	1.01	1 (5%)	26,32,35	1.56	5 (19%)
1	PSU	2A	1911	1	18,21,22	1.52	3 (16%)	22,30,33	1.47	5 (22%)
1	2MA	2A	2503	55,1	17,25,26	1.68	3 (17%)	17,37,40	1.53	3 (17%)
32	5MC	2a	1400	32	18,22,23	0.90	0	26,32,35	1.40	4 (15%)
32	MA6	1a	1518	32	19,26,27	0.94	2 (10%)	18,38,41	4.86	3 (16%)
1	5MC	2A	1962	55,1	18,22,23	1.48	2 (11%)	26,32,35	1.54	4 (15%)
1	OMG	2A	2251	55,1	18,26,27	1.77	5 (27%)	19,38,41	1.78	6 (31%)
32	7MG	2a	527	32	22,26,27	2.43	7 (31%)	29,39,42	1.87	7 (24%)
43	0TD	1l	92	43	7,9,10	2.25	2 (28%)	6,11,13	4.32	4 (66%)
1	5MU	1A	1961	55,1	19,22,23	1.04	2 (10%)	28,32,35	1.50	6 (21%)
32	PSU	2a	516	32	18,21,22	1.78	3 (16%)	22,30,33	2.23	5 (22%)
1	4OC	2A	1920	1	19,22,24	2.38	6 (31%)	26,31,35	1.14	3 (11%)
32	4OC	1a	1402	32	20,23,24	2.29	7 (35%)	26,32,35	1.00	2 (7%)
32	5MC	1a	1407	32	18,22,23	1.07	2 (11%)	26,32,35	1.43	5 (19%)
1	5MC	1A	1964	1	18,22,23	1.22	2 (11%)	26,32,35	1.39	3 (11%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	4.55	3 (16%)
32	5MC	2a	967	32	18,22,23	0.98	1 (5%)	26,32,35	1.70	7 (26%)
32	PSU	1a	516	55,32	18,21,22	1.55	4 (22%)	22,30,33	2.19	5 (22%)
1	PSU	2A	1917	1	18,21,22	1.12	1 (5%)	22,30,33	1.60	5 (22%)
1	OMU	2A	2552	55,1	19,22,23	6.61	10 (52%)	26,31,34	2.30	7 (26%)
1	PSU	2A	2605	1	18,21,22	1.53	1 (5%)	22,30,33	1.66	2 (9%)
32	4OC	2a	1402	32	20,23,24	2.63	7 (35%)	26,32,35	1.39	4 (15%)
1	5MU	2A	1915	1	19,22,23	1.82	3 (15%)	28,32,35	1.67	6 (21%)
32	MA6	2a	1519	32	19,26,27	1.12	2 (10%)	18,38,41	4.99	3 (16%)
32	M2G	1a	966	32	20,27,28	2.90	5 (25%)	22,40,43	1.73	6 (27%)
32	2MG	1a	1207	55,32	18,26,27	1.96	4 (22%)	16,38,41	1.97	6 (37%)
32	5MC	2a	1404	32	18,22,23	0.96	1 (5%)	26,32,35	1.46	4 (15%)
32	UR3	1a	1498	32	19,22,23	1.78	4 (21%)	26,32,35	1.29	2 (7%)
1	OMU	1A	2564	55,1	19,22,23	6.27	10 (52%)	26,31,34	2.62	9 (34%)
32	5MC	1a	1400	32	18,22,23	0.98	1 (5%)	26,32,35	1.61	6 (23%)
32	5MC	1a	1404	32	18,22,23	1.01	1 (5%)	26,32,35	1.55	4 (15%)
1	OMG	1A	2263	55,1	18,26,27	1.83	6 (33%)	19,38,41	1.82	6 (31%)
43	0TD	2l	92	43	7,9,10	1.67	1 (14%)	6,11,13	3.27	4 (66%)
32	7MG	1a	527	55,32	22,26,27	2.06	6 (27%)	29,39,42	1.66	8 (27%)
1	4OC	1A	1942	55,1	19,22,24	2.12	5 (26%)	26,31,35	1.29	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	1A	1937	1	19,22,23	1.56	3 (15%)	28,32,35	1.84	7 (25%)

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	2MA	1A	2515	55,1	-	1/3/25/26	0/3/3/3
1	5MU	2A	1939	55,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	55,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	1A	1984	55,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	55,1	-	2/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1962	55,1	-	2/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
32	7MG	2a	527	32	-	2/7/37/38	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
1	5MU	1A	1961	55,1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	2/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	55,32	-	1/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	55,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	2A	1915	1	-	4/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	2MG	1a	1207	55,32	-	2/5/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2564	55,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	55,1	-	1/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
32	7MG	1a	527	55,32	-	1/7/37/38	0/3/3/3
1	4OC	1A	1942	55,1	-	1/9/27/30	0/2/2/2
1	5MU	1A	1937	1	-	4/7/25/26	0/2/2/2

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-15.55	1.10	1.38
1	1A	2564	OMU	C4-N3	-14.51	1.12	1.38
1	2A	2552	OMU	C5-C4	14.17	1.75	1.43
1	1A	2564	OMU	C5-C4	13.91	1.74	1.43
1	2A	2552	OMU	C6-C5	-10.28	1.11	1.35

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	N1-C6-N6	-20.27	95.72	117.06
32	1a	1518	MA6	N1-C6-N6	-18.93	97.13	117.06
32	1a	1519	MA6	N1-C6-N6	-17.94	98.18	117.06
32	2a	1518	MA6	N1-C6-N6	-17.87	98.25	117.06
32	2a	516	PSU	C6-C5-C4	8.05	123.83	118.20

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C1'-N1-C2
1	1A	1937	5MU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	1A	1937	5MU	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C1'-C2'-O2'-CM2
32	1a	1402	4OC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2435 ligands modelled in this entry, 2431 are monoatomic and 2 are modelled with single atom - 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	$\# Z  > 2$
58	SF4	2d	501	35	0,12,12	-	-	-		
58	SF4	1d	501	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
58	SF4	2d	501	35	-	-	0/6/5/5
58	SF4	1d	501	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
1	2A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2A	2801(A):A	O3'	2802:G	P	3.50

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2861/2915 (98%)	0.04	136 (4%) 30 27	16, 34, 100, 113	0
1	2A	2856/2915 (97%)	0.02	141 (4%) 29 26	31, 56, 101, 114	0
2	1B	120/120 (100%)	-0.45	0 100 100	27, 51, 64, 93	0
2	2B	120/120 (100%)	-0.34	0 100 100	60, 79, 88, 96	0
3	1D	275/275 (100%)	-0.40	0 100 100	17, 34, 49, 74	0
3	2D	275/275 (100%)	-0.25	0 100 100	27, 49, 64, 83	0
4	1E	204/204 (100%)	-0.40	0 100 100	16, 37, 58, 73	0
4	2E	204/204 (100%)	-0.20	1 (0%) 91 91	31, 57, 73, 83	0
5	1F	203/203 (100%)	-0.29	1 (0%) 91 91	16, 38, 68, 92	0
5	2F	203/203 (100%)	-0.25	0 100 100	33, 66, 82, 91	0
6	1G	181/181 (100%)	-0.35	2 (1%) 80 80	47, 66, 83, 95	0
6	2G	181/181 (100%)	0.48	12 (6%) 18 14	76, 85, 92, 98	0
7	1H	174/174 (100%)	-0.42	1 (0%) 89 89	36, 51, 65, 70	0
7	2H	173/174 (99%)	0.77	28 (16%) 1 1	66, 85, 94, 98	0
8	1I	147/147 (100%)	-0.19	0 100 100	40, 71, 82, 87	0
8	2I	146/147 (99%)	0.35	7 (4%) 30 27	53, 80, 91, 97	0
9	1N	140/140 (100%)	-0.39	0 100 100	19, 33, 57, 73	0
9	2N	140/140 (100%)	-0.13	1 (0%) 87 87	46, 64, 76, 88	0
10	1O	122/122 (100%)	-0.40	0 100 100	26, 38, 55, 65	0
10	2O	122/122 (100%)	-0.36	0 100 100	41, 54, 68, 76	0
11	1P	149/149 (100%)	-0.27	0 100 100	17, 43, 64, 79	0
11	2P	149/149 (100%)	0.22	3 (2%) 65 63	38, 66, 83, 91	0
12	1Q	141/141 (100%)	-0.29	0 100 100	25, 38, 53, 68	0
12	2Q	141/141 (100%)	-0.30	1 (0%) 87 87	46, 63, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	-0.35	0 100 100	21, 32, 51, 61	0
13	2R	118/118 (100%)	-0.10	0 100 100	39, 53, 63, 76	0
14	1S	110/110 (100%)	-0.32	0 100 100	37, 51, 66, 69	0
14	2S	110/110 (100%)	0.31	5 (4%) 33 29	63, 75, 84, 86	0
15	1T	131/131 (100%)	-0.39	1 (0%) 86 86	32, 43, 70, 84	0
15	2T	131/131 (100%)	-0.31	0 100 100	48, 59, 79, 86	0
16	1U	116/116 (100%)	-0.46	0 100 100	19, 27, 42, 62	0
16	2U	116/116 (100%)	-0.15	0 100 100	41, 61, 77, 86	0
17	1V	101/101 (100%)	-0.39	0 100 100	17, 36, 54, 69	0
17	2V	101/101 (100%)	-0.11	1 (0%) 82 82	39, 72, 81, 89	0
18	1W	112/112 (100%)	-0.45	1 (0%) 84 84	19, 27, 50, 92	0
18	2W	112/112 (100%)	-0.25	0 100 100	38, 48, 67, 87	0
19	1X	95/95 (100%)	-0.37	0 100 100	22, 35, 62, 71	0
19	2X	95/95 (100%)	-0.06	1 (1%) 80 80	45, 61, 74, 78	0
20	1Y	107/107 (100%)	-0.32	1 (0%) 84 84	32, 47, 68, 78	0
20	2Y	107/107 (100%)	0.62	16 (14%) 2 1	55, 72, 84, 94	0
21	1Z	203/203 (100%)	-0.36	2 (0%) 82 82	40, 58, 77, 88	0
21	2Z	201/203 (99%)	0.18	7 (3%) 44 38	64, 79, 88, 95	0
22	10	77/77 (100%)	-0.29	1 (1%) 77 77	26, 35, 58, 65	0
22	20	77/77 (100%)	0.33	5 (6%) 18 14	53, 62, 74, 78	0
23	11	97/97 (100%)	-0.05	1 (1%) 82 82	25, 39, 67, 80	0
23	21	97/97 (100%)	-0.06	1 (1%) 82 82	40, 57, 79, 88	0
24	12	70/70 (100%)	-0.37	0 100 100	33, 47, 62, 82	0
24	22	70/70 (100%)	0.06	0 100 100	61, 71, 81, 83	0
25	13	59/59 (100%)	-0.35	0 100 100	21, 32, 58, 77	0
25	23	59/59 (100%)	0.62	6 (10%) 6 5	48, 62, 77, 82	0
26	14	69/69 (100%)	0.17	10 (14%) 2 1	63, 82, 96, 98	0
26	24	69/69 (100%)	1.04	17 (24%) 0 0	80, 92, 99, 100	0
27	15	59/59 (100%)	-0.41	0 100 100	15, 32, 48, 62	0
27	25	59/59 (100%)	-0.37	0 100 100	35, 52, 70, 76	0
28	16	53/53 (100%)	-0.40	0 100 100	32, 40, 55, 62	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/53 (100%)	-0.24	0 100 100	52, 62, 69, 76	0
29	17	48/48 (100%)	-0.20	1 (2%) 63 61	18, 24, 58, 65	0
29	27	48/48 (100%)	-0.12	0 100 100	32, 40, 66, 79	0
30	18	64/64 (100%)	-0.33	0 100 100	23, 30, 39, 48	0
30	28	64/64 (100%)	-0.02	0 100 100	41, 54, 64, 72	0
31	19	37/37 (100%)	-0.10	0 100 100	30, 40, 59, 71	0
31	29	37/37 (100%)	0.52	2 (5%) 25 22	61, 68, 79, 82	0
32	1a	1488/1521 (97%)	-0.02	48 (3%) 47 43	31, 74, 100, 114	0
32	2a	1492/1521 (98%)	-0.04	54 (3%) 42 37	41, 76, 100, 112	0
33	1b	231/231 (100%)	0.16	16 (6%) 16 13	67, 82, 92, 101	0
33	2b	231/231 (100%)	0.31	18 (7%) 13 10	68, 85, 94, 98	0
34	1c	206/206 (100%)	0.20	12 (5%) 23 19	70, 83, 92, 97	0
34	2c	206/206 (100%)	0.30	7 (3%) 45 40	77, 86, 93, 99	0
35	1d	208/208 (100%)	-0.06	5 (2%) 59 56	59, 76, 87, 91	0
35	2d	208/208 (100%)	-0.03	1 (0%) 91 91	61, 73, 84, 88	0
36	1e	148/148 (100%)	-0.14	1 (0%) 87 87	48, 69, 79, 96	0
36	2e	148/148 (100%)	-0.20	0 100 100	58, 71, 81, 89	0
37	1f	100/100 (100%)	-0.30	1 (1%) 82 82	53, 73, 80, 84	0
37	2f	100/100 (100%)	-0.44	0 100 100	57, 70, 82, 87	0
38	1g	155/155 (100%)	0.10	6 (3%) 39 35	67, 77, 86, 90	0
38	2g	155/155 (100%)	0.41	13 (8%) 11 8	73, 81, 89, 95	0
39	1h	137/137 (100%)	0.00	1 (0%) 87 87	55, 69, 77, 89	0
39	2h	137/137 (100%)	-0.12	1 (0%) 87 87	60, 72, 80, 87	0
40	1i	127/127 (100%)	0.56	11 (8%) 10 7	68, 86, 93, 97	0
40	2i	126/127 (99%)	1.03	22 (17%) 1 1	74, 88, 94, 97	0
41	1j	97/97 (100%)	1.13	21 (21%) 0 0	70, 87, 95, 98	0
41	2j	96/97 (98%)	1.08	20 (20%) 1 0	75, 89, 95, 97	0
42	1k	114/114 (100%)	-0.25	1 (0%) 84 84	40, 65, 81, 87	0
42	2k	114/114 (100%)	-0.06	1 (0%) 84 84	54, 71, 85, 91	0
43	1l	121/122 (99%)	-0.14	2 (1%) 70 69	47, 63, 75, 78	0
43	2l	121/122 (99%)	-0.14	0 100 100	54, 66, 75, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	116/116 (100%)	0.31	7 (6%) 21 18	71, 81, 88, 91	0
44	2m	114/116 (98%)	0.39	8 (7%) 16 12	76, 88, 93, 95	0
45	1n	60/60 (100%)	0.38	1 (1%) 70 69	71, 80, 88, 89	0
45	2n	60/60 (100%)	0.90	11 (18%) 1 0	76, 88, 92, 95	0
46	1o	88/88 (100%)	0.05	3 (3%) 45 40	46, 68, 80, 84	0
46	2o	88/88 (100%)	-0.10	0 100 100	55, 71, 83, 86	0
47	1p	82/82 (100%)	0.41	6 (7%) 15 11	64, 77, 86, 90	0
47	2p	82/82 (100%)	0.20	3 (3%) 41 37	58, 70, 79, 86	0
48	1q	99/99 (100%)	-0.04	1 (1%) 82 82	53, 68, 80, 84	0
48	2q	99/99 (100%)	-0.13	1 (1%) 82 82	57, 70, 79, 83	0
49	1r	68/68 (100%)	0.27	3 (4%) 34 30	55, 67, 80, 86	0
49	2r	68/68 (100%)	0.13	3 (4%) 34 30	61, 71, 82, 86	0
50	1s	83/83 (100%)	0.73	10 (12%) 4 3	76, 84, 91, 94	0
50	2s	83/83 (100%)	1.81	35 (42%) 0 0	84, 90, 97, 99	0
51	1t	96/98 (97%)	0.33	3 (3%) 49 44	64, 75, 86, 92	0
51	2t	98/98 (100%)	0.12	1 (1%) 82 82	56, 69, 83, 85	0
52	1u	23/23 (100%)	1.17	5 (21%) 0 0	72, 77, 83, 85	0
52	2u	23/23 (100%)	1.76	10 (43%) 0 0	79, 86, 89, 90	0
53	1x	97/97 (100%)	0.07	2 (2%) 63 61	52, 67, 81, 86	0
53	2x	96/97 (98%)	1.95	45 (46%) 0 0	72, 82, 93, 96	0
54	1y	10/10 (100%)	-0.26	0 100 100	30, 33, 40, 40	0
54	2y	10/10 (100%)	-0.13	0 100 100	43, 47, 58, 58	0
All	All	20786/20974 (99%)	0.01	833 (4%) 38 33	15, 64, 93, 114	0

The worst 5 of 833 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1133	G	17.7
1	1A	1118	C	12.5
1	1A	1135	G	12.5
1	1A	1137	G	12.0
1	1A	1121	C	11.6

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PSU	1A	1939	20/21	0.92	0.20	62,78,87,88	0
1	PSU	2A	1917	20/21	0.92	0.14	72,79,85,102	0
1	5MU	1A	1937	21/22	0.93	0.22	79,86,100,113	0
1	5MU	2A	1915	21/22	0.94	0.16	79,87,92,108	0
32	PSU	2a	516	20/21	0.94	0.16	72,83,88,90	0
32	2MG	2a	1207	24/25	0.94	0.17	81,90,95,99	0
32	5MC	2a	967	21/22	0.95	0.15	67,73,82,90	0
32	PSU	1a	516	20/21	0.95	0.15	66,74,77,77	0
1	PSU	2A	1911	20/21	0.96	0.11	65,73,80,81	0
32	M2G	1a	966	25/26	0.96	0.14	52,62,74,77	0
32	5MC	1a	967	21/22	0.96	0.14	57,65,75,83	0
32	2MG	1a	1207	24/25	0.96	0.12	76,81,85,85	0
32	7MG	2a	527	24/25	0.96	0.17	69,74,77,79	0
32	M2G	2a	966	25/26	0.96	0.14	67,71,86,94	0
32	5MC	1a	1407	21/22	0.96	0.14	44,53,58,61	0
43	0TD	1l	92	10/11	0.96	0.14	63,65,74,80	0
32	5MC	2a	1400	21/22	0.96	0.20	65,74,78,83	0
32	4OC	2a	1402	22/23	0.96	0.16	52,60,65,67	0
32	5MC	2a	1404	21/22	0.96	0.14	49,53,60,64	0
43	0TD	2l	92	10/11	0.96	0.15	71,73,77,92	0
1	PSU	2A	2605	20/21	0.97	0.17	33,35,41,41	0
1	4OC	1A	1942	21/23	0.97	0.16	47,59,64,65	0
32	UR3	1a	1498	21/22	0.97	0.19	41,50,56,59	0
1	PSU	1A	1933	20/21	0.97	0.15	57,70,74,76	0
32	7MG	1a	527	24/25	0.97	0.16	50,63,66,71	0
32	4OC	1a	1402	22/23	0.97	0.17	45,52,58,61	0
32	5MC	1a	1404	21/22	0.97	0.15	44,48,55,59	0
1	4OC	2A	1920	21/23	0.97	0.16	54,65,70,72	0
1	5MC	2A	1942	21/22	0.97	0.17	46,53,57,61	0
32	5MC	2a	1407	21/22	0.97	0.14	50,59,63,65	0
32	UR3	2a	1498	21/22	0.97	0.15	47,56,64,66	0
1	2MA	2A	2503	23/24	0.97	0.21	30,35,40,48	0
32	MA6	1a	1518	24/25	0.98	0.17	38,49,52,57	0
32	MA6	1a	1519	24/25	0.98	0.17	41,50,55,58	0
1	2MA	1A	2515	23/24	0.98	0.19	16,20,24,25	0
1	OMU	1A	2564	21/22	0.98	0.18	21,26,29,32	0
32	5MC	1a	1400	21/22	0.98	0.16	54,59,64,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	1A	2617	20/21	0.98	0.18	20,24,30,33	0
1	5MU	1A	1961	21/22	0.98	0.15	20,26,29,33	0
1	5MU	2A	1939	21/22	0.98	0.15	30,36,42,44	0
1	5MC	1A	1964	21/22	0.98	0.13	25,36,39,42	0
1	5MC	2A	1962	21/22	0.98	0.13	34,44,51,60	0
1	OMG	2A	2251	24/25	0.98	0.17	35,39,44,46	0
32	MA6	2a	1518	24/25	0.98	0.17	50,59,65,66	0
32	MA6	2a	1519	24/25	0.98	0.19	52,58,64,69	0
1	5MC	1A	1984	21/22	0.98	0.14	30,32,36,41	0
1	OMG	1A	2263	24/25	0.99	0.16	16,22,25,27	0
1	OMU	2A	2552	21/22	0.99	0.15	30,36,40,42	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3533	1/1	0.04	0.39	99,99,99,99	0
55	MG	2A	3768	1/1	0.23	0.36	95,95,95,95	0
55	MG	2A	3606	1/1	0.32	0.27	68,68,68,68	0
55	MG	1P	203	1/1	0.34	0.20	90,90,90,90	0
55	MG	2A	3090	1/1	0.38	0.41	76,76,76,76	0
55	MG	1a	3161	1/1	0.41	0.82	77,77,77,77	0
55	MG	1a	3005	1/1	0.41	0.19	81,81,81,81	0
55	MG	2A	3455	1/1	0.41	0.58	59,59,59,59	0
55	MG	2A	3792	1/1	0.41	1.02	79,79,79,79	0
55	MG	2A	3010	1/1	0.42	0.32	63,63,63,63	0
55	MG	1A	3246	1/1	0.45	0.19	78,78,78,78	0
55	MG	1A	3861	1/1	0.45	0.08	82,82,82,82	0
55	MG	2A	3800	1/1	0.45	0.27	112,112,112,112	0
55	MG	2A	3129	1/1	0.46	0.62	75,75,75,75	0
55	MG	2A	3553	1/1	0.46	1.09	89,89,89,89	0
55	MG	1a	3149	1/1	0.48	0.23	104,104,104,104	0
55	MG	1A	3702	1/1	0.48	0.72	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2B	3011	1/1	0.48	0.21	90,90,90,90	0
55	MG	2A	3101	1/1	0.49	0.22	74,74,74,74	0
55	MG	1F	314	1/1	0.49	0.30	53,53,53,53	0
55	MG	2B	3012	1/1	0.49	0.09	87,87,87,87	0
55	MG	1a	3215	1/1	0.50	0.25	86,86,86,86	0
55	MG	2A	3752	1/1	0.51	0.36	77,77,77,77	0
55	MG	2A	3502	1/1	0.51	0.31	70,70,70,70	0
55	MG	2a	1686	1/1	0.51	0.25	108,108,108,108	0
55	MG	2A	3172	1/1	0.53	0.34	69,69,69,69	0
55	MG	1A	3516	1/1	0.54	0.51	35,35,35,35	0
55	MG	2A	3511	1/1	0.55	0.14	90,90,90,90	0
55	MG	2A	3064	1/1	0.56	0.10	72,72,72,72	0
55	MG	2A	3142	1/1	0.56	0.97	60,60,60,60	0
55	MG	1Q	204	1/1	0.57	0.47	52,52,52,52	0
55	MG	2A	3162	1/1	0.57	0.36	82,82,82,82	0
55	MG	2d	504	1/1	0.57	0.14	90,90,90,90	0
55	MG	2n	502	1/1	0.57	0.42	82,82,82,82	0
55	MG	1A	3848	1/1	0.58	0.66	68,68,68,68	0
55	MG	1A	3181	1/1	0.59	0.24	51,51,51,51	0
55	MG	1A	3095	1/1	0.59	0.78	61,61,61,61	0
55	MG	1B	3006	1/1	0.60	0.21	59,59,59,59	0
55	MG	2A	3643	1/1	0.60	1.12	60,60,60,60	0
55	MG	2A	3706	1/1	0.60	0.13	90,90,90,90	0
55	MG	27	103	1/1	0.60	0.59	70,70,70,70	0
55	MG	2A	3080	1/1	0.60	0.41	69,69,69,69	0
55	MG	2A	3510	1/1	0.60	0.21	103,103,103,103	0
55	MG	2A	3563	1/1	0.60	0.65	77,77,77,77	0
55	MG	2a	1742	1/1	0.61	0.57	113,113,113,113	0
55	MG	2A	3672	1/1	0.61	0.28	59,59,59,59	0
55	MG	1A	3077	1/1	0.61	0.61	47,47,47,47	0
55	MG	1a	3058	1/1	0.62	0.69	82,82,82,82	0
55	MG	1A	3899	1/1	0.63	0.38	51,51,51,51	0
55	MG	1B	3002	1/1	0.63	0.28	69,69,69,69	0
55	MG	2e	3002	1/1	0.63	0.34	83,83,83,83	0
55	MG	2A	3019	1/1	0.63	0.22	45,45,45,45	0
55	MG	1A	3183	1/1	0.64	0.63	46,46,46,46	0
55	MG	2A	3574	1/1	0.64	0.23	98,98,98,98	0
55	MG	2A	3476	1/1	0.64	0.48	78,78,78,78	0
55	MG	2B	3013	1/1	0.64	0.12	84,84,84,84	0
55	MG	2D	302	1/1	0.64	0.45	58,58,58,58	0
55	MG	1A	3131	1/1	0.64	0.21	62,62,62,62	0
55	MG	2A	3507	1/1	0.64	0.56	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3074	1/1	0.64	0.45	48,48,48,48	0
55	MG	2a	1770	1/1	0.64	0.18	75,75,75,75	0
55	MG	1A	3396	1/1	0.64	0.48	66,66,66,66	0
55	MG	1A	3456	1/1	0.64	0.23	59,59,59,59	0
55	MG	2A	3320	1/1	0.64	0.13	79,79,79,79	0
55	MG	2a	1731	1/1	0.65	0.10	90,90,90,90	0
55	MG	2A	3582	1/1	0.65	0.61	64,64,64,64	0
55	MG	2a	1747	1/1	0.65	0.23	94,94,94,94	0
55	MG	1A	3244	1/1	0.65	0.81	72,72,72,72	0
55	MG	1a	3022	1/1	0.65	0.69	66,66,66,66	0
55	MG	1A	3165	1/1	0.65	0.30	80,80,80,80	0
55	MG	1a	3004	1/1	0.65	0.19	69,69,69,69	0
55	MG	1A	3498	1/1	0.66	0.10	70,70,70,70	0
55	MG	1A	3684	1/1	0.66	0.26	49,49,49,49	0
55	MG	1A	3503	1/1	0.66	0.40	77,77,77,77	0
55	MG	2G	3003	1/1	0.66	0.12	81,81,81,81	0
55	MG	1n	502	1/1	0.66	0.29	63,63,63,63	0
55	MG	2a	1637	1/1	0.66	1.07	71,71,71,71	0
55	MG	2A	3441	1/1	0.66	0.21	90,90,90,90	0
55	MG	2A	3184	1/1	0.67	0.38	73,73,73,73	0
55	MG	2A	3246	1/1	0.67	0.09	92,92,92,92	0
55	MG	2a	1653	1/1	0.67	0.44	85,85,85,85	0
55	MG	2a	1674	1/1	0.67	0.19	89,89,89,89	0
55	MG	2A	3813	1/1	0.67	0.46	57,57,57,57	0
55	MG	1A	3084	1/1	0.67	0.69	47,47,47,47	0
55	MG	1A	3192	1/1	0.68	0.33	42,42,42,42	0
55	MG	2A	3637	1/1	0.68	0.07	61,61,61,61	0
55	MG	2a	1724	1/1	0.68	0.29	93,93,93,93	0
55	MG	2G	3001	1/1	0.68	0.29	90,90,90,90	0
55	MG	1A	3105	1/1	0.68	0.30	46,46,46,46	0
55	MG	2Q	8004	1/1	0.68	0.62	66,66,66,66	0
55	MG	2A	3342	1/1	0.68	0.21	76,76,76,76	0
55	MG	2a	1631	1/1	0.68	0.57	85,85,85,85	0
55	MG	1A	3592	1/1	0.68	0.38	70,70,70,70	0
55	MG	2A	3194	1/1	0.68	0.09	84,84,84,84	0
55	MG	2A	3742	1/1	0.69	0.38	70,70,70,70	0
55	MG	1A	3501	1/1	0.69	0.18	64,64,64,64	0
55	MG	1A	3889	1/1	0.69	0.40	46,46,46,46	0
55	MG	2G	3002	1/1	0.69	0.26	90,90,90,90	0
55	MG	2a	1734	1/1	0.69	0.40	57,57,57,57	0
55	MG	1A	3118	1/1	0.69	0.28	63,63,63,63	0
55	MG	2A	3425	1/1	0.69	0.22	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1a	3218	1/1	0.69	0.30	72,72,72,72	0
55	MG	2A	3816	1/1	0.69	0.32	51,51,51,51	0
55	MG	1a	3034	1/1	0.69	0.22	84,84,84,84	0
55	MG	1A	3611	1/1	0.69	0.46	65,65,65,65	0
55	MG	1a	3074	1/1	0.70	0.35	65,65,65,65	0
55	MG	1a	3114	1/1	0.70	0.11	74,74,74,74	0
55	MG	18	3301	1/1	0.70	0.63	70,70,70,70	0
55	MG	2D	304	1/1	0.70	0.27	55,55,55,55	0
55	MG	1A	3917	1/1	0.70	0.31	36,36,36,36	0
55	MG	1a	3168	1/1	0.70	0.10	79,79,79,79	0
55	MG	1A	3230	1/1	0.70	0.34	50,50,50,50	0
55	MG	2A	3480	1/1	0.70	0.23	81,81,81,81	0
55	MG	2A	3489	1/1	0.70	0.16	81,81,81,81	0
55	MG	2a	1609	1/1	0.70	1.46	77,77,77,77	0
55	MG	1a	3064	1/1	0.70	0.25	78,78,78,78	0
55	MG	2A	3099	1/1	0.70	0.31	52,52,52,52	0
55	MG	1A	3259	1/1	0.71	0.19	52,52,52,52	0
55	MG	1a	3132	1/1	0.71	0.24	91,91,91,91	0
55	MG	1A	3552	1/1	0.71	0.39	45,45,45,45	0
55	MG	2a	1717	1/1	0.71	0.17	73,73,73,73	0
55	MG	2a	1719	1/1	0.71	0.22	75,75,75,75	0
55	MG	1A	3236	1/1	0.71	0.23	79,79,79,79	0
55	MG	2A	3105	1/1	0.71	0.26	82,82,82,82	0
55	MG	1B	3015	1/1	0.71	0.16	66,66,66,66	0
55	MG	2A	3642	1/1	0.71	0.12	82,82,82,82	0
55	MG	1A	3734	1/1	0.71	0.41	45,45,45,45	0
55	MG	2A	3150	1/1	0.71	0.42	49,49,49,49	0
55	MG	2a	1772	1/1	0.71	0.38	92,92,92,92	0
55	MG	2a	1787	1/1	0.71	0.18	80,80,80,80	0
55	MG	2a	1636	1/1	0.71	0.62	83,83,83,83	0
55	MG	2A	3155	1/1	0.71	0.85	50,50,50,50	0
55	MG	2a	1651	1/1	0.71	0.12	69,69,69,69	0
55	MG	2a	1730	1/1	0.72	0.27	92,92,92,92	0
55	MG	1A	3895	1/1	0.72	0.48	65,65,65,65	0
55	MG	1a	3073	1/1	0.72	0.19	74,74,74,74	0
55	MG	2A	3004	1/1	0.72	0.28	56,56,56,56	0
55	MG	1A	3578	1/1	0.72	0.15	86,86,86,86	0
55	MG	2A	3719	1/1	0.72	0.17	70,70,70,70	0
55	MG	1a	3108	1/1	0.72	0.06	81,81,81,81	0
55	MG	1A	3623	1/1	0.72	0.30	56,56,56,56	0
55	MG	2a	1625	1/1	0.72	0.32	70,70,70,70	0
55	MG	2a	1722	1/1	0.72	0.17	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3109	1/1	0.72	0.56	64,64,64,64	0
55	MG	2A	3104	1/1	0.73	0.16	56,56,56,56	0
55	MG	1A	3228	1/1	0.73	0.36	28,28,28,28	0
55	MG	2A	3445	1/1	0.73	0.32	48,48,48,48	0
55	MG	2A	3559	1/1	0.73	0.40	64,64,64,64	0
55	MG	1d	503	1/1	0.73	0.34	63,63,63,63	0
55	MG	1A	3659	1/1	0.73	0.12	57,57,57,57	0
55	MG	1A	3790	1/1	0.73	0.20	84,84,84,84	0
55	MG	2A	3586	1/1	0.73	0.17	101,101,101,101	0
55	MG	2A	3809	1/1	0.73	0.29	75,75,75,75	0
55	MG	2A	3307	1/1	0.73	0.10	54,54,54,54	0
55	MG	2a	1768	1/1	0.73	0.10	80,80,80,80	0
55	MG	2A	3627	1/1	0.73	0.24	66,66,66,66	0
55	MG	2A	3819	1/1	0.73	0.17	90,90,90,90	0
55	MG	15	104	1/1	0.73	0.30	26,26,26,26	0
55	MG	1A	3186	1/1	0.73	0.23	72,72,72,72	0
55	MG	2a	1656	1/1	0.73	0.41	72,72,72,72	0
55	MG	2A	3386	1/1	0.73	0.28	102,102,102,102	0
55	MG	2A	3471	1/1	0.74	0.15	79,79,79,79	0
55	MG	1A	3361	1/1	0.74	0.10	75,75,75,75	0
55	MG	1A	3837	1/1	0.74	0.07	84,84,84,84	0
55	MG	2a	1710	1/1	0.74	0.43	86,86,86,86	0
55	MG	1a	3150	1/1	0.74	0.32	99,99,99,99	0
55	MG	1A	3058	1/1	0.74	0.16	65,65,65,65	0
55	MG	1a	3038	1/1	0.74	0.78	79,79,79,79	0
55	MG	2A	3717	1/1	0.74	0.18	92,92,92,92	0
55	MG	2A	3257	1/1	0.74	0.50	68,68,68,68	0
55	MG	1A	3654	1/1	0.74	0.11	41,41,41,41	0
55	MG	1a	3063	1/1	0.74	0.98	64,64,64,64	0
55	MG	2A	3329	1/1	0.74	0.11	88,88,88,88	0
55	MG	1A	3220	1/1	0.74	0.71	77,77,77,77	0
55	MG	1A	3563	1/1	0.74	0.23	59,59,59,59	0
55	MG	1A	3143	1/1	0.74	0.50	45,45,45,45	0
55	MG	1A	3913	1/1	0.74	0.42	63,63,63,63	0
55	MG	2a	1642	1/1	0.74	0.14	68,68,68,68	0
55	MG	2a	1643	1/1	0.74	0.32	73,73,73,73	0
55	MG	1A	3119	1/1	0.74	0.39	33,33,33,33	0
55	MG	2A	3047	1/1	0.74	0.89	63,63,63,63	0
55	MG	2A	3030	1/1	0.75	0.21	69,69,69,69	0
55	MG	1A	3808	1/1	0.75	0.25	38,38,38,38	0
55	MG	1A	3148	1/1	0.75	0.25	58,58,58,58	0
55	MG	2A	3673	1/1	0.75	0.35	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3519	1/1	0.75	0.12	46,46,46,46	0
55	MG	2A	3138	1/1	0.75	0.71	48,48,48,48	0
55	MG	2a	1741	1/1	0.75	0.07	75,75,75,75	0
55	MG	2B	3015	1/1	0.75	0.15	85,85,85,85	0
55	MG	1A	3914	1/1	0.75	0.47	62,62,62,62	0
55	MG	2a	1652	1/1	0.75	0.35	90,90,90,90	0
55	MG	2A	3485	1/1	0.75	0.48	73,73,73,73	0
55	MG	1A	3509	1/1	0.75	0.34	38,38,38,38	0
55	MG	2A	3091	1/1	0.75	0.44	54,54,54,54	0
55	MG	1A	3602	1/1	0.75	0.23	76,76,76,76	0
55	MG	1a	3184	1/1	0.75	0.11	73,73,73,73	0
55	MG	2A	3641	1/1	0.75	0.13	77,77,77,77	0
55	MG	1A	3554	1/1	0.76	0.23	69,69,69,69	0
55	MG	2A	3478	1/1	0.76	0.18	94,94,94,94	0
55	MG	2A	3024	1/1	0.76	0.26	58,58,58,58	0
55	MG	2P	202	1/1	0.76	0.54	73,73,73,73	0
55	MG	2A	3154	1/1	0.76	0.89	61,61,61,61	0
55	MG	2A	3650	1/1	0.76	0.34	55,55,55,55	0
55	MG	28	101	1/1	0.76	1.05	64,64,64,64	0
55	MG	1a	3179	1/1	0.76	0.07	78,78,78,78	0
55	MG	2a	1614	1/1	0.76	1.41	75,75,75,75	0
55	MG	2A	3773	1/1	0.76	0.12	85,85,85,85	0
55	MG	2A	3777	1/1	0.76	0.22	83,83,83,83	0
55	MG	1a	3123	1/1	0.76	0.17	86,86,86,86	0
55	MG	2m	201	1/1	0.76	0.11	79,79,79,79	0
55	MG	2A	3685	1/1	0.76	0.29	54,54,54,54	0
55	MG	1A	3144	1/1	0.77	0.38	64,64,64,64	0
55	MG	1A	3624	1/1	0.77	0.31	68,68,68,68	0
55	MG	2A	3522	1/1	0.77	0.16	82,82,82,82	0
55	MG	1A	3193	1/1	0.77	0.42	42,42,42,42	0
55	MG	2a	1694	1/1	0.77	0.23	78,78,78,78	0
55	MG	1A	3506	1/1	0.77	0.17	71,71,71,71	0
55	MG	2H	201	1/1	0.77	0.81	108,108,108,108	0
55	MG	2A	3008	1/1	0.77	0.35	69,69,69,69	0
55	MG	2A	3113	1/1	0.77	0.20	66,66,66,66	0
55	MG	1A	3204	1/1	0.77	0.63	39,39,39,39	0
55	MG	2a	1727	1/1	0.77	0.39	91,91,91,91	0
55	MG	1A	3900	1/1	0.77	0.23	58,58,58,58	0
55	MG	28	102	1/1	0.77	0.70	59,59,59,59	0
55	MG	1a	3144	1/1	0.77	0.28	75,75,75,75	0
55	MG	1A	3905	1/1	0.77	0.74	45,45,45,45	0
55	MG	1A	3589	1/1	0.77	0.27	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3058	1/1	0.77	1.09	53,53,53,53	0
55	MG	1A	3733	1/1	0.77	0.39	27,27,27,27	0
55	MG	2A	3163	1/1	0.77	0.53	78,78,78,78	0
55	MG	1A	3210	1/1	0.77	0.25	45,45,45,45	0
55	MG	1A	3071	1/1	0.77	0.51	42,42,42,42	0
55	MG	2a	1644	1/1	0.77	0.18	67,67,67,67	0
55	MG	2a	1646	1/1	0.77	0.22	56,56,56,56	0
55	MG	1A	3604	1/1	0.77	0.13	52,52,52,52	0
55	MG	1A	3538	1/1	0.77	0.26	60,60,60,60	0
55	MG	2A	3131	1/1	0.78	0.31	65,65,65,65	0
55	MG	2A	3393	1/1	0.78	0.14	52,52,52,52	0
55	MG	2A	3423	1/1	0.78	0.10	79,79,79,79	0
55	MG	1A	3124	1/1	0.78	0.24	63,63,63,63	0
55	MG	2A	3629	1/1	0.78	0.10	74,74,74,74	0
55	MG	1A	3648	1/1	0.78	0.12	90,90,90,90	0
55	MG	1A	3526	1/1	0.78	0.14	64,64,64,64	0
55	MG	1a	3048	1/1	0.78	0.14	66,66,66,66	0
55	MG	1A	3031	1/1	0.78	0.21	22,22,22,22	0
55	MG	1A	3878	1/1	0.78	0.28	46,46,46,46	0
55	MG	1E	306	1/1	0.78	0.18	52,52,52,52	0
55	MG	1A	3599	1/1	0.78	0.07	50,50,50,50	0
55	MG	1A	3890	1/1	0.78	0.21	73,73,73,73	0
55	MG	2A	3192	1/1	0.78	1.03	64,64,64,64	0
55	MG	2A	3193	1/1	0.78	0.10	76,76,76,76	0
55	MG	1a	3076	1/1	0.78	0.22	74,74,74,74	0
55	MG	2A	3736	1/1	0.78	0.12	95,95,95,95	0
55	MG	1A	3548	1/1	0.78	0.26	39,39,39,39	0
55	MG	2A	3248	1/1	0.78	0.05	81,81,81,81	0
55	MG	2A	3252	1/1	0.78	0.21	69,69,69,69	0
55	MG	2A	3771	1/1	0.78	0.13	68,68,68,68	0
55	MG	1A	3725	1/1	0.78	0.54	44,44,44,44	0
55	MG	2A	3543	1/1	0.78	0.39	82,82,82,82	0
55	MG	2A	3108	1/1	0.78	0.29	84,84,84,84	0
55	MG	1A	3196	1/1	0.78	0.24	36,36,36,36	0
55	MG	1A	3457	1/1	0.78	0.10	24,24,24,24	0
55	MG	1A	3173	1/1	0.78	1.04	63,63,63,63	0
55	MG	2B	3005	1/1	0.79	0.10	69,69,69,69	0
55	MG	1A	3630	1/1	0.79	0.21	55,55,55,55	0
55	MG	1V	201	1/1	0.79	0.66	25,25,25,25	0
55	MG	1a	3028	1/1	0.79	0.23	55,55,55,55	0
55	MG	2A	3762	1/1	0.79	0.61	60,60,60,60	0
55	MG	2A	3765	1/1	0.79	0.55	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3375	1/1	0.79	0.48	49,49,49,49	0
55	MG	2A	3044	1/1	0.79	0.10	79,79,79,79	0
55	MG	1A	3634	1/1	0.79	0.23	38,38,38,38	0
55	MG	2A	3655	1/1	0.79	0.27	60,60,60,60	0
55	MG	1A	3853	1/1	0.79	0.10	25,25,25,25	0
55	MG	2A	3794	1/1	0.79	0.14	75,75,75,75	0
55	MG	2A	3136	1/1	0.79	0.48	55,55,55,55	0
55	MG	2X	102	1/1	0.79	0.47	82,82,82,82	0
55	MG	2A	3497	1/1	0.79	0.14	89,89,89,89	0
55	MG	2A	3431	1/1	0.79	0.32	77,77,77,77	0
55	MG	2A	3438	1/1	0.79	0.09	81,81,81,81	0
55	MG	1A	3189	1/1	0.79	0.32	43,43,43,43	0
55	MG	1h	3001	1/1	0.80	0.67	63,63,63,63	0
55	MG	1A	3433	1/1	0.80	0.32	51,51,51,51	0
55	MG	1A	3098	1/1	0.80	0.37	38,38,38,38	0
55	MG	2A	3487	1/1	0.80	0.38	68,68,68,68	0
55	MG	1A	3134	1/1	0.80	0.23	65,65,65,65	0
55	MG	2A	3290	1/1	0.80	0.18	64,64,64,64	0
55	MG	1A	3533	1/1	0.80	0.15	60,60,60,60	0
55	MG	1A	3459	1/1	0.80	0.34	50,50,50,50	0
55	MG	2A	3677	1/1	0.80	0.19	56,56,56,56	0
55	MG	1A	3167	1/1	0.80	0.30	52,52,52,52	0
55	MG	1A	3896	1/1	0.80	0.60	37,37,37,37	0
55	MG	2A	3520	1/1	0.80	0.60	65,65,65,65	0
55	MG	1A	3253	1/1	0.80	0.24	53,53,53,53	0
55	MG	1A	3745	1/1	0.80	0.07	54,54,54,54	0
55	MG	1A	3758	1/1	0.80	0.63	53,53,53,53	0
55	MG	1A	3760	1/1	0.80	0.27	65,65,65,65	0
55	MG	2R	202	1/1	0.80	0.37	74,74,74,74	0
55	MG	2S	201	1/1	0.80	0.37	67,67,67,67	0
55	MG	2A	3555	1/1	0.80	0.53	52,52,52,52	0
55	MG	2A	3161	1/1	0.80	0.61	54,54,54,54	0
55	MG	1A	3190	1/1	0.80	0.12	72,72,72,72	0
55	MG	1A	3041	1/1	0.80	0.37	62,62,62,62	0
55	MG	1A	3835	1/1	0.80	0.07	48,48,48,48	0
55	MG	1a	3186	1/1	0.80	0.08	69,69,69,69	0
55	MG	2A	3779	1/1	0.80	0.08	72,72,72,72	0
55	MG	2a	1629	1/1	0.80	0.15	90,90,90,90	0
55	MG	1A	3574	1/1	0.80	0.29	64,64,64,64	0
55	MG	1A	3106	1/1	0.80	0.43	42,42,42,42	0
55	MG	2h	8001	1/1	0.80	0.29	77,77,77,77	0
55	MG	2l	201	1/1	0.80	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1B	3021	1/1	0.80	0.11	66,66,66,66	0
55	MG	2A	3632	1/1	0.80	0.24	97,97,97,97	0
55	MG	2A	3195	1/1	0.81	0.14	55,55,55,55	0
55	MG	1A	3854	1/1	0.81	0.12	72,72,72,72	0
55	MG	1A	3855	1/1	0.81	0.27	48,48,48,48	0
55	MG	2a	1623	1/1	0.81	0.25	78,78,78,78	0
55	MG	1B	3003	1/1	0.81	0.14	64,64,64,64	0
55	MG	1A	3400	1/1	0.81	0.23	63,63,63,63	0
55	MG	2A	3530	1/1	0.81	0.86	52,52,52,52	0
55	MG	2A	3270	1/1	0.81	0.18	58,58,58,58	0
55	MG	1a	3040	1/1	0.81	0.25	75,75,75,75	0
55	MG	1A	3090	1/1	0.81	0.45	37,37,37,37	0
55	MG	1a	3057	1/1	0.81	0.34	81,81,81,81	0
55	MG	1b	3001	1/1	0.81	0.13	81,81,81,81	0
55	MG	2a	1645	1/1	0.81	0.32	63,63,63,63	0
55	MG	1A	3764	1/1	0.81	0.09	67,67,67,67	0
55	MG	1A	3175	1/1	0.81	0.55	56,56,56,56	0
55	MG	2A	3803	1/1	0.81	0.54	69,69,69,69	0
55	MG	2A	3804	1/1	0.81	0.20	35,35,35,35	0
55	MG	2A	3377	1/1	0.81	0.10	94,94,94,94	0
55	MG	2a	1670	1/1	0.81	0.12	84,84,84,84	0
55	MG	2A	3114	1/1	0.81	0.30	62,62,62,62	0
55	MG	2A	3117	1/1	0.81	0.25	58,58,58,58	0
55	MG	1F	303	1/1	0.81	0.63	43,43,43,43	0
55	MG	2a	1699	1/1	0.81	0.12	74,74,74,74	0
55	MG	1o	3001	1/1	0.81	0.26	52,52,52,52	0
55	MG	2A	3631	1/1	0.81	0.32	86,86,86,86	0
55	MG	1A	3794	1/1	0.81	0.22	59,59,59,59	0
55	MG	2A	3636	1/1	0.81	0.08	73,73,73,73	0
55	MG	1A	3164	1/1	0.81	0.31	59,59,59,59	0
55	MG	2B	3016	1/1	0.81	0.15	90,90,90,90	0
55	MG	2B	3018	1/1	0.81	0.39	92,92,92,92	0
55	MG	1A	3116	1/1	0.81	0.12	74,74,74,74	0
55	MG	1A	3315	1/1	0.81	0.28	45,45,45,45	0
55	MG	2a	1736	1/1	0.81	0.34	78,78,78,78	0
55	MG	2E	303	1/1	0.81	1.03	71,71,71,71	0
55	MG	2A	3022	1/1	0.81	0.14	68,68,68,68	0
55	MG	1W	3003	1/1	0.81	0.47	41,41,41,41	0
55	MG	2a	1766	1/1	0.81	0.10	91,91,91,91	0
55	MG	15	101	1/1	0.81	0.25	42,42,42,42	0
55	MG	1A	3901	1/1	0.81	0.16	42,42,42,42	0
55	MG	1a	3139	1/1	0.81	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3840	1/1	0.81	0.29	61,61,61,61	0
55	MG	2A	3059	1/1	0.81	0.56	64,64,64,64	0
55	MG	1A	3032	1/1	0.81	0.29	45,45,45,45	0
55	MG	2g	3001	1/1	0.81	0.18	72,72,72,72	0
55	MG	2A	3707	1/1	0.81	0.46	75,75,75,75	0
55	MG	20	101	1/1	0.81	0.43	64,64,64,64	0
55	MG	2A	3072	1/1	0.81	0.33	57,57,57,57	0
55	MG	1A	3202	1/1	0.81	0.24	63,63,63,63	0
55	MG	1A	3838	1/1	0.82	0.47	45,45,45,45	0
55	MG	1A	3839	1/1	0.82	0.15	59,59,59,59	0
55	MG	2A	3151	1/1	0.82	1.44	62,62,62,62	0
55	MG	1A	3660	1/1	0.82	0.36	56,56,56,56	0
55	MG	1D	308	1/1	0.82	0.09	58,58,58,58	0
55	MG	1A	3675	1/1	0.82	0.57	47,47,47,47	0
55	MG	1F	302	1/1	0.82	0.22	35,35,35,35	0
55	MG	2a	1641	1/1	0.82	0.23	77,77,77,77	0
55	MG	2A	3027	1/1	0.82	0.26	70,70,70,70	0
55	MG	1a	3077	1/1	0.82	0.44	81,81,81,81	0
55	MG	2A	3180	1/1	0.82	0.23	63,63,63,63	0
55	MG	2A	3034	1/1	0.82	0.20	54,54,54,54	0
55	MG	1A	3678	1/1	0.82	0.38	37,37,37,37	0
55	MG	1A	3248	1/1	0.82	0.41	51,51,51,51	0
55	MG	1A	3600	1/1	0.82	0.09	67,67,67,67	0
55	MG	1A	3703	1/1	0.82	0.50	30,30,30,30	0
55	MG	2A	3805	1/1	0.82	0.14	74,74,74,74	0
55	MG	2A	3201	1/1	0.82	0.23	48,48,48,48	0
55	MG	2A	3062	1/1	0.82	0.79	47,47,47,47	0
55	MG	2A	3815	1/1	0.82	0.46	67,67,67,67	0
55	MG	1A	3199	1/1	0.82	0.46	34,34,34,34	0
55	MG	2A	3068	1/1	0.82	0.33	56,56,56,56	0
55	MG	2A	3256	1/1	0.82	0.11	84,84,84,84	0
55	MG	1A	3404	1/1	0.82	0.09	60,60,60,60	0
55	MG	11	103	1/1	0.82	0.19	50,50,50,50	0
55	MG	1A	3610	1/1	0.82	0.20	70,70,70,70	0
55	MG	2A	3088	1/1	0.82	0.07	81,81,81,81	0
55	MG	1a	3160	1/1	0.82	0.25	84,84,84,84	0
55	MG	1A	3120	1/1	0.82	0.61	34,34,34,34	0
55	MG	1A	3753	1/1	0.82	0.17	67,67,67,67	0
55	MG	1A	3278	1/1	0.82	0.32	37,37,37,37	0
55	MG	1A	3569	1/1	0.82	0.16	43,43,43,43	0
55	MG	1a	3185	1/1	0.82	0.17	68,68,68,68	0
55	MG	1A	3573	1/1	0.82	0.68	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3199	1/1	0.82	0.07	68,68,68,68	0
55	MG	2a	1754	1/1	0.82	0.17	85,85,85,85	0
55	MG	1A	3631	1/1	0.82	0.18	59,59,59,59	0
55	MG	1A	3517	1/1	0.82	0.20	68,68,68,68	0
55	MG	1A	3806	1/1	0.82	0.12	65,65,65,65	0
55	MG	1A	3221	1/1	0.82	0.15	56,56,56,56	0
55	MG	2a	1774	1/1	0.82	0.10	91,91,91,91	0
55	MG	2A	3675	1/1	0.82	0.16	70,70,70,70	0
55	MG	1a	3041	1/1	0.82	0.18	72,72,72,72	0
55	MG	1A	3324	1/1	0.82	0.14	40,40,40,40	0
55	MG	2A	3456	1/1	0.82	0.36	70,70,70,70	0
55	MG	27	104	1/1	0.82	0.18	67,67,67,67	0
55	MG	2A	3462	1/1	0.82	0.19	62,62,62,62	0
55	MG	1A	3147	1/1	0.82	0.19	40,40,40,40	0
55	MG	2A	3140	1/1	0.82	0.33	61,61,61,61	0
55	MG	18	3302	1/1	0.83	0.54	40,40,40,40	0
55	MG	2A	3273	1/1	0.83	0.11	60,60,60,60	0
55	MG	1a	3001	1/1	0.83	0.05	76,76,76,76	0
55	MG	2A	3535	1/1	0.83	0.27	86,86,86,86	0
55	MG	2A	3304	1/1	0.83	0.09	48,48,48,48	0
55	MG	1B	3019	1/1	0.83	0.15	60,60,60,60	0
55	MG	2A	3784	1/1	0.83	0.14	94,94,94,94	0
55	MG	1a	3143	1/1	0.83	0.10	87,87,87,87	0
55	MG	1A	3111	1/1	0.83	0.41	42,42,42,42	0
55	MG	2A	3132	1/1	0.83	0.39	63,63,63,63	0
55	MG	1a	3012	1/1	0.83	0.15	68,68,68,68	0
55	MG	2A	3579	1/1	0.83	0.28	75,75,75,75	0
55	MG	1A	3464	1/1	0.83	0.64	35,35,35,35	0
55	MG	1D	315	1/1	0.83	0.35	68,68,68,68	0
55	MG	2A	3141	1/1	0.83	0.57	51,51,51,51	0
55	MG	2A	3610	1/1	0.83	0.11	81,81,81,81	0
55	MG	2A	3612	1/1	0.83	0.16	38,38,38,38	0
55	MG	1A	3490	1/1	0.83	0.18	62,62,62,62	0
55	MG	2B	3004	1/1	0.83	0.18	76,76,76,76	0
55	MG	2a	1697	1/1	0.83	0.08	80,80,80,80	0
55	MG	1A	3321	1/1	0.83	0.16	55,55,55,55	0
55	MG	1a	3169	1/1	0.83	0.37	95,95,95,95	0
55	MG	1a	3170	1/1	0.83	0.27	82,82,82,82	0
55	MG	1A	3676	1/1	0.83	0.22	70,70,70,70	0
55	MG	1a	3181	1/1	0.83	0.08	74,74,74,74	0
55	MG	1A	3089	1/1	0.83	0.37	37,37,37,37	0
55	MG	1A	3066	1/1	0.83	0.61	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3457	1/1	0.83	0.34	90,90,90,90	0
55	MG	2A	3646	1/1	0.83	0.38	53,53,53,53	0
55	MG	1A	3695	1/1	0.83	0.30	60,60,60,60	0
55	MG	2A	3078	1/1	0.83	0.61	51,51,51,51	0
55	MG	1A	3004	1/1	0.83	0.27	41,41,41,41	0
55	MG	2A	3477	1/1	0.83	0.29	68,68,68,68	0
55	MG	1A	3608	1/1	0.83	0.23	74,74,74,74	0
55	MG	10	104	1/1	0.83	0.11	50,50,50,50	0
55	MG	11	101	1/1	0.83	1.57	54,54,54,54	0
55	MG	2A	3094	1/1	0.83	0.82	59,59,59,59	0
55	MG	1A	3869	1/1	0.83	0.18	39,39,39,39	0
55	MG	2A	3224	1/1	0.83	0.17	69,69,69,69	0
55	MG	1d	504	1/1	0.83	0.27	75,75,75,75	0
55	MG	27	102	1/1	0.83	0.78	49,49,49,49	0
55	MG	1A	3875	1/1	0.83	0.26	44,44,44,44	0
55	MG	2d	505	1/1	0.83	0.38	101,101,101,101	0
55	MG	15	102	1/1	0.83	0.91	43,43,43,43	0
55	MG	2A	3747	1/1	0.83	0.08	75,75,75,75	0
55	MG	1A	3713	1/1	0.83	0.20	98,98,98,98	0
55	MG	2A	3754	1/1	0.83	0.24	101,101,101,101	0
55	MG	2A	3756	1/1	0.83	1.03	95,95,95,95	0
55	MG	1A	3722	1/1	0.83	0.14	62,62,62,62	0
55	MG	1a	3029	1/1	0.84	0.09	55,55,55,55	0
55	MG	1F	311	1/1	0.84	0.40	25,25,25,25	0
55	MG	1A	3135	1/1	0.84	0.20	37,37,37,37	0
55	MG	1a	3039	1/1	0.84	0.38	62,62,62,62	0
55	MG	1A	3570	1/1	0.84	0.28	48,48,48,48	0
55	MG	2A	3065	1/1	0.84	0.14	56,56,56,56	0
55	MG	2A	3469	1/1	0.84	0.13	68,68,68,68	0
55	MG	1A	3911	1/1	0.84	0.29	39,39,39,39	0
55	MG	2A	3175	1/1	0.84	0.99	69,69,69,69	0
55	MG	2a	1620	1/1	0.84	0.26	77,77,77,77	0
55	MG	1a	3047	1/1	0.84	0.20	68,68,68,68	0
55	MG	2A	3720	1/1	0.84	0.28	58,58,58,58	0
55	MG	1R	204	1/1	0.84	0.24	53,53,53,53	0
55	MG	1A	3150	1/1	0.84	0.15	39,39,39,39	0
55	MG	2A	3746	1/1	0.84	0.18	69,69,69,69	0
55	MG	2A	3482	1/1	0.84	0.39	54,54,54,54	0
55	MG	1a	3194	1/1	0.84	0.10	83,83,83,83	0
55	MG	2A	3486	1/1	0.84	1.38	57,57,57,57	0
55	MG	2A	3086	1/1	0.84	0.30	56,56,56,56	0
55	MG	1A	3227	1/1	0.84	0.41	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	10	101	1/1	0.84	0.66	52,52,52,52	0
55	MG	2A	3211	1/1	0.84	0.14	45,45,45,45	0
55	MG	2A	3221	1/1	0.84	0.25	52,52,52,52	0
55	MG	1a	3216	1/1	0.84	0.07	100,100,100,100	0
55	MG	2A	3228	1/1	0.84	0.21	51,51,51,51	0
55	MG	2A	3244	1/1	0.84	0.54	53,53,53,53	0
55	MG	1A	3783	1/1	0.84	0.10	55,55,55,55	0
55	MG	2A	3523	1/1	0.84	0.25	61,61,61,61	0
55	MG	1a	3222	1/1	0.84	0.44	62,62,62,62	0
55	MG	2A	3250	1/1	0.84	0.09	31,31,31,31	0
55	MG	1A	3180	1/1	0.84	0.37	48,48,48,48	0
55	MG	2A	3539	1/1	0.84	0.09	74,74,74,74	0
55	MG	2A	3542	1/1	0.84	0.16	88,88,88,88	0
55	MG	1A	3151	1/1	0.84	0.17	46,46,46,46	0
55	MG	2A	3812	1/1	0.84	0.23	60,60,60,60	0
55	MG	1A	3876	1/1	0.84	0.05	64,64,64,64	0
55	MG	1A	3011	1/1	0.84	0.36	41,41,41,41	0
55	MG	1A	3885	1/1	0.84	0.23	37,37,37,37	0
55	MG	1A	3184	1/1	0.84	0.48	37,37,37,37	0
55	MG	2A	3299	1/1	0.84	0.21	75,75,75,75	0
55	MG	1D	302	1/1	0.84	0.81	35,35,35,35	0
55	MG	2A	3305	1/1	0.84	0.07	84,84,84,84	0
55	MG	1A	3074	1/1	0.84	0.68	29,29,29,29	0
55	MG	2A	3590	1/1	0.84	0.47	65,65,65,65	0
55	MG	2B	3014	1/1	0.84	0.12	76,76,76,76	0
55	MG	1D	313	1/1	0.84	0.20	51,51,51,51	0
55	MG	1A	3205	1/1	0.84	0.51	44,44,44,44	0
55	MG	2A	3338	1/1	0.84	0.71	70,70,70,70	0
55	MG	1A	3658	1/1	0.84	0.50	38,38,38,38	0
55	MG	2A	3134	1/1	0.84	0.82	70,70,70,70	0
55	MG	1a	3148	1/1	0.84	0.13	82,82,82,82	0
55	MG	2a	1776	1/1	0.84	0.10	80,80,80,80	0
55	MG	1a	3017	1/1	0.84	0.31	65,65,65,65	0
55	MG	2A	3389	1/1	0.84	0.17	46,46,46,46	0
55	MG	1A	3092	1/1	0.84	0.28	37,37,37,37	0
55	MG	2A	3415	1/1	0.84	0.07	80,80,80,80	0
55	MG	1a	3152	1/1	0.84	0.16	91,91,91,91	0
55	MG	1A	3605	1/1	0.84	0.54	38,38,38,38	0
55	MG	2A	3146	1/1	0.84	0.62	53,53,53,53	0
55	MG	2A	3046	1/1	0.84	0.16	51,51,51,51	0
55	MG	2V	201	1/1	0.84	0.78	55,55,55,55	0
55	MG	2A	3054	1/1	0.85	0.63	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3055	1/1	0.85	0.32	49,49,49,49	0
55	MG	1P	204	1/1	0.85	0.12	35,35,35,35	0
55	MG	2A	3152	1/1	0.85	0.44	59,59,59,59	0
55	MG	1A	3219	1/1	0.85	0.19	49,49,49,49	0
55	MG	1A	3668	1/1	0.85	0.08	85,85,85,85	0
55	MG	2A	3159	1/1	0.85	0.77	58,58,58,58	0
55	MG	1A	3856	1/1	0.85	0.32	46,46,46,46	0
55	MG	2A	3420	1/1	0.85	0.09	60,60,60,60	0
55	MG	1A	3859	1/1	0.85	0.34	87,87,87,87	0
55	MG	1A	3072	1/1	0.85	0.17	43,43,43,43	0
55	MG	2A	3165	1/1	0.85	0.29	58,58,58,58	0
55	MG	1A	3398	1/1	0.85	0.24	37,37,37,37	0
55	MG	1A	3079	1/1	0.85	0.22	40,40,40,40	0
55	MG	1A	3681	1/1	0.85	0.07	38,38,38,38	0
55	MG	2a	1654	1/1	0.85	0.55	70,70,70,70	0
55	MG	1A	3101	1/1	0.85	0.68	63,63,63,63	0
55	MG	2A	3081	1/1	0.85	0.16	46,46,46,46	0
55	MG	1a	3075	1/1	0.85	0.18	48,48,48,48	0
55	MG	2a	1682	1/1	0.85	0.45	88,88,88,88	0
55	MG	2a	1683	1/1	0.85	0.16	67,67,67,67	0
55	MG	1B	3023	1/1	0.85	0.18	63,63,63,63	0
55	MG	2A	3463	1/1	0.85	0.33	76,76,76,76	0
55	MG	2A	3464	1/1	0.85	0.32	90,90,90,90	0
55	MG	1A	3262	1/1	0.85	0.20	84,84,84,84	0
55	MG	2a	1708	1/1	0.85	0.11	83,83,83,83	0
55	MG	17	105	1/1	0.85	0.25	52,52,52,52	0
55	MG	1D	307	1/1	0.85	0.74	44,44,44,44	0
55	MG	2A	3647	1/1	0.85	0.23	88,88,88,88	0
55	MG	1e	3002	1/1	0.85	0.50	58,58,58,58	0
55	MG	1A	3267	1/1	0.85	0.12	79,79,79,79	0
55	MG	2A	3661	1/1	0.85	0.07	85,85,85,85	0
55	MG	1a	3124	1/1	0.85	0.31	77,77,77,77	0
55	MG	1A	3815	1/1	0.85	0.58	51,51,51,51	0
55	MG	2F	309	1/1	0.85	0.21	60,60,60,60	0
55	MG	1A	3171	1/1	0.85	0.64	44,44,44,44	0
55	MG	1E	303	1/1	0.85	0.39	39,39,39,39	0
55	MG	2A	3681	1/1	0.85	0.10	71,71,71,71	0
55	MG	2A	3111	1/1	0.85	0.87	52,52,52,52	0
55	MG	1A	3053	1/1	0.85	0.30	58,58,58,58	0
55	MG	1A	3160	1/1	0.85	0.98	40,40,40,40	0
55	MG	1a	3018	1/1	0.85	0.16	64,64,64,64	0
55	MG	1A	3597	1/1	0.85	0.47	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3151	1/1	0.85	0.15	76,76,76,76	0
55	MG	2A	3726	1/1	0.85	0.09	41,41,41,41	0
55	MG	2A	3285	1/1	0.85	0.11	47,47,47,47	0
55	MG	2A	3513	1/1	0.85	0.71	47,47,47,47	0
55	MG	2b	3001	1/1	0.85	0.18	85,85,85,85	0
55	MG	2d	503	1/1	0.85	0.43	79,79,79,79	0
55	MG	1F	310	1/1	0.85	0.47	27,27,27,27	0
55	MG	1A	3534	1/1	0.85	0.12	52,52,52,52	0
55	MG	2A	3040	1/1	0.85	0.35	63,63,63,63	0
55	MG	1A	3465	1/1	0.85	0.24	54,54,54,54	0
55	MG	2a	1606	1/1	0.85	0.64	69,69,69,69	0
55	MG	1H	8001	1/1	0.85	0.11	76,76,76,76	0
55	MG	1A	3161	1/1	0.85	0.42	55,55,55,55	0
55	MG	2A	3050	1/1	0.85	0.42	64,64,64,64	0
55	MG	1A	3188	1/1	0.86	0.46	34,34,34,34	0
55	MG	2a	1602	1/1	0.86	0.51	55,55,55,55	0
55	MG	1a	3154	1/1	0.86	0.11	100,100,100,100	0
55	MG	1A	3377	1/1	0.86	0.06	70,70,70,70	0
55	MG	1A	3168	1/1	0.86	0.34	53,53,53,53	0
55	MG	1B	3009	1/1	0.86	0.26	60,60,60,60	0
55	MG	2a	1621	1/1	0.86	0.29	58,58,58,58	0
55	MG	2A	3525	1/1	0.86	0.07	50,50,50,50	0
55	MG	1A	3693	1/1	0.86	0.07	42,42,42,42	0
55	MG	2A	3328	1/1	0.86	0.27	72,72,72,72	0
55	MG	1B	3017	1/1	0.86	0.08	39,39,39,39	0
55	MG	2a	1633	1/1	0.86	0.28	79,79,79,79	0
55	MG	1a	3173	1/1	0.86	0.24	71,71,71,71	0
55	MG	2A	3148	1/1	0.86	0.32	57,57,57,57	0
55	MG	2A	3149	1/1	0.86	0.26	63,63,63,63	0
55	MG	1A	3485	1/1	0.86	0.21	47,47,47,47	0
55	MG	2A	3056	1/1	0.86	0.16	59,59,59,59	0
55	MG	1a	3180	1/1	0.86	0.21	102,102,102,102	0
55	MG	2A	3782	1/1	0.86	0.15	82,82,82,82	0
55	MG	1A	3883	1/1	0.86	0.08	58,58,58,58	0
55	MG	2a	1647	1/1	0.86	0.14	81,81,81,81	0
55	MG	2a	1648	1/1	0.86	0.13	63,63,63,63	0
55	MG	2A	3564	1/1	0.86	0.89	57,57,57,57	0
55	MG	2A	3394	1/1	0.86	0.18	65,65,65,65	0
55	MG	2A	3799	1/1	0.86	0.30	83,83,83,83	0
55	MG	2A	3060	1/1	0.86	0.80	52,52,52,52	0
55	MG	2A	3802	1/1	0.86	0.28	97,97,97,97	0
55	MG	1A	3169	1/1	0.86	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3585	1/1	0.86	0.17	68,68,68,68	0
55	MG	1B	3024	1/1	0.86	0.12	62,62,62,62	0
55	MG	1A	3831	1/1	0.86	0.42	51,51,51,51	0
55	MG	2A	3596	1/1	0.86	0.13	65,65,65,65	0
55	MG	2a	1692	1/1	0.86	0.29	85,85,85,85	0
55	MG	1a	3065	1/1	0.86	0.31	65,65,65,65	0
55	MG	1a	3197	1/1	0.86	0.15	82,82,82,82	0
55	MG	1a	3069	1/1	0.86	0.20	62,62,62,62	0
55	MG	2A	3614	1/1	0.86	0.06	58,58,58,58	0
55	MG	2B	3002	1/1	0.86	0.11	78,78,78,78	0
55	MG	1a	3213	1/1	0.86	0.29	64,64,64,64	0
55	MG	2A	3449	1/1	0.86	0.21	84,84,84,84	0
55	MG	1A	3590	1/1	0.86	0.11	48,48,48,48	0
55	MG	1A	3893	1/1	0.86	0.06	103,103,103,103	0
55	MG	1A	3034	1/1	0.86	0.16	57,57,57,57	0
55	MG	1A	3593	1/1	0.86	0.17	34,34,34,34	0
55	MG	1D	318	1/1	0.86	0.18	50,50,50,50	0
55	MG	1A	3206	1/1	0.86	0.39	32,32,32,32	0
55	MG	2A	3465	1/1	0.86	0.20	71,71,71,71	0
55	MG	1a	3003	1/1	0.86	0.17	65,65,65,65	0
55	MG	2A	3095	1/1	0.86	0.17	64,64,64,64	0
55	MG	2A	3475	1/1	0.86	0.13	76,76,76,76	0
55	MG	2a	1752	1/1	0.86	0.09	86,86,86,86	0
55	MG	1E	304	1/1	0.86	0.11	46,46,46,46	0
55	MG	2a	1756	1/1	0.86	0.13	69,69,69,69	0
55	MG	2a	1764	1/1	0.86	0.08	59,59,59,59	0
55	MG	2A	3660	1/1	0.86	0.20	71,71,71,71	0
55	MG	1A	3551	1/1	0.86	0.35	60,60,60,60	0
55	MG	2A	3664	1/1	0.86	0.10	75,75,75,75	0
55	MG	1A	3046	1/1	0.86	0.28	38,38,38,38	0
55	MG	1a	3137	1/1	0.86	0.29	68,68,68,68	0
55	MG	1a	3016	1/1	0.86	0.41	80,80,80,80	0
55	MG	2a	1779	1/1	0.86	0.48	75,75,75,75	0
55	MG	2a	1785	1/1	0.86	0.07	68,68,68,68	0
55	MG	1A	3452	1/1	0.86	0.46	76,76,76,76	0
55	MG	2a	1792	1/1	0.86	0.33	52,52,52,52	0
55	MG	1A	3194	1/1	0.86	0.48	34,34,34,34	0
55	MG	1a	3020	1/1	0.86	0.19	58,58,58,58	0
55	MG	2A	3705	1/1	0.86	0.20	75,75,75,75	0
55	MG	1A	3672	1/1	0.86	0.17	49,49,49,49	0
55	MG	25	101	1/1	0.86	0.45	58,58,58,58	0
55	MG	25	103	1/1	0.86	0.64	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3568	1/1	0.86	0.21	63,63,63,63	0
55	MG	2A	3025	1/1	0.86	0.20	38,38,38,38	0
55	MG	2A	3130	1/1	0.86	0.19	58,58,58,58	0
55	MG	1A	3146	1/1	0.86	0.12	54,54,54,54	0
55	MG	1A	3641	1/1	0.87	0.47	35,35,35,35	0
55	MG	2a	1635	1/1	0.87	0.49	77,77,77,77	0
55	MG	1a	3117	1/1	0.87	0.23	61,61,61,61	0
55	MG	2A	3589	1/1	0.87	0.25	82,82,82,82	0
55	MG	1d	502	1/1	0.87	0.10	80,80,80,80	0
55	MG	2A	3593	1/1	0.87	0.20	68,68,68,68	0
55	MG	1A	3532	1/1	0.87	0.22	69,69,69,69	0
55	MG	2A	3605	1/1	0.87	0.26	63,63,63,63	0
55	MG	2A	3186	1/1	0.87	0.87	61,61,61,61	0
55	MG	2A	3454	1/1	0.87	0.13	81,81,81,81	0
55	MG	1A	3730	1/1	0.87	0.12	65,65,65,65	0
55	MG	1e	3001	1/1	0.87	0.20	55,55,55,55	0
55	MG	2a	1650	1/1	0.87	0.68	55,55,55,55	0
55	MG	1F	306	1/1	0.87	0.24	39,39,39,39	0
55	MG	1A	3057	1/1	0.87	0.07	54,54,54,54	0
55	MG	1A	3172	1/1	0.87	0.37	50,50,50,50	0
55	MG	1a	3140	1/1	0.87	0.20	84,84,84,84	0
55	MG	1F	312	1/1	0.87	0.30	44,44,44,44	0
55	MG	2a	1660	1/1	0.87	0.16	79,79,79,79	0
55	MG	1a	3019	1/1	0.87	0.22	54,54,54,54	0
55	MG	1A	3245	1/1	0.87	0.51	46,46,46,46	0
55	MG	2A	3015	1/1	0.87	0.69	50,50,50,50	0
55	MG	1A	3331	1/1	0.87	0.10	22,22,22,22	0
55	MG	2A	3021	1/1	0.87	0.43	43,43,43,43	0
55	MG	1a	3026	1/1	0.87	0.24	58,58,58,58	0
55	MG	1N	8003	1/1	0.87	0.18	69,69,69,69	0
55	MG	2B	3017	1/1	0.87	0.13	84,84,84,84	0
55	MG	1P	201	1/1	0.87	0.98	30,30,30,30	0
55	MG	1A	3549	1/1	0.87	0.33	31,31,31,31	0
55	MG	2D	303	1/1	0.87	0.57	50,50,50,50	0
55	MG	2a	1711	1/1	0.87	0.74	80,80,80,80	0
55	MG	2A	3268	1/1	0.87	0.15	69,69,69,69	0
55	MG	2a	1718	1/1	0.87	0.13	88,88,88,88	0
55	MG	2D	308	1/1	0.87	0.53	55,55,55,55	0
55	MG	1a	3159	1/1	0.87	0.12	65,65,65,65	0
55	MG	2F	306	1/1	0.87	0.54	43,43,43,43	0
55	MG	1A	3670	1/1	0.87	0.24	53,53,53,53	0
55	MG	2A	3039	1/1	0.87	0.80	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3135	1/1	0.87	0.94	71,71,71,71	0
55	MG	1B	3013	1/1	0.87	0.12	58,58,58,58	0
55	MG	2A	3509	1/1	0.87	1.02	53,53,53,53	0
55	MG	1A	3761	1/1	0.87	0.13	64,64,64,64	0
55	MG	1A	3212	1/1	0.87	0.41	43,43,43,43	0
55	MG	1A	3767	1/1	0.87	0.06	51,51,51,51	0
55	MG	1A	3247	1/1	0.87	0.11	86,86,86,86	0
55	MG	1A	3087	1/1	0.87	0.77	33,33,33,33	0
55	MG	2X	101	1/1	0.87	0.20	61,61,61,61	0
55	MG	1A	3174	1/1	0.87	0.16	44,44,44,44	0
55	MG	2A	3337	1/1	0.87	0.13	79,79,79,79	0
55	MG	20	104	1/1	0.87	0.24	81,81,81,81	0
55	MG	20	106	1/1	0.87	0.48	78,78,78,78	0
55	MG	1A	3255	1/1	0.87	0.17	34,34,34,34	0
55	MG	1A	3201	1/1	0.87	0.34	41,41,41,41	0
55	MG	2A	3534	1/1	0.87	0.67	80,80,80,80	0
55	MG	2A	3357	1/1	0.87	0.14	50,50,50,50	0
55	MG	2A	3538	1/1	0.87	0.59	62,62,62,62	0
55	MG	1A	3156	1/1	0.87	0.78	54,54,54,54	0
55	MG	1A	3443	1/1	0.87	0.14	22,22,22,22	0
55	MG	2A	3380	1/1	0.87	0.20	81,81,81,81	0
55	MG	2A	3547	1/1	0.87	0.16	41,41,41,41	0
55	MG	15	107	1/1	0.87	0.13	52,52,52,52	0
55	MG	1A	3834	1/1	0.87	0.11	61,61,61,61	0
55	MG	2e	3001	1/1	0.87	0.28	67,67,67,67	0
55	MG	2A	3158	1/1	0.87	0.30	72,72,72,72	0
55	MG	2f	8001	1/1	0.87	0.17	56,56,56,56	0
55	MG	1A	3009	1/1	0.87	0.24	28,28,28,28	0
55	MG	1A	3455	1/1	0.87	0.10	49,49,49,49	0
55	MG	19	101	1/1	0.87	0.31	41,41,41,41	0
55	MG	1a	3078	1/1	0.87	0.66	78,78,78,78	0
55	MG	1A	3149	1/1	0.87	0.68	43,43,43,43	0
55	MG	2o	3001	1/1	0.87	0.18	60,60,60,60	0
55	MG	2A	3032	1/1	0.88	0.63	66,66,66,66	0
55	MG	2A	3432	1/1	0.88	0.21	74,74,74,74	0
55	MG	1A	3759	1/1	0.88	0.24	61,61,61,61	0
55	MG	1A	3026	1/1	0.88	0.14	63,63,63,63	0
55	MG	1A	3577	1/1	0.88	0.74	40,40,40,40	0
55	MG	2A	3446	1/1	0.88	0.30	62,62,62,62	0
55	MG	2A	3652	1/1	0.88	0.63	53,53,53,53	0
55	MG	2A	3653	1/1	0.88	0.23	77,77,77,77	0
55	MG	1F	305	1/1	0.88	0.25	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3021	1/1	0.88	0.16	42,42,42,42	0
55	MG	1a	3153	1/1	0.88	0.14	57,57,57,57	0
55	MG	1F	307	1/1	0.88	0.76	29,29,29,29	0
55	MG	1a	3024	1/1	0.88	0.21	57,57,57,57	0
55	MG	2a	1603	1/1	0.88	0.24	69,69,69,69	0
55	MG	2A	3459	1/1	0.88	0.31	71,71,71,71	0
55	MG	2a	1607	1/1	0.88	0.25	52,52,52,52	0
55	MG	1A	3579	1/1	0.88	0.14	64,64,64,64	0
55	MG	2A	3171	1/1	0.88	0.21	74,74,74,74	0
55	MG	2a	1615	1/1	0.88	0.16	47,47,47,47	0
55	MG	1A	3771	1/1	0.88	0.06	71,71,71,71	0
55	MG	1A	3781	1/1	0.88	0.63	28,28,28,28	0
55	MG	2A	3704	1/1	0.88	0.06	62,62,62,62	0
55	MG	2A	3468	1/1	0.88	0.11	80,80,80,80	0
55	MG	2A	3176	1/1	0.88	0.46	51,51,51,51	0
55	MG	1A	3581	1/1	0.88	0.53	35,35,35,35	0
55	MG	1A	3787	1/1	0.88	0.16	59,59,59,59	0
55	MG	1A	3136	1/1	0.88	0.10	68,68,68,68	0
55	MG	1a	3175	1/1	0.88	0.14	85,85,85,85	0
55	MG	2A	3721	1/1	0.88	0.26	42,42,42,42	0
55	MG	1A	3063	1/1	0.88	0.23	49,49,49,49	0
55	MG	2A	3727	1/1	0.88	0.51	65,65,65,65	0
55	MG	1A	3804	1/1	0.88	0.08	87,87,87,87	0
55	MG	2A	3071	1/1	0.88	0.57	62,62,62,62	0
55	MG	1A	3523	1/1	0.88	0.20	56,56,56,56	0
55	MG	1a	3183	1/1	0.88	0.18	84,84,84,84	0
55	MG	2A	3748	1/1	0.88	0.14	68,68,68,68	0
55	MG	2A	3215	1/1	0.88	0.24	80,80,80,80	0
55	MG	2a	1649	1/1	0.88	0.23	83,83,83,83	0
55	MG	1A	3524	1/1	0.88	0.17	52,52,52,52	0
55	MG	2A	3222	1/1	0.88	0.41	62,62,62,62	0
55	MG	1a	3052	1/1	0.88	0.22	51,51,51,51	0
55	MG	2A	3506	1/1	0.88	0.47	47,47,47,47	0
55	MG	2A	3225	1/1	0.88	0.09	51,51,51,51	0
55	MG	1a	3053	1/1	0.88	0.24	82,82,82,82	0
55	MG	2A	3240	1/1	0.88	0.16	34,34,34,34	0
55	MG	2A	3776	1/1	0.88	0.15	43,43,43,43	0
55	MG	1a	3056	1/1	0.88	0.10	69,69,69,69	0
55	MG	1A	3163	1/1	0.88	0.20	65,65,65,65	0
55	MG	1S	201	1/1	0.88	0.39	55,55,55,55	0
55	MG	1a	3208	1/1	0.88	0.23	75,75,75,75	0
55	MG	1U	207	1/1	0.88	0.23	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3825	1/1	0.88	0.09	68,68,68,68	0
55	MG	2A	3796	1/1	0.88	0.68	67,67,67,67	0
55	MG	1A	3048	1/1	0.88	0.70	33,33,33,33	0
55	MG	2A	3258	1/1	0.88	0.08	59,59,59,59	0
55	MG	1a	3217	1/1	0.88	0.13	87,87,87,87	0
55	MG	2A	3102	1/1	0.88	0.40	56,56,56,56	0
55	MG	2a	1716	1/1	0.88	0.16	73,73,73,73	0
55	MG	1a	3067	1/1	0.88	0.14	65,65,65,65	0
55	MG	1A	3281	1/1	0.88	0.10	54,54,54,54	0
55	MG	2A	3541	1/1	0.88	0.07	78,78,78,78	0
55	MG	2A	3810	1/1	0.88	0.32	51,51,51,51	0
55	MG	1A	3293	1/1	0.88	0.09	75,75,75,75	0
55	MG	1A	3313	1/1	0.88	0.20	55,55,55,55	0
55	MG	2A	3302	1/1	0.88	0.15	44,44,44,44	0
55	MG	1A	3200	1/1	0.88	0.91	37,37,37,37	0
55	MG	1A	3182	1/1	0.88	0.83	46,46,46,46	0
55	MG	2A	3822	1/1	0.88	0.31	53,53,53,53	0
55	MG	1A	3709	1/1	0.88	0.18	49,49,49,49	0
55	MG	2A	3319	1/1	0.88	0.06	78,78,78,78	0
55	MG	2a	1745	1/1	0.88	0.28	67,67,67,67	0
55	MG	1A	3478	1/1	0.88	0.16	44,44,44,44	0
55	MG	2B	3007	1/1	0.88	0.12	81,81,81,81	0
55	MG	1a	3092	1/1	0.88	0.07	85,85,85,85	0
55	MG	1A	3239	1/1	0.88	0.24	35,35,35,35	0
55	MG	2a	1758	1/1	0.88	0.24	70,70,70,70	0
55	MG	2a	1759	1/1	0.88	0.15	72,72,72,72	0
55	MG	1A	3097	1/1	0.88	0.52	48,48,48,48	0
55	MG	2A	3583	1/1	0.88	0.23	72,72,72,72	0
55	MG	2A	3001	1/1	0.88	0.18	55,55,55,55	0
55	MG	1A	3555	1/1	0.88	0.10	61,61,61,61	0
55	MG	2A	3587	1/1	0.88	0.08	68,68,68,68	0
55	MG	2a	1773	1/1	0.88	0.25	89,89,89,89	0
55	MG	2A	3348	1/1	0.88	0.10	76,76,76,76	0
55	MG	1A	3731	1/1	0.88	0.12	72,72,72,72	0
55	MG	2a	1777	1/1	0.88	0.11	77,77,77,77	0
55	MG	1A	3070	1/1	0.88	0.49	32,32,32,32	0
55	MG	1A	3038	1/1	0.88	0.50	66,66,66,66	0
55	MG	1a	3134	1/1	0.88	0.26	78,78,78,78	0
55	MG	2A	3381	1/1	0.88	0.08	77,77,77,77	0
55	MG	2F	304	1/1	0.88	0.58	49,49,49,49	0
55	MG	1A	3128	1/1	0.88	0.16	31,31,31,31	0
55	MG	1A	3088	1/1	0.88	0.64	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3144	1/1	0.88	0.14	73,73,73,73	0
55	MG	2A	3625	1/1	0.88	0.09	74,74,74,74	0
55	MG	1A	3757	1/1	0.88	0.20	37,37,37,37	0
55	MG	2A	3147	1/1	0.88	0.11	78,78,78,78	0
55	MG	1a	3006	1/1	0.88	0.48	74,74,74,74	0
55	MG	2A	3421	1/1	0.88	0.30	58,58,58,58	0
55	MG	2A	3634	1/1	0.88	0.18	83,83,83,83	0
55	MG	1A	3507	1/1	0.88	0.28	48,48,48,48	0
55	MG	2U	201	1/1	0.88	0.46	64,64,64,64	0
55	MG	1a	3146	1/1	0.88	0.07	80,80,80,80	0
55	MG	1A	3287	1/1	0.89	0.23	45,45,45,45	0
55	MG	2A	3686	1/1	0.89	0.08	95,95,95,95	0
55	MG	2A	3692	1/1	0.89	0.07	54,54,54,54	0
55	MG	1A	3625	1/1	0.89	0.46	35,35,35,35	0
55	MG	1A	3877	1/1	0.89	0.20	63,63,63,63	0
55	MG	2A	3218	1/1	0.89	0.07	52,52,52,52	0
55	MG	2A	3479	1/1	0.89	0.22	40,40,40,40	0
55	MG	2A	3716	1/1	0.89	0.15	92,92,92,92	0
55	MG	1A	3747	1/1	0.89	0.07	45,45,45,45	0
55	MG	1a	3055	1/1	0.89	0.58	47,47,47,47	0
55	MG	1a	3191	1/1	0.89	0.13	47,47,47,47	0
55	MG	1A	3093	1/1	0.89	0.33	43,43,43,43	0
55	MG	1A	3756	1/1	0.89	0.19	40,40,40,40	0
55	MG	2A	3089	1/1	0.89	0.10	56,56,56,56	0
55	MG	2A	3731	1/1	0.89	0.16	70,70,70,70	0
55	MG	2A	3732	1/1	0.89	0.74	61,61,61,61	0
55	MG	2A	3241	1/1	0.89	0.16	49,49,49,49	0
55	MG	2a	1632	1/1	0.89	0.23	75,75,75,75	0
55	MG	1A	3887	1/1	0.89	0.28	44,44,44,44	0
55	MG	2A	3504	1/1	0.89	0.21	55,55,55,55	0
55	MG	1A	3301	1/1	0.89	0.21	41,41,41,41	0
55	MG	1A	3302	1/1	0.89	0.10	42,42,42,42	0
55	MG	2A	3751	1/1	0.89	0.18	67,67,67,67	0
55	MG	1A	3640	1/1	0.89	0.40	34,34,34,34	0
55	MG	2A	3753	1/1	0.89	0.15	71,71,71,71	0
55	MG	1A	3484	1/1	0.89	0.12	47,47,47,47	0
55	MG	1A	3642	1/1	0.89	0.54	36,36,36,36	0
55	MG	2A	3761	1/1	0.89	0.12	38,38,38,38	0
55	MG	1a	3071	1/1	0.89	0.17	53,53,53,53	0
55	MG	1A	3646	1/1	0.89	0.20	31,31,31,31	0
55	MG	2A	3259	1/1	0.89	0.12	34,34,34,34	0
55	MG	1A	3126	1/1	0.89	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3106	1/1	0.89	0.53	60,60,60,60	0
55	MG	1A	3060	1/1	0.89	0.12	36,36,36,36	0
55	MG	1A	3317	1/1	0.89	0.12	73,73,73,73	0
55	MG	1A	3178	1/1	0.89	0.29	39,39,39,39	0
55	MG	1A	3179	1/1	0.89	0.60	38,38,38,38	0
55	MG	2a	1658	1/1	0.89	0.08	74,74,74,74	0
55	MG	1A	3788	1/1	0.89	0.07	48,48,48,48	0
55	MG	2a	1666	1/1	0.89	0.20	79,79,79,79	0
55	MG	2A	3790	1/1	0.89	0.05	71,71,71,71	0
55	MG	2A	3115	1/1	0.89	0.17	66,66,66,66	0
55	MG	2a	1677	1/1	0.89	0.22	71,71,71,71	0
55	MG	1a	3107	1/1	0.89	0.18	67,67,67,67	0
55	MG	2A	3128	1/1	0.89	0.11	61,61,61,61	0
55	MG	2A	3798	1/1	0.89	0.19	93,93,93,93	0
55	MG	1A	3662	1/1	0.89	0.09	52,52,52,52	0
55	MG	1A	3130	1/1	0.89	0.25	33,33,33,33	0
55	MG	2a	1696	1/1	0.89	0.09	77,77,77,77	0
55	MG	1A	3359	1/1	0.89	0.10	64,64,64,64	0
55	MG	1A	3145	1/1	0.89	0.39	29,29,29,29	0
55	MG	2A	3331	1/1	0.89	0.10	61,61,61,61	0
55	MG	1B	3007	1/1	0.89	0.13	51,51,51,51	0
55	MG	1a	3129	1/1	0.89	0.08	66,66,66,66	0
55	MG	1A	3807	1/1	0.89	0.26	48,48,48,48	0
55	MG	2A	3345	1/1	0.89	0.20	81,81,81,81	0
55	MG	1B	3012	1/1	0.89	0.07	44,44,44,44	0
55	MG	2A	3020	1/1	0.89	0.10	42,42,42,42	0
55	MG	1A	3580	1/1	0.89	0.14	61,61,61,61	0
55	MG	1A	3812	1/1	0.89	0.11	28,28,28,28	0
55	MG	1A	3514	1/1	0.89	0.12	35,35,35,35	0
55	MG	1A	3214	1/1	0.89	0.21	40,40,40,40	0
55	MG	1A	3216	1/1	0.89	0.24	52,52,52,52	0
55	MG	1a	3145	1/1	0.89	0.24	77,77,77,77	0
55	MG	1A	3254	1/1	0.89	0.33	50,50,50,50	0
55	MG	2A	3602	1/1	0.89	0.06	73,73,73,73	0
55	MG	1A	3690	1/1	0.89	0.11	67,67,67,67	0
55	MG	2A	3403	1/1	0.89	0.26	79,79,79,79	0
55	MG	2A	3035	1/1	0.89	0.42	32,32,32,32	0
55	MG	2A	3038	1/1	0.89	0.11	49,49,49,49	0
55	MG	1A	3195	1/1	0.89	0.34	46,46,46,46	0
55	MG	2A	3621	1/1	0.89	0.51	54,54,54,54	0
55	MG	2A	3622	1/1	0.89	0.35	49,49,49,49	0
55	MG	1D	304	1/1	0.89	0.37	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3157	1/1	0.89	0.16	57,57,57,57	0
55	MG	2A	3045	1/1	0.89	0.25	46,46,46,46	0
55	MG	1A	3408	1/1	0.89	0.20	43,43,43,43	0
55	MG	2A	3435	1/1	0.89	0.28	76,76,76,76	0
55	MG	1A	3530	1/1	0.89	0.13	44,44,44,44	0
55	MG	1A	3847	1/1	0.89	0.12	58,58,58,58	0
55	MG	2A	3442	1/1	0.89	0.23	81,81,81,81	0
55	MG	2A	3053	1/1	0.89	0.18	57,57,57,57	0
55	MG	2A	3167	1/1	0.89	0.26	56,56,56,56	0
55	MG	1A	3708	1/1	0.89	0.50	53,53,53,53	0
55	MG	2A	3451	1/1	0.89	0.30	67,67,67,67	0
55	MG	1A	3260	1/1	0.89	0.51	36,36,36,36	0
55	MG	2a	1788	1/1	0.89	0.04	86,86,86,86	0
55	MG	2A	3174	1/1	0.89	0.17	58,58,58,58	0
55	MG	2a	1793	1/1	0.89	0.15	61,61,61,61	0
55	MG	1A	3198	1/1	0.89	0.59	28,28,28,28	0
55	MG	1A	3264	1/1	0.89	0.14	37,37,37,37	0
55	MG	1A	3222	1/1	0.89	0.56	36,36,36,36	0
55	MG	1a	3035	1/1	0.89	1.15	64,64,64,64	0
55	MG	2W	3001	1/1	0.89	0.22	60,60,60,60	0
55	MG	2A	3185	1/1	0.89	0.80	62,62,62,62	0
55	MG	2A	3061	1/1	0.89	0.21	62,62,62,62	0
55	MG	1A	3857	1/1	0.89	0.28	71,71,71,71	0
55	MG	1A	3019	1/1	0.89	0.66	39,39,39,39	0
55	MG	1A	3054	1/1	0.89	0.31	49,49,49,49	0
55	MG	1A	3550	1/1	0.89	0.27	44,44,44,44	0
55	MG	2A	3678	1/1	0.89	0.09	92,92,92,92	0
55	MG	2A	3472	1/1	0.89	0.35	88,88,88,88	0
56	A	1B	3025	1/23	0.89	0.61	57,57,57,57	0
55	MG	1A	3866	1/1	0.90	0.21	61,61,61,61	0
55	MG	28	103	1/1	0.90	0.10	77,77,77,77	0
55	MG	1A	3348	1/1	0.90	0.09	71,71,71,71	0
55	MG	1A	3001	1/1	0.90	0.10	32,32,32,32	0
55	MG	1a	3066	1/1	0.90	0.11	68,68,68,68	0
55	MG	1A	3094	1/1	0.90	0.72	30,30,30,30	0
55	MG	2A	3537	1/1	0.90	0.16	61,61,61,61	0
55	MG	2A	3346	1/1	0.90	0.06	77,77,77,77	0
55	MG	2A	3347	1/1	0.90	0.09	80,80,80,80	0
55	MG	2A	3057	1/1	0.90	1.07	49,49,49,49	0
55	MG	15	105	1/1	0.90	0.32	43,43,43,43	0
55	MG	2A	3366	1/1	0.90	0.05	92,92,92,92	0
55	MG	1A	3133	1/1	0.90	0.56	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	17	103	1/1	0.90	0.84	43,43,43,43	0
55	MG	1A	3467	1/1	0.90	0.23	32,32,32,32	0
55	MG	1A	3792	1/1	0.90	0.21	55,55,55,55	0
55	MG	2A	3766	1/1	0.90	0.18	81,81,81,81	0
55	MG	1a	3203	1/1	0.90	0.12	67,67,67,67	0
55	MG	1A	3002	1/1	0.90	0.21	48,48,48,48	0
55	MG	2A	3571	1/1	0.90	0.12	41,41,41,41	0
55	MG	1A	3802	1/1	0.90	0.17	39,39,39,39	0
55	MG	2A	3069	1/1	0.90	0.83	52,52,52,52	0
55	MG	1A	3231	1/1	0.90	0.72	31,31,31,31	0
55	MG	2A	3412	1/1	0.90	0.54	70,70,70,70	0
55	MG	2A	3413	1/1	0.90	0.13	70,70,70,70	0
55	MG	2A	3786	1/1	0.90	0.11	49,49,49,49	0
55	MG	2A	3788	1/1	0.90	0.17	88,88,88,88	0
55	MG	2A	3789	1/1	0.90	0.21	62,62,62,62	0
55	MG	1A	3715	1/1	0.90	0.04	85,85,85,85	0
55	MG	1a	3095	1/1	0.90	0.14	62,62,62,62	0
55	MG	2A	3075	1/1	0.90	0.26	53,53,53,53	0
55	MG	1A	3721	1/1	0.90	0.18	50,50,50,50	0
55	MG	1A	3258	1/1	0.90	0.67	44,44,44,44	0
55	MG	2A	3429	1/1	0.90	0.10	64,64,64,64	0
55	MG	2A	3598	1/1	0.90	0.12	62,62,62,62	0
55	MG	1A	3487	1/1	0.90	0.33	57,57,57,57	0
55	MG	2a	1659	1/1	0.90	0.12	71,71,71,71	0
55	MG	1a	3007	1/1	0.90	0.17	74,74,74,74	0
55	MG	1A	3729	1/1	0.90	0.20	47,47,47,47	0
55	MG	1A	3817	1/1	0.90	0.37	72,72,72,72	0
55	MG	1A	3073	1/1	0.90	0.73	43,43,43,43	0
55	MG	1A	3539	1/1	0.90	0.17	62,62,62,62	0
55	MG	2A	3615	1/1	0.90	0.20	56,56,56,56	0
55	MG	1a	3133	1/1	0.90	0.32	74,74,74,74	0
55	MG	2A	3814	1/1	0.90	0.91	68,68,68,68	0
55	MG	2A	3207	1/1	0.90	0.12	70,70,70,70	0
55	MG	2A	3624	1/1	0.90	0.82	62,62,62,62	0
55	MG	2A	3208	1/1	0.90	0.15	60,60,60,60	0
55	MG	1A	3907	1/1	0.90	0.29	46,46,46,46	0
55	MG	1a	3136	1/1	0.90	0.36	79,79,79,79	0
55	MG	2B	3003	1/1	0.90	0.35	73,73,73,73	0
55	MG	1t	3001	1/1	0.90	0.36	76,76,76,76	0
55	MG	1A	3656	1/1	0.90	0.25	79,79,79,79	0
55	MG	2B	3006	1/1	0.90	0.41	80,80,80,80	0
55	MG	1a	3021	1/1	0.90	0.22	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2B	3008	1/1	0.90	0.11	83,83,83,83	0
55	MG	2B	3010	1/1	0.90	0.07	72,72,72,72	0
55	MG	1A	3491	1/1	0.90	0.29	55,55,55,55	0
55	MG	1A	3742	1/1	0.90	0.89	71,71,71,71	0
55	MG	2a	1726	1/1	0.90	0.09	78,78,78,78	0
55	MG	2A	3639	1/1	0.90	0.19	76,76,76,76	0
55	MG	2a	1729	1/1	0.90	0.14	60,60,60,60	0
55	MG	2A	3107	1/1	0.90	0.17	57,57,57,57	0
55	MG	2A	3232	1/1	0.90	0.09	67,67,67,67	0
55	MG	2A	3011	1/1	0.90	0.43	58,58,58,58	0
55	MG	1A	3113	1/1	0.90	0.33	41,41,41,41	0
55	MG	2A	3110	1/1	0.90	0.54	53,53,53,53	0
55	MG	2A	3649	1/1	0.90	0.41	49,49,49,49	0
55	MG	2a	1744	1/1	0.90	0.15	76,76,76,76	0
55	MG	2A	3470	1/1	0.90	0.12	63,63,63,63	0
55	MG	2A	3245	1/1	0.90	0.32	78,78,78,78	0
55	MG	2D	307	1/1	0.90	1.69	64,64,64,64	0
55	MG	1a	3027	1/1	0.90	0.46	70,70,70,70	0
55	MG	1A	3432	1/1	0.90	0.07	49,49,49,49	0
55	MG	2a	1757	1/1	0.90	0.11	71,71,71,71	0
55	MG	2E	307	1/1	0.90	0.08	73,73,73,73	0
55	MG	1A	3138	1/1	0.90	0.13	52,52,52,52	0
55	MG	2a	1760	1/1	0.90	0.06	90,90,90,90	0
55	MG	2a	1761	1/1	0.90	0.21	67,67,67,67	0
55	MG	1A	3139	1/1	0.90	0.22	59,59,59,59	0
55	MG	2F	307	1/1	0.90	0.87	60,60,60,60	0
55	MG	1Q	201	1/1	0.90	0.50	44,44,44,44	0
55	MG	2A	3121	1/1	0.90	0.15	81,81,81,81	0
55	MG	1A	3027	1/1	0.90	0.31	31,31,31,31	0
55	MG	2A	3026	1/1	0.90	0.32	73,73,73,73	0
55	MG	1A	3454	1/1	0.90	0.08	56,56,56,56	0
55	MG	1A	3607	1/1	0.90	0.07	60,60,60,60	0
55	MG	1U	204	1/1	0.90	0.70	29,29,29,29	0
55	MG	2A	3684	1/1	0.90	0.12	57,57,57,57	0
55	MG	2A	3277	1/1	0.90	0.25	36,36,36,36	0
55	MG	1a	3043	1/1	0.90	0.43	68,68,68,68	0
55	MG	2U	203	1/1	0.90	0.10	71,71,71,71	0
55	MG	2A	3690	1/1	0.90	0.20	84,84,84,84	0
55	MG	2V	202	1/1	0.90	1.02	55,55,55,55	0
55	MG	1A	3556	1/1	0.90	0.15	14,14,14,14	0
55	MG	2A	3295	1/1	0.90	0.27	71,71,71,71	0
55	MG	2A	3036	1/1	0.90	0.52	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2X	103	1/1	0.90	0.11	58,58,58,58	0
55	MG	1A	3510	1/1	0.90	0.10	70,70,70,70	0
55	MG	20	103	1/1	0.90	0.30	59,59,59,59	0
55	MG	1W	3001	1/1	0.90	0.23	38,38,38,38	0
55	MG	1B	3016	1/1	0.90	0.07	51,51,51,51	0
55	MG	1A	3272	1/1	0.90	0.26	56,56,56,56	0
55	MG	2A	3143	1/1	0.90	0.28	53,53,53,53	0
55	MG	10	103	1/1	0.90	0.22	65,65,65,65	0
55	MG	2A	3521	1/1	0.90	0.19	68,68,68,68	0
55	MG	1A	3612	1/1	0.90	0.07	78,78,78,78	0
55	MG	1A	3338	1/1	0.90	0.16	20,20,20,20	0
55	MG	1A	3728	1/1	0.91	0.10	54,54,54,54	0
55	MG	1D	309	1/1	0.91	0.51	41,41,41,41	0
55	MG	2A	3448	1/1	0.91	0.25	51,51,51,51	0
55	MG	1D	311	1/1	0.91	0.22	38,38,38,38	0
55	MG	1A	3017	1/1	0.91	0.40	31,31,31,31	0
55	MG	2A	3654	1/1	0.91	0.08	34,34,34,34	0
55	MG	1D	314	1/1	0.91	0.27	34,34,34,34	0
55	MG	2A	3659	1/1	0.91	0.17	73,73,73,73	0
55	MG	1A	3633	1/1	0.91	0.24	79,79,79,79	0
55	MG	2A	3196	1/1	0.91	0.18	77,77,77,77	0
55	MG	2A	3197	1/1	0.91	0.20	48,48,48,48	0
55	MG	2A	3666	1/1	0.91	0.05	70,70,70,70	0
55	MG	2A	3458	1/1	0.91	0.10	78,78,78,78	0
55	MG	2A	3200	1/1	0.91	0.99	65,65,65,65	0
55	MG	1D	316	1/1	0.91	0.10	73,73,73,73	0
55	MG	1A	3052	1/1	0.91	0.81	36,36,36,36	0
55	MG	1A	3635	1/1	0.91	0.26	39,39,39,39	0
55	MG	1A	3636	1/1	0.91	0.11	38,38,38,38	0
55	MG	2A	3212	1/1	0.91	0.16	60,60,60,60	0
55	MG	1A	3008	1/1	0.91	0.26	46,46,46,46	0
55	MG	1A	3033	1/1	0.91	0.59	45,45,45,45	0
55	MG	2A	3689	1/1	0.91	0.19	67,67,67,67	0
55	MG	1A	3005	1/1	0.91	0.21	22,22,22,22	0
55	MG	1a	3178	1/1	0.91	0.15	75,75,75,75	0
55	MG	2A	3697	1/1	0.91	0.07	57,57,57,57	0
55	MG	2A	3703	1/1	0.91	0.25	93,93,93,93	0
55	MG	1F	304	1/1	0.91	0.96	39,39,39,39	0
55	MG	1a	3036	1/1	0.91	0.12	49,49,49,49	0
55	MG	2a	1611	1/1	0.91	0.10	58,58,58,58	0
55	MG	1A	3870	1/1	0.91	0.26	54,54,54,54	0
55	MG	1a	3182	1/1	0.91	0.50	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1617	1/1	0.91	0.38	65,65,65,65	0
55	MG	1A	3645	1/1	0.91	0.31	54,54,54,54	0
55	MG	1A	3122	1/1	0.91	0.53	30,30,30,30	0
55	MG	2A	3481	1/1	0.91	0.23	67,67,67,67	0
55	MG	1F	309	1/1	0.91	0.11	28,28,28,28	0
55	MG	2A	3483	1/1	0.91	0.65	55,55,55,55	0
55	MG	2A	3722	1/1	0.91	0.08	67,67,67,67	0
55	MG	2A	3724	1/1	0.91	0.11	45,45,45,45	0
55	MG	2A	3725	1/1	0.91	0.05	64,64,64,64	0
55	MG	1A	3440	1/1	0.91	0.15	47,47,47,47	0
55	MG	1A	3511	1/1	0.91	0.15	26,26,26,26	0
55	MG	1A	3882	1/1	0.91	0.13	62,62,62,62	0
55	MG	2a	1640	1/1	0.91	0.72	61,61,61,61	0
55	MG	1a	3049	1/1	0.91	0.45	69,69,69,69	0
55	MG	2A	3096	1/1	0.91	0.14	46,46,46,46	0
55	MG	1A	3513	1/1	0.91	0.09	27,27,27,27	0
55	MG	1A	3314	1/1	0.91	0.12	52,52,52,52	0
55	MG	1a	3207	1/1	0.91	0.12	76,76,76,76	0
55	MG	1N	8002	1/1	0.91	0.15	64,64,64,64	0
55	MG	2A	3750	1/1	0.91	0.33	63,63,63,63	0
55	MG	2A	3260	1/1	0.91	0.12	66,66,66,66	0
55	MG	1A	3445	1/1	0.91	0.17	65,65,65,65	0
55	MG	1A	3449	1/1	0.91	0.17	21,21,21,21	0
55	MG	1A	3076	1/1	0.91	0.23	63,63,63,63	0
55	MG	1a	3062	1/1	0.91	0.38	79,79,79,79	0
55	MG	2A	3758	1/1	0.91	0.15	77,77,77,77	0
55	MG	2A	3759	1/1	0.91	0.30	88,88,88,88	0
55	MG	2A	3278	1/1	0.91	0.11	56,56,56,56	0
55	MG	1A	3891	1/1	0.91	0.18	64,64,64,64	0
55	MG	1A	3666	1/1	0.91	0.23	45,45,45,45	0
55	MG	1A	3778	1/1	0.91	0.07	83,83,83,83	0
55	MG	1A	3218	1/1	0.91	0.43	35,35,35,35	0
55	MG	2A	3769	1/1	0.91	0.17	75,75,75,75	0
55	MG	2a	1673	1/1	0.91	0.15	63,63,63,63	0
55	MG	2A	3301	1/1	0.91	0.14	49,49,49,49	0
55	MG	1R	205	1/1	0.91	0.28	34,34,34,34	0
55	MG	1A	3023	1/1	0.91	0.14	21,21,21,21	0
55	MG	1A	3595	1/1	0.91	0.10	67,67,67,67	0
55	MG	2a	1684	1/1	0.91	0.07	76,76,76,76	0
55	MG	1A	3078	1/1	0.91	0.56	39,39,39,39	0
55	MG	1f	8001	1/1	0.91	0.21	60,60,60,60	0
55	MG	1A	3598	1/1	0.91	0.13	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3099	1/1	0.91	0.30	62,62,62,62	0
55	MG	1A	3007	1/1	0.91	0.12	38,38,38,38	0
55	MG	1A	3154	1/1	0.91	0.64	28,28,28,28	0
55	MG	2a	1701	1/1	0.91	0.23	90,90,90,90	0
55	MG	1A	3349	1/1	0.91	0.17	25,25,25,25	0
55	MG	1A	3350	1/1	0.91	0.16	46,46,46,46	0
55	MG	2A	3556	1/1	0.91	0.71	57,57,57,57	0
55	MG	2A	3557	1/1	0.91	0.14	67,67,67,67	0
55	MG	2A	3340	1/1	0.91	0.27	52,52,52,52	0
55	MG	2A	3560	1/1	0.91	0.19	53,53,53,53	0
55	MG	1a	3094	1/1	0.91	0.10	46,46,46,46	0
55	MG	2a	1720	1/1	0.91	0.10	73,73,73,73	0
55	MG	2a	1721	1/1	0.91	0.17	84,84,84,84	0
55	MG	1A	3694	1/1	0.91	0.10	35,35,35,35	0
55	MG	2A	3569	1/1	0.91	0.65	48,48,48,48	0
55	MG	2A	3570	1/1	0.91	0.14	57,57,57,57	0
55	MG	1a	3103	1/1	0.91	0.17	72,72,72,72	0
55	MG	2A	3808	1/1	0.91	0.22	44,44,44,44	0
55	MG	1A	3474	1/1	0.91	0.20	69,69,69,69	0
55	MG	2A	3575	1/1	0.91	0.20	48,48,48,48	0
55	MG	2A	3811	1/1	0.91	0.17	67,67,67,67	0
55	MG	1A	3696	1/1	0.91	0.10	29,29,29,29	0
55	MG	2a	1739	1/1	0.91	0.08	86,86,86,86	0
55	MG	1A	3102	1/1	0.91	0.33	42,42,42,42	0
55	MG	2A	3363	1/1	0.91	0.14	50,50,50,50	0
55	MG	2A	3584	1/1	0.91	0.23	62,62,62,62	0
55	MG	1a	3116	1/1	0.91	0.44	76,76,76,76	0
55	MG	1A	3479	1/1	0.91	0.13	39,39,39,39	0
55	MG	2a	1750	1/1	0.91	0.11	83,83,83,83	0
55	MG	1a	3118	1/1	0.91	0.08	70,70,70,70	0
55	MG	1a	3120	1/1	0.91	0.10	65,65,65,65	0
55	MG	1A	3824	1/1	0.91	0.15	47,47,47,47	0
55	MG	1A	3707	1/1	0.91	0.22	72,72,72,72	0
55	MG	2A	3595	1/1	0.91	0.11	52,52,52,52	0
55	MG	2A	3387	1/1	0.91	0.15	68,68,68,68	0
55	MG	17	101	1/1	0.91	0.42	35,35,35,35	0
55	MG	2A	3600	1/1	0.91	0.50	54,54,54,54	0
55	MG	2A	3031	1/1	0.91	0.35	59,59,59,59	0
55	MG	1a	3130	1/1	0.91	0.30	62,62,62,62	0
55	MG	2a	1767	1/1	0.91	0.17	79,79,79,79	0
55	MG	2A	3401	1/1	0.91	0.19	66,66,66,66	0
55	MG	1A	3042	1/1	0.91	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3404	1/1	0.91	0.05	63,63,63,63	0
55	MG	2A	3406	1/1	0.91	0.56	62,62,62,62	0
55	MG	1A	3833	1/1	0.91	0.21	69,69,69,69	0
55	MG	2A	3618	1/1	0.91	0.21	55,55,55,55	0
55	MG	1A	3371	1/1	0.91	0.19	63,63,63,63	0
55	MG	2D	301	1/1	0.91	0.78	47,47,47,47	0
55	MG	1a	3135	1/1	0.91	0.13	77,77,77,77	0
55	MG	1A	3711	1/1	0.91	0.26	39,39,39,39	0
55	MG	1A	3618	1/1	0.91	0.24	72,72,72,72	0
55	MG	2a	1791	1/1	0.91	0.21	71,71,71,71	0
55	MG	2D	305	1/1	0.91	0.95	59,59,59,59	0
55	MG	1A	3376	1/1	0.91	0.06	72,72,72,72	0
55	MG	2a	1795	1/1	0.91	0.17	57,57,57,57	0
55	MG	1A	3488	1/1	0.91	0.46	43,43,43,43	0
55	MG	2A	3426	1/1	0.91	0.20	70,70,70,70	0
55	MG	2A	3427	1/1	0.91	0.13	61,61,61,61	0
55	MG	2A	3633	1/1	0.91	0.11	82,82,82,82	0
55	MG	2F	305	1/1	0.91	0.13	46,46,46,46	0
55	MG	2A	3428	1/1	0.91	0.28	71,71,71,71	0
55	MG	1A	3064	1/1	0.91	0.33	29,29,29,29	0
55	MG	1D	303	1/1	0.91	0.30	52,52,52,52	0
55	MG	2A	3048	1/1	0.91	0.24	56,56,56,56	0
55	MG	1A	3014	1/1	0.91	0.64	41,41,41,41	0
55	MG	1D	306	1/1	0.91	0.28	35,35,35,35	0
55	MG	1a	3009	1/1	0.91	0.31	69,69,69,69	0
55	MG	2N	201	1/1	0.91	0.63	82,82,82,82	0
55	MG	1A	3726	1/1	0.91	0.24	29,29,29,29	0
55	MG	2A	3359	1/1	0.92	0.07	51,51,51,51	0
55	MG	2A	3360	1/1	0.92	0.11	64,64,64,64	0
55	MG	2A	3164	1/1	0.92	0.40	56,56,56,56	0
55	MG	2A	3740	1/1	0.92	0.26	68,68,68,68	0
55	MG	1A	3727	1/1	0.92	0.23	40,40,40,40	0
55	MG	2a	1605	1/1	0.92	0.30	56,56,56,56	0
55	MG	2A	3743	1/1	0.92	0.26	59,59,59,59	0
55	MG	2A	3549	1/1	0.92	0.05	74,74,74,74	0
55	MG	2a	1608	1/1	0.92	0.08	51,51,51,51	0
55	MG	1A	3836	1/1	0.92	0.12	54,54,54,54	0
55	MG	2A	3168	1/1	0.92	0.28	53,53,53,53	0
55	MG	1A	3446	1/1	0.92	0.21	49,49,49,49	0
55	MG	1a	3189	1/1	0.92	0.25	84,84,84,84	0
55	MG	2a	1616	1/1	0.92	0.14	68,68,68,68	0
55	MG	2A	3383	1/1	0.92	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1619	1/1	0.92	0.33	72,72,72,72	0
55	MG	10	105	1/1	0.92	0.10	57,57,57,57	0
55	MG	1A	3237	1/1	0.92	0.15	53,53,53,53	0
55	MG	2A	3755	1/1	0.92	0.12	63,63,63,63	0
55	MG	1a	3196	1/1	0.92	0.09	77,77,77,77	0
55	MG	2a	1626	1/1	0.92	0.12	60,60,60,60	0
55	MG	2A	3757	1/1	0.92	0.35	53,53,53,53	0
55	MG	2A	3568	1/1	0.92	0.24	68,68,68,68	0
55	MG	1A	3451	1/1	0.92	0.06	43,43,43,43	0
55	MG	2A	3181	1/1	0.92	0.23	79,79,79,79	0
55	MG	2A	3398	1/1	0.92	0.17	81,81,81,81	0
55	MG	2A	3573	1/1	0.92	0.13	71,71,71,71	0
55	MG	1A	3341	1/1	0.92	0.12	20,20,20,20	0
55	MG	1A	3582	1/1	0.92	0.30	69,69,69,69	0
55	MG	1A	3586	1/1	0.92	0.07	59,59,59,59	0
55	MG	1A	3849	1/1	0.92	0.26	89,89,89,89	0
55	MG	1A	3741	1/1	0.92	0.11	56,56,56,56	0
55	MG	2A	3774	1/1	0.92	0.21	79,79,79,79	0
55	MG	1A	3036	1/1	0.92	0.15	28,28,28,28	0
55	MG	1A	3243	1/1	0.92	1.04	44,44,44,44	0
55	MG	2A	3416	1/1	0.92	0.17	56,56,56,56	0
55	MG	2A	3418	1/1	0.92	0.11	55,55,55,55	0
55	MG	2A	3588	1/1	0.92	0.22	67,67,67,67	0
55	MG	1A	3037	1/1	0.92	0.08	56,56,56,56	0
55	MG	1A	3750	1/1	0.92	0.09	52,52,52,52	0
55	MG	2A	3198	1/1	0.92	0.17	27,27,27,27	0
55	MG	1A	3123	1/1	0.92	0.57	27,27,27,27	0
55	MG	1a	3223	1/1	0.92	0.19	54,54,54,54	0
55	MG	2A	3793	1/1	0.92	0.27	67,67,67,67	0
55	MG	2A	3597	1/1	0.92	0.10	51,51,51,51	0
55	MG	1A	3285	1/1	0.92	0.28	47,47,47,47	0
55	MG	2A	3797	1/1	0.92	0.15	75,75,75,75	0
55	MG	2A	3599	1/1	0.92	0.12	75,75,75,75	0
55	MG	2a	1668	1/1	0.92	0.08	51,51,51,51	0
55	MG	1A	3863	1/1	0.92	0.24	58,58,58,58	0
55	MG	1A	3596	1/1	0.92	0.22	58,58,58,58	0
55	MG	2A	3430	1/1	0.92	0.20	74,74,74,74	0
55	MG	1A	3525	1/1	0.92	0.19	57,57,57,57	0
55	MG	2A	3608	1/1	0.92	0.16	62,62,62,62	0
55	MG	1A	3671	1/1	0.92	0.20	46,46,46,46	0
55	MG	1A	3363	1/1	0.92	0.08	26,26,26,26	0
55	MG	2A	3436	1/1	0.92	0.12	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1688	1/1	0.92	0.09	56,56,56,56	0
55	MG	2A	3100	1/1	0.92	0.20	58,58,58,58	0
55	MG	1A	3012	1/1	0.92	0.18	22,22,22,22	0
55	MG	1E	302	1/1	0.92	0.93	39,39,39,39	0
55	MG	1l	201	1/1	0.92	0.22	74,74,74,74	0
55	MG	1A	3051	1/1	0.92	0.57	30,30,30,30	0
55	MG	2A	3447	1/1	0.92	0.17	73,73,73,73	0
55	MG	2a	1707	1/1	0.92	0.19	92,92,92,92	0
55	MG	2A	3229	1/1	0.92	0.16	82,82,82,82	0
55	MG	2A	3230	1/1	0.92	0.36	51,51,51,51	0
55	MG	1A	3470	1/1	0.92	0.10	28,28,28,28	0
55	MG	2A	3237	1/1	0.92	0.17	67,67,67,67	0
55	MG	1A	3294	1/1	0.92	0.06	33,33,33,33	0
55	MG	1A	3772	1/1	0.92	0.17	37,37,37,37	0
55	MG	2A	3635	1/1	0.92	0.05	92,92,92,92	0
55	MG	1A	3775	1/1	0.92	0.16	72,72,72,72	0
55	MG	2A	3005	1/1	0.92	0.13	44,44,44,44	0
55	MG	1A	3477	1/1	0.92	0.12	20,20,20,20	0
55	MG	2A	3640	1/1	0.92	0.22	78,78,78,78	0
55	MG	1A	3381	1/1	0.92	0.11	62,62,62,62	0
55	MG	1A	3691	1/1	0.92	0.13	26,26,26,26	0
55	MG	1a	3023	1/1	0.92	0.27	53,53,53,53	0
55	MG	1A	3547	1/1	0.92	0.44	35,35,35,35	0
55	MG	1A	3892	1/1	0.92	0.22	62,62,62,62	0
55	MG	2a	1733	1/1	0.92	0.17	67,67,67,67	0
55	MG	2A	3125	1/1	0.92	1.07	58,58,58,58	0
55	MG	1A	3384	1/1	0.92	0.47	58,58,58,58	0
55	MG	1A	3385	1/1	0.92	0.12	57,57,57,57	0
55	MG	1A	3115	1/1	0.92	0.07	54,54,54,54	0
55	MG	1a	3032	1/1	0.92	0.14	45,45,45,45	0
55	MG	1A	3701	1/1	0.92	0.49	40,40,40,40	0
55	MG	2A	3276	1/1	0.92	0.14	48,48,48,48	0
55	MG	2A	3133	1/1	0.92	0.37	60,60,60,60	0
55	MG	1G	3002	1/1	0.92	0.07	62,62,62,62	0
55	MG	2a	1751	1/1	0.92	0.17	107,107,107,107	0
55	MG	2A	3028	1/1	0.92	0.30	64,64,64,64	0
55	MG	1A	3039	1/1	0.92	0.32	55,55,55,55	0
55	MG	2E	304	1/1	0.92	0.83	46,46,46,46	0
55	MG	2A	3670	1/1	0.92	0.08	84,84,84,84	0
55	MG	2F	301	1/1	0.92	1.03	47,47,47,47	0
55	MG	2F	303	1/1	0.92	0.48	62,62,62,62	0
55	MG	2A	3294	1/1	0.92	0.16	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3226	1/1	0.92	0.46	31,31,31,31	0
55	MG	2A	3297	1/1	0.92	0.14	78,78,78,78	0
55	MG	2A	3676	1/1	0.92	0.38	73,73,73,73	0
55	MG	1A	3903	1/1	0.92	0.23	59,59,59,59	0
55	MG	1A	3904	1/1	0.92	0.31	17,17,17,17	0
55	MG	1A	3402	1/1	0.92	0.29	43,43,43,43	0
55	MG	1A	3117	1/1	0.92	0.11	44,44,44,44	0
55	MG	1A	3494	1/1	0.92	0.19	59,59,59,59	0
55	MG	1a	3165	1/1	0.92	0.61	75,75,75,75	0
55	MG	2A	3310	1/1	0.92	0.10	57,57,57,57	0
55	MG	2Q	8002	1/1	0.92	0.08	62,62,62,62	0
55	MG	2A	3317	1/1	0.92	0.15	55,55,55,55	0
55	MG	2R	201	1/1	0.92	0.79	56,56,56,56	0
55	MG	2a	1786	1/1	0.92	0.07	90,90,90,90	0
55	MG	1a	3166	1/1	0.92	0.09	80,80,80,80	0
55	MG	2A	3041	1/1	0.92	0.09	73,73,73,73	0
55	MG	2A	3321	1/1	0.92	0.18	34,34,34,34	0
55	MG	1A	3710	1/1	0.92	0.10	42,42,42,42	0
55	MG	1A	3257	1/1	0.92	0.23	40,40,40,40	0
55	MG	1A	3916	1/1	0.92	0.41	29,29,29,29	0
55	MG	2V	203	1/1	0.92	0.15	59,59,59,59	0
55	MG	1A	3499	1/1	0.92	0.12	59,59,59,59	0
55	MG	2A	3712	1/1	0.92	0.16	63,63,63,63	0
55	MG	1U	201	1/1	0.92	0.27	34,34,34,34	0
55	MG	1A	3316	1/1	0.92	0.11	58,58,58,58	0
55	MG	2A	3528	1/1	0.92	0.17	34,34,34,34	0
55	MG	2A	3157	1/1	0.92	0.29	62,62,62,62	0
55	MG	1A	3132	1/1	0.92	0.17	35,35,35,35	0
55	MG	1A	3208	1/1	0.92	0.23	37,37,37,37	0
55	MG	1A	3020	1/1	0.92	0.59	39,39,39,39	0
55	MG	1W	3002	1/1	0.92	0.20	49,49,49,49	0
55	MG	2A	3350	1/1	0.92	0.09	49,49,49,49	0
55	MG	1A	3104	1/1	0.92	0.67	37,37,37,37	0
55	MG	2A	3729	1/1	0.92	0.14	70,70,70,70	0
55	MG	2A	3339	1/1	0.93	0.05	71,71,71,71	0
55	MG	2A	3531	1/1	0.93	0.09	83,83,83,83	0
55	MG	1a	3163	1/1	0.93	0.10	74,74,74,74	0
55	MG	2A	3728	1/1	0.93	0.11	34,34,34,34	0
55	MG	1a	3044	1/1	0.93	0.10	66,66,66,66	0
55	MG	2A	3343	1/1	0.93	0.04	73,73,73,73	0
55	MG	1A	3481	1/1	0.93	0.10	23,23,23,23	0
55	MG	2A	3733	1/1	0.93	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3167	1/1	0.93	0.11	86,86,86,86	0
55	MG	1U	206	1/1	0.93	0.26	28,28,28,28	0
55	MG	1A	3679	1/1	0.93	0.22	44,44,44,44	0
55	MG	2a	1610	1/1	0.93	0.55	74,74,74,74	0
55	MG	2A	3049	1/1	0.93	0.21	38,38,38,38	0
55	MG	1a	3050	1/1	0.93	0.15	45,45,45,45	0
55	MG	2A	3544	1/1	0.93	0.06	90,90,90,90	0
55	MG	1a	3172	1/1	0.93	0.17	77,77,77,77	0
55	MG	2A	3169	1/1	0.93	0.81	50,50,50,50	0
55	MG	1A	3406	1/1	0.93	0.19	46,46,46,46	0
55	MG	1A	3407	1/1	0.93	0.05	48,48,48,48	0
55	MG	2A	3369	1/1	0.93	0.12	58,58,58,58	0
55	MG	1A	3069	1/1	0.93	0.17	38,38,38,38	0
55	MG	1A	3411	1/1	0.93	0.17	52,52,52,52	0
55	MG	1A	3346	1/1	0.93	0.10	52,52,52,52	0
55	MG	2A	3177	1/1	0.93	0.15	62,62,62,62	0
55	MG	2a	1630	1/1	0.93	0.50	50,50,50,50	0
55	MG	2A	3382	1/1	0.93	0.19	65,65,65,65	0
55	MG	2A	3565	1/1	0.93	0.07	56,56,56,56	0
55	MG	10	102	1/1	0.93	0.45	52,52,52,52	0
55	MG	2A	3385	1/1	0.93	0.18	32,32,32,32	0
55	MG	1A	3865	1/1	0.93	0.14	75,75,75,75	0
55	MG	2A	3182	1/1	0.93	0.27	72,72,72,72	0
55	MG	1A	3080	1/1	0.93	0.59	36,36,36,36	0
55	MG	2A	3392	1/1	0.93	0.19	31,31,31,31	0
55	MG	1A	3620	1/1	0.93	0.05	50,50,50,50	0
55	MG	2A	3772	1/1	0.93	0.08	63,63,63,63	0
55	MG	2A	3577	1/1	0.93	0.10	56,56,56,56	0
55	MG	10	108	1/1	0.93	0.68	43,43,43,43	0
55	MG	2A	3187	1/1	0.93	0.61	73,73,73,73	0
55	MG	2A	3399	1/1	0.93	0.16	45,45,45,45	0
55	MG	2A	3190	1/1	0.93	0.47	68,68,68,68	0
55	MG	2A	3191	1/1	0.93	0.17	61,61,61,61	0
55	MG	2A	3783	1/1	0.93	0.12	78,78,78,78	0
55	MG	1D	305	1/1	0.93	0.63	42,42,42,42	0
55	MG	2A	3785	1/1	0.93	0.09	60,60,60,60	0
55	MG	1A	3436	1/1	0.93	0.17	49,49,49,49	0
55	MG	2A	3410	1/1	0.93	0.10	83,83,83,83	0
55	MG	13	102	1/1	0.93	0.35	44,44,44,44	0
55	MG	1a	3193	1/1	0.93	0.21	74,74,74,74	0
55	MG	2A	3592	1/1	0.93	0.17	89,89,89,89	0
55	MG	2A	3414	1/1	0.93	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1662	1/1	0.93	0.09	74,74,74,74	0
55	MG	2A	3594	1/1	0.93	0.11	56,56,56,56	0
55	MG	1A	3215	1/1	0.93	0.42	38,38,38,38	0
55	MG	1A	3233	1/1	0.93	0.36	63,63,63,63	0
55	MG	2A	3417	1/1	0.93	0.76	58,58,58,58	0
55	MG	1A	3444	1/1	0.93	0.10	75,75,75,75	0
55	MG	1A	3706	1/1	0.93	0.16	54,54,54,54	0
55	MG	2a	1681	1/1	0.93	0.12	84,84,84,84	0
55	MG	1A	3358	1/1	0.93	0.13	19,19,19,19	0
55	MG	2A	3204	1/1	0.93	0.30	54,54,54,54	0
55	MG	1A	3256	1/1	0.93	0.20	41,41,41,41	0
55	MG	2A	3082	1/1	0.93	0.14	56,56,56,56	0
55	MG	1A	3235	1/1	0.93	0.37	38,38,38,38	0
55	MG	2a	1689	1/1	0.93	0.10	58,58,58,58	0
55	MG	2a	1690	1/1	0.93	0.24	83,83,83,83	0
55	MG	1a	3210	1/1	0.93	0.15	78,78,78,78	0
55	MG	1a	3087	1/1	0.93	0.06	57,57,57,57	0
55	MG	1A	3886	1/1	0.93	0.16	61,61,61,61	0
55	MG	1D	317	1/1	0.93	0.24	57,57,57,57	0
55	MG	1A	3155	1/1	0.93	0.59	27,27,27,27	0
55	MG	2A	3619	1/1	0.93	0.12	50,50,50,50	0
55	MG	2a	1706	1/1	0.93	0.28	63,63,63,63	0
55	MG	1A	3575	1/1	0.93	0.31	23,23,23,23	0
55	MG	1a	3220	1/1	0.93	0.09	65,65,65,65	0
55	MG	1a	3106	1/1	0.93	0.06	60,60,60,60	0
55	MG	1A	3137	1/1	0.93	0.96	46,46,46,46	0
55	MG	2a	1712	1/1	0.93	0.33	69,69,69,69	0
55	MG	2a	1713	1/1	0.93	0.06	69,69,69,69	0
55	MG	1A	3022	1/1	0.93	0.42	31,31,31,31	0
55	MG	1a	3109	1/1	0.93	0.24	53,53,53,53	0
55	MG	2A	3103	1/1	0.93	0.51	65,65,65,65	0
55	MG	1a	3112	1/1	0.93	0.17	86,86,86,86	0
55	MG	1A	3805	1/1	0.93	0.07	65,65,65,65	0
55	MG	1F	301	1/1	0.93	0.31	28,28,28,28	0
55	MG	1A	3718	1/1	0.93	0.21	67,67,67,67	0
55	MG	2a	1723	1/1	0.93	0.23	110,110,110,110	0
55	MG	1A	3719	1/1	0.93	0.10	45,45,45,45	0
55	MG	1a	3008	1/1	0.93	0.43	60,60,60,60	0
55	MG	2A	3638	1/1	0.93	0.16	86,86,86,86	0
55	MG	2a	1728	1/1	0.93	0.13	86,86,86,86	0
55	MG	1A	3512	1/1	0.93	0.28	46,46,46,46	0
55	MG	1a	3010	1/1	0.93	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1a	3128	1/1	0.93	0.18	71,71,71,71	0
55	MG	2a	1732	1/1	0.93	0.10	74,74,74,74	0
55	MG	1A	3898	1/1	0.93	0.38	63,63,63,63	0
55	MG	1A	3159	1/1	0.93	0.27	30,30,30,30	0
55	MG	2a	1735	1/1	0.93	0.08	81,81,81,81	0
55	MG	2A	3002	1/1	0.93	0.12	63,63,63,63	0
55	MG	2a	1737	1/1	0.93	0.24	69,69,69,69	0
55	MG	1A	3724	1/1	0.93	0.06	71,71,71,71	0
55	MG	2A	3265	1/1	0.93	0.16	59,59,59,59	0
55	MG	1A	3378	1/1	0.93	0.12	20,20,20,20	0
55	MG	2A	3126	1/1	0.93	0.14	55,55,55,55	0
55	MG	1A	3515	1/1	0.93	0.20	54,54,54,54	0
55	MG	2A	3009	1/1	0.93	0.49	59,59,59,59	0
55	MG	2a	1748	1/1	0.93	0.05	79,79,79,79	0
55	MG	1A	3044	1/1	0.93	0.31	33,33,33,33	0
55	MG	2A	3657	1/1	0.93	0.08	66,66,66,66	0
55	MG	2A	3474	1/1	0.93	0.10	70,70,70,70	0
55	MG	2a	1753	1/1	0.93	0.50	69,69,69,69	0
55	MG	1A	3207	1/1	0.93	0.35	45,45,45,45	0
55	MG	2A	3281	1/1	0.93	0.10	61,61,61,61	0
55	MG	2A	3013	1/1	0.93	0.11	60,60,60,60	0
55	MG	2A	3287	1/1	0.93	0.09	39,39,39,39	0
55	MG	2A	3668	1/1	0.93	0.12	66,66,66,66	0
55	MG	1A	3270	1/1	0.93	0.17	18,18,18,18	0
55	MG	2A	3018	1/1	0.93	1.18	52,52,52,52	0
55	MG	2F	308	1/1	0.93	0.41	59,59,59,59	0
55	MG	1a	3138	1/1	0.93	0.12	58,58,58,58	0
55	MG	1A	3386	1/1	0.93	0.08	61,61,61,61	0
55	MG	1A	3387	1/1	0.93	0.13	70,70,70,70	0
55	MG	2A	3484	1/1	0.93	0.48	46,46,46,46	0
55	MG	1H	8002	1/1	0.93	0.10	46,46,46,46	0
55	MG	1A	3323	1/1	0.93	0.20	46,46,46,46	0
55	MG	2A	3303	1/1	0.93	0.12	88,88,88,88	0
55	MG	1A	3471	1/1	0.93	0.13	65,65,65,65	0
55	MG	2A	3494	1/1	0.93	0.10	77,77,77,77	0
55	MG	2a	1778	1/1	0.93	0.06	79,79,79,79	0
55	MG	2A	3688	1/1	0.93	0.13	66,66,66,66	0
55	MG	2a	1781	1/1	0.93	0.26	76,76,76,76	0
55	MG	2a	1784	1/1	0.93	0.09	80,80,80,80	0
55	MG	1A	3140	1/1	0.93	0.17	37,37,37,37	0
55	MG	2A	3499	1/1	0.93	0.09	65,65,65,65	0
55	MG	2A	3691	1/1	0.93	0.12	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2U	202	1/1	0.93	0.62	46,46,46,46	0
55	MG	2a	1789	1/1	0.93	0.11	86,86,86,86	0
55	MG	2a	1790	1/1	0.93	0.46	80,80,80,80	0
55	MG	2A	3500	1/1	0.93	0.31	41,41,41,41	0
55	MG	1a	3031	1/1	0.93	0.09	61,61,61,61	0
55	MG	1A	3476	1/1	0.93	0.21	45,45,45,45	0
55	MG	1A	3327	1/1	0.93	0.14	18,18,18,18	0
55	MG	2A	3318	1/1	0.93	0.21	67,67,67,67	0
55	MG	1B	3005	1/1	0.93	0.11	54,54,54,54	0
55	MG	1Q	203	1/1	0.93	0.21	38,38,38,38	0
55	MG	2A	3708	1/1	0.93	0.16	66,66,66,66	0
55	MG	1A	3842	1/1	0.93	0.08	84,84,84,84	0
55	MG	20	102	1/1	0.93	0.17	75,75,75,75	0
55	MG	2A	3324	1/1	0.93	0.17	61,61,61,61	0
55	MG	1A	3129	1/1	0.93	0.27	36,36,36,36	0
55	MG	1a	3158	1/1	0.93	0.07	88,88,88,88	0
55	MG	2I	101	1/1	0.93	0.76	61,61,61,61	0
55	MG	1A	3748	1/1	0.93	0.09	50,50,50,50	0
55	MG	2A	3334	1/1	0.93	0.17	45,45,45,45	0
55	MG	1A	3279	1/1	0.93	0.11	56,56,56,56	0
55	MG	1A	3480	1/1	0.93	0.27	34,34,34,34	0
56	A	2A	3821	1/23	0.93	0.16	79,79,79,79	0
55	MG	1A	3289	1/1	0.94	0.13	53,53,53,53	0
55	MG	1A	3698	1/1	0.94	0.13	48,48,48,48	0
55	MG	2D	311	1/1	0.94	0.16	53,53,53,53	0
55	MG	1A	3820	1/1	0.94	0.60	41,41,41,41	0
55	MG	2A	3335	1/1	0.94	0.07	71,71,71,71	0
55	MG	1A	3822	1/1	0.94	0.09	58,58,58,58	0
55	MG	1A	3823	1/1	0.94	0.12	28,28,28,28	0
55	MG	1A	3520	1/1	0.94	0.18	56,56,56,56	0
55	MG	2A	3112	1/1	0.94	0.62	77,77,77,77	0
55	MG	1A	3521	1/1	0.94	0.20	45,45,45,45	0
55	MG	1a	3187	1/1	0.94	0.07	89,89,89,89	0
55	MG	1a	3188	1/1	0.94	0.18	64,64,64,64	0
55	MG	1A	3829	1/1	0.94	0.20	60,60,60,60	0
55	MG	2A	3118	1/1	0.94	0.32	52,52,52,52	0
55	MG	2A	3120	1/1	0.94	0.81	56,56,56,56	0
55	MG	1A	3177	1/1	0.94	0.57	52,52,52,52	0
55	MG	2A	3356	1/1	0.94	0.19	43,43,43,43	0
55	MG	2A	3123	1/1	0.94	0.24	43,43,43,43	0
55	MG	1D	312	1/1	0.94	0.24	15,15,15,15	0
55	MG	2P	201	1/1	0.94	0.56	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	2A	3609	1/1	0.94	0.12	38,38,38,38	0
55	MG	1A	3704	1/1	0.94	0.06	42,42,42,42	0
55	MG	2A	3361	1/1	0.94	0.07	64,64,64,64	0
55	MG	2A	3362	1/1	0.94	0.18	61,61,61,61	0
55	MG	1A	3368	1/1	0.94	0.19	29,29,29,29	0
55	MG	2A	3617	1/1	0.94	0.09	33,33,33,33	0
55	MG	1A	3370	1/1	0.94	0.16	41,41,41,41	0
55	MG	1A	3209	1/1	0.94	0.17	72,72,72,72	0
55	MG	2A	3371	1/1	0.94	0.17	36,36,36,36	0
55	MG	2A	3374	1/1	0.94	0.16	62,62,62,62	0
55	MG	1a	3200	1/1	0.94	0.08	93,93,93,93	0
55	MG	1A	3528	1/1	0.94	0.15	57,57,57,57	0
55	MG	2A	3626	1/1	0.94	0.17	60,60,60,60	0
55	MG	2A	3379	1/1	0.94	0.09	61,61,61,61	0
55	MG	2A	3628	1/1	0.94	0.32	63,63,63,63	0
55	MG	1a	3204	1/1	0.94	0.06	72,72,72,72	0
55	MG	2A	3630	1/1	0.94	0.32	58,58,58,58	0
55	MG	1A	3373	1/1	0.94	0.12	58,58,58,58	0
55	MG	1A	3375	1/1	0.94	0.14	51,51,51,51	0
55	MG	1a	3209	1/1	0.94	0.12	52,52,52,52	0
55	MG	1A	3298	1/1	0.94	0.19	27,27,27,27	0
55	MG	2A	3139	1/1	0.94	0.51	53,53,53,53	0
55	MG	1a	3211	1/1	0.94	0.23	59,59,59,59	0
55	MG	25	102	1/1	0.94	0.35	62,62,62,62	0
55	MG	1a	3212	1/1	0.94	0.05	51,51,51,51	0
55	MG	1A	3714	1/1	0.94	0.10	68,68,68,68	0
55	MG	1a	3046	1/1	0.94	0.26	54,54,54,54	0
55	MG	1E	305	1/1	0.94	0.16	26,26,26,26	0
55	MG	2A	3396	1/1	0.94	0.19	71,71,71,71	0
55	MG	2A	3397	1/1	0.94	0.09	76,76,76,76	0
55	MG	2A	3145	1/1	0.94	0.16	79,79,79,79	0
55	MG	1A	3845	1/1	0.94	0.18	43,43,43,43	0
55	MG	1A	3049	1/1	0.94	0.53	45,45,45,45	0
55	MG	1A	3469	1/1	0.94	0.18	39,39,39,39	0
55	MG	1A	3030	1/1	0.94	0.12	30,30,30,30	0
55	MG	2A	3651	1/1	0.94	0.22	56,56,56,56	0
55	MG	1A	3545	1/1	0.94	0.49	36,36,36,36	0
55	MG	2A	3408	1/1	0.94	0.14	67,67,67,67	0
55	MG	2A	3409	1/1	0.94	0.13	48,48,48,48	0
55	MG	1A	3308	1/1	0.94	0.08	42,42,42,42	0
55	MG	2a	1613	1/1	0.94	0.41	61,61,61,61	0
55	MG	2A	3656	1/1	0.94	0.11	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3628	1/1	0.94	0.07	50,50,50,50	0
55	MG	2A	3658	1/1	0.94	0.18	76,76,76,76	0
55	MG	1A	3383	1/1	0.94	0.12	20,20,20,20	0
55	MG	1F	308	1/1	0.94	0.53	32,32,32,32	0
55	MG	1d	505	1/1	0.94	0.06	74,74,74,74	0
55	MG	1d	506	1/1	0.94	0.09	91,91,91,91	0
55	MG	2a	1622	1/1	0.94	0.44	50,50,50,50	0
55	MG	2A	3665	1/1	0.94	0.09	59,59,59,59	0
55	MG	1a	3060	1/1	0.94	0.21	69,69,69,69	0
55	MG	1A	3309	1/1	0.94	0.17	32,32,32,32	0
55	MG	1A	3858	1/1	0.94	0.11	56,56,56,56	0
55	MG	1g	3001	1/1	0.94	0.20	66,66,66,66	0
55	MG	1A	3311	1/1	0.94	0.06	34,34,34,34	0
55	MG	1A	3860	1/1	0.94	0.14	53,53,53,53	0
55	MG	1A	3312	1/1	0.94	0.07	64,64,64,64	0
55	MG	1F	315	1/1	0.94	0.45	43,43,43,43	0
55	MG	1F	316	1/1	0.94	0.10	69,69,69,69	0
55	MG	1a	3070	1/1	0.94	0.18	62,62,62,62	0
55	MG	1A	3062	1/1	0.94	0.22	37,37,37,37	0
55	MG	1A	3392	1/1	0.94	0.14	35,35,35,35	0
55	MG	1A	3395	1/1	0.94	0.11	44,44,44,44	0
55	MG	2A	3434	1/1	0.94	0.11	65,65,65,65	0
55	MG	1N	8001	1/1	0.94	0.44	51,51,51,51	0
55	MG	1A	3121	1/1	0.94	0.15	43,43,43,43	0
55	MG	2A	3179	1/1	0.94	0.99	48,48,48,48	0
55	MG	2A	3439	1/1	0.94	0.39	64,64,64,64	0
55	MG	2A	3694	1/1	0.94	0.04	65,65,65,65	0
55	MG	2A	3696	1/1	0.94	0.09	62,62,62,62	0
55	MG	1A	3560	1/1	0.94	0.06	72,72,72,72	0
55	MG	1A	3873	1/1	0.94	0.10	49,49,49,49	0
55	MG	1a	3082	1/1	0.94	0.20	62,62,62,62	0
55	MG	1a	3084	1/1	0.94	0.29	64,64,64,64	0
55	MG	2A	3017	1/1	0.94	0.53	54,54,54,54	0
55	MG	1A	3735	1/1	0.94	0.35	27,27,27,27	0
55	MG	1a	3090	1/1	0.94	0.06	40,40,40,40	0
55	MG	2A	3188	1/1	0.94	0.17	45,45,45,45	0
55	MG	1A	3737	1/1	0.94	0.11	14,14,14,14	0
55	MG	1A	3643	1/1	0.94	0.11	34,34,34,34	0
55	MG	2A	3718	1/1	0.94	0.08	83,83,83,83	0
55	MG	1A	3561	1/1	0.94	0.09	47,47,47,47	0
55	MG	1a	3097	1/1	0.94	0.10	61,61,61,61	0
55	MG	1A	3880	1/1	0.94	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3104	1/1	0.94	0.30	82,82,82,82	0
55	MG	2a	1676	1/1	0.94	0.17	55,55,55,55	0
55	MG	1a	3105	1/1	0.94	0.14	58,58,58,58	0
55	MG	1A	3018	1/1	0.94	0.41	23,23,23,23	0
55	MG	1A	3567	1/1	0.94	0.23	30,30,30,30	0
55	MG	1A	3884	1/1	0.94	0.07	18,18,18,18	0
55	MG	1A	3650	1/1	0.94	0.37	49,49,49,49	0
55	MG	1A	3653	1/1	0.94	0.13	62,62,62,62	0
55	MG	1A	3238	1/1	0.94	0.39	38,38,38,38	0
55	MG	1a	3115	1/1	0.94	0.40	66,66,66,66	0
55	MG	2A	3210	1/1	0.94	0.09	95,95,95,95	0
55	MG	1A	3217	1/1	0.94	0.42	45,45,45,45	0
55	MG	2A	3737	1/1	0.94	0.07	80,80,80,80	0
55	MG	2A	3738	1/1	0.94	0.10	86,86,86,86	0
55	MG	1A	3265	1/1	0.94	0.18	44,44,44,44	0
55	MG	2A	3213	1/1	0.94	0.16	33,33,33,33	0
55	MG	1A	3266	1/1	0.94	0.17	70,70,70,70	0
55	MG	2a	1703	1/1	0.94	0.08	61,61,61,61	0
55	MG	2a	1704	1/1	0.94	0.14	68,68,68,68	0
55	MG	1a	3119	1/1	0.94	0.10	81,81,81,81	0
55	MG	2A	3042	1/1	0.94	0.17	27,27,27,27	0
55	MG	1A	3242	1/1	0.94	0.42	29,29,29,29	0
55	MG	2A	3749	1/1	0.94	0.05	85,85,85,85	0
55	MG	1A	3268	1/1	0.94	0.18	35,35,35,35	0
55	MG	1A	3894	1/1	0.94	0.82	38,38,38,38	0
55	MG	1A	3664	1/1	0.94	0.13	59,59,59,59	0
55	MG	2a	1715	1/1	0.94	0.14	82,82,82,82	0
55	MG	1A	3762	1/1	0.94	0.65	48,48,48,48	0
55	MG	1A	3075	1/1	0.94	0.76	41,41,41,41	0
55	MG	1A	3765	1/1	0.94	0.10	39,39,39,39	0
55	MG	2A	3236	1/1	0.94	0.08	80,80,80,80	0
55	MG	2A	3051	1/1	0.94	0.84	61,61,61,61	0
55	MG	2A	3493	1/1	0.94	0.27	51,51,51,51	0
55	MG	10	106	1/1	0.94	0.07	58,58,58,58	0
55	MG	10	107	1/1	0.94	0.18	57,57,57,57	0
55	MG	2A	3242	1/1	0.94	0.24	40,40,40,40	0
55	MG	2a	1725	1/1	0.94	0.12	86,86,86,86	0
55	MG	2A	3764	1/1	0.94	0.12	72,72,72,72	0
55	MG	1A	3420	1/1	0.94	0.14	27,27,27,27	0
55	MG	1A	3045	1/1	0.94	0.18	12,12,12,12	0
55	MG	1A	3339	1/1	0.94	0.15	18,18,18,18	0
55	MG	13	101	1/1	0.94	0.36	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3435	1/1	0.94	0.08	69,69,69,69	0
55	MG	2A	3508	1/1	0.94	0.56	57,57,57,57	0
55	MG	1A	3674	1/1	0.94	0.15	26,26,26,26	0
55	MG	2A	3253	1/1	0.94	0.16	56,56,56,56	0
55	MG	2A	3775	1/1	0.94	0.16	57,57,57,57	0
55	MG	1a	3141	1/1	0.94	0.10	75,75,75,75	0
55	MG	2A	3512	1/1	0.94	0.19	61,61,61,61	0
55	MG	1A	3780	1/1	0.94	0.04	58,58,58,58	0
55	MG	2A	3780	1/1	0.94	0.11	40,40,40,40	0
55	MG	2A	3515	1/1	0.94	0.23	52,52,52,52	0
55	MG	2A	3517	1/1	0.94	0.12	64,64,64,64	0
55	MG	1A	3908	1/1	0.94	0.36	33,33,33,33	0
55	MG	1A	3276	1/1	0.94	0.24	3,3,3,3	0
55	MG	2A	3066	1/1	0.94	0.40	58,58,58,58	0
55	MG	2A	3261	1/1	0.94	0.11	88,88,88,88	0
55	MG	2A	3524	1/1	0.94	0.09	67,67,67,67	0
55	MG	1A	3912	1/1	0.94	0.14	43,43,43,43	0
55	MG	2A	3526	1/1	0.94	0.13	73,73,73,73	0
55	MG	2A	3527	1/1	0.94	0.31	73,73,73,73	0
55	MG	1A	3035	1/1	0.94	0.15	37,37,37,37	0
55	MG	2A	3529	1/1	0.94	0.13	75,75,75,75	0
55	MG	17	102	1/1	0.94	0.49	36,36,36,36	0
55	MG	2A	3271	1/1	0.94	0.15	36,36,36,36	0
55	MG	2A	3272	1/1	0.94	0.10	41,41,41,41	0
55	MG	1A	3784	1/1	0.94	0.07	42,42,42,42	0
55	MG	2A	3073	1/1	0.94	0.56	48,48,48,48	0
55	MG	1A	3786	1/1	0.94	0.14	23,23,23,23	0
55	MG	1A	3588	1/1	0.94	0.14	62,62,62,62	0
55	MG	2A	3279	1/1	0.94	0.15	45,45,45,45	0
55	MG	2A	3806	1/1	0.94	0.20	73,73,73,73	0
55	MG	2A	3540	1/1	0.94	0.18	64,64,64,64	0
55	MG	2A	3076	1/1	0.94	0.28	55,55,55,55	0
55	MG	2A	3282	1/1	0.94	0.12	34,34,34,34	0
55	MG	1A	3067	1/1	0.94	1.04	37,37,37,37	0
55	MG	2A	3286	1/1	0.94	0.11	42,42,42,42	0
55	MG	1A	3055	1/1	0.94	0.24	53,53,53,53	0
55	MG	2A	3548	1/1	0.94	0.07	65,65,65,65	0
55	MG	1A	3682	1/1	0.94	0.27	61,61,61,61	0
55	MG	2A	3291	1/1	0.94	0.15	34,34,34,34	0
55	MG	2A	3818	1/1	0.94	0.24	57,57,57,57	0
55	MG	2A	3554	1/1	0.94	0.22	58,58,58,58	0
55	MG	1A	3591	1/1	0.94	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3800	1/1	0.94	0.16	64,64,64,64	0
55	MG	1B	3008	1/1	0.94	0.18	57,57,57,57	0
55	MG	2A	3558	1/1	0.94	0.08	59,59,59,59	0
55	MG	1A	3801	1/1	0.94	0.04	56,56,56,56	0
55	MG	1A	3686	1/1	0.94	0.08	35,35,35,35	0
55	MG	1A	3803	1/1	0.94	0.07	39,39,39,39	0
55	MG	2A	3093	1/1	0.94	0.39	46,46,46,46	0
55	MG	2a	1796	1/1	0.94	0.14	60,60,60,60	0
55	MG	1A	3689	1/1	0.94	0.10	68,68,68,68	0
55	MG	1A	3283	1/1	0.94	0.12	25,25,25,25	0
55	MG	1a	3011	1/1	0.94	0.15	32,32,32,32	0
55	MG	2A	3098	1/1	0.94	0.19	53,53,53,53	0
55	MG	2A	3311	1/1	0.94	0.15	42,42,42,42	0
55	MG	2A	3313	1/1	0.94	0.09	40,40,40,40	0
55	MG	1A	3352	1/1	0.94	0.10	22,22,22,22	0
55	MG	1A	3029	1/1	0.94	0.19	38,38,38,38	0
55	MG	1B	3020	1/1	0.94	0.27	73,73,73,73	0
55	MG	1A	3450	1/1	0.94	0.13	19,19,19,19	0
55	MG	1a	3176	1/1	0.94	0.14	92,92,92,92	0
55	MG	1A	3809	1/1	0.94	0.16	13,13,13,13	0
55	MG	2A	3327	1/1	0.94	0.35	67,67,67,67	0
55	MG	1A	3082	1/1	0.94	0.73	37,37,37,37	0
55	MG	2D	306	1/1	0.94	0.21	57,57,57,57	0
55	MG	2R	203	1/1	0.95	0.20	39,39,39,39	0
55	MG	1A	3687	1/1	0.95	0.17	56,56,56,56	0
55	MG	1A	3688	1/1	0.95	0.09	26,26,26,26	0
55	MG	2A	3063	1/1	0.95	1.28	49,49,49,49	0
55	MG	1a	3155	1/1	0.95	0.11	78,78,78,78	0
55	MG	2U	204	1/1	0.95	0.19	55,55,55,55	0
55	MG	2A	3450	1/1	0.95	0.16	40,40,40,40	0
55	MG	2A	3233	1/1	0.95	0.16	73,73,73,73	0
55	MG	1a	3156	1/1	0.95	0.18	69,69,69,69	0
55	MG	2V	205	1/1	0.95	0.31	73,73,73,73	0
55	MG	1a	3157	1/1	0.95	0.07	82,82,82,82	0
55	MG	1A	3431	1/1	0.95	0.12	40,40,40,40	0
55	MG	1A	3213	1/1	0.95	0.85	32,32,32,32	0
55	MG	1B	3018	1/1	0.95	0.10	37,37,37,37	0
55	MG	1A	3162	1/1	0.95	0.64	37,37,37,37	0
55	MG	2A	3461	1/1	0.95	0.11	34,34,34,34	0
55	MG	1a	3162	1/1	0.95	0.07	77,77,77,77	0
55	MG	1A	3297	1/1	0.95	0.16	15,15,15,15	0
55	MG	1A	3813	1/1	0.95	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3674	1/1	0.95	0.17	66,66,66,66	0
55	MG	23	101	1/1	0.95	0.88	64,64,64,64	0
55	MG	1A	3261	1/1	0.95	0.36	28,28,28,28	0
55	MG	2A	3077	1/1	0.95	0.19	56,56,56,56	0
55	MG	1A	3025	1/1	0.95	0.61	33,33,33,33	0
55	MG	27	101	1/1	0.95	0.22	55,55,55,55	0
55	MG	2A	3255	1/1	0.95	0.19	62,62,62,62	0
55	MG	1A	3819	1/1	0.95	0.12	58,58,58,58	0
55	MG	1A	3442	1/1	0.95	0.07	49,49,49,49	0
55	MG	1A	3821	1/1	0.95	0.10	54,54,54,54	0
55	MG	1A	3114	1/1	0.95	0.27	37,37,37,37	0
55	MG	2A	3687	1/1	0.95	0.17	49,49,49,49	0
55	MG	2a	1601	1/1	0.95	0.32	79,79,79,79	0
55	MG	1A	3700	1/1	0.95	0.12	24,24,24,24	0
55	MG	1A	3303	1/1	0.95	0.15	13,13,13,13	0
55	MG	2A	3262	1/1	0.95	0.23	74,74,74,74	0
55	MG	1A	3367	1/1	0.95	0.19	30,30,30,30	0
55	MG	1a	3177	1/1	0.95	0.08	74,74,74,74	0
55	MG	2A	3092	1/1	0.95	0.66	49,49,49,49	0
55	MG	1A	3827	1/1	0.95	0.12	64,64,64,64	0
55	MG	1D	310	1/1	0.95	0.52	42,42,42,42	0
55	MG	2A	3702	1/1	0.95	0.16	34,34,34,34	0
55	MG	1A	3241	1/1	0.95	0.23	30,30,30,30	0
55	MG	1a	3030	1/1	0.95	0.93	61,61,61,61	0
55	MG	1A	3050	1/1	0.95	0.36	29,29,29,29	0
55	MG	1A	3310	1/1	0.95	0.26	41,41,41,41	0
55	MG	1A	3166	1/1	0.95	0.44	46,46,46,46	0
55	MG	2a	1618	1/1	0.95	0.42	81,81,81,81	0
55	MG	1A	3609	1/1	0.95	0.10	62,62,62,62	0
55	MG	1A	3127	1/1	0.95	0.21	14,14,14,14	0
55	MG	2A	3715	1/1	0.95	0.08	66,66,66,66	0
55	MG	2A	3496	1/1	0.95	0.16	43,43,43,43	0
55	MG	1A	3269	1/1	0.95	0.07	62,62,62,62	0
55	MG	1A	3100	1/1	0.95	0.25	25,25,25,25	0
55	MG	1A	3615	1/1	0.95	0.14	19,19,19,19	0
55	MG	1A	3616	1/1	0.95	0.05	48,48,48,48	0
55	MG	1a	3192	1/1	0.95	0.11	49,49,49,49	0
55	MG	1a	3042	1/1	0.95	0.20	53,53,53,53	0
55	MG	1A	3841	1/1	0.95	0.08	64,64,64,64	0
55	MG	1a	3195	1/1	0.95	0.10	62,62,62,62	0
55	MG	2a	1634	1/1	0.95	0.56	81,81,81,81	0
55	MG	2A	3298	1/1	0.95	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3056	1/1	0.95	0.20	28,28,28,28	0
55	MG	1A	3716	1/1	0.95	0.07	46,46,46,46	0
55	MG	2a	1639	1/1	0.95	0.55	50,50,50,50	0
55	MG	1A	3187	1/1	0.95	0.09	52,52,52,52	0
55	MG	1A	3621	1/1	0.95	0.12	40,40,40,40	0
55	MG	1a	3201	1/1	0.95	0.13	92,92,92,92	0
55	MG	1A	3720	1/1	0.95	0.06	65,65,65,65	0
55	MG	2A	3519	1/1	0.95	0.10	73,73,73,73	0
55	MG	1A	3852	1/1	0.95	0.22	24,24,24,24	0
55	MG	1A	3622	1/1	0.95	0.09	76,76,76,76	0
55	MG	1A	3531	1/1	0.95	0.05	46,46,46,46	0
55	MG	2A	3741	1/1	0.95	0.05	70,70,70,70	0
55	MG	1A	3458	1/1	0.95	0.10	46,46,46,46	0
55	MG	1A	3277	1/1	0.95	0.16	30,30,30,30	0
55	MG	1A	3462	1/1	0.95	0.04	40,40,40,40	0
55	MG	1A	3463	1/1	0.95	0.10	28,28,28,28	0
55	MG	1a	3059	1/1	0.95	0.16	80,80,80,80	0
55	MG	1A	3318	1/1	0.95	0.26	61,61,61,61	0
55	MG	2A	3322	1/1	0.95	0.07	62,62,62,62	0
55	MG	1a	3061	1/1	0.95	0.17	74,74,74,74	0
55	MG	1A	3543	1/1	0.95	0.17	63,63,63,63	0
55	MG	2A	3532	1/1	0.95	0.06	84,84,84,84	0
55	MG	1F	313	1/1	0.95	0.16	32,32,32,32	0
55	MG	2a	1664	1/1	0.95	0.34	69,69,69,69	0
55	MG	1A	3320	1/1	0.95	0.15	62,62,62,62	0
55	MG	2A	3330	1/1	0.95	0.14	57,57,57,57	0
55	MG	2A	3536	1/1	0.95	0.06	64,64,64,64	0
55	MG	2a	1672	1/1	0.95	0.13	57,57,57,57	0
55	MG	1A	3862	1/1	0.95	0.12	59,59,59,59	0
55	MG	2A	3332	1/1	0.95	0.08	46,46,46,46	0
55	MG	1A	3006	1/1	0.95	0.11	21,21,21,21	0
55	MG	1A	3016	1/1	0.95	0.50	19,19,19,19	0
55	MG	2a	1679	1/1	0.95	0.10	63,63,63,63	0
55	MG	2A	3763	1/1	0.95	0.12	41,41,41,41	0
55	MG	1A	3637	1/1	0.95	0.17	38,38,38,38	0
55	MG	1A	3868	1/1	0.95	0.09	29,29,29,29	0
55	MG	1A	3638	1/1	0.95	0.43	31,31,31,31	0
55	MG	1A	3158	1/1	0.95	0.15	37,37,37,37	0
55	MG	2A	3545	1/1	0.95	0.17	97,97,97,97	0
55	MG	2A	3770	1/1	0.95	0.04	79,79,79,79	0
55	MG	2A	3341	1/1	0.95	0.17	34,34,34,34	0
55	MG	1A	3871	1/1	0.95	0.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3738	1/1	0.95	0.13	14,14,14,14	0
55	MG	2A	3344	1/1	0.95	0.11	55,55,55,55	0
55	MG	1A	3393	1/1	0.95	0.11	53,53,53,53	0
55	MG	1A	3472	1/1	0.95	0.17	58,58,58,58	0
55	MG	1A	3743	1/1	0.95	0.11	45,45,45,45	0
55	MG	1a	3079	1/1	0.95	0.17	55,55,55,55	0
55	MG	1A	3473	1/1	0.95	0.05	63,63,63,63	0
55	MG	2a	1705	1/1	0.95	0.21	69,69,69,69	0
55	MG	2A	3352	1/1	0.95	0.18	59,59,59,59	0
55	MG	2A	3353	1/1	0.95	0.07	72,72,72,72	0
55	MG	2A	3561	1/1	0.95	0.08	59,59,59,59	0
55	MG	1m	201	1/1	0.95	0.16	72,72,72,72	0
55	MG	1A	3746	1/1	0.95	0.14	31,31,31,31	0
55	MG	1Q	205	1/1	0.95	0.12	43,43,43,43	0
55	MG	2A	3566	1/1	0.95	0.33	64,64,64,64	0
55	MG	1R	201	1/1	0.95	0.97	46,46,46,46	0
55	MG	1R	203	1/1	0.95	0.23	19,19,19,19	0
55	MG	1A	3881	1/1	0.95	0.25	43,43,43,43	0
55	MG	1A	3644	1/1	0.95	0.12	18,18,18,18	0
55	MG	2A	3795	1/1	0.95	0.13	72,72,72,72	0
55	MG	2A	3365	1/1	0.95	0.22	39,39,39,39	0
55	MG	1a	3096	1/1	0.95	0.16	78,78,78,78	0
55	MG	2A	3006	1/1	0.95	0.12	36,36,36,36	0
55	MG	2A	3007	1/1	0.95	0.19	61,61,61,61	0
55	MG	1A	3553	1/1	0.95	0.24	37,37,37,37	0
55	MG	1a	3102	1/1	0.95	0.09	48,48,48,48	0
55	MG	1A	3394	1/1	0.95	0.20	50,50,50,50	0
55	MG	2A	3166	1/1	0.95	0.41	44,44,44,44	0
55	MG	1U	202	1/1	0.95	0.19	43,43,43,43	0
55	MG	1U	203	1/1	0.95	0.52	42,42,42,42	0
55	MG	1A	3751	1/1	0.95	0.20	39,39,39,39	0
55	MG	1A	3475	1/1	0.95	0.99	32,32,32,32	0
55	MG	1A	3649	1/1	0.95	0.12	33,33,33,33	0
55	MG	1A	3282	1/1	0.95	0.10	26,26,26,26	0
55	MG	1A	3651	1/1	0.95	0.15	40,40,40,40	0
55	MG	1a	3113	1/1	0.95	0.29	66,66,66,66	0
55	MG	2A	3391	1/1	0.95	0.07	43,43,43,43	0
55	MG	1A	3083	1/1	0.95	0.06	57,57,57,57	0
55	MG	2a	1738	1/1	0.95	0.80	85,85,85,85	0
55	MG	2A	3178	1/1	0.95	0.68	38,38,38,38	0
55	MG	1A	3335	1/1	0.95	0.18	19,19,19,19	0
55	MG	2A	3395	1/1	0.95	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3820	1/1	0.95	0.11	69,69,69,69	0
55	MG	1A	3336	1/1	0.95	0.11	21,21,21,21	0
55	MG	1A	3566	1/1	0.95	0.11	23,23,23,23	0
55	MG	2A	3601	1/1	0.95	0.11	58,58,58,58	0
55	MG	2a	1749	1/1	0.95	0.05	80,80,80,80	0
55	MG	1A	3401	1/1	0.95	0.06	62,62,62,62	0
55	MG	2A	3604	1/1	0.95	0.33	65,65,65,65	0
55	MG	2A	3183	1/1	0.95	0.20	75,75,75,75	0
55	MG	1A	3068	1/1	0.95	0.29	27,27,27,27	0
55	MG	2A	3607	1/1	0.95	0.12	80,80,80,80	0
55	MG	2B	3009	1/1	0.95	0.09	71,71,71,71	0
55	MG	1A	3766	1/1	0.95	0.07	39,39,39,39	0
55	MG	1A	3403	1/1	0.95	0.09	53,53,53,53	0
55	MG	1A	3768	1/1	0.95	0.10	46,46,46,46	0
55	MG	2A	3611	1/1	0.95	0.42	83,83,83,83	0
55	MG	1a	3127	1/1	0.95	0.10	53,53,53,53	0
55	MG	1A	3663	1/1	0.95	0.09	26,26,26,26	0
55	MG	1A	3211	1/1	0.95	0.77	31,31,31,31	0
55	MG	2A	3616	1/1	0.95	0.12	53,53,53,53	0
55	MG	2A	3037	1/1	0.95	0.18	24,24,24,24	0
55	MG	1A	3572	1/1	0.95	0.12	41,41,41,41	0
55	MG	1a	3131	1/1	0.95	0.15	76,76,76,76	0
55	MG	1A	3010	1/1	0.95	0.41	37,37,37,37	0
55	MG	1A	3669	1/1	0.95	0.26	56,56,56,56	0
55	MG	2A	3623	1/1	0.95	0.31	66,66,66,66	0
55	MG	1A	3344	1/1	0.95	0.08	25,25,25,25	0
55	MG	1A	3910	1/1	0.95	0.51	35,35,35,35	0
55	MG	1A	3291	1/1	0.95	0.16	30,30,30,30	0
55	MG	2D	309	1/1	0.95	0.20	30,30,30,30	0
55	MG	2D	310	1/1	0.95	0.10	55,55,55,55	0
55	MG	1A	3347	1/1	0.95	0.12	18,18,18,18	0
55	MG	2A	3422	1/1	0.95	0.09	52,52,52,52	0
55	MG	2A	3203	1/1	0.95	1.10	63,63,63,63	0
55	MG	2A	3424	1/1	0.95	0.20	50,50,50,50	0
55	MG	1A	3414	1/1	0.95	0.15	19,19,19,19	0
55	MG	2F	302	1/1	0.95	0.62	55,55,55,55	0
55	MG	1A	3495	1/1	0.95	0.14	49,49,49,49	0
55	MG	1A	3497	1/1	0.95	0.14	66,66,66,66	0
55	MG	1A	3789	1/1	0.95	0.10	31,31,31,31	0
55	MG	17	104	1/1	0.95	0.32	61,61,61,61	0
55	MG	1A	3677	1/1	0.95	0.09	56,56,56,56	0
55	MG	1A	3292	1/1	0.95	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3214	1/1	0.95	0.14	37,37,37,37	0
55	MG	2F	310	1/1	0.95	0.15	75,75,75,75	0
55	MG	1A	3424	1/1	0.95	0.04	62,62,62,62	0
55	MG	2A	3217	1/1	0.95	0.15	32,32,32,32	0
55	MG	1A	3680	1/1	0.95	0.10	59,59,59,59	0
55	MG	1A	3425	1/1	0.95	0.14	20,20,20,20	0
55	MG	1A	3427	1/1	0.95	0.08	42,42,42,42	0
55	MG	2A	3440	1/1	0.95	0.17	74,74,74,74	0
55	MG	1A	3505	1/1	0.95	0.18	31,31,31,31	0
55	MG	1A	3428	1/1	0.95	0.10	68,68,68,68	0
55	MG	2Q	8003	1/1	0.95	0.18	57,57,57,57	0
55	MG	2n	503	1/1	0.95	0.32	85,85,85,85	0
55	MG	2A	3443	1/1	0.95	0.17	63,63,63,63	0
55	MG	2A	3444	1/1	0.95	0.15	31,31,31,31	0
55	MG	2A	3227	1/1	0.95	0.15	65,65,65,65	0
57	ZN	1n	501	1/1	0.95	0.15	88,88,88,88	0
57	ZN	2n	501	1/1	0.95	0.08	108,108,108,108	0
55	MG	1A	3110	1/1	0.96	0.25	38,38,38,38	0
55	MG	2A	3223	1/1	0.96	0.13	68,68,68,68	0
55	MG	2A	3744	1/1	0.96	0.21	64,64,64,64	0
55	MG	2A	3745	1/1	0.96	0.18	70,70,70,70	0
55	MG	1A	3657	1/1	0.96	0.06	50,50,50,50	0
55	MG	1A	3736	1/1	0.96	0.18	55,55,55,55	0
55	MG	2A	3226	1/1	0.96	0.12	44,44,44,44	0
55	MG	2A	3562	1/1	0.96	0.16	74,74,74,74	0
55	MG	1A	3362	1/1	0.96	0.15	20,20,20,20	0
55	MG	2A	3097	1/1	0.96	0.16	35,35,35,35	0
55	MG	1a	3098	1/1	0.96	0.18	61,61,61,61	0
55	MG	2A	3400	1/1	0.96	0.12	43,43,43,43	0
55	MG	2A	3567	1/1	0.96	0.43	51,51,51,51	0
55	MG	1a	3101	1/1	0.96	0.14	39,39,39,39	0
55	MG	1A	3583	1/1	0.96	0.23	37,37,37,37	0
55	MG	1a	3221	1/1	0.96	0.26	71,71,71,71	0
55	MG	2A	3234	1/1	0.96	0.19	45,45,45,45	0
55	MG	2a	1628	1/1	0.96	0.15	54,54,54,54	0
55	MG	2A	3235	1/1	0.96	0.08	69,69,69,69	0
55	MG	2A	3760	1/1	0.96	0.08	40,40,40,40	0
55	MG	15	103	1/1	0.96	0.33	34,34,34,34	0
55	MG	1A	3584	1/1	0.96	0.07	37,37,37,37	0
55	MG	1B	3022	1/1	0.96	0.40	63,63,63,63	0
55	MG	1A	3518	1/1	0.96	0.12	77,77,77,77	0
55	MG	2A	3580	1/1	0.96	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3581	1/1	0.96	0.08	72,72,72,72	0
55	MG	1A	3153	1/1	0.96	0.19	49,49,49,49	0
55	MG	2A	3243	1/1	0.96	0.07	72,72,72,72	0
55	MG	1A	3249	1/1	0.96	0.14	21,21,21,21	0
55	MG	1A	3846	1/1	0.96	0.12	53,53,53,53	0
55	MG	1A	3251	1/1	0.96	0.54	34,34,34,34	0
55	MG	2A	3419	1/1	0.96	0.08	33,33,33,33	0
55	MG	1A	3522	1/1	0.96	0.13	26,26,26,26	0
55	MG	1A	3326	1/1	0.96	0.12	24,24,24,24	0
55	MG	1A	3850	1/1	0.96	0.08	21,21,21,21	0
55	MG	18	3303	1/1	0.96	0.07	52,52,52,52	0
55	MG	2A	3254	1/1	0.96	0.27	54,54,54,54	0
55	MG	1A	3413	1/1	0.96	0.09	43,43,43,43	0
55	MG	1h	3002	1/1	0.96	0.08	76,76,76,76	0
55	MG	2A	3116	1/1	0.96	0.13	43,43,43,43	0
55	MG	1k	3001	1/1	0.96	0.16	48,48,48,48	0
55	MG	19	103	1/1	0.96	0.08	61,61,61,61	0
55	MG	1A	3594	1/1	0.96	0.16	24,24,24,24	0
55	MG	2A	3787	1/1	0.96	0.13	61,61,61,61	0
55	MG	2a	1657	1/1	0.96	0.12	65,65,65,65	0
55	MG	1A	3234	1/1	0.96	0.12	48,48,48,48	0
55	MG	2A	3122	1/1	0.96	0.38	46,46,46,46	0
55	MG	2A	3263	1/1	0.96	0.18	46,46,46,46	0
55	MG	2A	3791	1/1	0.96	0.09	45,45,45,45	0
55	MG	2a	1663	1/1	0.96	0.29	63,63,63,63	0
55	MG	2A	3603	1/1	0.96	0.11	61,61,61,61	0
55	MG	2A	3264	1/1	0.96	0.11	65,65,65,65	0
55	MG	1a	3122	1/1	0.96	0.32	71,71,71,71	0
55	MG	2a	1669	1/1	0.96	0.10	46,46,46,46	0
55	MG	2A	3437	1/1	0.96	0.20	78,78,78,78	0
55	MG	1A	3755	1/1	0.96	0.07	69,69,69,69	0
55	MG	2A	3269	1/1	0.96	0.08	45,45,45,45	0
55	MG	1A	3418	1/1	0.96	0.14	26,26,26,26	0
55	MG	2a	1675	1/1	0.96	0.09	51,51,51,51	0
55	MG	2A	3127	1/1	0.96	0.37	60,60,60,60	0
55	MG	1A	3527	1/1	0.96	0.08	35,35,35,35	0
55	MG	1A	3419	1/1	0.96	0.14	37,37,37,37	0
55	MG	2A	3274	1/1	0.96	0.05	61,61,61,61	0
55	MG	1A	3372	1/1	0.96	0.18	29,29,29,29	0
55	MG	1A	3271	1/1	0.96	0.10	22,22,22,22	0
55	MG	1A	3601	1/1	0.96	0.34	37,37,37,37	0
55	MG	2A	3807	1/1	0.96	0.38	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3332	1/1	0.96	0.14	28,28,28,28	0
55	MG	1E	301	1/1	0.96	0.12	15,15,15,15	0
55	MG	1a	3013	1/1	0.96	0.05	72,72,72,72	0
55	MG	2a	1691	1/1	0.96	0.15	56,56,56,56	0
55	MG	2A	3283	1/1	0.96	0.09	37,37,37,37	0
55	MG	2A	3284	1/1	0.96	0.10	37,37,37,37	0
55	MG	1A	3763	1/1	0.96	0.16	22,22,22,22	0
55	MG	2A	3012	1/1	0.96	0.17	38,38,38,38	0
55	MG	2a	1698	1/1	0.96	0.66	58,58,58,58	0
55	MG	1A	3203	1/1	0.96	0.30	35,35,35,35	0
55	MG	1A	3275	1/1	0.96	0.16	27,27,27,27	0
55	MG	2a	1702	1/1	0.96	0.06	67,67,67,67	0
55	MG	2A	3016	1/1	0.96	0.75	46,46,46,46	0
55	MG	2A	3460	1/1	0.96	0.10	55,55,55,55	0
55	MG	2A	3293	1/1	0.96	0.12	40,40,40,40	0
55	MG	1A	3535	1/1	0.96	0.13	38,38,38,38	0
55	MG	1A	3536	1/1	0.96	0.08	44,44,44,44	0
55	MG	1A	3537	1/1	0.96	0.28	38,38,38,38	0
55	MG	2a	1709	1/1	0.96	0.15	82,82,82,82	0
55	MG	1A	3305	1/1	0.96	0.15	16,16,16,16	0
55	MG	2A	3467	1/1	0.96	0.08	57,57,57,57	0
55	MG	1A	3380	1/1	0.96	0.18	52,52,52,52	0
55	MG	1A	3541	1/1	0.96	0.61	34,34,34,34	0
55	MG	1a	3025	1/1	0.96	0.11	55,55,55,55	0
55	MG	1A	3777	1/1	0.96	0.05	41,41,41,41	0
55	MG	1A	3482	1/1	0.96	0.20	43,43,43,43	0
55	MG	1A	3692	1/1	0.96	0.08	43,43,43,43	0
55	MG	2A	3306	1/1	0.96	0.21	39,39,39,39	0
55	MG	1A	3879	1/1	0.96	0.10	41,41,41,41	0
55	MG	2A	3644	1/1	0.96	0.14	63,63,63,63	0
55	MG	2A	3309	1/1	0.96	0.09	65,65,65,65	0
55	MG	1A	3483	1/1	0.96	0.19	38,38,38,38	0
55	MG	1A	3047	1/1	0.96	0.15	24,24,24,24	0
55	MG	1A	3382	1/1	0.96	0.16	52,52,52,52	0
55	MG	1A	3486	1/1	0.96	0.14	63,63,63,63	0
55	MG	1A	3340	1/1	0.96	0.12	22,22,22,22	0
55	MG	1A	3438	1/1	0.96	0.09	57,57,57,57	0
55	MG	1A	3489	1/1	0.96	0.09	33,33,33,33	0
55	MG	1A	3191	1/1	0.96	0.18	66,66,66,66	0
55	MG	1A	3112	1/1	0.96	0.18	42,42,42,42	0
55	MG	1A	3629	1/1	0.96	0.22	42,42,42,42	0
55	MG	1A	3796	1/1	0.96	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3490	1/1	0.96	0.22	33,33,33,33	0
55	MG	1A	3705	1/1	0.96	0.27	48,48,48,48	0
55	MG	1A	3345	1/1	0.96	0.17	45,45,45,45	0
55	MG	2E	301	1/1	0.96	0.27	43,43,43,43	0
55	MG	2A	3495	1/1	0.96	0.09	59,59,59,59	0
55	MG	1a	3045	1/1	0.96	0.26	57,57,57,57	0
55	MG	2E	306	1/1	0.96	0.14	49,49,49,49	0
55	MG	1A	3061	1/1	0.96	0.28	47,47,47,47	0
55	MG	2A	3498	1/1	0.96	0.10	39,39,39,39	0
55	MG	1A	3557	1/1	0.96	0.10	24,24,24,24	0
55	MG	2A	3333	1/1	0.96	0.13	42,42,42,42	0
55	MG	2A	3173	1/1	0.96	0.56	42,42,42,42	0
55	MG	1P	202	1/1	0.96	0.39	28,28,28,28	0
55	MG	2A	3505	1/1	0.96	0.18	44,44,44,44	0
55	MG	1A	3559	1/1	0.96	0.19	26,26,26,26	0
55	MG	1A	3388	1/1	0.96	0.20	48,48,48,48	0
55	MG	1A	3389	1/1	0.96	0.17	48,48,48,48	0
55	MG	2A	3680	1/1	0.96	0.10	66,66,66,66	0
55	MG	1A	3712	1/1	0.96	0.16	52,52,52,52	0
55	MG	2A	3682	1/1	0.96	0.18	67,67,67,67	0
55	MG	1a	3054	1/1	0.96	0.14	82,82,82,82	0
55	MG	1A	3448	1/1	0.96	0.16	23,23,23,23	0
55	MG	1A	3902	1/1	0.96	0.13	56,56,56,56	0
55	MG	1A	3564	1/1	0.96	0.16	43,43,43,43	0
55	MG	2a	1763	1/1	0.96	0.09	55,55,55,55	0
55	MG	1A	3810	1/1	0.96	0.11	27,27,27,27	0
55	MG	1A	3639	1/1	0.96	0.11	47,47,47,47	0
55	MG	1A	3906	1/1	0.96	0.10	59,59,59,59	0
55	MG	1A	3390	1/1	0.96	0.14	23,23,23,23	0
55	MG	2a	1769	1/1	0.96	0.27	76,76,76,76	0
55	MG	1T	201	1/1	0.96	0.19	54,54,54,54	0
55	MG	2A	3693	1/1	0.96	0.06	95,95,95,95	0
55	MG	2A	3351	1/1	0.96	0.11	68,68,68,68	0
55	MG	2A	3695	1/1	0.96	0.10	97,97,97,97	0
55	MG	1A	3103	1/1	0.96	0.55	35,35,35,35	0
55	MG	1A	3504	1/1	0.96	0.19	19,19,19,19	0
55	MG	2A	3700	1/1	0.96	0.16	87,87,87,87	0
55	MG	1A	3818	1/1	0.96	0.06	24,24,24,24	0
55	MG	1A	3040	1/1	0.96	0.17	37,37,37,37	0
55	MG	2a	1782	1/1	0.96	0.21	70,70,70,70	0
55	MG	2a	1783	1/1	0.96	0.17	53,53,53,53	0
55	MG	1A	3125	1/1	0.96	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3068	1/1	0.96	0.29	73,73,73,73	0
55	MG	1A	3028	1/1	0.96	0.53	37,37,37,37	0
55	MG	1A	3263	1/1	0.96	0.18	17,17,17,17	0
55	MG	1A	3647	1/1	0.96	0.12	39,39,39,39	0
55	MG	2A	3364	1/1	0.96	0.07	60,60,60,60	0
55	MG	2A	3713	1/1	0.96	0.03	79,79,79,79	0
55	MG	1a	3072	1/1	0.96	0.06	65,65,65,65	0
55	MG	1A	3355	1/1	0.96	0.13	53,53,53,53	0
55	MG	2A	3367	1/1	0.96	0.15	37,37,37,37	0
55	MG	1A	3399	1/1	0.96	0.20	15,15,15,15	0
55	MG	2A	3370	1/1	0.96	0.11	76,76,76,76	0
55	MG	2A	3202	1/1	0.96	0.15	56,56,56,56	0
55	MG	1X	8001	1/1	0.96	0.10	31,31,31,31	0
55	MG	1A	3826	1/1	0.96	0.12	59,59,59,59	0
55	MG	2A	3723	1/1	0.96	0.05	73,73,73,73	0
55	MG	1A	3357	1/1	0.96	0.18	20,20,20,20	0
55	MG	2A	3378	1/1	0.96	0.15	51,51,51,51	0
55	MG	1A	3828	1/1	0.96	0.17	61,61,61,61	0
55	MG	1A	3013	1/1	0.96	0.07	51,51,51,51	0
55	MG	2A	3083	1/1	0.96	0.31	57,57,57,57	0
55	MG	2A	3546	1/1	0.96	0.06	87,87,87,87	0
55	MG	1A	3652	1/1	0.96	0.11	34,34,34,34	0
55	MG	2A	3087	1/1	0.96	0.18	62,62,62,62	0
55	MG	1B	3010	1/1	0.96	0.04	59,59,59,59	0
55	MG	2A	3550	1/1	0.96	0.10	48,48,48,48	0
55	MG	1a	3085	1/1	0.96	0.27	64,64,64,64	0
55	MG	1A	3832	1/1	0.96	0.11	55,55,55,55	0
55	MG	1A	3461	1/1	0.96	0.09	63,63,63,63	0
57	ZN	24	501	1/1	0.96	0.03	129,129,129,129	0
57	ZN	26	101	1/1	0.96	0.12	64,64,64,64	0
55	MG	1A	3108	1/1	0.96	0.20	24,24,24,24	0
55	MG	1A	3299	1/1	0.97	0.18	28,28,28,28	0
55	MG	1A	3558	1/1	0.97	0.12	27,27,27,27	0
55	MG	1A	3613	1/1	0.97	0.04	82,82,82,82	0
55	MG	2A	3572	1/1	0.97	0.13	55,55,55,55	0
55	MG	1A	3415	1/1	0.97	0.07	20,20,20,20	0
55	MG	1A	3416	1/1	0.97	0.14	26,26,26,26	0
55	MG	1G	3003	1/1	0.97	0.08	47,47,47,47	0
55	MG	2A	3576	1/1	0.97	0.41	52,52,52,52	0
55	MG	1A	3417	1/1	0.97	0.10	22,22,22,22	0
55	MG	1A	3085	1/1	0.97	0.35	34,34,34,34	0
55	MG	1A	3322	1/1	0.97	0.24	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3565	1/1	0.97	0.14	20,20,20,20	0
55	MG	1A	3091	1/1	0.97	0.29	16,16,16,16	0
55	MG	1a	3033	1/1	0.97	0.10	50,50,50,50	0
55	MG	2A	3266	1/1	0.97	0.15	65,65,65,65	0
55	MG	2A	3267	1/1	0.97	0.26	61,61,61,61	0
55	MG	2A	3014	1/1	0.97	0.26	66,66,66,66	0
55	MG	1A	3421	1/1	0.97	0.12	28,28,28,28	0
55	MG	1A	3683	1/1	0.97	0.30	51,51,51,51	0
55	MG	1A	3422	1/1	0.97	0.10	30,30,30,30	0
55	MG	2A	3137	1/1	0.97	0.84	60,60,60,60	0
55	MG	2A	3591	1/1	0.97	0.19	53,53,53,53	0
55	MG	2a	1638	1/1	0.97	0.16	73,73,73,73	0
55	MG	1A	3830	1/1	0.97	0.04	47,47,47,47	0
55	MG	1a	3147	1/1	0.97	0.13	85,85,85,85	0
55	MG	2A	3433	1/1	0.97	0.11	66,66,66,66	0
55	MG	2A	3275	1/1	0.97	0.10	47,47,47,47	0
55	MG	1A	3685	1/1	0.97	0.13	52,52,52,52	0
55	MG	1Q	202	1/1	0.97	0.07	39,39,39,39	0
55	MG	1A	3626	1/1	0.97	0.13	44,44,44,44	0
55	MG	1A	3754	1/1	0.97	0.05	39,39,39,39	0
55	MG	2A	3280	1/1	0.97	0.07	51,51,51,51	0
55	MG	2A	3778	1/1	0.97	0.22	50,50,50,50	0
55	MG	1A	3627	1/1	0.97	0.49	44,44,44,44	0
55	MG	1A	3423	1/1	0.97	0.13	20,20,20,20	0
55	MG	2A	3781	1/1	0.97	0.07	51,51,51,51	0
55	MG	1R	202	1/1	0.97	0.18	46,46,46,46	0
55	MG	1A	3915	1/1	0.97	0.20	60,60,60,60	0
55	MG	2A	3029	1/1	0.97	0.25	61,61,61,61	0
55	MG	2a	1655	1/1	0.97	0.06	84,84,84,84	0
55	MG	1A	3351	1/1	0.97	0.30	54,54,54,54	0
55	MG	1A	3185	1/1	0.97	0.66	32,32,32,32	0
55	MG	1A	3354	1/1	0.97	0.09	36,36,36,36	0
55	MG	2A	3033	1/1	0.97	0.09	59,59,59,59	0
55	MG	2A	3292	1/1	0.97	0.28	77,77,77,77	0
55	MG	2a	1661	1/1	0.97	0.26	63,63,63,63	0
55	MG	1A	3632	1/1	0.97	0.11	49,49,49,49	0
55	MG	1B	3004	1/1	0.97	0.11	44,44,44,44	0
55	MG	2A	3453	1/1	0.97	0.18	81,81,81,81	0
55	MG	2A	3156	1/1	0.97	0.52	39,39,39,39	0
55	MG	2a	1667	1/1	0.97	0.11	64,64,64,64	0
55	MG	2A	3296	1/1	0.97	0.15	42,42,42,42	0
55	MG	1A	3250	1/1	0.97	0.17	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3356	1/1	0.97	0.15	25,25,25,25	0
55	MG	2a	1671	1/1	0.97	0.08	80,80,80,80	0
55	MG	1A	3576	1/1	0.97	0.51	47,47,47,47	0
55	MG	2A	3620	1/1	0.97	0.10	45,45,45,45	0
55	MG	1a	3164	1/1	0.97	0.14	61,61,61,61	0
55	MG	1A	3843	1/1	0.97	0.21	49,49,49,49	0
55	MG	1A	3844	1/1	0.97	0.07	27,27,27,27	0
55	MG	1A	3307	1/1	0.97	0.06	63,63,63,63	0
55	MG	2A	3043	1/1	0.97	0.12	72,72,72,72	0
55	MG	2a	1680	1/1	0.97	0.09	55,55,55,55	0
55	MG	1V	202	1/1	0.97	0.25	25,25,25,25	0
55	MG	1V	203	1/1	0.97	0.12	60,60,60,60	0
55	MG	2A	3308	1/1	0.97	0.23	52,52,52,52	0
55	MG	1A	3330	1/1	0.97	0.11	37,37,37,37	0
55	MG	1A	3699	1/1	0.97	0.08	38,38,38,38	0
55	MG	2a	1687	1/1	0.97	0.23	55,55,55,55	0
55	MG	2A	3170	1/1	0.97	0.23	73,73,73,73	0
55	MG	2A	3312	1/1	0.97	0.16	53,53,53,53	0
55	MG	1A	3434	1/1	0.97	0.21	16,16,16,16	0
55	MG	2A	3473	1/1	0.97	0.09	61,61,61,61	0
55	MG	2A	3315	1/1	0.97	0.16	67,67,67,67	0
55	MG	2a	1693	1/1	0.97	0.21	54,54,54,54	0
55	MG	1a	3174	1/1	0.97	0.11	70,70,70,70	0
55	MG	1A	3391	1/1	0.97	0.16	18,18,18,18	0
55	MG	1Y	502	1/1	0.97	0.10	74,74,74,74	0
55	MG	2A	3052	1/1	0.97	0.42	42,42,42,42	0
55	MG	1A	3770	1/1	0.97	0.14	34,34,34,34	0
55	MG	1A	3851	1/1	0.97	0.07	21,21,21,21	0
55	MG	2B	3001	1/1	0.97	0.12	64,64,64,64	0
55	MG	1A	3086	1/1	0.97	0.06	50,50,50,50	0
55	MG	2A	3326	1/1	0.97	0.10	35,35,35,35	0
55	MG	1A	3529	1/1	0.97	0.15	58,58,58,58	0
55	MG	1A	3773	1/1	0.97	0.17	44,44,44,44	0
55	MG	1A	3774	1/1	0.97	0.25	45,45,45,45	0
55	MG	2A	3648	1/1	0.97	0.06	34,34,34,34	0
55	MG	1A	3176	1/1	0.97	0.27	52,52,52,52	0
55	MG	1A	3776	1/1	0.97	0.10	43,43,43,43	0
55	MG	2A	3488	1/1	0.97	0.13	58,58,58,58	0
55	MG	1D	301	1/1	0.97	0.22	32,32,32,32	0
55	MG	1A	3333	1/1	0.97	0.18	17,17,17,17	0
55	MG	2a	1714	1/1	0.97	0.14	71,71,71,71	0
55	MG	2A	3491	1/1	0.97	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3286	1/1	0.97	0.11	64,64,64,64	0
55	MG	1A	3366	1/1	0.97	0.12	26,26,26,26	0
55	MG	2A	3336	1/1	0.97	0.22	56,56,56,56	0
55	MG	1A	3024	1/1	0.97	0.36	30,30,30,30	0
55	MG	2A	3189	1/1	0.97	0.16	43,43,43,43	0
55	MG	1A	3109	1/1	0.97	0.12	30,30,30,30	0
55	MG	1a	3080	1/1	0.97	0.12	69,69,69,69	0
55	MG	2A	3662	1/1	0.97	0.07	68,68,68,68	0
55	MG	2A	3663	1/1	0.97	0.08	50,50,50,50	0
55	MG	1a	3081	1/1	0.97	0.23	69,69,69,69	0
55	MG	2A	3501	1/1	0.97	0.11	76,76,76,76	0
55	MG	2A	3070	1/1	0.97	0.18	35,35,35,35	0
55	MG	2A	3667	1/1	0.97	0.12	57,57,57,57	0
55	MG	2A	3503	1/1	0.97	0.23	53,53,53,53	0
55	MG	2A	3669	1/1	0.97	0.13	40,40,40,40	0
55	MG	1A	3369	1/1	0.97	0.07	14,14,14,14	0
55	MG	1a	3083	1/1	0.97	0.26	67,67,67,67	0
55	MG	2E	302	1/1	0.97	0.06	35,35,35,35	0
55	MG	1A	3864	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3015	1/1	0.97	0.42	23,23,23,23	0
55	MG	2E	305	1/1	0.97	0.12	34,34,34,34	0
55	MG	1a	3198	1/1	0.97	0.05	47,47,47,47	0
55	MG	2A	3199	1/1	0.97	0.27	65,65,65,65	0
55	MG	2A	3349	1/1	0.97	0.06	77,77,77,77	0
55	MG	1a	3086	1/1	0.97	0.34	68,68,68,68	0
55	MG	1A	3493	1/1	0.97	0.12	30,30,30,30	0
55	MG	2a	1743	1/1	0.97	0.04	55,55,55,55	0
55	MG	1a	3088	1/1	0.97	0.37	63,63,63,63	0
55	MG	2A	3514	1/1	0.97	0.48	53,53,53,53	0
55	MG	2a	1746	1/1	0.97	0.06	69,69,69,69	0
55	MG	1A	3867	1/1	0.97	0.67	37,37,37,37	0
55	MG	2A	3354	1/1	0.97	0.17	26,26,26,26	0
55	MG	1A	3170	1/1	0.97	0.54	34,34,34,34	0
55	MG	2A	3205	1/1	0.97	0.68	52,52,52,52	0
55	MG	1a	3205	1/1	0.97	0.07	77,77,77,77	0
55	MG	1a	3206	1/1	0.97	0.04	68,68,68,68	0
55	MG	2A	3209	1/1	0.97	0.09	81,81,81,81	0
55	MG	2A	3085	1/1	0.97	0.26	62,62,62,62	0
55	MG	2a	1755	1/1	0.97	0.73	81,81,81,81	0
55	MG	1a	3093	1/1	0.97	0.06	73,73,73,73	0
55	MG	1A	3229	1/1	0.97	0.23	62,62,62,62	0
55	MG	1A	3496	1/1	0.97	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3342	1/1	0.97	0.09	21,21,21,21	0
55	MG	2Q	8001	1/1	0.97	0.03	79,79,79,79	0
55	MG	1A	3872	1/1	0.97	0.08	29,29,29,29	0
55	MG	2a	1762	1/1	0.97	0.10	74,74,74,74	0
55	MG	1A	3793	1/1	0.97	0.06	52,52,52,52	0
55	MG	2A	3698	1/1	0.97	0.14	42,42,42,42	0
55	MG	2a	1765	1/1	0.97	0.10	71,71,71,71	0
55	MG	2Q	8005	1/1	0.97	0.09	62,62,62,62	0
55	MG	2A	3699	1/1	0.97	0.12	38,38,38,38	0
55	MG	1a	3100	1/1	0.97	0.31	60,60,60,60	0
55	MG	2A	3219	1/1	0.97	0.37	22,22,22,22	0
55	MG	2A	3373	1/1	0.97	0.11	48,48,48,48	0
55	MG	1A	3874	1/1	0.97	0.17	59,59,59,59	0
55	MG	1A	3717	1/1	0.97	0.10	35,35,35,35	0
55	MG	2A	3376	1/1	0.97	0.11	31,31,31,31	0
55	MG	1A	3795	1/1	0.97	0.35	46,46,46,46	0
55	MG	1A	3655	1/1	0.97	0.32	41,41,41,41	0
55	MG	2A	3710	1/1	0.97	0.10	60,60,60,60	0
55	MG	2A	3711	1/1	0.97	0.08	70,70,70,70	0
55	MG	2a	1780	1/1	0.97	0.06	68,68,68,68	0
55	MG	2V	204	1/1	0.97	0.39	77,77,77,77	0
55	MG	1a	3002	1/1	0.97	0.15	82,82,82,82	0
55	MG	1A	3546	1/1	0.97	0.33	25,25,25,25	0
55	MG	2A	3714	1/1	0.97	0.10	49,49,49,49	0
55	MG	1A	3343	1/1	0.97	0.09	26,26,26,26	0
55	MG	1A	3081	1/1	0.97	0.51	33,33,33,33	0
55	MG	1E	307	1/1	0.97	0.19	33,33,33,33	0
55	MG	1E	308	1/1	0.97	0.15	49,49,49,49	0
55	MG	2A	3231	1/1	0.97	0.19	48,48,48,48	0
55	MG	1A	3500	1/1	0.97	0.37	65,65,65,65	0
55	MG	1A	3723	1/1	0.97	0.10	47,47,47,47	0
55	MG	1A	3096	1/1	0.97	0.54	34,34,34,34	0
55	MG	1A	3603	1/1	0.97	0.08	49,49,49,49	0
55	MG	1A	3409	1/1	0.97	0.08	49,49,49,49	0
55	MG	2A	3551	1/1	0.97	0.06	71,71,71,71	0
55	MG	1A	3410	1/1	0.97	0.20	42,42,42,42	0
55	MG	1a	3014	1/1	0.97	0.32	81,81,81,81	0
55	MG	1a	3015	1/1	0.97	0.21	74,74,74,74	0
55	MG	1a	3121	1/1	0.97	0.51	62,62,62,62	0
55	MG	2A	3730	1/1	0.97	0.12	56,56,56,56	0
55	MG	1A	3665	1/1	0.97	0.26	51,51,51,51	0
55	MG	1A	3232	1/1	0.97	0.99	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	1A	3412	1/1	0.97	0.16	12,12,12,12	0
55	MG	2A	3735	1/1	0.97	0.18	49,49,49,49	0
55	MG	1a	3126	1/1	0.97	0.15	74,74,74,74	0
55	MG	2A	3247	1/1	0.97	0.17	35,35,35,35	0
55	MG	1A	3379	1/1	0.97	0.15	43,43,43,43	0
55	MG	2A	3739	1/1	0.97	0.07	69,69,69,69	0
55	MG	2A	3249	1/1	0.97	0.25	43,43,43,43	0
55	MG	2A	3407	1/1	0.97	0.32	74,74,74,74	0
55	MG	1A	3508	1/1	0.97	0.13	51,51,51,51	0
57	ZN	14	501	1/1	0.97	0.04	109,109,109,109	0
55	MG	1A	3816	1/1	0.97	0.11	19,19,19,19	0
57	ZN	2Y	501	1/1	0.97	0.06	95,95,95,95	0
55	MG	2A	3119	1/1	0.97	0.54	49,49,49,49	0
55	MG	2a	1612	1/1	0.97	0.12	51,51,51,51	0
55	MG	2A	3411	1/1	0.97	0.11	63,63,63,63	0
55	MG	2a	1695	1/1	0.98	0.26	58,58,58,58	0
55	MG	1A	3430	1/1	0.98	0.12	16,16,16,16	0
55	MG	2A	3153	1/1	0.98	0.10	52,52,52,52	0
55	MG	2A	3552	1/1	0.98	0.32	52,52,52,52	0
55	MG	1a	3142	1/1	0.98	0.09	85,85,85,85	0
55	MG	2a	1700	1/1	0.98	0.13	76,76,76,76	0
55	MG	1A	3397	1/1	0.98	0.03	64,64,64,64	0
55	MG	1A	3003	1/1	0.98	0.09	20,20,20,20	0
55	MG	1A	3296	1/1	0.98	0.15	20,20,20,20	0
55	MG	1A	3141	1/1	0.98	0.31	37,37,37,37	0
55	MG	1A	3280	1/1	0.98	0.09	29,29,29,29	0
55	MG	2A	3452	1/1	0.98	0.07	51,51,51,51	0
55	MG	2A	3160	1/1	0.98	0.39	46,46,46,46	0
55	MG	2A	3251	1/1	0.98	0.04	79,79,79,79	0
55	MG	1A	3319	1/1	0.98	0.20	34,34,34,34	0
55	MG	20	105	1/1	0.98	0.12	81,81,81,81	0
55	MG	2A	3671	1/1	0.98	0.25	73,73,73,73	0
55	MG	1A	3437	1/1	0.98	0.07	34,34,34,34	0
55	MG	21	102	1/1	0.98	0.07	60,60,60,60	0
55	MG	1A	3142	1/1	0.98	0.92	32,32,32,32	0
55	MG	1A	3439	1/1	0.98	0.07	54,54,54,54	0
55	MG	1A	3606	1/1	0.98	0.17	56,56,56,56	0
55	MG	2A	3355	1/1	0.98	0.03	76,76,76,76	0
55	MG	1A	3374	1/1	0.98	0.09	62,62,62,62	0
55	MG	1A	3562	1/1	0.98	0.23	20,20,20,20	0
55	MG	2A	3679	1/1	0.98	0.08	52,52,52,52	0
55	MG	1A	3441	1/1	0.98	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3405	1/1	0.98	0.09	42,42,42,42	0
55	MG	2A	3084	1/1	0.98	0.27	45,45,45,45	0
55	MG	1A	3300	1/1	0.98	0.07	44,44,44,44	0
55	MG	1A	3661	1/1	0.98	0.08	33,33,33,33	0
55	MG	1A	3909	1/1	0.98	0.16	32,32,32,32	0
55	MG	1A	3240	1/1	0.98	0.18	58,58,58,58	0
55	MG	2a	1604	1/1	0.98	0.15	53,53,53,53	0
55	MG	1A	3223	1/1	0.98	0.08	42,42,42,42	0
55	MG	2A	3578	1/1	0.98	0.06	61,61,61,61	0
55	MG	1A	3614	1/1	0.98	0.15	70,70,70,70	0
55	MG	2A	3368	1/1	0.98	0.05	42,42,42,42	0
55	MG	1G	3001	1/1	0.98	0.10	67,67,67,67	0
55	MG	1A	3284	1/1	0.98	0.12	43,43,43,43	0
55	MG	1A	3779	1/1	0.98	0.10	24,24,24,24	0
55	MG	1A	3325	1/1	0.98	0.06	28,28,28,28	0
55	MG	1A	3667	1/1	0.98	0.19	46,46,46,46	0
55	MG	1A	3782	1/1	0.98	0.06	33,33,33,33	0
55	MG	1B	3001	1/1	0.98	0.23	55,55,55,55	0
55	MG	2a	1740	1/1	0.98	0.05	70,70,70,70	0
55	MG	1a	3089	1/1	0.98	0.06	52,52,52,52	0
55	MG	1a	3171	1/1	0.98	0.10	50,50,50,50	0
55	MG	2A	3701	1/1	0.98	0.06	60,60,60,60	0
55	MG	2A	3817	1/1	0.98	0.12	65,65,65,65	0
55	MG	1A	3617	1/1	0.98	0.05	38,38,38,38	0
55	MG	1A	3304	1/1	0.98	0.08	45,45,45,45	0
55	MG	1A	3785	1/1	0.98	0.09	25,25,25,25	0
55	MG	1A	3619	1/1	0.98	0.16	44,44,44,44	0
55	MG	1A	3571	1/1	0.98	0.31	54,54,54,54	0
55	MG	2A	3384	1/1	0.98	0.09	68,68,68,68	0
55	MG	1A	3225	1/1	0.98	0.10	34,34,34,34	0
55	MG	1A	3673	1/1	0.98	0.13	35,35,35,35	0
55	MG	1A	3353	1/1	0.98	0.12	67,67,67,67	0
55	MG	2A	3492	1/1	0.98	0.08	52,52,52,52	0
55	MG	2A	3388	1/1	0.98	0.14	60,60,60,60	0
55	MG	2A	3023	1/1	0.98	0.32	47,47,47,47	0
55	MG	2A	3390	1/1	0.98	0.14	49,49,49,49	0
55	MG	1A	3791	1/1	0.98	0.06	33,33,33,33	0
55	MG	1B	3011	1/1	0.98	0.15	48,48,48,48	0
55	MG	2A	3289	1/1	0.98	0.13	46,46,46,46	0
55	MG	1A	3328	1/1	0.98	0.12	22,22,22,22	0
55	MG	1A	3492	1/1	0.98	0.16	50,50,50,50	0
55	MG	1B	3014	1/1	0.98	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3329	1/1	0.98	0.11	40,40,40,40	0
55	MG	1A	3252	1/1	0.98	0.50	36,36,36,36	0
55	MG	1A	3273	1/1	0.98	0.25	19,19,19,19	0
55	MG	1A	3797	1/1	0.98	0.06	28,28,28,28	0
55	MG	2A	3613	1/1	0.98	0.08	55,55,55,55	0
55	MG	1A	3798	1/1	0.98	0.09	48,48,48,48	0
55	MG	1a	3110	1/1	0.98	0.08	52,52,52,52	0
55	MG	2a	1771	1/1	0.98	0.07	55,55,55,55	0
55	MG	2A	3206	1/1	0.98	0.10	39,39,39,39	0
55	MG	2A	3405	1/1	0.98	0.08	43,43,43,43	0
55	MG	2A	3300	1/1	0.98	0.12	36,36,36,36	0
55	MG	2a	1775	1/1	0.98	0.08	63,63,63,63	0
55	MG	1A	3799	1/1	0.98	0.11	49,49,49,49	0
55	MG	1A	3288	1/1	0.98	0.14	26,26,26,26	0
55	MG	2A	3734	1/1	0.98	0.04	67,67,67,67	0
55	MG	1A	3274	1/1	0.98	0.18	27,27,27,27	0
55	MG	1U	205	1/1	0.98	0.36	29,29,29,29	0
55	MG	1A	3360	1/1	0.98	0.12	21,21,21,21	0
55	MG	2A	3516	1/1	0.98	0.09	45,45,45,45	0
55	MG	1A	3290	1/1	0.98	0.04	49,49,49,49	0
55	MG	1A	3059	1/1	0.98	0.19	35,35,35,35	0
55	MG	1A	3739	1/1	0.98	0.17	22,22,22,22	0
55	MG	1A	3740	1/1	0.98	0.04	26,26,26,26	0
55	MG	2A	3216	1/1	0.98	0.24	41,41,41,41	0
55	MG	1A	3337	1/1	0.98	0.10	39,39,39,39	0
55	MG	1A	3585	1/1	0.98	0.25	59,59,59,59	0
55	MG	1A	3542	1/1	0.98	0.11	77,77,77,77	0
55	MG	2A	3220	1/1	0.98	0.10	66,66,66,66	0
55	MG	2A	3316	1/1	0.98	0.17	43,43,43,43	0
55	MG	1A	3744	1/1	0.98	0.06	55,55,55,55	0
55	MG	2a	1794	1/1	0.98	0.07	70,70,70,70	0
55	MG	1a	3125	1/1	0.98	0.30	74,74,74,74	0
55	MG	1A	3811	1/1	0.98	0.05	56,56,56,56	0
55	MG	1A	3587	1/1	0.98	0.06	50,50,50,50	0
55	MG	1A	3502	1/1	0.98	0.11	62,62,62,62	0
55	MG	1A	3814	1/1	0.98	0.10	18,18,18,18	0
55	MG	1A	3544	1/1	0.98	0.30	34,34,34,34	0
55	MG	2A	3325	1/1	0.98	0.07	51,51,51,51	0
55	MG	1a	3051	1/1	0.98	0.42	57,57,57,57	0
55	MG	2a	1678	1/1	0.98	0.47	65,65,65,65	0
55	MG	1A	3364	1/1	0.98	0.25	36,36,36,36	0
55	MG	2A	3645	1/1	0.98	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3214	1/1	0.98	0.04	71,71,71,71	0
55	MG	1A	3365	1/1	0.98	0.11	40,40,40,40	0
55	MG	1A	3466	1/1	0.98	0.08	46,46,46,46	0
55	MG	1A	3752	1/1	0.98	0.07	22,22,22,22	0
55	MG	1A	3043	1/1	0.98	0.30	10,10,10,10	0
55	MG	1a	3219	1/1	0.98	0.16	63,63,63,63	0
55	MG	1A	3468	1/1	0.98	0.06	49,49,49,49	0
55	MG	2A	3767	1/1	0.98	0.06	65,65,65,65	0
55	MG	1A	3888	1/1	0.98	0.11	47,47,47,47	0
55	MG	2A	3238	1/1	0.98	0.10	38,38,38,38	0
55	MG	2A	3239	1/1	0.98	0.10	38,38,38,38	0
55	MG	1A	3107	1/1	0.98	0.47	36,36,36,36	0
57	ZN	29	501	1/1	0.98	0.10	75,75,75,75	0
55	MG	1A	3697	1/1	0.98	0.13	19,19,19,19	0
55	MG	1A	3453	1/1	0.99	0.13	19,19,19,19	0
55	MG	2A	3801	1/1	0.99	0.26	21,21,21,21	0
55	MG	2A	3402	1/1	0.99	0.11	37,37,37,37	0
55	MG	1A	3334	1/1	0.99	0.14	20,20,20,20	0
55	MG	1A	3749	1/1	0.99	0.06	36,36,36,36	0
55	MG	1A	3426	1/1	0.99	0.06	18,18,18,18	0
55	MG	2T	201	1/1	0.99	0.12	47,47,47,47	0
55	MG	2A	3372	1/1	0.99	0.13	38,38,38,38	0
55	MG	1a	3111	1/1	0.99	0.14	56,56,56,56	0
55	MG	1A	3540	1/1	0.99	0.17	19,19,19,19	0
55	MG	1a	3202	1/1	0.99	0.07	47,47,47,47	0
55	MG	1a	3091	1/1	0.99	0.08	37,37,37,37	0
55	MG	1A	3065	1/1	0.99	0.19	32,32,32,32	0
55	MG	2A	3314	1/1	0.99	0.14	60,60,60,60	0
55	MG	1l	102	1/1	0.99	0.05	56,56,56,56	0
55	MG	2A	3518	1/1	0.99	0.14	71,71,71,71	0
55	MG	1A	3295	1/1	0.99	0.13	13,13,13,13	0
55	MG	1a	3037	1/1	0.99	0.18	68,68,68,68	0
55	MG	2A	3288	1/1	0.99	0.07	30,30,30,30	0
55	MG	1A	3897	1/1	0.99	0.20	11,11,11,11	0
55	MG	2A	3067	1/1	0.99	0.09	62,62,62,62	0
55	MG	2a	1665	1/1	0.99	0.09	74,74,74,74	0
55	MG	2d	502	1/1	0.99	0.13	74,74,74,74	0
55	MG	1A	3769	1/1	0.99	0.07	61,61,61,61	0
55	MG	2a	1624	1/1	0.99	0.20	53,53,53,53	0
55	MG	1A	3447	1/1	0.99	0.15	17,17,17,17	0
55	MG	2A	3323	1/1	0.99	0.22	66,66,66,66	0
55	MG	2a	1627	1/1	0.99	0.26	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3124	1/1	0.99	0.23	47,47,47,47	0
55	MG	2A	3709	1/1	0.99	0.09	45,45,45,45	0
55	MG	1a	3099	1/1	0.99	0.14	61,61,61,61	0
55	MG	1A	3429	1/1	0.99	0.10	26,26,26,26	0
55	MG	2A	3358	1/1	0.99	0.16	45,45,45,45	0
55	MG	1A	3460	1/1	0.99	0.13	20,20,20,20	0
55	MG	1a	3190	1/1	0.99	0.04	79,79,79,79	0
55	MG	1A	3306	1/1	0.99	0.12	14,14,14,14	0
55	MG	1A	3152	1/1	0.99	0.08	53,53,53,53	0
55	MG	1A	3224	1/1	0.99	0.07	73,73,73,73	0
57	ZN	1Y	501	1/1	0.99	0.13	61,61,61,61	0
55	MG	1A	3197	1/1	0.99	0.13	25,25,25,25	0
57	ZN	15	106	1/1	0.99	0.16	47,47,47,47	0
57	ZN	16	101	1/1	0.99	0.12	44,44,44,44	0
55	MG	2A	3466	1/1	0.99	0.10	37,37,37,37	0
55	MG	1A	3732	1/1	0.99	0.09	21,21,21,21	0
55	MG	2A	3683	1/1	0.99	0.06	60,60,60,60	0
57	ZN	25	104	1/1	0.99	0.11	54,54,54,54	0
55	MG	2a	1685	1/1	0.99	0.15	56,56,56,56	0
55	MG	2A	3079	1/1	0.99	0.28	50,50,50,50	0
55	MG	2A	3003	1/1	0.99	0.11	31,31,31,31	0
58	SF4	1d	501	8/8	0.99	0.14	65,70,75,78	0
58	SF4	2d	501	8/8	0.99	0.12	65,69,77,88	0
57	ZN	19	102	1/1	1.00	0.12	43,43,43,43	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.