



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2016 – 02:26 PM EDT

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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

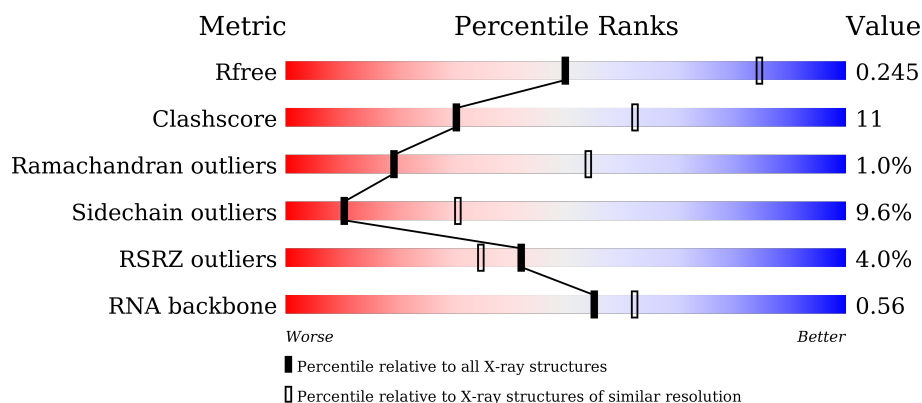
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>5%</div> <div>23% 50% 21% . .</div> </div>
1	2A	2915	<div> <div>5%</div> <div>36% 43% 17% . .</div> </div>
2	1B	120	<div> <div>35% 50% 14% .</div> </div>
2	2B	120	<div> <div>40% 43% 15% .</div> </div>


























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Mol	Chain	Length	Quality of chain
3	1D	275	
3	2D	275	
4	1E	204	
4	2E	204	
5	1F	203	
5	2F	203	
6	1G	181	
6	2G	181	
7	1H	174	
7	2H	174	
8	1I	147	
8	2I	147	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	149	
11	2P	149	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	110	
14	2S	110	
15	1T	131	

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Mol	Chain	Length	Quality of chain
15	2T	131	
16	1U	116	
16	2U	116	
17	1V	101	
17	2V	101	
18	1W	112	
18	2W	112	
19	1X	95	
19	2X	95	
20	1Y	107	
20	2Y	107	
21	1Z	203	
21	2Z	203	
22	10	77	
22	20	77	
23	11	97	
23	21	97	
24	12	70	
24	22	70	
25	13	59	
25	23	59	
26	14	69	
26	24	69	
27	15	59	
27	25	59	

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Mol	Chain	Length	Quality of chain
28	16	53	
28	26	53	
29	17	48	
29	27	48	
30	18	64	
30	28	64	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	231	
33	2b	231	
34	1c	206	
34	2c	206	
35	1d	208	
35	2d	208	
36	1e	148	
36	2e	148	
37	1f	100	
37	2f	100	
38	1g	155	
38	2g	155	
39	1h	137	
39	2h	137	
40	1i	127	

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Mol	Chain	Length	Quality of chain
40	2i	127	<div> <div>17%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
41	1j	97	<div> <div>22%</div> <div>90%</div> <div>10%</div> </div>
41	2j	97	<div> <div>21%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
42	1k	114	<div> <div>%</div> <div>96%</div> <div>.</div> </div>
42	2k	114	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>
43	1l	122	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>
43	2l	122	<div> <div></div> <div>93%</div> <div>7%</div> </div>
44	1m	116	<div> <div>6%</div> <div>90%</div> <div>10%</div> </div>
44	2m	116	<div> <div>7%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
45	1n	60	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
45	2n	60	<div> <div>18%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
46	1o	88	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
46	2o	88	<div> <div></div> <div>92%</div> <div>8%</div> </div>
47	1p	82	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
47	2p	82	<div> <div>4%</div> <div>90%</div> <div>10%</div> </div>
48	1q	99	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
48	2q	99	<div> <div>%</div> <div>93%</div> <div>7%</div> </div>
49	1r	68	<div> <div>4%</div> <div>91%</div> <div>9%</div> </div>
49	2r	68	<div> <div>3%</div> <div>87%</div> <div>13%</div> </div>
50	1s	83	<div> <div>12%</div> <div>90%</div> <div>10%</div> </div>
50	2s	83	<div> <div>42%</div> <div>93%</div> <div>7%</div> </div>
51	1t	98	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
51	2t	98	<div> <div>%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
52	1u	23	<div> <div>22%</div> <div>87%</div> <div>13%</div> </div>
52	2u	23	<div> <div>43%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
53	1x	97	
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	10	102	-	-	-	X
55	MG	10	103	-	-	-	X
55	MG	11	101	-	-	-	X
55	MG	13	101	-	-	-	X
55	MG	13	102	-	-	-	X
55	MG	15	101	-	-	-	X
55	MG	15	102	-	-	-	X
55	MG	15	103	-	-	-	X
55	MG	15	104	-	-	-	X
55	MG	17	101	-	-	-	X
55	MG	17	102	-	-	-	X
55	MG	17	103	-	-	-	X
55	MG	18	3302	-	-	-	X
55	MG	1A	3005	-	-	-	X
55	MG	1A	3018	-	-	-	X
55	MG	1A	3019	-	-	-	X
55	MG	1A	3020	-	-	-	X
55	MG	1A	3021	-	-	-	X
55	MG	1A	3025	-	-	-	X
55	MG	1A	3027	-	-	-	X
55	MG	1A	3028	-	-	-	X
55	MG	1A	3031	-	-	-	X
55	MG	1A	3040	-	-	-	X
55	MG	1A	3068	-	-	-	X
55	MG	1A	3070	-	-	-	X
55	MG	1A	3077	-	-	-	X
55	MG	1A	3080	-	-	-	X
55	MG	1A	3082	-	-	-	X
55	MG	1A	3085	-	-	-	X
55	MG	1A	3087	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1A	3102	-	-	-	X
55	MG	1A	3103	-	-	-	X
55	MG	1A	3104	-	-	-	X
55	MG	1A	3107	-	-	-	X
55	MG	1A	3110	-	-	-	X
55	MG	1A	3113	-	-	-	X
55	MG	1A	3119	-	-	-	X
55	MG	1A	3122	-	-	-	X
55	MG	1A	3123	-	-	-	X
55	MG	1A	3124	-	-	-	X
55	MG	1A	3127	-	-	-	X
55	MG	1A	3129	-	-	-	X
55	MG	1A	3141	-	-	-	X
55	MG	1A	3142	-	-	-	X
55	MG	1A	3147	-	-	-	X
55	MG	1A	3154	-	-	-	X
55	MG	1A	3155	-	-	-	X
55	MG	1A	3159	-	-	-	X
55	MG	1A	3160	-	-	-	X
55	MG	1A	3170	-	-	-	X
55	MG	1A	3175	-	-	-	X
55	MG	1A	3177	-	-	-	X
55	MG	1A	3184	-	-	-	X
55	MG	1A	3185	-	-	-	X
55	MG	1A	3188	-	-	-	X
55	MG	1A	3189	-	-	-	X
55	MG	1A	3193	-	-	-	X
55	MG	1A	3198	-	-	-	X
55	MG	1A	3199	-	-	-	X
55	MG	1A	3201	-	-	-	X
55	MG	1A	3202	-	-	-	X
55	MG	1A	3206	-	-	-	X
55	MG	1A	3208	-	-	-	X
55	MG	1A	3211	-	-	-	X
55	MG	1A	3228	-	-	-	X
55	MG	1A	3231	-	-	-	X
55	MG	1A	3233	-	-	-	X
55	MG	1A	3242	-	-	-	X
55	MG	1A	3243	-	-	-	X
55	MG	1A	3252	-	-	-	X
55	MG	1A	3256	-	-	-	X
55	MG	1A	3257	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1A	3258	-	-	-	X
55	MG	1A	3260	-	-	-	X
55	MG	1A	3261	-	-	-	X
55	MG	1A	3265	-	-	-	X
55	MG	1A	3273	-	-	-	X
55	MG	1A	3276	-	-	-	X
55	MG	1A	3278	-	-	-	X
55	MG	1A	3285	-	-	-	X
55	MG	1A	3313	-	-	-	X
55	MG	1A	3315	-	-	-	X
55	MG	1A	3372	-	-	-	X
55	MG	1A	3446	-	-	-	X
55	MG	1A	3459	-	-	-	X
55	MG	1A	3464	-	-	-	X
55	MG	1A	3467	-	-	-	X
55	MG	1A	3475	-	-	-	X
55	MG	1A	3480	-	-	-	X
55	MG	1A	3482	-	-	-	X
55	MG	1A	3494	-	-	-	X
55	MG	1A	3509	-	-	-	X
55	MG	1A	3516	-	-	-	X
55	MG	1A	3545	-	-	-	X
55	MG	1A	3549	-	-	-	X
55	MG	1A	3551	-	-	-	X
55	MG	1A	3553	-	-	-	X
55	MG	1A	3573	-	-	-	X
55	MG	1A	3577	-	-	-	X
55	MG	1A	3581	-	-	-	X
55	MG	1A	3589	-	-	-	X
55	MG	1A	3593	-	-	-	X
55	MG	1A	3597	-	-	-	X
55	MG	1A	3605	-	-	-	X
55	MG	1A	3627	-	-	-	X
55	MG	1A	3638	-	-	-	X
55	MG	1A	3640	-	-	-	X
55	MG	1A	3641	-	-	-	X
55	MG	1A	3642	-	-	-	X
55	MG	1A	3646	-	-	-	X
55	MG	1A	3655	-	-	-	X
55	MG	1A	3666	-	-	-	X
55	MG	1A	3708	-	-	-	X
55	MG	1A	3709	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1A	3711	-	-	-	X
55	MG	1A	3725	-	-	-	X
55	MG	1A	3726	-	-	-	X
55	MG	1A	3733	-	-	-	X
55	MG	1A	3762	-	-	-	X
55	MG	1A	3773	-	-	-	X
55	MG	1A	3808	-	-	-	X
55	MG	1A	3838	-	-	-	X
55	MG	1A	3857	-	-	-	X
55	MG	1A	3863	-	-	-	X
55	MG	1A	3867	-	-	-	X
55	MG	1A	3877	-	-	-	X
55	MG	1A	3878	-	-	-	X
55	MG	1A	3885	-	-	-	X
55	MG	1A	3894	-	-	-	X
55	MG	1A	3896	-	-	-	X
55	MG	1A	3904	-	-	-	X
55	MG	1A	3905	-	-	-	X
55	MG	1A	3908	-	-	-	X
55	MG	1A	3910	-	-	-	X
55	MG	1B	3008	-	-	-	X
55	MG	1B	3023	-	-	-	X
55	MG	1D	301	-	-	-	X
55	MG	1D	302	-	-	-	X
55	MG	1D	303	-	-	-	X
55	MG	1D	304	-	-	-	X
55	MG	1D	305	-	-	-	X
55	MG	1D	307	-	-	-	X
55	MG	1D	309	-	-	-	X
55	MG	1D	310	-	-	-	X
55	MG	1D	311	-	-	-	X
55	MG	1D	312	-	-	-	X
55	MG	1D	313	-	-	-	X
55	MG	1D	314	-	-	-	X
55	MG	1E	302	-	-	-	X
55	MG	1E	303	-	-	-	X
55	MG	1F	301	-	-	-	X
55	MG	1F	302	-	-	-	X
55	MG	1F	303	-	-	-	X
55	MG	1F	304	-	-	-	X
55	MG	1F	305	-	-	-	X
55	MG	1F	306	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	1F	308	-	-	-	X
55	MG	1F	310	-	-	-	X
55	MG	1F	311	-	-	-	X
55	MG	1F	314	-	-	-	X
55	MG	1F	315	-	-	-	X
55	MG	1N	8001	-	-	-	X
55	MG	1P	201	-	-	-	X
55	MG	1P	202	-	-	-	X
55	MG	1Q	201	-	-	-	X
55	MG	1R	201	-	-	-	X
55	MG	1R	203	-	-	-	X
55	MG	1U	201	-	-	-	X
55	MG	1U	204	-	-	-	X
55	MG	1U	205	-	-	-	X
55	MG	1U	206	-	-	-	X
55	MG	1V	201	-	-	-	X
55	MG	1V	202	-	-	-	X
55	MG	1a	3015	-	-	-	X
55	MG	1a	3016	-	-	-	X
55	MG	1a	3020	-	-	-	X
55	MG	1a	3021	-	-	-	X
55	MG	1a	3023	-	-	-	X
55	MG	1a	3024	-	-	-	X
55	MG	1a	3042	-	-	-	X
55	MG	1a	3052	-	-	-	X
55	MG	1a	3057	-	-	-	X
55	MG	1a	3075	-	-	-	X
55	MG	1a	3088	-	-	-	X
55	MG	1a	3104	-	-	-	X
55	MG	1a	3136	-	-	-	X
55	MG	1a	3137	-	-	-	X
55	MG	1a	3144	-	-	-	X
55	MG	1a	3182	-	-	-	X
55	MG	1a	3208	-	-	-	X
55	MG	1a	3211	-	-	-	X
55	MG	1e	3002	-	-	-	X
55	MG	1n	502	-	-	-	X
55	MG	20	101	-	-	-	X
55	MG	21	101	-	-	-	X
55	MG	23	101	-	-	-	X
55	MG	25	101	-	-	-	X
55	MG	25	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	25	103	-	-	-	X
55	MG	27	101	-	-	-	X
55	MG	27	102	-	-	-	X
55	MG	28	102	-	-	-	X
55	MG	2A	3001	-	-	-	X
55	MG	2A	3017	-	-	-	X
55	MG	2A	3018	-	-	-	X
55	MG	2A	3019	-	-	-	X
55	MG	2A	3023	-	-	-	X
55	MG	2A	3025	-	-	-	X
55	MG	2A	3032	-	-	-	X
55	MG	2A	3034	-	-	-	X
55	MG	2A	3040	-	-	-	X
55	MG	2A	3052	-	-	-	X
55	MG	2A	3054	-	-	-	X
55	MG	2A	3055	-	-	-	X
55	MG	2A	3062	-	-	-	X
55	MG	2A	3066	-	-	-	X
55	MG	2A	3078	-	-	-	X
55	MG	2A	3083	-	-	-	X
55	MG	2A	3086	-	-	-	X
55	MG	2A	3092	-	-	-	X
55	MG	2A	3094	-	-	-	X
55	MG	2A	3095	-	-	-	X
55	MG	2A	3097	-	-	-	X
55	MG	2A	3099	-	-	-	X
55	MG	2A	3103	-	-	-	X
55	MG	2A	3107	-	-	-	X
55	MG	2A	3110	-	-	-	X
55	MG	2A	3111	-	-	-	X
55	MG	2A	3119	-	-	-	X
55	MG	2A	3120	-	-	-	X
55	MG	2A	3123	-	-	-	X
55	MG	2A	3124	-	-	-	X
55	MG	2A	3138	-	-	-	X
55	MG	2A	3143	-	-	-	X
55	MG	2A	3146	-	-	-	X
55	MG	2A	3150	-	-	-	X
55	MG	2A	3154	-	-	-	X
55	MG	2A	3155	-	-	-	X
55	MG	2A	3157	-	-	-	X
55	MG	2A	3158	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3160	-	-	-	X
55	MG	2A	3164	-	-	-	X
55	MG	2A	3165	-	-	-	X
55	MG	2A	3178	-	-	-	X
55	MG	2A	3190	-	-	-	X
55	MG	2A	3199	-	-	-	X
55	MG	2A	3200	-	-	-	X
55	MG	2A	3203	-	-	-	X
55	MG	2A	3205	-	-	-	X
55	MG	2A	3216	-	-	-	X
55	MG	2A	3219	-	-	-	X
55	MG	2A	3221	-	-	-	X
55	MG	2A	3222	-	-	-	X
55	MG	2A	3228	-	-	-	X
55	MG	2A	3242	-	-	-	X
55	MG	2A	3249	-	-	-	X
55	MG	2A	3252	-	-	-	X
55	MG	2A	3277	-	-	-	X
55	MG	2A	3315	-	-	-	X
55	MG	2A	3365	-	-	-	X
55	MG	2A	3406	-	-	-	X
55	MG	2A	3412	-	-	-	X
55	MG	2A	3414	-	-	-	X
55	MG	2A	3417	-	-	-	X
55	MG	2A	3432	-	-	-	X
55	MG	2A	3445	-	-	-	X
55	MG	2A	3448	-	-	-	X
55	MG	2A	3455	-	-	-	X
55	MG	2A	3479	-	-	-	X
55	MG	2A	3482	-	-	-	X
55	MG	2A	3483	-	-	-	X
55	MG	2A	3486	-	-	-	X
55	MG	2A	3490	-	-	-	X
55	MG	2A	3502	-	-	-	X
55	MG	2A	3506	-	-	-	X
55	MG	2A	3509	-	-	-	X
55	MG	2A	3513	-	-	-	X
55	MG	2A	3523	-	-	-	X
55	MG	2A	3527	-	-	-	X
55	MG	2A	3530	-	-	-	X
55	MG	2A	3538	-	-	-	X
55	MG	2A	3556	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2A	3566	-	-	-	X
55	MG	2A	3567	-	-	-	X
55	MG	2A	3568	-	-	-	X
55	MG	2A	3569	-	-	-	X
55	MG	2A	3579	-	-	-	X
55	MG	2A	3585	-	-	-	X
55	MG	2A	3590	-	-	-	X
55	MG	2A	3630	-	-	-	X
55	MG	2A	3643	-	-	-	X
55	MG	2A	3649	-	-	-	X
55	MG	2A	3655	-	-	-	X
55	MG	2A	3676	-	-	-	X
55	MG	2A	3720	-	-	-	X
55	MG	2A	3721	-	-	-	X
55	MG	2A	3732	-	-	-	X
55	MG	2A	3742	-	-	-	X
55	MG	2A	3750	-	-	-	X
55	MG	2A	3756	-	-	-	X
55	MG	2A	3759	-	-	-	X
55	MG	2A	3766	-	-	-	X
55	MG	2A	3777	-	-	-	X
55	MG	2A	3801	-	-	-	X
55	MG	2A	3807	-	-	-	X
55	MG	2A	3810	-	-	-	X
55	MG	2A	3814	-	-	-	X
55	MG	2A	3822	-	-	-	X
55	MG	2B	3003	-	-	-	X
55	MG	2B	3006	-	-	-	X
55	MG	2B	3011	-	-	-	X
55	MG	2D	302	-	-	-	X
55	MG	2D	305	-	-	-	X
55	MG	2D	306	-	-	-	X
55	MG	2D	307	-	-	-	X
55	MG	2D	308	-	-	-	X
55	MG	2E	301	-	-	-	X
55	MG	2E	303	-	-	-	X
55	MG	2E	304	-	-	-	X
55	MG	2F	301	-	-	-	X
55	MG	2F	302	-	-	-	X
55	MG	2F	303	-	-	-	X
55	MG	2F	304	-	-	-	X
55	MG	2F	306	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	2F	307	-	-	-	X
55	MG	2H	201	-	-	-	X
55	MG	2P	201	-	-	-	X
55	MG	2Q	8004	-	-	-	X
55	MG	2R	201	-	-	-	X
55	MG	2U	201	-	-	-	X
55	MG	2U	202	-	-	-	X
55	MG	2V	201	-	-	-	X
55	MG	2V	202	-	-	-	X
55	MG	2V	204	-	-	-	X
55	MG	2X	102	-	-	-	X
55	MG	2a	1602	-	-	-	X
55	MG	2a	1603	-	-	-	X
55	MG	2a	1621	-	-	-	X
55	MG	2a	1634	-	-	-	X
55	MG	2a	1639	-	-	-	X
55	MG	2a	1646	-	-	-	X
55	MG	2a	1663	-	-	-	X
55	MG	2a	1666	-	-	-	X
55	MG	2a	1682	-	-	-	X
55	MG	2a	1694	-	-	-	X
55	MG	2a	1711	-	-	-	X
55	MG	2a	1719	-	-	-	X
55	MG	2a	1722	-	-	-	X
55	MG	2a	1753	-	-	-	X
55	MG	2a	1772	-	-	-	X
55	MG	2a	1781	-	-	-	X
55	MG	2d	503	-	-	-	X
55	MG	2d	505	-	-	-	X
55	MG	2e	3002	-	-	-	X
55	MG	2n	502	-	-	-	X
55	MG	2n	503	-	-	-	X

## 2 Entry composition

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
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
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
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
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
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			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
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			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	2E	7	Total	Mg	0	0
			7	7		
55	17	5	Total	Mg	0	0
			5	5		
55	2d	4	Total	Mg	0	0
			4	4		
55	1T	1	Total	Mg	0	0
			1	1		
55	1N	3	Total	Mg	0	0
			3	3		
55	20	6	Total	Mg	0	0
			6	6		
55	18	3	Total	Mg	0	0
			3	3		
55	1o	1	Total	Mg	0	0
			1	1		
55	2W	1	Total	Mg	0	0
			1	1		
55	1Y	1	Total	Mg	0	0
			1	1		
55	13	2	Total	Mg	0	0
			2	2		
55	1f	1	Total	Mg	0	0
			1	1		
55	2h	1	Total	Mg	0	0
			1	1		
55	1P	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2B	18	Total 18	Mg 18	0	0
55	2a	196	Total 196	Mg 196	0	0
55	1k	1	Total 1	Mg 1	0	0
55	1E	8	Total 8	Mg 8	0	0
55	1b	1	Total 1	Mg 1	0	0
55	2l	1	Total 1	Mg 1	0	0
55	2F	10	Total 10	Mg 10	0	0
55	28	3	Total 3	Mg 3	0	0
55	2e	2	Total 2	Mg 2	0	0
55	1W	3	Total 3	Mg 3	0	0
55	1A	917	Total 917	Mg 917	0	0
55	1t	1	Total 1	Mg 1	0	0
55	1n	1	Total 1	Mg 1	0	0
55	2P	2	Total 2	Mg 2	0	0
55	1X	1	Total 1	Mg 1	0	0
55	1S	1	Total 1	Mg 1	0	0
55	25	3	Total 3	Mg 3	0	0
55	2b	1	Total 1	Mg 1	0	0
55	2T	1	Total 1	Mg 1	0	0
55	1D	18	Total 18	Mg 18	0	0
55	2N	1	Total 1	Mg 1	0	0

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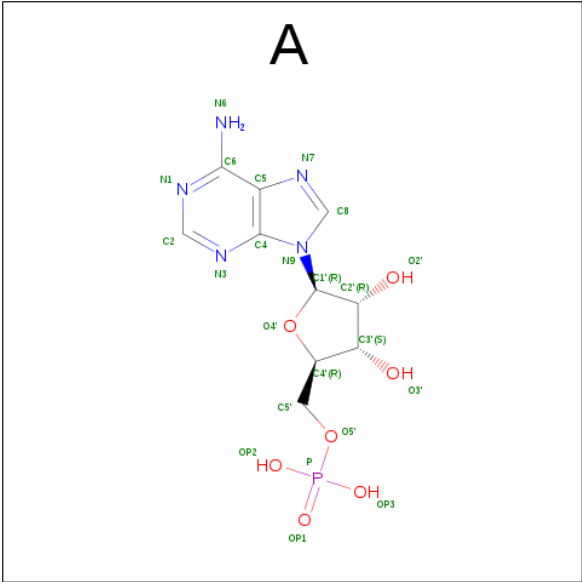
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	1e	2	Total 2	Mg 2	0	0
55	2m	1	Total 1	Mg 1	0	0
55	2G	3	Total 3	Mg 3	0	0
55	2f	1	Total 1	Mg 1	0	0
55	1V	3	Total 3	Mg 3	0	0
55	2X	3	Total 3	Mg 3	0	0
55	1a	223	Total 223	Mg 223	0	0
55	2Q	5	Total 5	Mg 5	0	0
55	15	6	Total 6	Mg 6	0	0
55	1R	5	Total 5	Mg 5	0	0
55	1m	1	Total 1	Mg 1	0	0
55	2U	4	Total 4	Mg 4	0	0
55	1G	3	Total 3	Mg 3	0	0
55	11	3	Total 3	Mg 3	0	0
55	1d	5	Total 5	Mg 5	0	0
55	2n	2	Total 2	Mg 2	0	0
55	1H	2	Total 2	Mg 2	0	0
55	21	2	Total 2	Mg 2	0	0
55	2g	1	Total 1	Mg 1	0	0
55	23	1	Total 1	Mg 1	0	0
55	2R	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	2D	11	Total 11	Mg 11	0	0
55	1U	7	Total 7	Mg 7	0	0
55	27	4	Total 4	Mg 4	0	0
55	19	2	Total 2	Mg 2	0	0
55	1l	1	Total 1	Mg 1	0	0
55	2V	5	Total 5	Mg 5	0	0
55	1F	16	Total 16	Mg 16	0	0
55	2H	1	Total 1	Mg 1	0	0
55	10	8	Total 8	Mg 8	0	0
55	1g	1	Total 1	Mg 1	0	0
55	2o	1	Total 1	Mg 1	0	0
55	1Q	5	Total 5	Mg 5	0	0
55	2A	821	Total 821	Mg 821	0	0
55	1h	2	Total 2	Mg 2	0	0
55	1B	24	Total 24	Mg 24	0	0
55	2S	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).

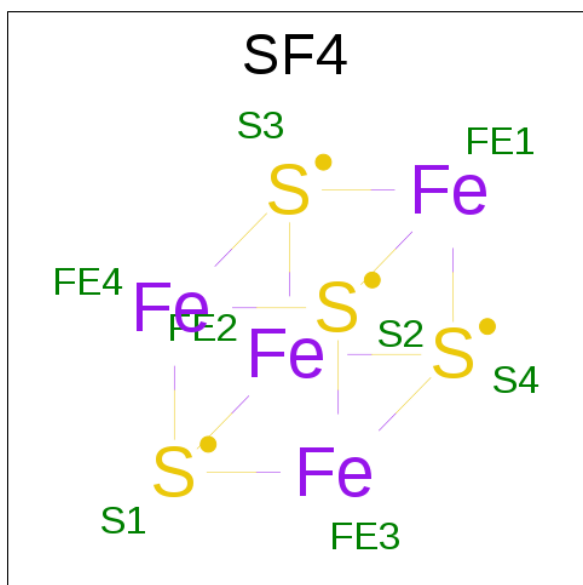
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1Y	1	Total Zn 1 1	0	0
57	14	1	Total Zn 1 1	0	0
57	1n	1	Total Zn 1 1	0	0
57	15	1	Total Zn 1 1	0	0
57	29	1	Total Zn 1 1	0	0
57	19	1	Total Zn 1 1	0	0
57	26	1	Total Zn 1 1	0	0
57	25	1	Total Zn 1 1	0	0
57	24	1	Total Zn 1 1	0	0
57	2n	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2Y	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

- 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	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

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

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

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

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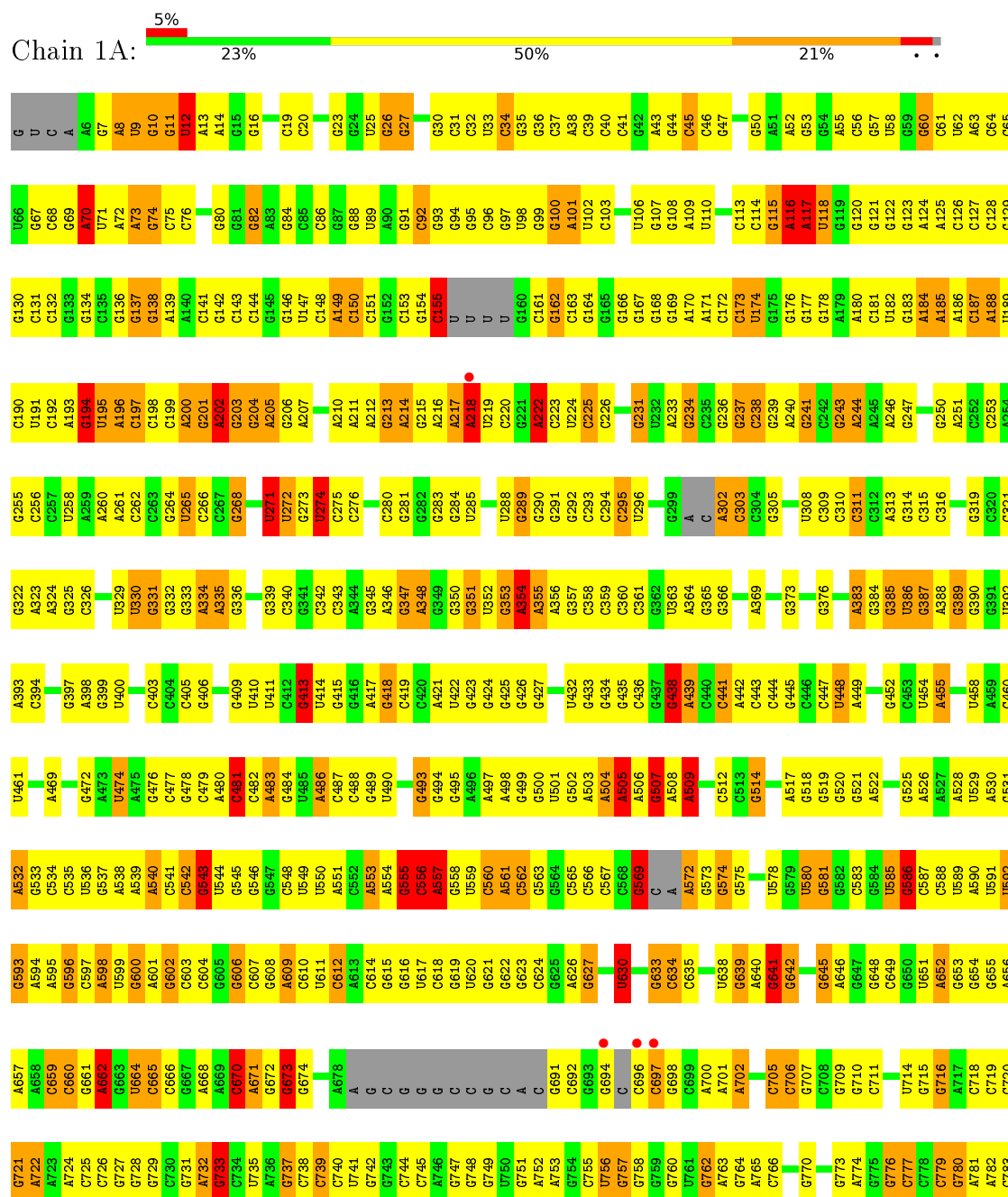
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2l	3	Total 3	O 3	0	0
59	2m	3	Total 3	O 3	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	1	Total 1	O 1	0	0
59	2t	1	Total 1	O 1	0	0

### 3 Residue-property plots

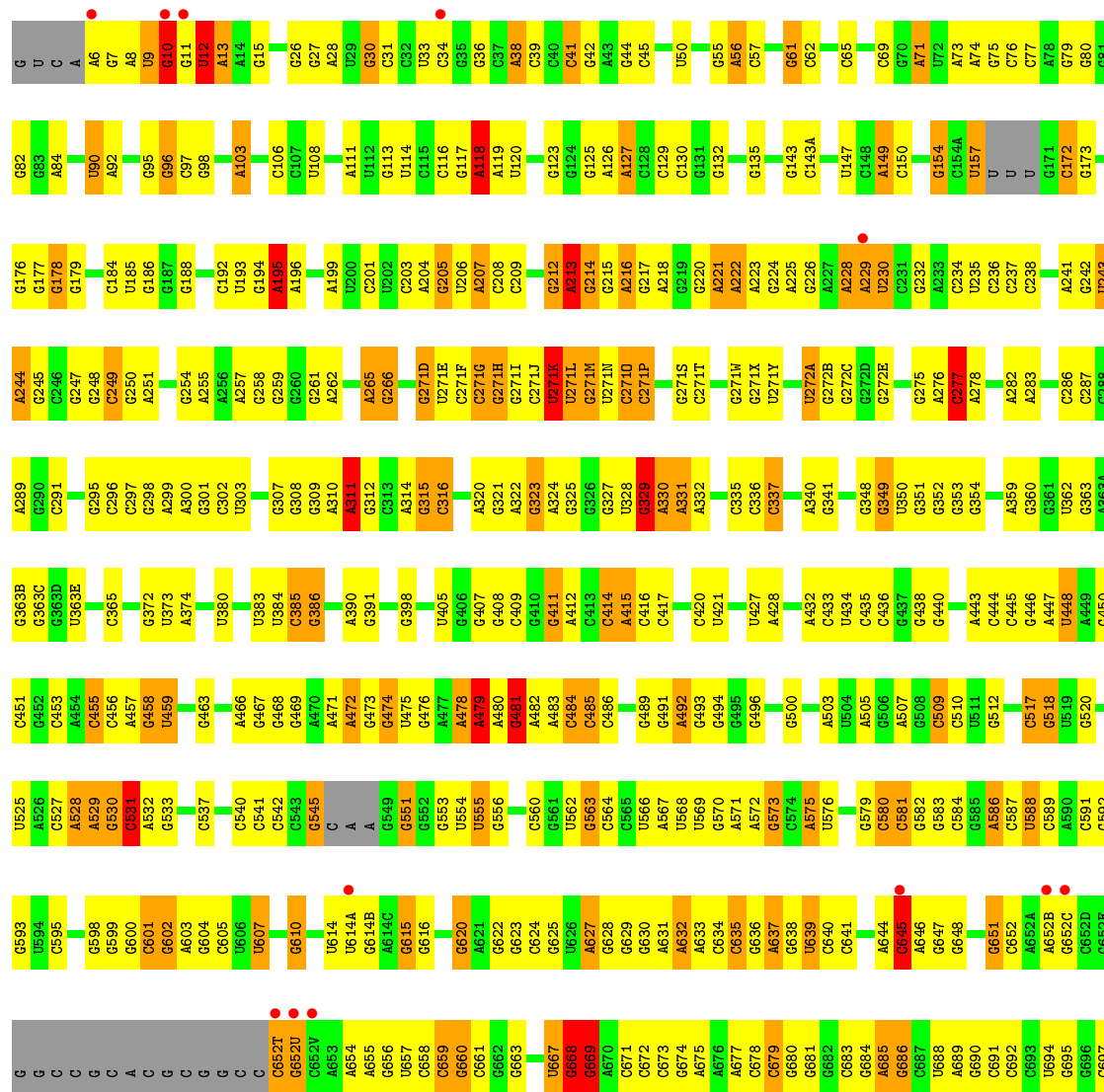
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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



G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	A1676	A1677	G1680	A1681	G1682	G1683	G1684	G1685	U1686	G1687	A1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	A1701	A1702	G1705	U1706	G1707	G1708	G1709	G1710	G1713	G1714	A1715	G1716	G1717	G1718	U1719	U1720	G1721	G1722	A1723	A1724	G1725	U1726	U1727	G1728	G1729					
G1607	G1608	A1609	G1610	G1611	G1612	A1613	A1614	G1615	A1616	A1617	A1618	A1619	G1620	G1621	G1622	G1623	G1624	U1625	A1626	A1627	G1628	G1629	G1630	G1631	A1632	G1633	G1634	G1635	U1636	G1637	G1638	U1639	A1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	U1648	A1649	G1650	G1651	G1652	G1653	A1654	U1655	A1656	G1657	G1658	A1659	G1660	G1661	A1662	G1663	A1664	G1665	G1666	U1667
A1541	A1542	U1543	C1544	G1545	G1546	C1547	C1548	U1549	C1552	A1553	A1554	C1555	A1556	A1557	G1558	C1559	U1560	A1561	G1562	G1563	U1566	G1567	G1568	G1569	A1570	G1571	G1572	U1573	G1574	G1575	G1576	G1577	G1578	G1579	G	U	A	C	G1584	G1585	G1586	A1589	G1592	A1593	C1594	G1597	G1598	G1599	A1600	C1603	G1604	A1605	G1606	U1607						
A1473	C1474	G1475	C1476	U1477	C1478	G1481	G1482	A1485	G1486	A1487	A1488	A1489	G1490	C1491	C1492	G1493	G1494	A1495	A1496	A1497	A1500	U1501	G1502	C1503	A1504	G1505	A1506	U1507	A1508	C1509	A1510	G1511	U1512	G1513	C1514	C1515	A1516	G1517	A1518	A1519	G1520	C1521	G1522	C1523	A1524	G1525	G1529	G1530	G1531	A1532	G1533	A1536	G1537	G1538	G1539	A1540				
C1408	C1409	G1410	A1411	G1412	A1413	G1414	G1415	G1416	G1417	U1418	A1419	G1420	C1421	C1422	G1423	A1424	A1425	G1426	G1427	G1428	G1429	A1430	G1431	C1432	C1433	U1434	U1439	U1440	A1441	U1442	U1443	G1444	C1445	G1446	G1447	C1450	U1451	U1452	C1453	C1454	G1455	G1456	C1457	U1461	C1462	C1463	G1464	A1465	U1466	G1467	U1470	G1471	G1472							
G1284	G1285	U1286	A1287	G1288	G1289	G1290	G1291	A1292	A1293	G1294	U1295	G1296	C1297	G1298	A1299	U1300	A1301	G1302	C1303	C1304	G1305	G1306	C1307	A1308	U1309	G1310	A1311	G1312	U1313	A1314	A1315	C1316	G1317	A1318	U1319	A1320	A1321	A1322	G1323	A1324	G1325	G1326	G1329	A1330	G1331	A1332	A1333	U1334	C1335	C1336	U1337	U1338	C1339	U1340	C1341	G1342	C1343	C1344		
G1217	G1218	A1219	U1220	G1221	A1222	C1223	C1224	G1228	G1229	G1230	G1231	G1232	U1233	A1234	G1235	A1236	G1237	U1238	A1239	G1242	U1243	U1244	G1245	G1246	C1247	A1255	C1256	G1257	A1258	G1261	C1262	C1263	G1264	C1265	C1266	C1267	C1268	G1269	C1270	G1271	A1272	G1273	G1274	G1277	G1278	C1279	U1280	G1281	C1282	A1283										
C1155	G1156	A1157	G1158	U1159	G1160	G1161	C1162	G1166	C1167	G1168	C1169	C1170	G1171	A1172	A1173	A1174	U1175	U1176	U1177	U1178	U1179	G1180	G1181	G1182	G1183	G1184	C1185	U1186	U1187	A1188	A1189	C1190	C1191	C1192	C1193	A1194	G1195	C1196	G1197	C1198	C1199	G1200	A1201	A1202	G1203	C1204	U1205	G1206	C1207	G1208	G1209	G1210	U1211	C1212	U1213	G1214	G1215	G1216		
C1095	A1096	G1097	A1098	C1099	A1100	G1101	C1102	A1103	G1104	G1105	U1106	U1107	G1108	C1109	U1110	U1111	U1112	A1113	G1114	A1115	A1116	G1117	C1118	G1119	G1120	C1121	C1122	G1123	U1124	C1125	C1126	U1127	U1128	C1129	A1130	A1131	C1132	G1133	A1134	G1135	U1136	G1137	C1138	G1139	U1140	A1141	A1142	U1143	A1144	C1145	C1146	U1147	C1148	A1149	C1150	U1151	G1152	U1154		
G1033	A1034	A1035	C1036	C1037	G1038	G1039	C1040	C1041	A1042	G1043	C1044	U1045	A1046	A1047	G1048	G1049	C1050	C1051	C1052	C1053	C1054	A1055	A1056	G1057	U1058	C1059	U1060	A1065	A1067	G1068	U1069	C1070	G1071	U1072	A1073	A1074	A1075	G1076	G1077	A1078	U1079	G1080	U1081	G1082	G1083	C1087	G1088	A1026	C1089	G1090	U1091	A1092	A1094							
G973	G974	U975	G976	G977	G978	G979	C981	C982	G983	G984	G985	G986	G987	G988	G989	G990	A991	G992	G993	G994	G995	G996	G997	A998	G999	C1000	U1001	A1002	U1003	C1004	A1005	U1006	G1007	U1008	C1009	C1010	G1011	C1012	G1013	C954	A955	A956	G1016	G1017	A1018	G1019	C1020	C961	G1022	G1023	G1024	G965	G1025	G966	A1027	C1028	A1029	A1030	C1032	
U907	A908	G909	A910	G911	G912	A913	C914	U915	G916	A917	U918	A919	G922	C923	U924	A925	G926	G927	C932	C933	A934	C935	C936	C872	U873	U874	U875	U876	A877	G878	G879	U880	C881	A882	G883	C884	U886	C887	A888	G889	G890	C958	G959	G962	A963	A964	G965	G966	G967	U968	C969	C970	G1083	A972						
G845	G846	A847	G848	A849	U850	A851	G852	C853	U854	G855	G856	U857	U858	C859	U860	C861	C864	G865	A866	A867	A868	U869	G870	A871	G872	U873	U874	U875	A876	G877	G878	G879	U880	C881	A882	G883	C884	U886	C887	A888	G889	G890	C958	G959	G962	A963	A964	G965	G966	G967	U968	C969	C970	G1083	A972					
G784	G785	G786	U787	G788	U789	G790	G791	G792	C793	U794	G795	G796	A797	A798	U799	C800	C801	C802	C803	U804	C805	C806	G807	A808	U809	G810	A811	G812	C813	U814	G815	G816	G817	G818	A821	G822	G823	A824	U825	U826	G827	A828	A829	A830	A831	G832	C833	U834	A835	A836	C837	C838	A839	G841	C842	C843	G906			

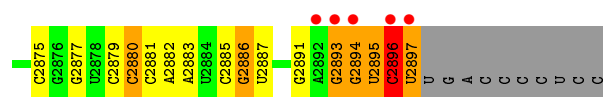




G1681	G1686	U1518	G1444	G1371	A1308	G1245	A	G109	C1049	A988	A910	C940	C772	C698
C1607	G1606	G1519	A1444	U1372	G1309	A1246	C1178	G1110	A1050	G889	A911	C943	U773	A699
A1608	A1609	G1525	C1445A	A1373	G1310	A1247	U1179	A1111	C1051	A990	C912	G843	A774	G700
A1610	G1687	G1528	A1448	G1375	G1311	G1248	C1180	G1112	C1052	G991	A917	C944	G775	G701
G1613	A1528A	A1528	G1450	C1376	U1312	U1249	C1181	U1113	A1053	G992	A918	G845	G776	G702
A1614	G1688	G1529	G1450A	G1377	U1316	C1251	A1183	G1115	C1055	G993	A919	G848	A777	U703
A1615	A1689	C1530	C1451	A1378	A1317	A1252	G1184	C1116	G1056	C994	G920	A849	U778	G704
C1616	G1691	C1531	A1452	G1380	G1318	A1253	C1185	G1117	A1057	A996	G921	A852	U779	A705
C1617	G1692	C1532	G1459	A1384	G1319	G1256	G1186	C1118	G1058	G998	G922	G853	G788	G706
A1618	U1693	G1533	A1460	A1385	C1320	C1257	G1191	C1123	U	U	G927	G854	G789	A707
G1623	G1696	U	A1461	G1386	A1321	C1258	U1198	G1124	G1062	A1001	G928	G855	G790	G713
G1626	G1697	C1536	G1467	C1387	A1322	G1259	U1199	G1125	G1063	G1002	G929	G857	G791	G717
G1627	A1698	G1537	C1467	G1388	G1324	C1261	C1200	A1126	U1065	C1004	G932	G858	G792	A718
G1628	G1699	G1539	G1470	A1392	C1327	A1262	C1201	A1127	U1066	C1005	G936	G859	G793	G729
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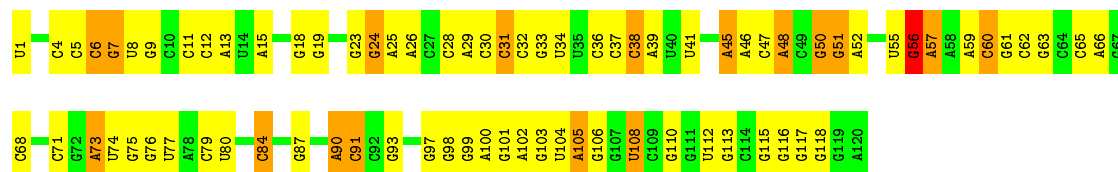


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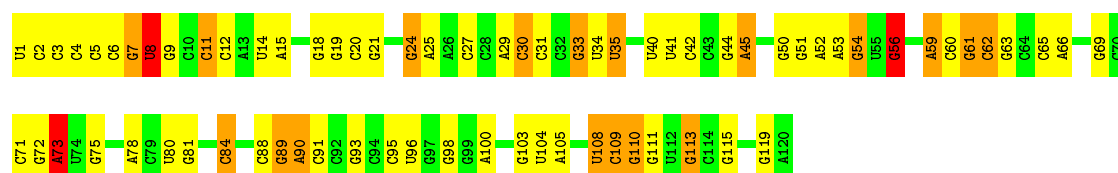
- Molecule 2: 5S ribosomal RNA

Chain 1B: 35% 50% 14%



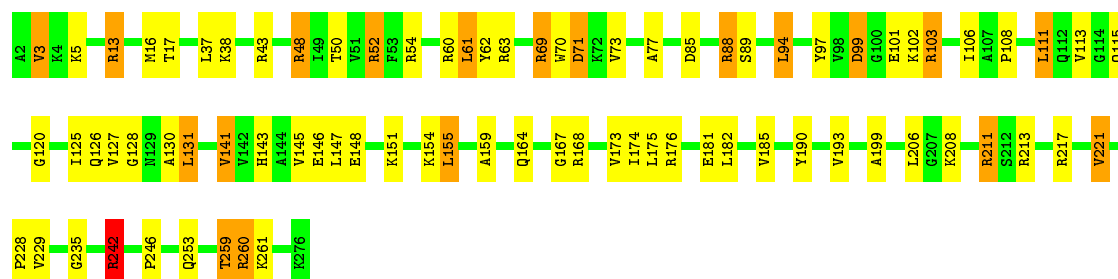
- Molecule 2: 5S ribosomal RNA

Chain 2B: 40% 43% 15%



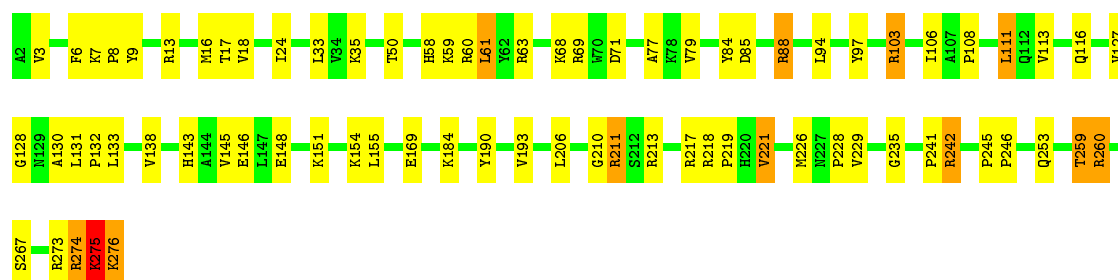
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 71% 22% 7%

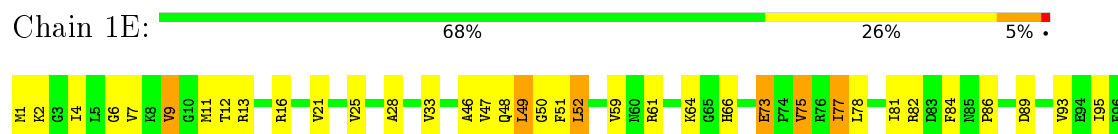


- Molecule 3: 50S ribosomal protein L2

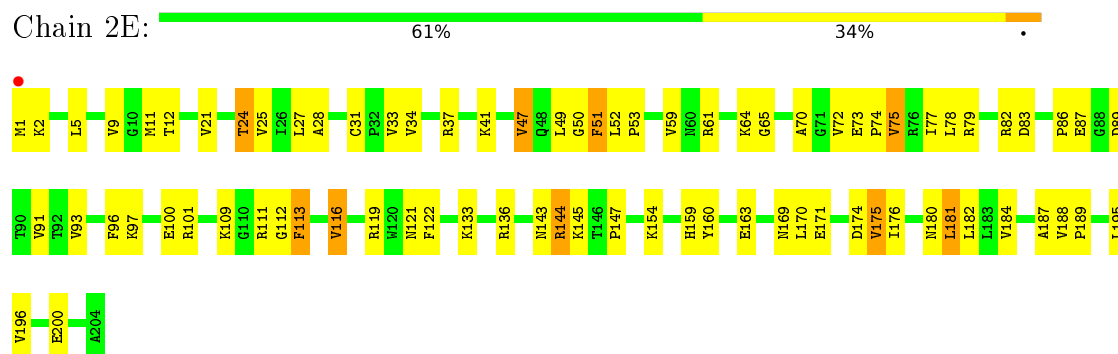
Chain 2D: 72% 23%



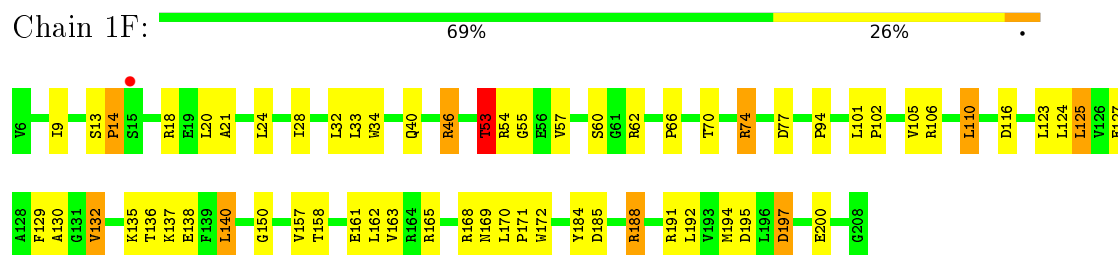
- Molecule 4: 50S ribosomal protein L3



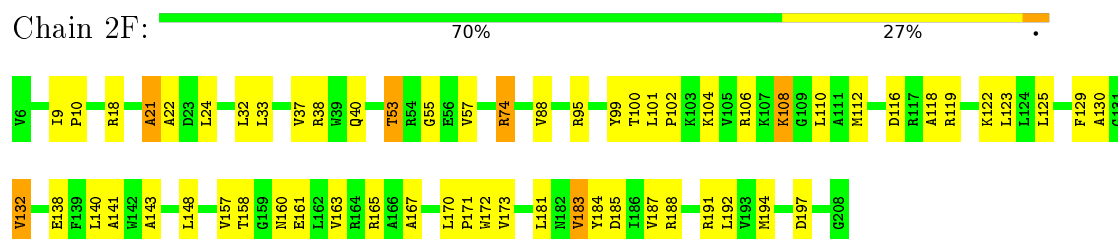
• Molecule 4: 50S ribosomal protein L3



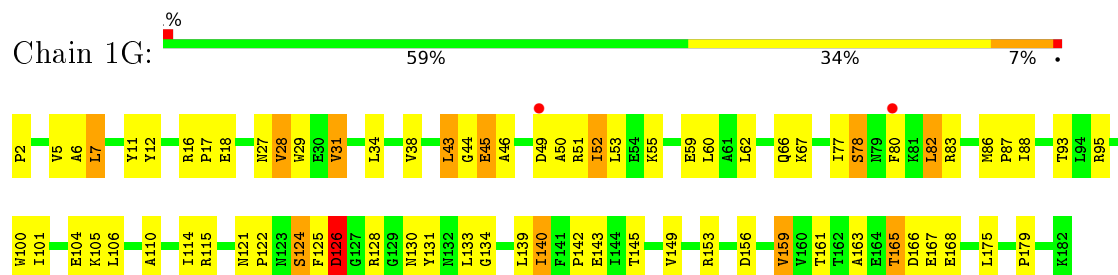
• Molecule 5: 50S ribosomal protein L4



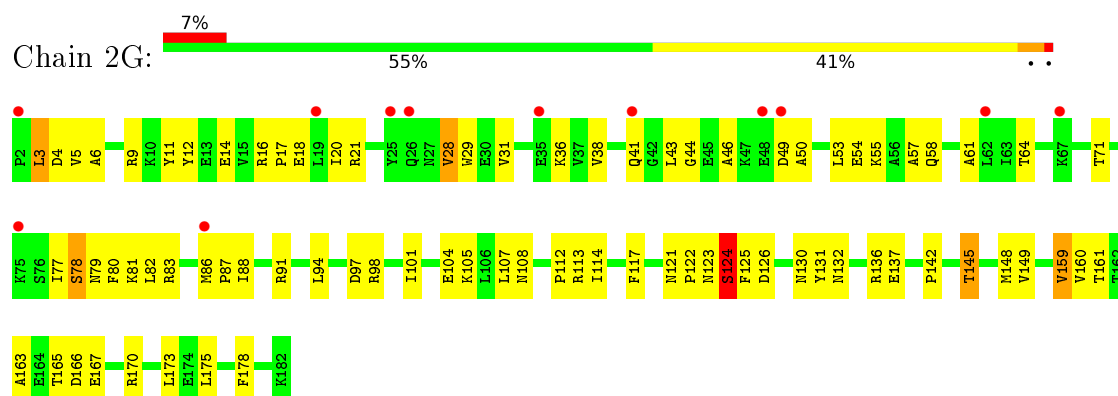
• Molecule 5: 50S ribosomal protein L4



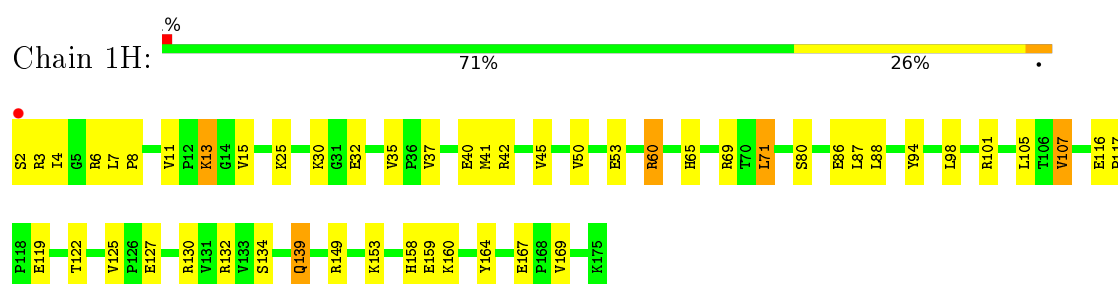
• Molecule 6: 50S ribosomal protein L5



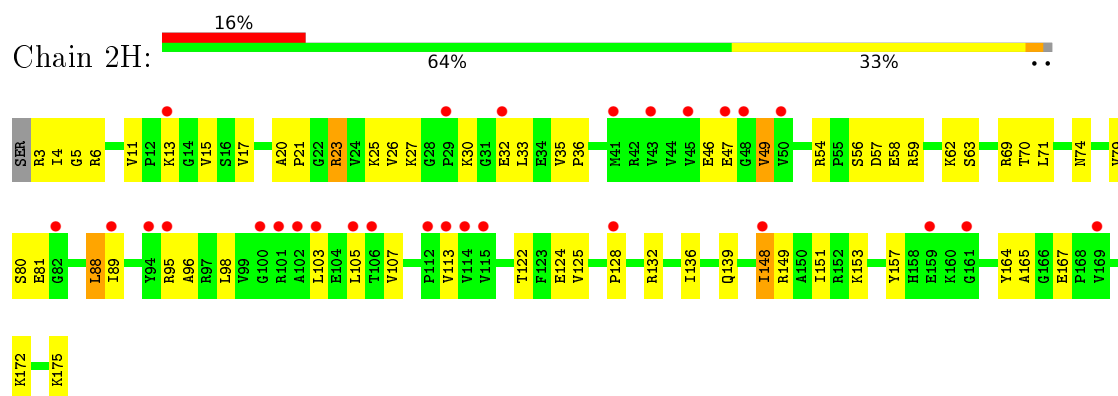
- Molecule 6: 50S ribosomal protein L5



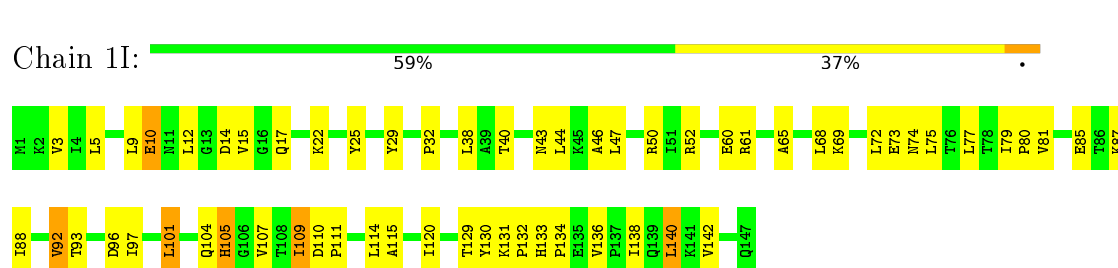
- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6

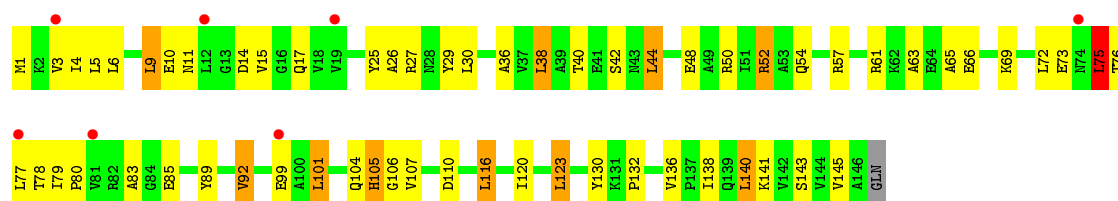


- Molecule 8: 50S ribosomal protein L9



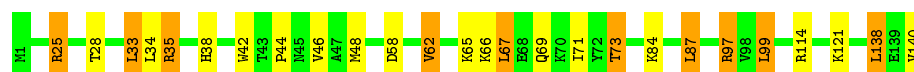
- Molecule 8: 50S ribosomal protein L9





• Molecule 9: 50S ribosomal protein L13

Chain 1N: 81% 11% 7%



• Molecule 9: 50S ribosomal protein L13

Chain 2N: 74% 22% .



• Molecule 10: 50S ribosomal protein L14

Chain 1O: 75% 20% .



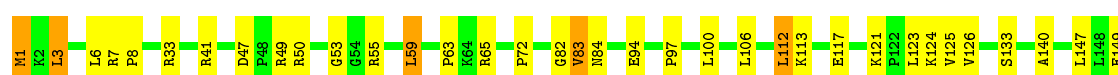
• Molecule 10: 50S ribosomal protein L14

Chain 2O: 72% 28%



• Molecule 11: 50S ribosomal protein L15

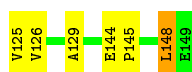
Chain 1P: 77% 20% .



• Molecule 11: 50S ribosomal protein L15

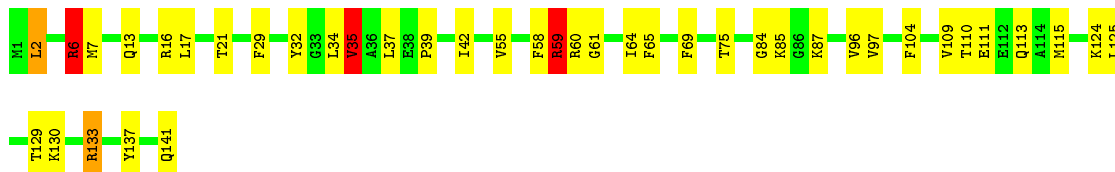
Chain 2P: 74% 22% .





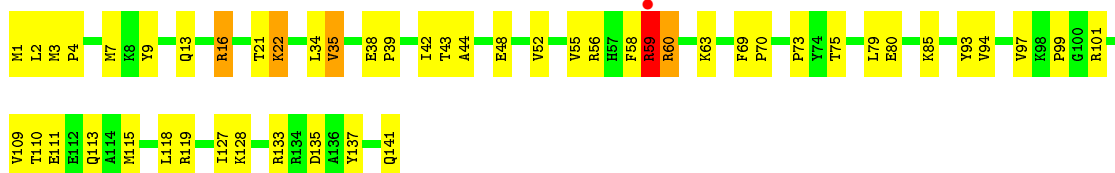
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 71% 26% ..



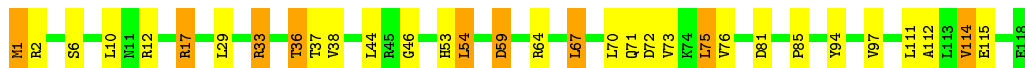
- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 65% 32% ..



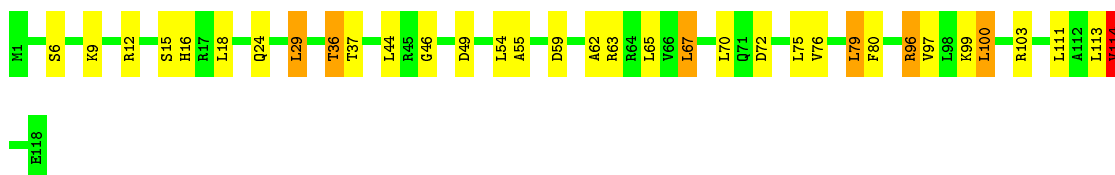
- Molecule 13: 50S ribosomal protein L17

Chain 1R: 73% 19% 8%



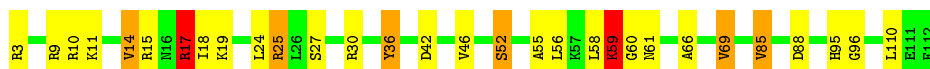
- Molecule 13: 50S ribosomal protein L17

Chain 2R: 71% 23% 5%



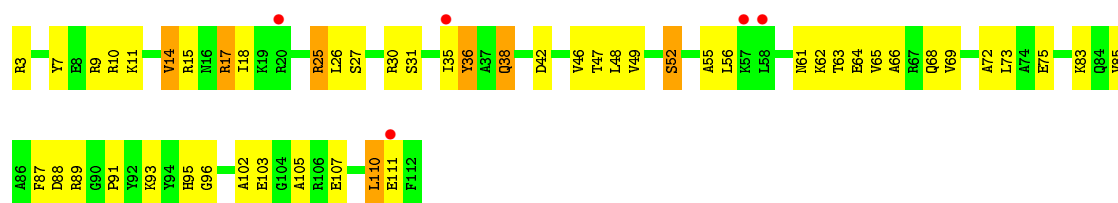
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 73% 20% 5%

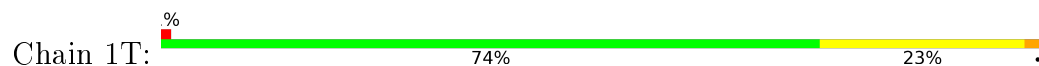


- Molecule 14: 50S ribosomal protein L18

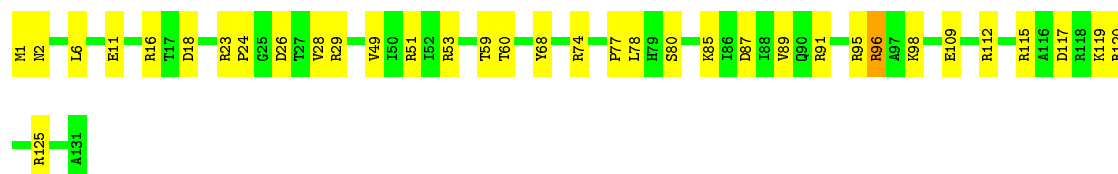
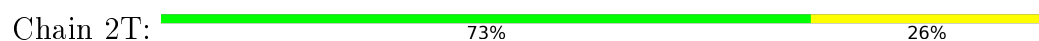
Chain 2S: 54% 40% 6%



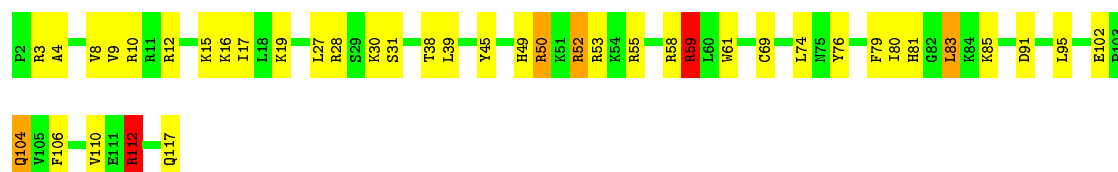
- Molecule 15: 50S ribosomal protein L19



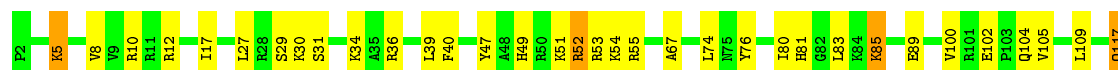
- Molecule 15: 50S ribosomal protein L19



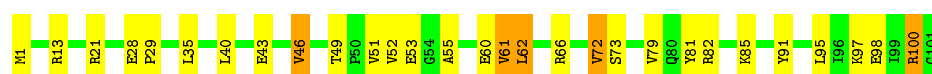
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

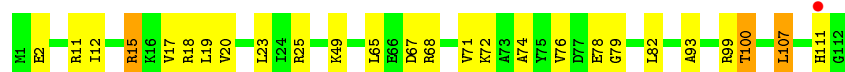
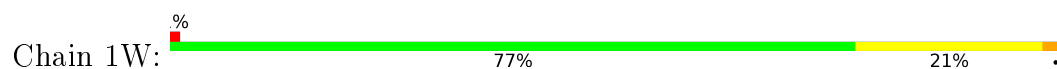


- Molecule 17: 50S ribosomal protein L21

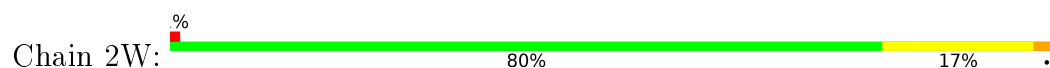




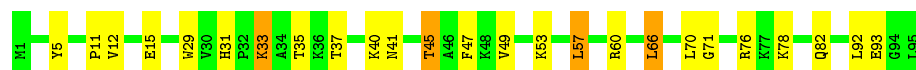
- Molecule 18: 50S ribosomal protein L22



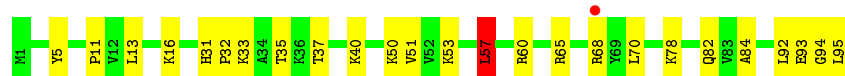
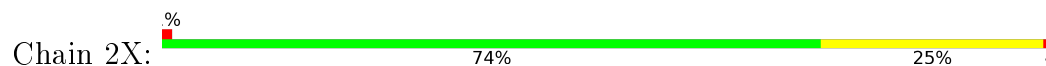
- Molecule 18: 50S ribosomal protein L22



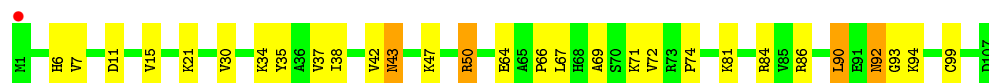
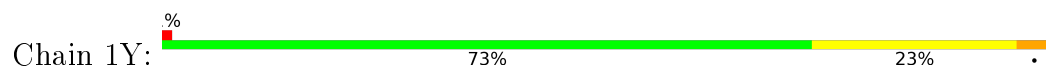
- Molecule 19: 50S ribosomal protein L23



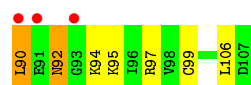
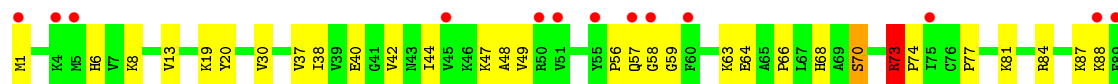
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

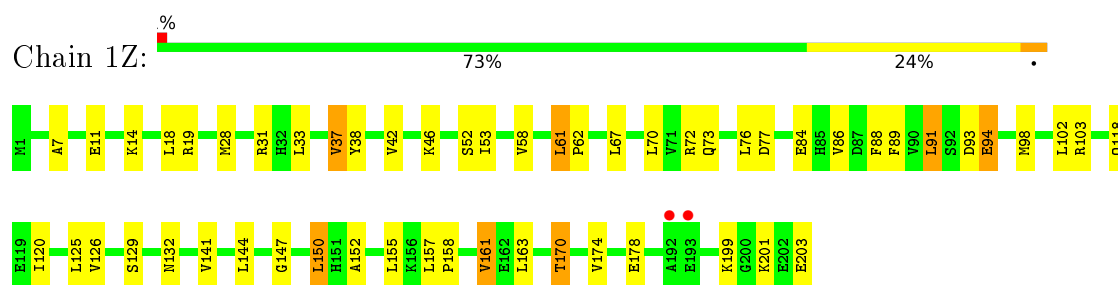


- Molecule 20: 50S ribosomal protein L24

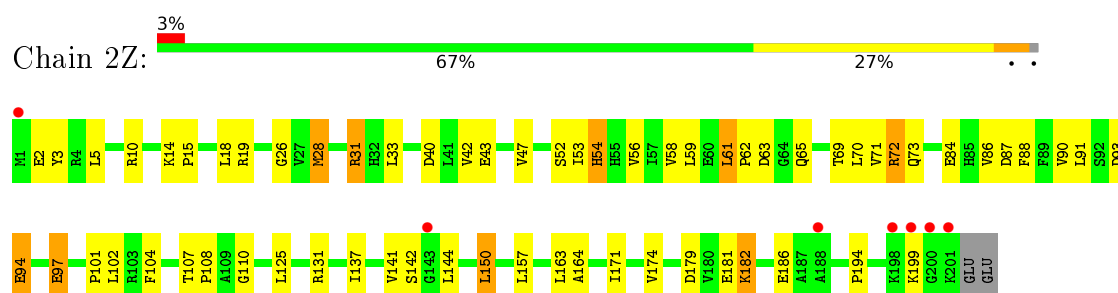


- Molecule 21: 50S ribosomal protein L25

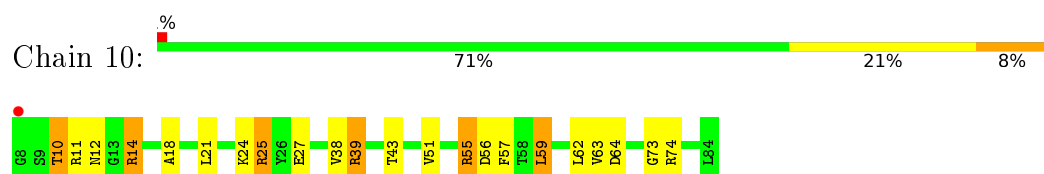




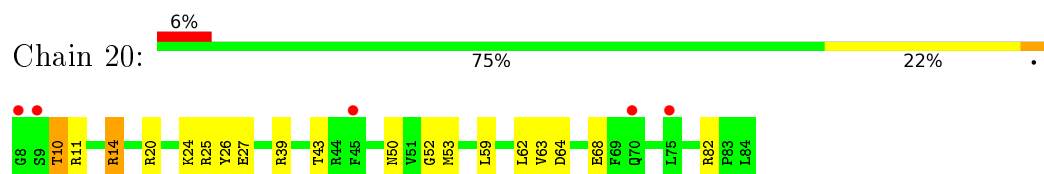
- Molecule 21: 50S ribosomal protein L25



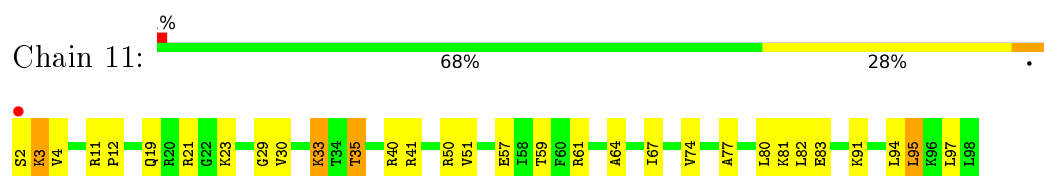
- Molecule 22: 50S ribosomal protein L27



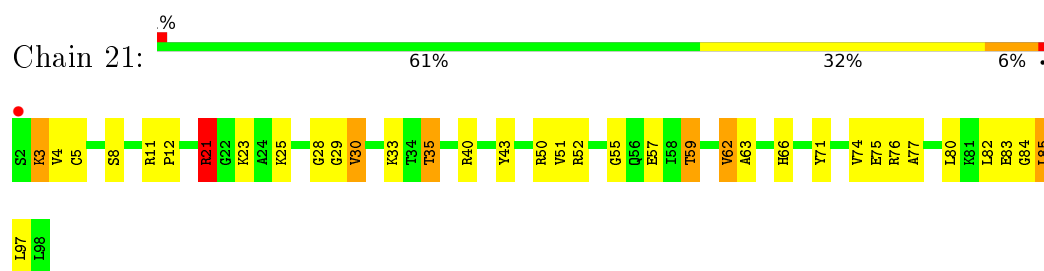
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28




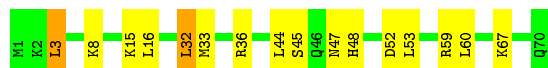
- Molecule 24: 50S ribosomal protein L29

Chain 12:  70% 29% .




- Molecule 24: 50S ribosomal protein L29

Chain 22:  77% 20% .



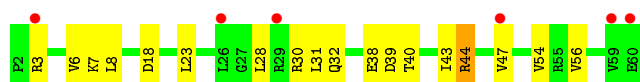
- Molecule 25: 50S ribosomal protein L30

Chain 13:  76% 22% .



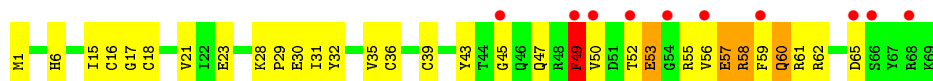
- Molecule 25: 50S ribosomal protein L30

Chain 23:  10% 69% 29% .




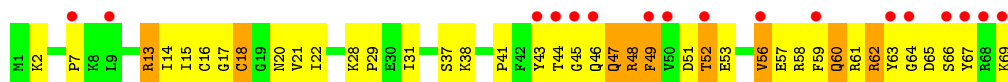
- Molecule 26: 50S ribosomal protein L31

Chain 14:  14% 54% 39% 6% .



- Molecule 26: 50S ribosomal protein L31

Chain 24:  25% 42% 45% 13% .



- Molecule 27: 50S ribosomal protein L32

Chain 15:  69% 17% 10% .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  73% 20% 7%



- Molecule 28: 50S ribosomal protein L33

Chain 16:  66% 26% 8%




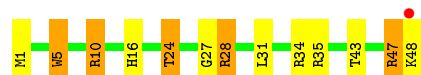
- Molecule 28: 50S ribosomal protein L33

Chain 26:  68% 25% 8%




- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 73% 17% 10%



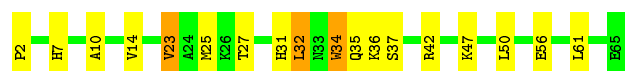
- Molecule 29: 50S ribosomal protein L34

Chain 27:  79% 19% 2%



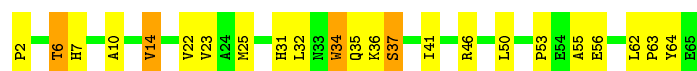
- Molecule 30: 50S ribosomal protein L35

Chain 18:  72% 23% 5%



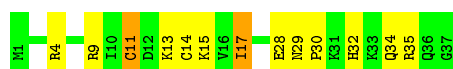
- Molecule 30: 50S ribosomal protein L35

Chain 28:  64% 30% 6%



- Molecule 31: 50S ribosomal protein L36

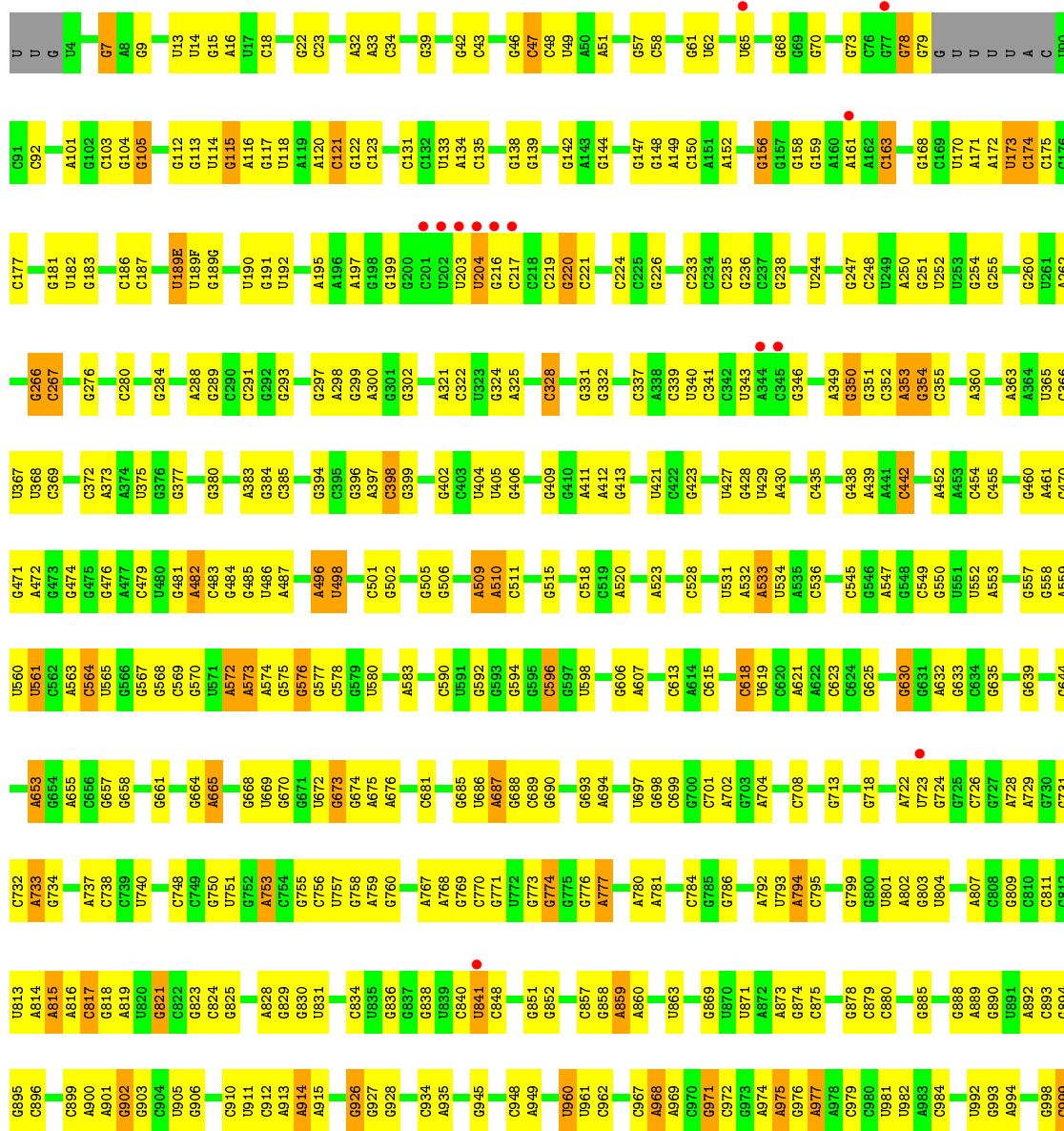
Chain 19:  65% 30% 5%

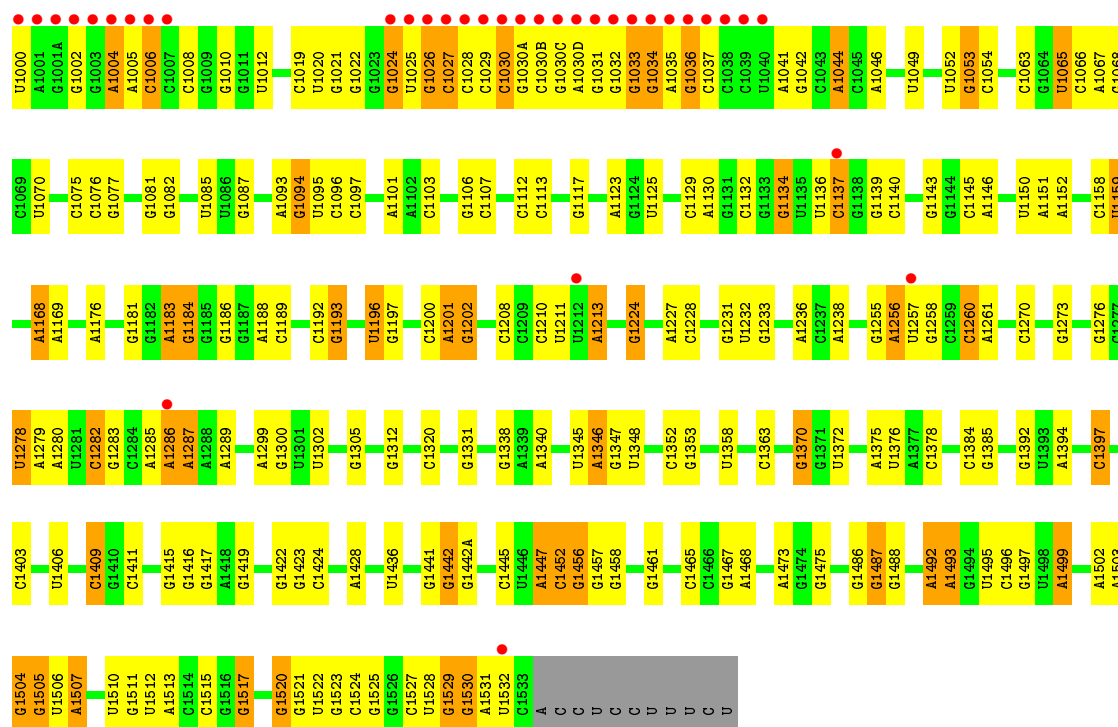


- Molecule 31: 50S ribosomal protein L36

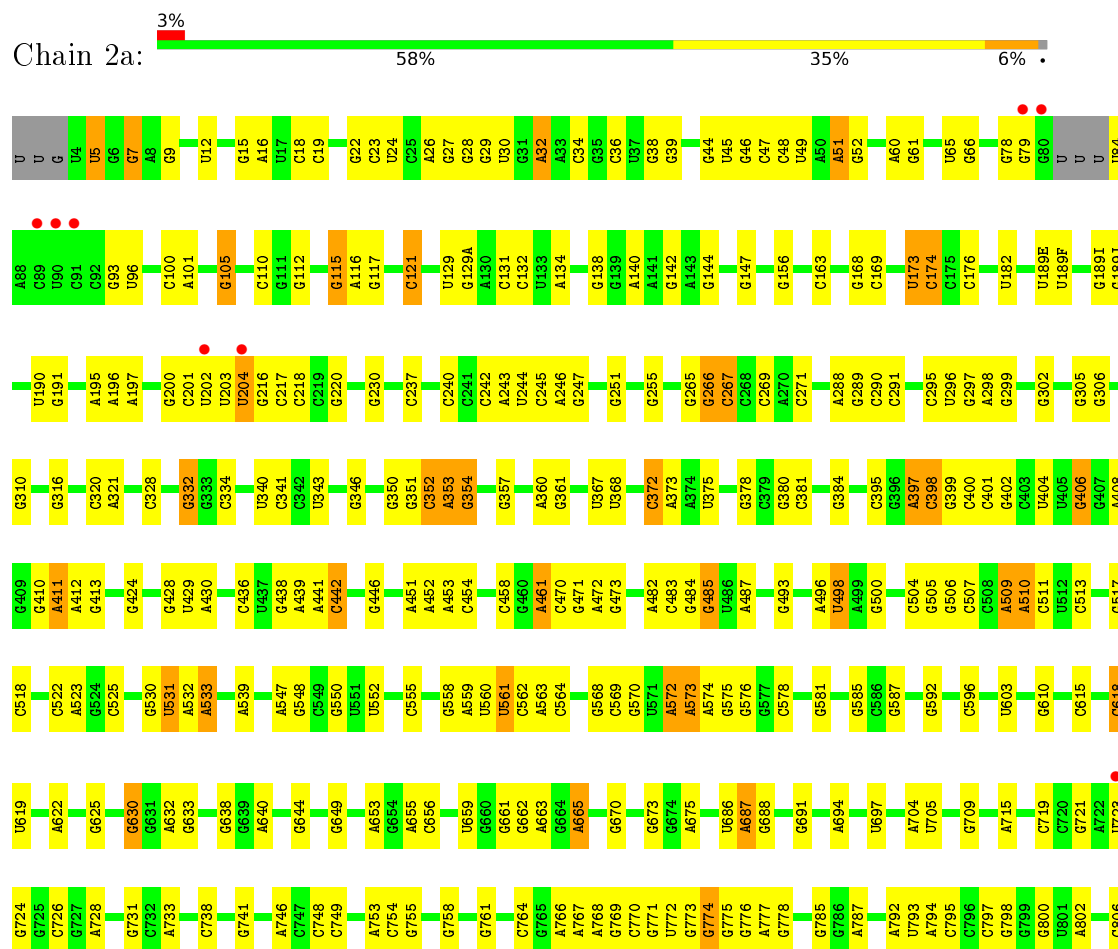


- Molecule 32: 16S ribosomal RNA

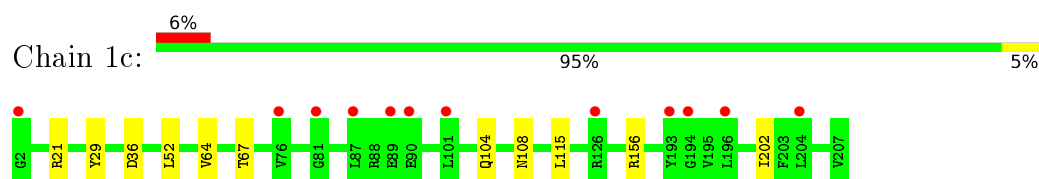




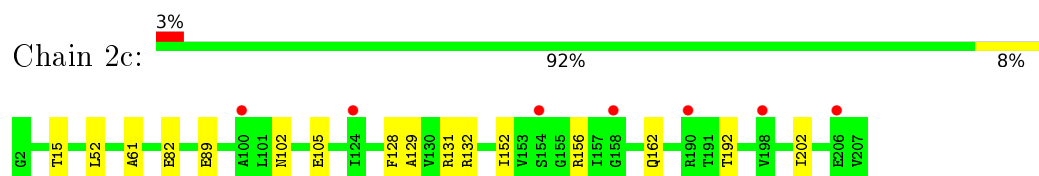
### • Molecule 32: 16S ribosomal RNA



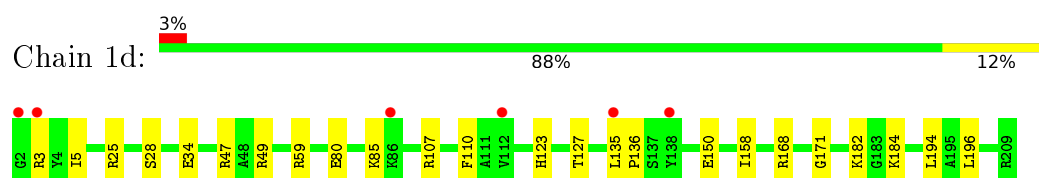




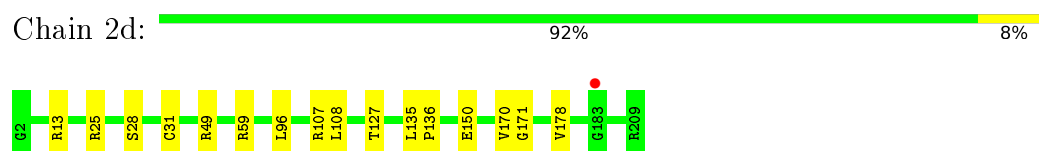
- Molecule 34: 30S ribosomal protein S3



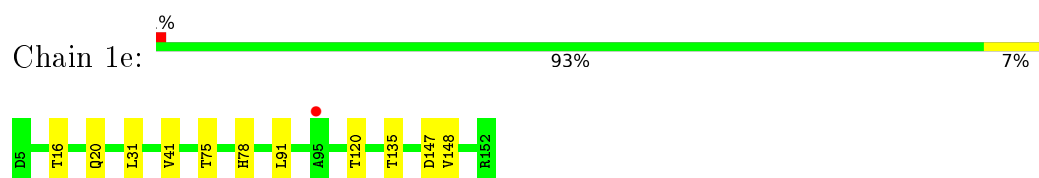
- Molecule 35: 30S ribosomal protein S4



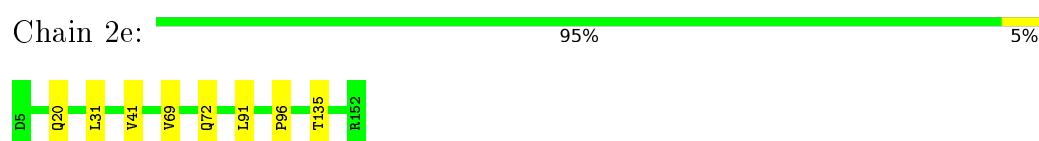
- Molecule 35: 30S ribosomal protein S4



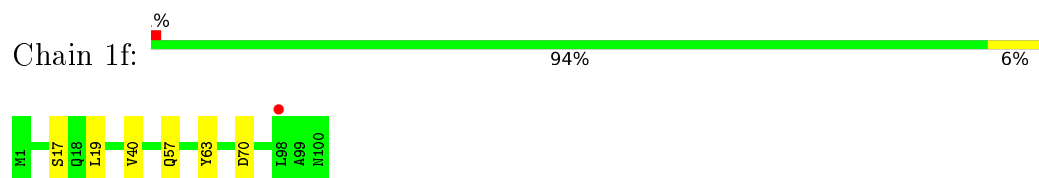
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



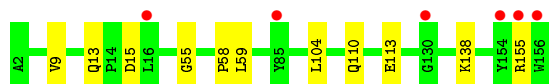
- Molecule 37: 30S ribosomal protein S6

Chain 2f:  96% .



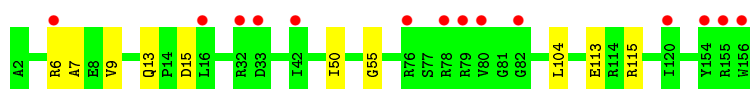
- Molecule 38: 30S ribosomal protein S7

Chain 1g:  4% 93% 7%



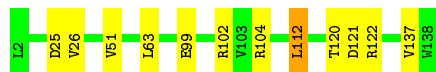
- Molecule 38: 30S ribosomal protein S7

Chain 2g:  9% 94% 6%



- Molecule 39: 30S ribosomal protein S8

Chain 1h:  91% 8% .




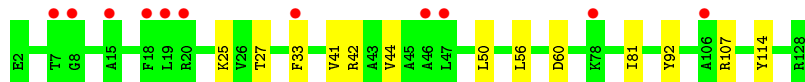
- Molecule 39: 30S ribosomal protein S8

Chain 2h:  % 94% 6%




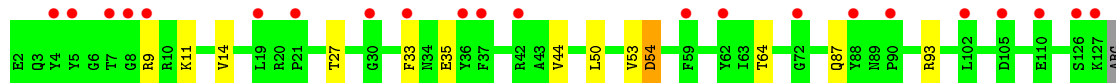
- Molecule 40: 30S ribosomal protein S9

Chain 1i:  9% 90% 10%



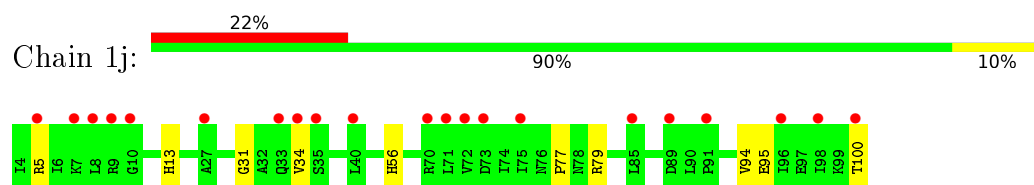
- Molecule 40: 30S ribosomal protein S9

Chain 2i:  17% 89% 9% ..

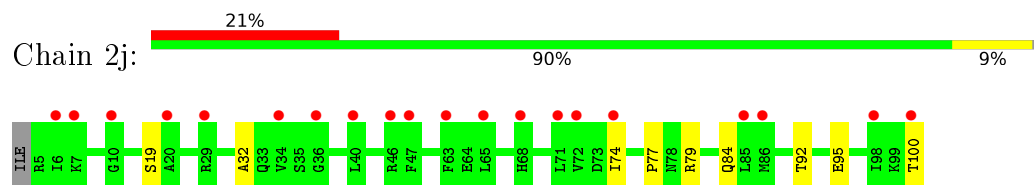


- Molecule 41: 30S ribosomal protein S10

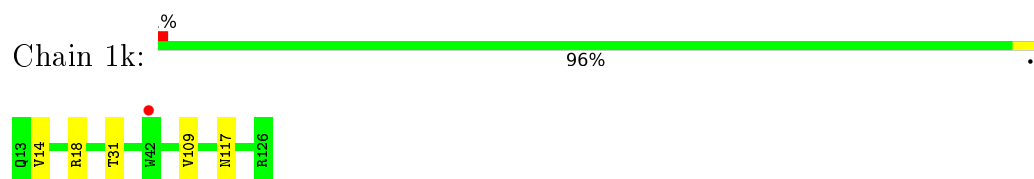




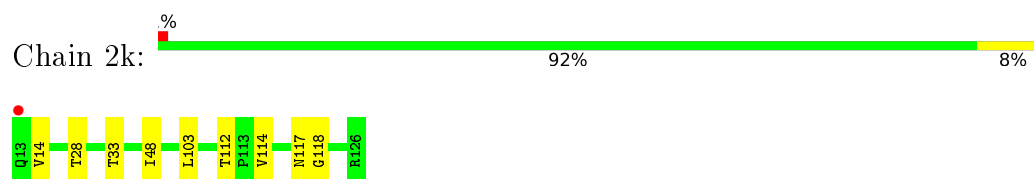
- Molecule 41: 30S ribosomal protein S10



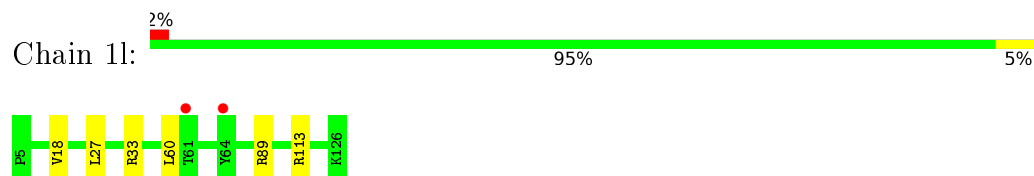
- Molecule 42: 30S ribosomal protein S11



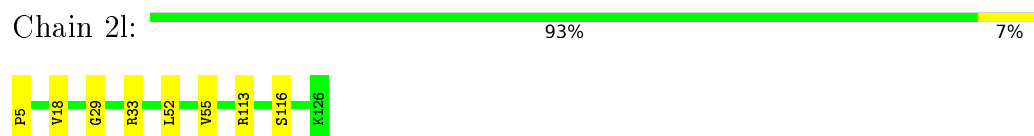
- Molecule 42: 30S ribosomal protein S11



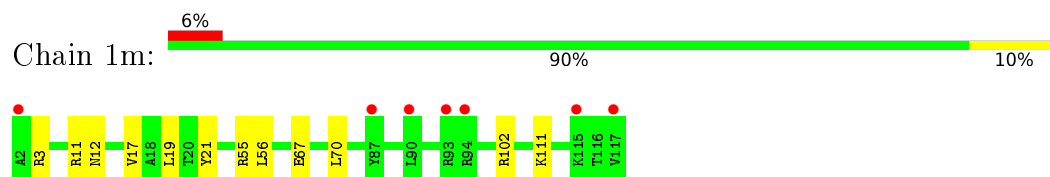
- Molecule 43: 30S ribosomal protein S12



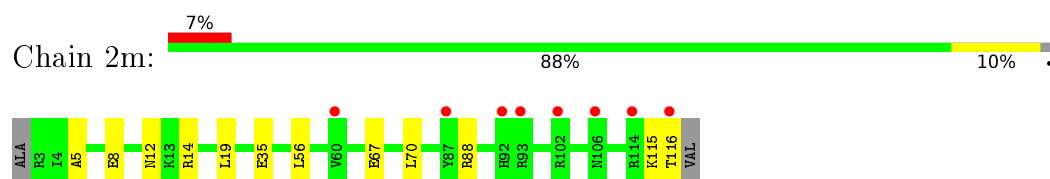
- Molecule 43: 30S ribosomal protein S12



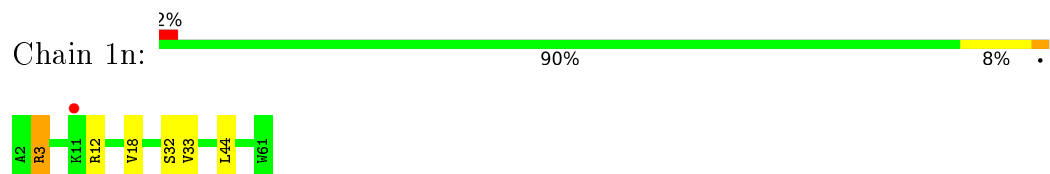
- Molecule 44: 30S ribosomal protein S13



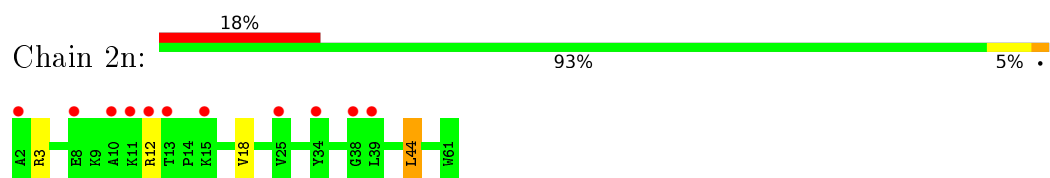
- Molecule 44: 30S ribosomal protein S13



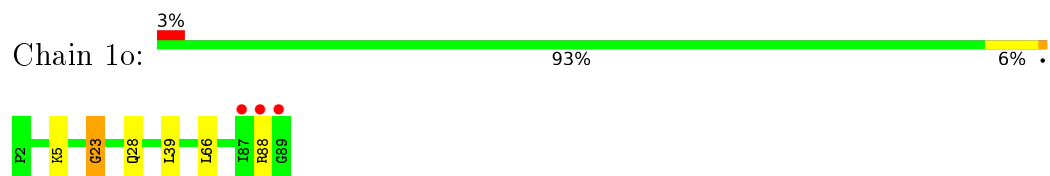
- Molecule 45: 30S ribosomal protein S14 type Z



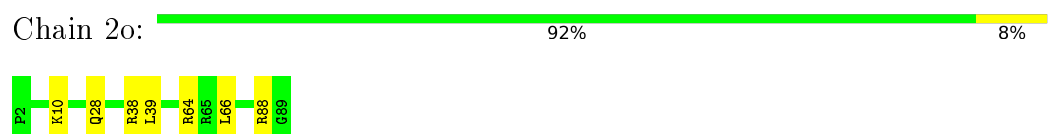
- Molecule 45: 30S ribosomal protein S14 type Z



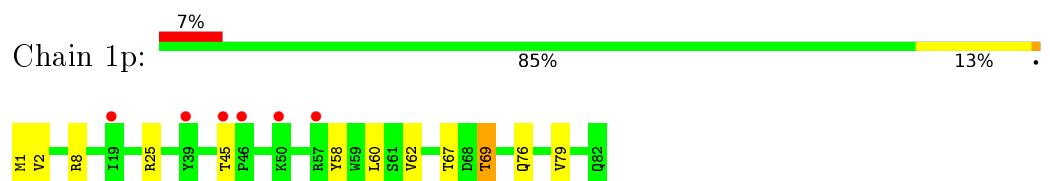
- Molecule 46: 30S ribosomal protein S15



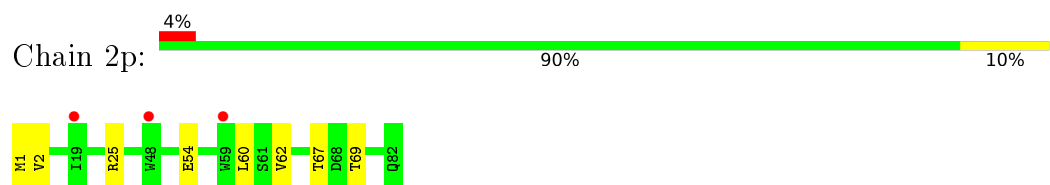
- Molecule 46: 30S ribosomal protein S15



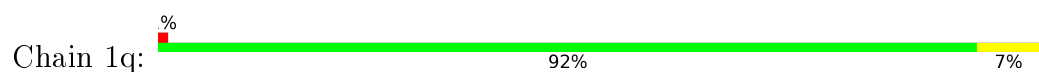
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



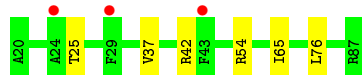
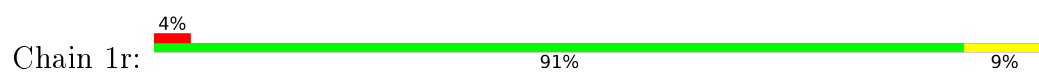
- Molecule 48: 30S ribosomal protein S17



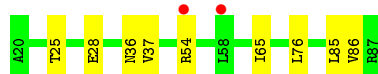
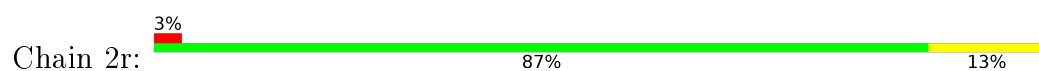
- Molecule 48: 30S ribosomal protein S17



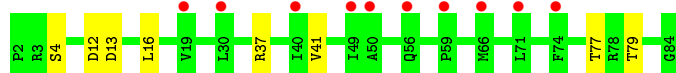
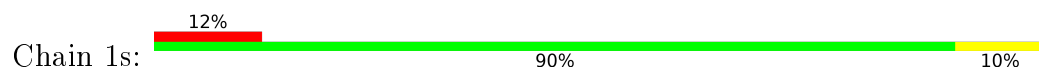
- Molecule 49: 30S ribosomal protein S18



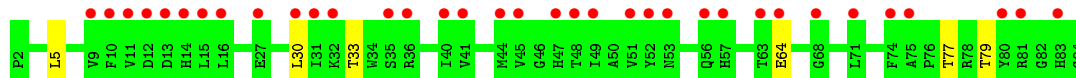
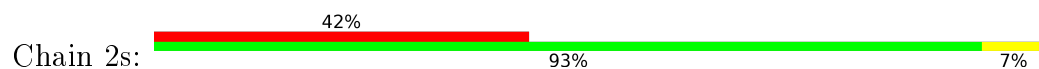
- Molecule 49: 30S ribosomal protein S18



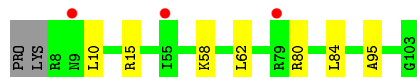
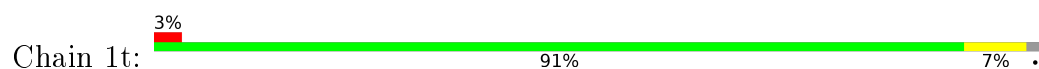
- Molecule 50: 30S ribosomal protein S19



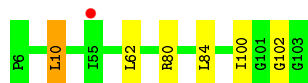
- Molecule 50: 30S ribosomal protein S19



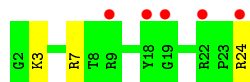
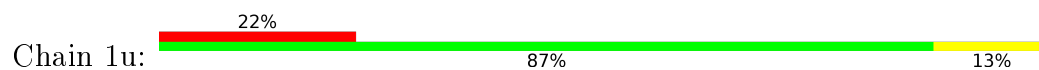
- Molecule 51: 30S ribosomal protein S20



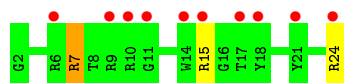
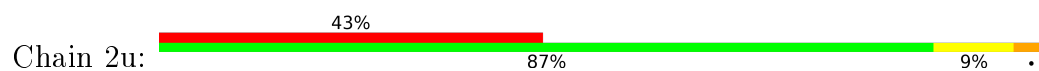
- Molecule 51: 30S ribosomal protein S20



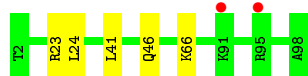
- Molecule 52: 30S ribosomal protein Thx



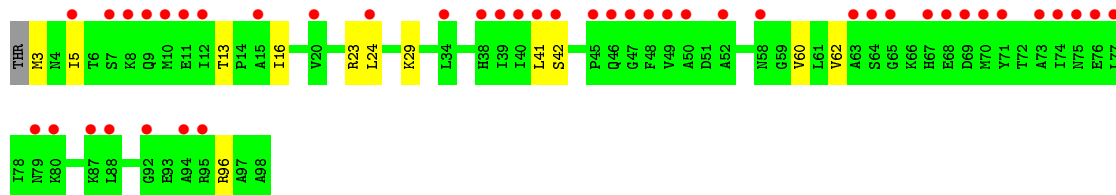
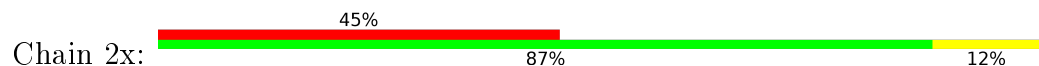
- Molecule 52: 30S ribosomal protein Thx



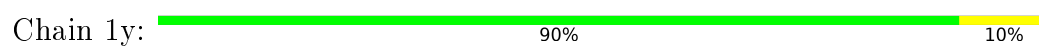
- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 54: Metalnikowin I



- Molecule 54: Metalnikowin I



## 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)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.183 , 0.234 0.201 , 0.245	Depositor DCC
$R_{free}$ test set	69999 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 1427008 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	293484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61862	0	31140	704	0
1	2A	61751	0	31143	819	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1B	2575	0	1304	26	0
2	2B	2571	0	1308	40	0
3	1D	2131	0	2207	63	0
3	2D	2136	0	2218	59	0
4	1E	1559	0	1618	44	0
4	2E	1559	0	1618	54	0
5	1F	1584	0	1625	39	0
5	2F	1574	0	1608	42	0
6	1G	1426	0	1445	55	0
6	2G	1424	0	1441	63	0
7	1H	1330	0	1407	30	0
7	2H	1324	0	1402	35	0
8	1I	1094	0	1127	44	0
8	2I	1076	0	1094	51	0
9	1N	1121	0	1195	18	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	19	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	30	0
12	1Q	1122	0	1179	29	0
12	2Q	1122	0	1179	40	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	21	0
14	1S	877	0	938	28	0
14	2S	870	0	923	40	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	30	0
16	1U	959	0	1019	26	0
16	2U	959	0	1019	32	0
17	1V	775	0	841	14	0
17	2V	771	0	830	19	0
18	1W	880	0	929	12	0
18	2W	877	0	927	15	0
19	1X	750	0	814	27	0
19	2X	750	0	814	22	0
20	1Y	810	0	892	23	0
20	2Y	810	0	887	24	0
21	1Z	1587	0	1598	31	0
21	2Z	1557	0	1564	46	0
22	10	608	0	622	24	0
22	20	608	0	622	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	11	754	0	823	24	0
23	21	759	0	837	31	0
24	12	588	0	643	13	0
24	22	592	0	654	10	0
25	13	469	0	518	10	0
25	23	464	0	514	11	0
26	14	546	0	522	19	0
26	24	536	0	514	32	0
27	15	459	0	476	18	0
27	25	455	0	465	16	0
28	16	453	0	473	10	0
28	26	449	0	469	11	0
29	17	418	0	467	15	0
29	27	418	0	467	9	0
30	18	517	0	582	11	0
30	28	517	0	582	17	0
31	19	307	0	335	11	0
31	29	307	0	335	9	0
32	1a	32246	0	16296	0	0
32	2a	32331	0	16339	0	0
33	1b	1842	0	1862	0	0
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0
34	2c	1542	0	1517	0	0
35	1d	1665	0	1687	0	0
35	2d	1668	0	1703	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	986	0	990	0	0
40	2i	966	0	953	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1m	914	0	954	0	0
44	2m	895	0	920	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	648	0	658	0	0
50	2s	645	0	635	0	0
51	1t	732	0	809	0	0
51	2t	733	0	795	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1x	764	0	786	0	0
53	2x	749	0	757	0	0
54	1y	87	0	88	0	0
54	2y	87	0	88	0	0
55	10	8	0	0	0	0
55	11	3	0	0	0	0
55	13	2	0	0	0	0
55	15	6	0	0	0	0
55	17	5	0	0	0	0
55	18	3	0	0	0	0
55	19	2	0	0	0	0
55	1A	917	0	0	0	0
55	1B	24	0	0	0	0
55	1D	18	0	0	0	0
55	1E	8	0	0	0	0
55	1F	16	0	0	0	0
55	1G	3	0	0	0	0
55	1H	2	0	0	0	0
55	1N	3	0	0	0	0
55	1P	4	0	0	0	0
55	1Q	5	0	0	0	0
55	1R	5	0	0	0	0
55	1S	1	0	0	0	0
55	1T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	1U	7	0	0	0	0
55	1V	3	0	0	0	0
55	1W	3	0	0	0	0
55	1X	1	0	0	0	0
55	1Y	1	0	0	0	0
55	1a	223	0	0	0	0
55	1b	1	0	0	0	0
55	1d	5	0	0	0	0
55	1e	2	0	0	0	0
55	1f	1	0	0	0	0
55	1g	1	0	0	0	0
55	1h	2	0	0	0	0
55	1k	1	0	0	0	0
55	1l	1	0	0	0	0
55	1m	1	0	0	0	0
55	1n	1	0	0	0	0
55	1o	1	0	0	0	0
55	1t	1	0	0	0	0
55	20	6	0	0	0	0
55	21	2	0	0	0	0
55	23	1	0	0	0	0
55	25	3	0	0	0	0
55	27	4	0	0	0	0
55	28	3	0	0	0	0
55	2A	821	0	0	0	0
55	2B	18	0	0	0	0
55	2D	11	0	0	0	0
55	2E	7	0	0	0	0
55	2F	10	0	0	0	0
55	2G	3	0	0	0	0
55	2H	1	0	0	0	0
55	2N	1	0	0	0	0
55	2P	2	0	0	0	0
55	2Q	5	0	0	0	0
55	2R	3	0	0	0	0
55	2S	1	0	0	0	0
55	2T	1	0	0	0	0
55	2U	4	0	0	0	0
55	2V	5	0	0	0	0
55	2W	1	0	0	0	0
55	2X	3	0	0	0	0
55	2a	196	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	2b	1	0	0	0	0
55	2d	4	0	0	0	0
55	2e	2	0	0	0	0
55	2f	1	0	0	0	0
55	2g	1	0	0	0	0
55	2h	1	0	0	0	0
55	2l	1	0	0	0	0
55	2m	1	0	0	0	0
55	2n	2	0	0	0	0
55	2o	1	0	0	0	0
56	1B	1	0	0	5	0
56	2A	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	4	0	0	0	0
59	11	2	0	0	0	0
59	13	1	0	0	0	0
59	15	2	0	0	0	0
59	16	3	0	0	0	0
59	17	1	0	0	0	0
59	18	7	0	0	0	0
59	19	2	0	0	0	0
59	1A	1740	0	0	5	0
59	1B	42	0	0	0	0
59	1D	14	0	0	0	0
59	1E	18	0	0	0	0
59	1F	11	0	0	0	0
59	1G	2	0	0	0	0
59	1H	3	0	0	0	0
59	1N	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1P	13	0	0	0	0
59	1Q	5	0	0	0	0
59	1R	3	0	0	0	0
59	1T	5	0	0	0	0
59	1U	6	0	0	1	0
59	1V	4	0	0	0	0
59	1W	2	0	0	0	0
59	1X	1	0	0	0	0
59	1Y	5	0	0	1	0
59	1a	393	0	0	0	0
59	1d	10	0	0	0	0
59	1e	3	0	0	0	0
59	1f	1	0	0	0	0
59	1h	1	0	0	0	0
59	1j	1	0	0	0	0
59	1l	3	0	0	0	0
59	1m	2	0	0	0	0
59	1n	1	0	0	0	0
59	1o	1	0	0	0	0
59	1t	2	0	0	0	0
59	20	6	0	0	0	0
59	21	3	0	0	0	0
59	23	1	0	0	0	0
59	25	2	0	0	0	0
59	26	2	0	0	0	0
59	27	1	0	0	0	0
59	28	5	0	0	0	0
59	29	1	0	0	0	0
59	2A	1666	0	0	8	0
59	2B	35	0	0	1	0
59	2D	12	0	0	0	0
59	2E	17	0	0	1	0
59	2F	11	0	0	0	0
59	2G	2	0	0	0	0
59	2H	3	0	0	2	0
59	2N	1	0	0	0	0
59	2P	9	0	0	0	0
59	2Q	5	0	0	0	0
59	2R	3	0	0	0	0
59	2T	3	0	0	0	0
59	2U	2	0	0	1	0
59	2V	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2W	2	0	0	0	0
59	2X	6	0	0	0	0
59	2Y	3	0	0	0	0
59	2a	384	0	0	0	0
59	2c	1	0	0	0	0
59	2d	7	0	0	0	0
59	2e	4	0	0	0	0
59	2f	1	0	0	0	0
59	2h	1	0	0	0	0
59	2j	1	0	0	0	0
59	2l	3	0	0	0	0
59	2m	3	0	0	0	0
59	2o	1	0	0	0	0
59	2p	1	0	0	0	0
59	2t	1	0	0	0	0
All	All	293484	0	194466	2745	0

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

The worst 5 of 2745 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2552:OMU:C4	1:2A:2552:OMU:C5	1.75	1.57
1:1A:1405:A:N6	1:1A:1418:U:H3	1.21	1.38
1:1A:9:U:N3	1:1A:2641:A:H2	1.35	1.19
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.05	1.12
1:1A:1405:A:N1	1:1A:1418:U:O4	1.84	1.10

There are no symmetry-related clashes.

## 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%)	34	71
4	2E	202/204 (99%)	191 (95%)	10 (5%)	1 (0%)	34	71
5	1F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
5	2F	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	19	54
6	1G	179/181 (99%)	163 (91%)	12 (7%)	4 (2%)	8	31
6	2G	179/181 (99%)	163 (91%)	13 (7%)	3 (2%)	11	38
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%)	9	32
8	2I	144/147 (98%)	125 (87%)	16 (11%)	3 (2%)	9	32
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%)	24	60
10	2O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	24	60
11	1P	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	26	63
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	26	63
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	26	63
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%)	21	57
14	2S	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	21	57
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%)	19	54
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	54
18	1W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/112 (98%)	109 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	17	51
23	21	95/97 (98%)	93 (98%)	1 (1%)	1 (1%)	17	51
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%)	2	6
26	24	67/69 (97%)	52 (78%)	10 (15%)	5 (8%)	1	3
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	8
33	2b	229/231 (99%)	192 (84%)	27 (12%)	10 (4%)	3	12
34	1c	204/206 (99%)	171 (84%)	31 (15%)	2 (1%)	19	54
34	2c	204/206 (99%)	176 (86%)	25 (12%)	3 (2%)	13	42
35	1d	206/208 (99%)	183 (89%)	19 (9%)	4 (2%)	10	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/208 (99%)	186 (90%)	17 (8%)	3 (2%)	13	42
36	1e	146/148 (99%)	126 (86%)	19 (13%)	1 (1%)	26	63
36	2e	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	26	63
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%)	26	63
38	2g	153/155 (99%)	142 (93%)	8 (5%)	3 (2%)	9	33
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%)	7	29
40	2i	124/127 (98%)	105 (85%)	15 (12%)	4 (3%)	5	20
41	1j	95/97 (98%)	79 (83%)	13 (14%)	3 (3%)	5	20
41	2j	94/97 (97%)	79 (84%)	12 (13%)	3 (3%)	5	20
42	1k	112/114 (98%)	100 (89%)	11 (10%)	1 (1%)	21	57
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%)	3	12
44	2m	112/116 (97%)	103 (92%)	7 (6%)	2 (2%)	11	37
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%)	16	48
46	2o	86/88 (98%)	82 (95%)	3 (4%)	1 (1%)	16	48
47	1p	80/82 (98%)	67 (84%)	12 (15%)	1 (1%)	15	46
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%)	13	42
49	2r	66/68 (97%)	62 (94%)	3 (4%)	1 (2%)	13	42
50	1s	81/83 (98%)	73 (90%)	6 (7%)	2 (2%)	7	27
50	2s	81/83 (98%)	74 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/98 (96%)	87 (93%)	6 (6%)	1 (1%)	17	51
51	2t	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	5	21
52	1u	21/23 (91%)	19 (90%)	0	2 (10%)	1	2
52	2u	21/23 (91%)	17 (81%)	3 (14%)	1 (5%)	3	10
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%)	19	54

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 ⓘ

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%)	7	22
3	2D	215/217 (99%)	195 (91%)	20 (9%)	11	32
4	1E	164/165 (99%)	147 (90%)	17 (10%)	9	26
4	2E	164/165 (99%)	144 (88%)	20 (12%)	6	18
5	1F	160/161 (99%)	136 (85%)	24 (15%)	3	11
5	2F	158/161 (98%)	142 (90%)	16 (10%)	9	28
6	1G	144/155 (93%)	127 (88%)	17 (12%)	6	19
6	2G	142/155 (92%)	133 (94%)	9 (6%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	144/145 (99%)	132 (92%)	12 (8%)	14	38
7	2H	143/145 (99%)	121 (85%)	22 (15%)	3	10
8	1I	111/123 (90%)	97 (87%)	14 (13%)	5	16
8	2I	108/123 (88%)	95 (88%)	13 (12%)	6	18
9	1N	119/119 (100%)	105 (88%)	14 (12%)	6	19
9	2N	118/119 (99%)	105 (89%)	13 (11%)	8	23
10	1O	100/100 (100%)	91 (91%)	9 (9%)	12	34
10	2O	100/100 (100%)	94 (94%)	6 (6%)	24	57
11	1P	115/116 (99%)	107 (93%)	8 (7%)	19	47
11	2P	115/116 (99%)	106 (92%)	9 (8%)	16	41
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	18	46
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	10	29
13	1R	101/101 (100%)	88 (87%)	13 (13%)	5	16
13	2R	101/101 (100%)	87 (86%)	14 (14%)	4	12
14	1S	87/87 (100%)	77 (88%)	10 (12%)	7	21
14	2S	85/87 (98%)	75 (88%)	10 (12%)	6	19
15	1T	115/115 (100%)	109 (95%)	6 (5%)	29	64
15	2T	113/115 (98%)	108 (96%)	5 (4%)	35	70
16	1U	93/93 (100%)	82 (88%)	11 (12%)	6	19
16	2U	93/93 (100%)	86 (92%)	7 (8%)	17	44
17	1V	81/82 (99%)	70 (86%)	11 (14%)	5	13
17	2V	80/82 (98%)	69 (86%)	11 (14%)	4	13
18	1W	89/91 (98%)	81 (91%)	8 (9%)	12	34
18	2W	88/91 (97%)	83 (94%)	5 (6%)	25	59
19	1X	77/77 (100%)	71 (92%)	6 (8%)	16	41
19	2X	77/77 (100%)	75 (97%)	2 (3%)	54	85
20	1Y	86/88 (98%)	79 (92%)	7 (8%)	15	39
20	2Y	86/88 (98%)	76 (88%)	10 (12%)	7	20
21	1Z	169/176 (96%)	147 (87%)	22 (13%)	5	15
21	2Z	165/176 (94%)	149 (90%)	16 (10%)	10	30
22	10	61/62 (98%)	56 (92%)	5 (8%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	61/62 (98%)	58 (95%)	3 (5%)	31	67
23	11	79/82 (96%)	72 (91%)	7 (9%)	12	35
23	21	81/82 (99%)	72 (89%)	9 (11%)	8	22
24	12	65/66 (98%)	61 (94%)	4 (6%)	23	55
24	22	66/66 (100%)	60 (91%)	6 (9%)	12	34
25	13	51/51 (100%)	49 (96%)	2 (4%)	39	75
25	23	50/51 (98%)	46 (92%)	4 (8%)	15	40
26	14	58/62 (94%)	49 (84%)	9 (16%)	3	10
26	24	54/62 (87%)	45 (83%)	9 (17%)	3	8
27	15	51/51 (100%)	45 (88%)	6 (12%)	6	19
27	25	50/51 (98%)	47 (94%)	3 (6%)	24	57
28	16	51/51 (100%)	46 (90%)	5 (10%)	10	30
28	26	50/51 (98%)	45 (90%)	5 (10%)	9	28
29	17	41/41 (100%)	36 (88%)	5 (12%)	6	18
29	27	41/41 (100%)	38 (93%)	3 (7%)	17	45
30	18	54/54 (100%)	48 (89%)	6 (11%)	8	22
30	28	54/54 (100%)	47 (87%)	7 (13%)	5	15
31	19	34/34 (100%)	32 (94%)	2 (6%)	24	58
31	29	34/34 (100%)	32 (94%)	2 (6%)	24	58
33	1b	191/199 (96%)	170 (89%)	21 (11%)	8	23
33	2b	187/199 (94%)	156 (83%)	31 (17%)	3	8
34	1c	144/160 (90%)	135 (94%)	9 (6%)	22	54
34	2c	140/160 (88%)	127 (91%)	13 (9%)	11	32
35	1d	171/180 (95%)	151 (88%)	20 (12%)	7	19
35	2d	172/180 (96%)	159 (92%)	13 (8%)	16	43
36	1e	114/114 (100%)	104 (91%)	10 (9%)	12	35
36	2e	114/114 (100%)	107 (94%)	7 (6%)	23	56
37	1f	85/90 (94%)	80 (94%)	5 (6%)	24	58
37	2f	85/90 (94%)	81 (95%)	4 (5%)	32	68
38	1g	120/126 (95%)	111 (92%)	9 (8%)	17	44
38	2g	119/126 (94%)	112 (94%)	7 (6%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	116/118 (98%)	104 (90%)	12 (10%)	9	26
39	2h	114/118 (97%)	106 (93%)	8 (7%)	19	47
40	1i	91/98 (93%)	81 (89%)	10 (11%)	8	23
40	2i	88/98 (90%)	79 (90%)	9 (10%)	9	27
41	1j	68/87 (78%)	61 (90%)	7 (10%)	9	26
41	2j	68/87 (78%)	62 (91%)	6 (9%)	12	35
42	1k	83/86 (96%)	79 (95%)	4 (5%)	31	67
42	2k	83/86 (96%)	75 (90%)	8 (10%)	10	31
43	1l	96/102 (94%)	90 (94%)	6 (6%)	22	54
43	2l	96/102 (94%)	89 (93%)	7 (7%)	17	45
44	1m	90/94 (96%)	83 (92%)	7 (8%)	16	41
44	2m	87/94 (93%)	77 (88%)	10 (12%)	7	21
45	1n	49/49 (100%)	43 (88%)	6 (12%)	6	18
45	2n	49/49 (100%)	45 (92%)	4 (8%)	14	39
46	1o	78/79 (99%)	73 (94%)	5 (6%)	22	53
46	2o	78/79 (99%)	72 (92%)	6 (8%)	16	42
47	1p	69/71 (97%)	57 (83%)	12 (17%)	2	7
47	2p	68/71 (96%)	61 (90%)	7 (10%)	9	26
48	1q	94/94 (100%)	88 (94%)	6 (6%)	22	53
48	2q	94/94 (100%)	88 (94%)	6 (6%)	22	53
49	1r	59/59 (100%)	54 (92%)	5 (8%)	13	37
49	2r	59/59 (100%)	51 (86%)	8 (14%)	5	13
50	1s	68/72 (94%)	62 (91%)	6 (9%)	12	35
50	2s	67/72 (93%)	62 (92%)	5 (8%)	17	44
51	1t	71/76 (93%)	65 (92%)	6 (8%)	13	37
51	2t	70/76 (92%)	66 (94%)	4 (6%)	25	59
52	1u	18/18 (100%)	17 (94%)	1 (6%)	26	60
52	2u	18/18 (100%)	15 (83%)	3 (17%)	3	8
53	1x	82/83 (99%)	77 (94%)	5 (6%)	23	56
53	2x	79/83 (95%)	67 (85%)	12 (15%)	3	10
54	1y	10/10 (100%)	9 (90%)	1 (10%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	2y	10/10 (100%)	9 (90%)	1 (10%)	9	28
All	All	9540/9882 (96%)	8626 (90%)	914 (10%)	10	31

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

Mol	Chain	Res	Type
45	1n	12	ARG
5	2F	74	ARG
43	2l	52	LEU
47	1p	8	ARG
54	1y	6	TYR

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

Mol	Chain	Res	Type
48	1q	16	GLN
7	2H	74	ASN
42	2k	117	ASN
50	1s	23	ASN
3	2D	126	GLN

### 5.3.3 RNA ⓘ

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	2434	A
1	2A	249	C
1	2A	2308	G
1	1A	2442	A
1	1A	2701	U

## 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	PSU	1A	1933	1	15,21,22	1.91	3 (20%)	16,30,33	3.01	4 (25%)
1	5MU	1A	1937	1	13,22,23	1.48	1 (7%)	16,32,35	3.49	3 (18%)
1	PSU	1A	1939	1,55	15,21,22	2.09	4 (26%)	16,30,33	2.98	6 (37%)
1	4OC	1A	1942	1,55	15,22,24	1.78	5 (33%)	20,31,35	1.88	4 (20%)
1	5MU	1A	1961	1,55	13,22,23	1.59	1 (7%)	16,32,35	3.34	3 (18%)
1	5MC	1A	1964	1	14,22,23	1.01	1 (7%)	17,32,35	0.85	0
1	5MC	1A	1984	1,55	14,22,23	1.25	2 (14%)	17,32,35	1.02	1 (5%)
1	OMG	1A	2263	1,55	18,26,27	2.21	8 (44%)	21,38,41	2.20	6 (28%)
1	2MA	1A	2515	1,55	17,25,26	2.24	5 (29%)	18,37,40	3.77	5 (27%)
1	OMU	1A	2564	1,55	14,22,23	7.42	8 (57%)	19,31,34	1.83	3 (15%)
1	PSU	1A	2617	1	15,21,22	2.14	4 (26%)	16,30,33	3.34	6 (37%)
32	2MG	1a	1207	55,32	18,26,27	2.85	5 (27%)	21,38,41	3.62	10 (47%)
32	5MC	1a	1400	32	14,22,23	1.01	0	17,32,35	1.05	2 (11%)
32	4OC	1a	1402	32	15,23,24	1.86	6 (40%)	21,32,35	1.61	3 (14%)
32	5MC	1a	1404	32	14,22,23	1.17	1 (7%)	17,32,35	0.82	1 (5%)
32	5MC	1a	1407	32	14,22,23	1.18	1 (7%)	17,32,35	1.18	2 (11%)
32	UR3	1a	1498	32	13,22,23	1.68	3 (23%)	18,32,35	0.75	0
32	MA6	1a	1518	32	18,26,27	0.86	2 (11%)	15,38,41	3.83	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	MA6	1a	1519	32	18,26,27	1.07	2 (11%)	15,38,41	3.04	3 (20%)
32	PSU	1a	516	55,32	15,21,22	2.19	4 (26%)	16,30,33	3.43	5 (31%)
32	7MG	1a	527	55,32	20,26,27	2.62	7 (35%)	23,39,42	1.75	6 (26%)
32	M2G	1a	966	32	18,27,28	2.79	6 (33%)	22,40,43	1.89	7 (31%)
32	5MC	1a	967	32	14,22,23	0.81	0	17,32,35	0.93	2 (11%)
43	0TD	1l	92	43	4,9,10	1.98	2 (50%)	4,11,13	4.99	2 (50%)
1	PSU	2A	1911	1	15,21,22	2.02	4 (26%)	16,30,33	2.95	5 (31%)
1	5MU	2A	1915	1	13,22,23	1.72	2 (15%)	16,32,35	3.62	3 (18%)
1	PSU	2A	1917	1	15,21,22	1.67	3 (20%)	16,30,33	2.85	6 (37%)
1	4OC	2A	1920	1	15,22,24	2.13	5 (33%)	20,31,35	2.27	2 (10%)
1	5MU	2A	1939	1,55	13,22,23	1.58	3 (23%)	16,32,35	2.98	2 (12%)
1	5MC	2A	1942	1	14,22,23	0.78	0	17,32,35	0.87	1 (5%)
1	5MC	2A	1962	1,55	14,22,23	1.60	2 (14%)	17,32,35	0.77	0
1	OMG	2A	2251	1,55	18,26,27	2.43	5 (27%)	21,38,41	2.71	6 (28%)
1	2MA	2A	2503	1,55	17,25,26	2.26	6 (35%)	18,37,40	3.33	4 (22%)
1	OMU	2A	2552	1,55	14,22,23	7.75	8 (57%)	19,31,34	2.02	2 (10%)
1	PSU	2A	2605	1	15,21,22	2.12	5 (33%)	16,30,33	2.83	6 (37%)
32	2MG	2a	1207	32	18,26,27	2.83	7 (38%)	21,38,41	3.03	8 (38%)
32	5MC	2a	1400	32	14,22,23	0.97	0	17,32,35	0.95	1 (5%)
32	4OC	2a	1402	32	15,23,24	2.14	5 (33%)	21,32,35	2.90	3 (14%)
32	5MC	2a	1404	32	14,22,23	0.98	1 (7%)	17,32,35	0.93	1 (5%)
32	5MC	2a	1407	32	14,22,23	0.84	0	17,32,35	0.96	1 (5%)
32	UR3	2a	1498	32	13,22,23	1.81	3 (23%)	18,32,35	0.88	0
32	MA6	2a	1518	32	18,26,27	0.85	0	15,38,41	3.32	3 (20%)
32	MA6	2a	1519	32	18,26,27	1.02	2 (11%)	15,38,41	2.87	3 (20%)
32	PSU	2a	516	32	15,21,22	2.63	5 (33%)	16,30,33	3.57	5 (31%)
32	7MG	2a	527	32	20,26,27	2.88	7 (35%)	23,39,42	2.04	6 (26%)
32	M2G	2a	966	32	18,27,28	3.11	6 (33%)	22,40,43	2.36	6 (27%)
32	5MC	2a	967	32	14,22,23	1.37	1 (7%)	17,32,35	1.14	2 (11%)
43	0TD	2l	92	43	4,9,10	1.58	1 (25%)	4,11,13	3.65	2 (50%)

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	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1939	1,55	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1,55	-	0/5/27/30	0/2/2/2
1	5MU	1A	1961	1,55	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1,55	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,55	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,55	-	0/3/25/26	0/3/3/3
1	OMU	1A	2564	1,55	-	0/5/27/28	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	55,32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	55,32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	55,32	-	0/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	0/2/12/14	0/0/0/0
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	2A	1939	1,55	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1,55	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,55	-	0/3/25/26	0/3/3/3
1	OMU	2A	2552	1,55	-	0/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	0/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	0/2/12/14	0/0/0/0

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C4-N3	-12.37	1.10	1.33
1	2A	2552	OMU	C6-C5	-12.37	1.11	1.38
1	1A	2564	OMU	C6-C5	-12.19	1.11	1.38
1	1A	2564	OMU	C4-N3	-11.34	1.12	1.33
1	2A	2552	OMU	C3'-C2'	-8.59	1.33	1.53

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C1'-N9-C4	-11.20	114.31	126.81
32	1a	1518	MA6	C1'-N9-C4	-10.18	115.45	126.81
1	2A	1915	5MU	C5-C4-N3	-9.94	117.00	125.35
32	1a	1518	MA6	N3-C2-N1	-9.89	121.10	128.87
32	1a	1519	MA6	N3-C2-N1	-9.69	121.26	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1933	PSU	1	0
1	1A	1942	4OC	1	0
1	1A	1961	5MU	1	0
1	1A	2515	2MA	1	0
1	2A	1915	5MU	1	0
1	2A	1917	PSU	1	0
1	2A	1920	4OC	1	0
1	2A	1942	5MC	1	0
1	2A	2251	OMG	1	0
1	2A	2503	2MA	2	0
1	2A	2552	OMU	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2435 ligands modelled in this entry, 2 are modelled with single atom and 2431 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
58	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-
58	SF4	2d	501	35	0,12,12	0.00	-	0,24,24	0.00	-

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	1d	501	35	-	0/0/48/48	0/6/5/5
58	SF4	2d	501	35	-	0/0/48/48	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.01	135 (4%) 35 29	16, 34, 100, 113	0
1	2A	2856/2915 (97%)	-0.01	140 (4%) 33 27	31, 56, 101, 114	0
2	1B	120/120 (100%)	-0.47	0 100 100	27, 51, 64, 93	0
2	2B	120/120 (100%)	-0.36	0 100 100	60, 79, 88, 96	0
3	1D	275/275 (100%)	-0.42	0 100 100	17, 34, 49, 74	0
3	2D	275/275 (100%)	-0.27	0 100 100	27, 49, 64, 83	0
4	1E	204/204 (100%)	-0.42	0 100 100	16, 37, 58, 73	0
4	2E	204/204 (100%)	-0.22	1 (0%) 91 90	31, 57, 73, 83	0
5	1F	203/203 (100%)	-0.31	1 (0%) 91 90	16, 38, 68, 92	0
5	2F	203/203 (100%)	-0.27	0 100 100	33, 66, 82, 91	0
6	1G	181/181 (100%)	-0.36	2 (1%) 82 80	47, 66, 83, 95	0
6	2G	181/181 (100%)	0.47	12 (6%) 22 16	76, 85, 92, 98	0
7	1H	174/174 (100%)	-0.43	1 (0%) 90 89	36, 51, 65, 70	0
7	2H	173/174 (99%)	0.76	28 (16%) 3 1	66, 85, 94, 98	0
8	1I	147/147 (100%)	-0.21	0 100 100	40, 71, 82, 87	0
8	2I	146/147 (99%)	0.32	7 (4%) 34 28	53, 80, 91, 97	0
9	1N	140/140 (100%)	-0.41	0 100 100	19, 33, 57, 73	0
9	2N	140/140 (100%)	-0.13	1 (0%) 89 88	46, 64, 76, 88	0
10	1O	122/122 (100%)	-0.43	0 100 100	26, 38, 55, 65	0
10	2O	122/122 (100%)	-0.37	0 100 100	41, 54, 68, 76	0
11	1P	149/149 (100%)	-0.30	0 100 100	17, 43, 64, 79	0
11	2P	149/149 (100%)	0.20	3 (2%) 68 64	38, 66, 83, 91	0
12	1Q	141/141 (100%)	-0.32	0 100 100	25, 38, 53, 68	0
12	2Q	141/141 (100%)	-0.31	1 (0%) 89 88	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%)	-0.38	0 100 100	21, 32, 51, 61	0
13	2R	118/118 (100%)	-0.11	0 100 100	39, 53, 63, 76	0
14	1S	110/110 (100%)	-0.34	0 100 100	37, 51, 66, 69	0
14	2S	110/110 (100%)	0.29	5 (4%) 37 31	63, 75, 84, 86	0
15	1T	131/131 (100%)	-0.41	1 (0%) 87 86	32, 43, 70, 84	0
15	2T	131/131 (100%)	-0.32	0 100 100	48, 59, 79, 86	0
16	1U	116/116 (100%)	-0.49	0 100 100	19, 27, 42, 62	0
16	2U	116/116 (100%)	-0.16	0 100 100	41, 61, 77, 86	0
17	1V	101/101 (100%)	-0.41	0 100 100	17, 36, 54, 69	0
17	2V	101/101 (100%)	-0.12	1 (0%) 84 82	39, 72, 81, 89	0
18	1W	112/112 (100%)	-0.47	1 (0%) 85 84	19, 27, 50, 92	0
18	2W	112/112 (100%)	-0.26	1 (0%) 85 84	38, 48, 67, 87	0
19	1X	95/95 (100%)	-0.39	0 100 100	22, 35, 62, 71	0
19	2X	95/95 (100%)	-0.07	1 (1%) 82 80	45, 61, 74, 78	0
20	1Y	107/107 (100%)	-0.33	1 (0%) 85 84	32, 47, 68, 78	0
20	2Y	107/107 (100%)	0.61	16 (14%) 3 2	55, 72, 84, 94	0
21	1Z	203/203 (100%)	-0.37	2 (0%) 84 82	40, 58, 77, 88	0
21	2Z	201/203 (99%)	0.17	7 (3%) 48 40	64, 79, 88, 95	0
22	10	77/77 (100%)	-0.31	1 (1%) 79 78	26, 35, 58, 65	0
22	20	77/77 (100%)	0.31	5 (6%) 22 16	53, 62, 74, 78	0
23	11	97/97 (100%)	-0.06	1 (1%) 84 82	25, 39, 67, 80	0
23	21	97/97 (100%)	-0.07	1 (1%) 84 82	40, 57, 79, 88	0
24	12	70/70 (100%)	-0.38	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%)	-0.37	0 100 100	21, 32, 58, 77	0
25	23	59/59 (100%)	0.61	6 (10%) 9 5	48, 62, 77, 82	0
26	14	69/69 (100%)	0.17	10 (14%) 3 2	63, 82, 96, 98	0
26	24	69/69 (100%)	1.03	17 (24%) 1 0	80, 92, 99, 100	0
27	15	59/59 (100%)	-0.44	0 100 100	15, 32, 48, 62	0
27	25	59/59 (100%)	-0.40	0 100 100	35, 52, 70, 76	0
28	16	53/53 (100%)	-0.42	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%)	-0.25	0 100 100	52, 62, 69, 76	0
29	17	48/48 (100%)	-0.22	1 (2%) 67 62	18, 24, 58, 65	0
29	27	48/48 (100%)	-0.13	0 100 100	32, 40, 66, 79	0
30	18	64/64 (100%)	-0.35	0 100 100	23, 30, 39, 48	0
30	28	64/64 (100%)	-0.04	0 100 100	41, 54, 64, 72	0
31	19	37/37 (100%)	-0.12	0 100 100	30, 40, 59, 71	0
31	29	37/37 (100%)	0.52	2 (5%) 29 23	61, 68, 79, 82	0
32	1a	1488/1521 (97%)	-0.04	48 (3%) 51 43	31, 74, 100, 114	0
32	2a	1492/1521 (98%)	-0.05	52 (3%) 48 40	41, 76, 100, 112	0
33	1b	231/231 (100%)	0.15	15 (6%) 22 16	67, 82, 92, 101	0
33	2b	231/231 (100%)	0.30	17 (7%) 17 11	68, 85, 94, 98	0
34	1c	206/206 (100%)	0.19	12 (5%) 26 20	70, 83, 92, 97	0
34	2c	206/206 (100%)	0.28	7 (3%) 49 41	77, 86, 93, 99	0
35	1d	208/208 (100%)	-0.07	6 (2%) 55 49	59, 76, 87, 91	0
35	2d	208/208 (100%)	-0.03	1 (0%) 91 90	61, 73, 84, 88	0
36	1e	148/148 (100%)	-0.16	1 (0%) 89 88	48, 69, 79, 96	0
36	2e	148/148 (100%)	-0.21	0 100 100	58, 71, 81, 89	0
37	1f	100/100 (100%)	-0.30	1 (1%) 84 82	53, 73, 80, 84	0
37	2f	100/100 (100%)	-0.45	0 100 100	57, 70, 82, 87	0
38	1g	155/155 (100%)	0.09	6 (3%) 43 36	67, 77, 86, 90	0
38	2g	155/155 (100%)	0.40	14 (9%) 12 7	73, 81, 89, 95	0
39	1h	137/137 (100%)	-0.01	0 100 100	55, 69, 77, 89	0
39	2h	137/137 (100%)	-0.13	1 (0%) 89 88	60, 72, 80, 87	0
40	1i	127/127 (100%)	0.55	11 (8%) 13 8	68, 86, 93, 97	0
40	2i	126/127 (99%)	1.02	22 (17%) 2 1	74, 88, 94, 97	0
41	1j	97/97 (100%)	1.12	21 (21%) 1 0	70, 87, 95, 98	0
41	2j	96/97 (98%)	1.07	20 (20%) 1 1	75, 89, 95, 97	0
42	1k	114/114 (100%)	-0.26	1 (0%) 85 84	40, 65, 81, 87	0
42	2k	114/114 (100%)	-0.07	1 (0%) 85 84	54, 71, 85, 91	0
43	1l	121/122 (99%)	-0.15	2 (1%) 73 70	47, 63, 75, 78	0
43	2l	121/122 (99%)	-0.15	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%)	0.30	7 (6%) 25 18	71, 81, 88, 91	0
44	2m	114/116 (98%)	0.38	8 (7%) 19 13	76, 88, 93, 95	0
45	1n	60/60 (100%)	0.38	1 (1%) 73 70	71, 80, 88, 89	0
45	2n	60/60 (100%)	0.89	11 (18%) 2 1	76, 88, 92, 95	0
46	1o	88/88 (100%)	0.05	3 (3%) 49 41	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%)	0.40	6 (7%) 18 12	64, 77, 86, 90	0
47	2p	82/82 (100%)	0.18	3 (3%) 45 38	58, 70, 79, 87	0
48	1q	99/99 (100%)	-0.05	1 (1%) 84 82	53, 68, 80, 84	0
48	2q	99/99 (100%)	-0.14	1 (1%) 84 82	57, 70, 79, 83	0
49	1r	68/68 (100%)	0.25	3 (4%) 38 32	55, 67, 80, 86	0
49	2r	68/68 (100%)	0.11	2 (2%) 55 49	61, 71, 82, 86	0
50	1s	83/83 (100%)	0.72	10 (12%) 6 3	76, 84, 91, 94	0
50	2s	83/83 (100%)	1.80	35 (42%) 0 0	84, 91, 97, 99	0
51	1t	96/98 (97%)	0.32	3 (3%) 52 45	64, 75, 86, 92	0
51	2t	98/98 (100%)	0.12	1 (1%) 84 82	56, 69, 83, 85	0
52	1u	23/23 (100%)	1.16	5 (21%) 1 0	72, 77, 83, 85	0
52	2u	23/23 (100%)	1.75	10 (43%) 0 0	79, 86, 89, 90	0
53	1x	97/97 (100%)	0.07	2 (2%) 67 62	52, 67, 81, 86	0
53	2x	96/97 (98%)	1.94	44 (45%) 0 0	73, 82, 93, 96	0
54	1y	10/10 (100%)	-0.27	0 100 100	30, 33, 40, 40	0
54	2y	10/10 (100%)	-0.16	0 100 100	43, 47, 58, 58	0
All	All	20786/20974 (99%)	-0.01	827 (3%) 42 35	15, 64, 93, 114	0

The worst 5 of 827 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	PSU	1a	516	20/21	0.95	0.15	-	66,74,77,77	0
1	5MC	1A	1964	21/22	0.98	0.13	-	25,36,39,42	0
1	5MU	2A	1939	21/22	0.98	0.15	-	30,36,42,44	0
32	MA6	1a	1519	24/25	0.98	0.16	-	41,50,55,58	0
32	4OC	1a	1402	22/23	0.97	0.17	-	45,52,58,61	0
32	M2G	2a	966	25/26	0.96	0.13	-	67,71,86,94	0
1	PSU	1A	2617	20/21	0.98	0.18	-	20,24,30,33	0
1	5MC	2A	1962	21/22	0.98	0.13	-	34,44,51,60	0
32	5MC	1a	1407	21/22	0.97	0.14	-	44,53,58,61	0
1	5MU	2A	1915	21/22	0.94	0.15	-	79,87,92,108	0
1	2MA	1A	2515	23/24	0.98	0.19	-	16,20,24,25	0
1	4OC	1A	1942	21/23	0.97	0.16	-	47,59,64,65	0
1	OMG	1A	2263	24/25	0.99	0.16	-	16,22,25,27	0
32	2MG	1a	1207	24/25	0.96	0.12	-	76,81,85,85	0
32	2MG	2a	1207	24/25	0.94	0.17	-	81,90,95,99	0
1	PSU	1A	1939	20/21	0.93	0.20	-	62,78,87,88	0
1	PSU	2A	1917	20/21	0.92	0.14	-	72,79,85,102	0
1	OMG	2A	2251	24/25	0.98	0.16	-	35,39,44,46	0
1	PSU	2A	2605	20/21	0.97	0.17	-	33,35,41,41	0
32	5MC	1a	1400	21/22	0.98	0.16	-	54,59,64,67	0
1	5MU	1A	1937	21/22	0.93	0.22	-	79,86,100,113	0
32	M2G	1a	966	25/26	0.96	0.14	-	52,62,74,77	0
1	OMU	2A	2552	21/22	0.99	0.14	-	30,36,40,42	0
32	5MC	1a	967	21/22	0.96	0.14	-	57,65,75,83	0
43	0TD	2l	92	10/11	0.96	0.15	-	71,73,77,92	0
32	5MC	2a	1404	21/22	0.96	0.14	-	49,53,60,64	0
32	PSU	2a	516	20/21	0.94	0.16	-	72,83,88,90	0
32	7MG	2a	527	24/25	0.96	0.17	-	69,74,77,79	0
43	0TD	1l	92	10/11	0.96	0.14	-	63,65,74,80	0
32	4OC	2a	1402	22/23	0.96	0.16	-	52,60,65,67	0
1	2MA	2A	2503	23/24	0.97	0.20	-	30,35,40,48	0
32	5MC	2a	1407	21/22	0.97	0.14	-	50,59,63,65	0
32	5MC	2a	967	21/22	0.95	0.15	-	67,73,82,90	0
1	5MU	1A	1961	21/22	0.98	0.15	-	20,26,29,33	0
1	5MC	1A	1984	21/22	0.98	0.14	-	30,32,36,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UR3	1a	1498	21/22	0.97	0.19	-	41,50,56,59	0
32	5MC	2a	1400	21/22	0.96	0.20	-	65,74,78,83	0
32	7MG	1a	527	24/25	0.97	0.16	-	50,63,66,71	0
32	MA6	1a	1518	24/25	0.98	0.17	-	38,49,52,57	0
32	MA6	2a	1519	24/25	0.98	0.18	-	52,58,64,69	0
1	5MC	2A	1942	21/22	0.97	0.17	-	46,53,57,61	0
32	MA6	2a	1518	24/25	0.98	0.17	-	50,59,65,66	0
32	5MC	1a	1404	21/22	0.97	0.15	-	44,48,55,59	0
32	UR3	2a	1498	21/22	0.97	0.15	-	47,56,64,66	0
1	OMU	1A	2564	21/22	0.98	0.18	-	21,26,29,32	0
1	PSU	2A	1911	20/21	0.96	0.11	-	65,73,80,81	0
1	4OC	2A	1920	21/23	0.97	0.16	-	54,65,70,72	0
1	PSU	1A	1933	20/21	0.97	0.14	-	57,70,74,76	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3231	1/1	0.90	0.72	154.66	31,31,31,31	0
55	MG	1A	3475	1/1	0.95	0.99	102.88	32,32,32,32	0
55	MG	2A	3509	1/1	0.86	1.03	102.30	53,53,53,53	0
55	MG	2A	3643	1/1	0.60	1.12	96.19	60,60,60,60	0
55	MG	1A	3243	1/1	0.92	1.05	87.58	44,44,44,44	0
55	MG	2F	301	1/1	0.92	1.03	85.74	47,47,47,47	0
55	MG	1A	3573	1/1	0.82	0.68	80.55	37,37,37,37	0
55	MG	2A	3018	1/1	0.93	1.17	79.11	52,52,52,52	0
55	MG	1A	3211	1/1	0.95	0.77	74.05	31,31,31,31	0
55	MG	1E	302	1/1	0.92	0.93	70.67	39,39,39,39	0
55	MG	1A	3193	1/1	0.77	0.42	68.21	42,42,42,42	0
55	MG	1A	3160	1/1	0.85	0.98	67.31	40,40,40,40	0
55	MG	1A	3087	1/1	0.87	0.77	66.60	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3894	1/1	0.94	0.83	65.57	38,38,38,38	0
55	MG	1A	3198	1/1	0.89	0.60	65.44	28,28,28,28	0
55	MG	1A	3233	1/1	0.93	0.35	65.15	63,63,63,63	0
55	MG	2E	303	1/1	0.81	1.02	62.26	71,71,71,71	0
55	MG	2A	3054	1/1	0.85	0.63	60.97	51,51,51,51	0
55	MG	2A	3094	1/1	0.83	0.82	57.86	59,59,59,59	0
55	MG	1A	3082	1/1	0.94	0.72	56.69	37,37,37,37	0
55	MG	1P	201	1/1	0.87	0.98	56.28	30,30,30,30	0
55	MG	1V	201	1/1	0.79	0.66	56.15	25,25,25,25	0
55	MG	2A	3417	1/1	0.93	0.75	55.64	58,58,58,58	0
55	MG	1A	3867	1/1	0.98	0.66	54.34	37,37,37,37	0
55	MG	2A	3062	1/1	0.82	0.79	52.88	47,47,47,47	0
55	MG	2A	3146	1/1	0.83	0.62	52.63	53,53,53,53	0
55	MG	2D	305	1/1	0.91	0.96	52.56	59,59,59,59	0
55	MG	2A	3569	1/1	0.91	0.65	50.24	48,48,48,48	0
55	MG	1A	3070	1/1	0.88	0.49	50.23	32,32,32,32	0
55	MG	1A	3170	1/1	0.97	0.54	50.18	34,34,34,34	0
55	MG	2A	3178	1/1	0.95	0.68	49.45	38,38,38,38	0
55	MG	1A	3640	1/1	0.90	0.41	49.23	34,34,34,34	0
55	MG	1A	3154	1/1	0.91	0.65	48.63	28,28,28,28	0
55	MG	1D	305	1/1	0.93	0.62	48.25	42,42,42,42	0
55	MG	1A	3142	1/1	0.98	0.92	47.82	32,32,32,32	0
55	MG	2Q	8004	1/1	0.69	0.63	47.76	66,66,66,66	0
55	MG	1F	303	1/1	0.81	0.63	46.02	43,43,43,43	0
55	MG	2A	3756	1/1	0.83	1.03	45.59	95,95,95,95	0
55	MG	2A	3154	1/1	0.76	0.90	45.48	61,61,61,61	0
55	MG	17	103	1/1	0.90	0.84	45.25	43,43,43,43	0
55	MG	1F	304	1/1	0.91	0.95	45.17	39,39,39,39	0
55	MG	1A	3019	1/1	0.89	0.66	45.07	39,39,39,39	0
55	MG	1A	3762	1/1	0.94	0.66	44.65	48,48,48,48	0
55	MG	2A	3513	1/1	0.85	0.72	44.52	47,47,47,47	0
55	MG	2A	3486	1/1	0.84	1.38	43.96	57,57,57,57	0
55	MG	1A	3028	1/1	0.96	0.53	42.87	37,37,37,37	0
55	MG	2A	3120	1/1	0.94	0.82	42.53	56,56,56,56	0
55	MG	2A	3092	1/1	0.95	0.66	42.33	49,49,49,49	0
55	MG	1A	3577	1/1	0.88	0.74	41.92	40,40,40,40	0
55	MG	1A	3122	1/1	0.91	0.53	41.63	30,30,30,30	0
55	MG	1A	3185	1/1	0.97	0.66	41.12	32,32,32,32	0
55	MG	2A	3155	1/1	0.71	0.85	40.82	50,50,50,50	0
55	MG	2A	3732	1/1	0.89	0.74	40.29	61,61,61,61	0
55	MG	2A	3119	1/1	0.97	0.53	40.03	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3206	1/1	0.86	0.39	39.80	32,32,32,32	0
55	MG	1A	3896	1/1	0.80	0.60	39.16	37,37,37,37	0
55	MG	10	102	1/1	0.94	0.45	38.73	52,52,52,52	0
55	MG	2A	3530	1/1	0.81	0.86	38.51	52,52,52,52	0
55	MG	2E	304	1/1	0.92	0.83	38.31	46,46,46,46	0
55	MG	1A	3123	1/1	0.92	0.58	37.84	27,27,27,27	0
55	MG	1A	3102	1/1	0.91	0.33	36.37	42,42,42,42	0
55	MG	2V	202	1/1	0.91	1.01	35.70	55,55,55,55	0
55	MG	1A	3545	1/1	0.94	0.48	35.21	36,36,36,36	0
55	MG	2A	3138	1/1	0.75	0.72	33.85	48,48,48,48	0
55	MG	2D	302	1/1	0.64	0.45	33.77	58,58,58,58	0
55	MG	1D	302	1/1	0.84	0.82	32.51	35,35,35,35	0
55	MG	1A	3905	1/1	0.77	0.74	32.32	45,45,45,45	0
55	MG	1A	3020	1/1	0.92	0.60	31.90	39,39,39,39	0
55	MG	1A	3025	1/1	0.95	0.61	31.03	33,33,33,33	0
55	MG	1A	3104	1/1	0.92	0.66	30.81	37,37,37,37	0
55	MG	1A	3077	1/1	0.61	0.62	30.73	47,47,47,47	0
55	MG	15	102	1/1	0.82	0.91	30.51	43,43,43,43	0
55	MG	1A	3199	1/1	0.82	0.46	30.38	34,34,34,34	0
55	MG	2A	3742	1/1	0.69	0.38	30.28	70,70,70,70	0
55	MG	1U	204	1/1	0.90	0.70	30.02	29,29,29,29	0
55	MG	1A	3103	1/1	0.96	0.55	29.95	35,35,35,35	0
55	MG	2R	201	1/1	0.93	0.78	29.64	56,56,56,56	0
55	MG	1A	3189	1/1	0.79	0.32	29.29	43,43,43,43	0
55	MG	1D	307	1/1	0.85	0.74	29.19	44,44,44,44	0
55	MG	1A	3175	1/1	0.81	0.53	29.17	56,56,56,56	0
55	MG	1A	3725	1/1	0.78	0.54	28.92	44,44,44,44	0
55	MG	2a	1602	1/1	0.86	0.50	28.90	55,55,55,55	0
55	MG	2A	3103	1/1	0.93	0.51	28.87	65,65,65,65	0
55	MG	2A	3150	1/1	0.71	0.42	28.04	49,49,49,49	0
55	MG	1A	3464	1/1	0.83	0.64	27.86	35,35,35,35	0
55	MG	2F	307	1/1	0.90	0.87	27.85	60,60,60,60	0
55	MG	1A	3638	1/1	0.94	0.43	27.50	31,31,31,31	0
55	MG	1D	309	1/1	0.91	0.52	27.48	41,41,41,41	0
55	MG	2A	3111	1/1	0.84	0.86	27.38	52,52,52,52	0
55	MG	2A	3017	1/1	0.94	0.54	27.15	54,54,54,54	0
55	MG	25	101	1/1	0.86	0.46	26.68	58,58,58,58	0
55	MG	1R	201	1/1	0.95	0.97	26.65	46,46,46,46	0
55	MG	2F	302	1/1	0.95	0.61	26.65	55,55,55,55	0
55	MG	2A	3590	1/1	0.84	0.46	26.18	65,65,65,65	0
55	MG	1F	308	1/1	0.94	0.53	25.90	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2V	201	1/1	0.84	0.78	25.77	55,55,55,55	0
55	MG	27	102	1/1	0.83	0.77	25.76	49,49,49,49	0
55	MG	25	103	1/1	0.86	0.64	25.56	62,62,62,62	0
55	MG	1A	3581	1/1	0.88	0.53	25.09	35,35,35,35	0
55	MG	1a	3182	1/1	0.91	0.49	25.02	71,71,71,71	0
55	MG	1A	3107	1/1	0.98	0.47	24.99	36,36,36,36	0
55	MG	1A	3910	1/1	0.94	0.52	24.73	35,35,35,35	0
55	MG	1A	3177	1/1	0.94	0.58	24.35	52,52,52,52	0
55	MG	1A	3184	1/1	0.84	0.48	24.28	37,37,37,37	0
55	MG	2A	3506	1/1	0.88	0.46	24.26	47,47,47,47	0
55	MG	1A	3242	1/1	0.94	0.42	24.09	29,29,29,29	0
55	MG	17	102	1/1	0.94	0.49	23.75	36,36,36,36	0
55	MG	1A	3627	1/1	0.97	0.48	23.69	44,44,44,44	0
55	MG	1A	3597	1/1	0.85	0.47	23.68	38,38,38,38	0
55	MG	20	101	1/1	0.82	0.42	23.60	64,64,64,64	0
55	MG	2A	3579	1/1	0.83	0.28	23.01	75,75,75,75	0
55	MG	1A	3188	1/1	0.85	0.45	22.63	34,34,34,34	0
55	MG	1E	303	1/1	0.85	0.38	22.49	39,39,39,39	0
55	MG	1A	3080	1/1	0.92	0.60	22.33	36,36,36,36	0
55	MG	2D	308	1/1	0.87	0.53	22.18	55,55,55,55	0
55	MG	2A	3110	1/1	0.90	0.55	21.82	53,53,53,53	0
55	MG	2A	3483	1/1	0.91	0.65	21.72	55,55,55,55	0
55	MG	1A	3838	1/1	0.82	0.47	21.63	45,45,45,45	0
55	MG	1A	3252	1/1	0.98	0.51	21.37	36,36,36,36	0
55	MG	2A	3200	1/1	0.91	0.99	20.85	65,65,65,65	0
55	MG	2a	1711	1/1	0.87	0.73	20.78	80,80,80,80	0
55	MG	1A	3509	1/1	0.75	0.33	20.74	38,38,38,38	0
55	MG	1F	310	1/1	0.85	0.48	20.53	27,27,27,27	0
55	MG	11	101	1/1	0.83	1.58	20.35	54,54,54,54	0
55	MG	2A	3556	1/1	0.91	0.71	20.04	57,57,57,57	0
55	MG	1A	3516	1/1	0.54	0.52	19.87	35,35,35,35	0
55	MG	2F	306	1/1	0.87	0.54	19.75	43,43,43,43	0
55	MG	1F	315	1/1	0.94	0.45	19.56	43,43,43,43	0
55	MG	1a	3144	1/1	0.77	0.28	19.29	75,75,75,75	0
55	MG	2A	3406	1/1	0.91	0.56	19.20	62,62,62,62	0
55	MG	2D	307	1/1	0.90	1.68	19.19	64,64,64,64	0
55	MG	1A	3258	1/1	0.90	0.67	18.91	44,44,44,44	0
55	MG	2A	3814	1/1	0.90	0.90	18.71	68,68,68,68	0
55	MG	1A	3605	1/1	0.84	0.54	18.51	38,38,38,38	0
55	MG	1A	3119	1/1	0.75	0.39	18.36	33,33,33,33	0
55	MG	15	104	1/1	0.73	0.30	18.30	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3857	1/1	0.89	0.28	18.26	71,71,71,71	0
55	MG	2A	3023	1/1	0.98	0.32	18.22	47,47,47,47	0
55	MG	2A	3205	1/1	0.97	0.66	18.17	52,52,52,52	0
55	MG	1A	3733	1/1	0.77	0.40	18.10	27,27,27,27	0
55	MG	2F	303	1/1	0.92	0.48	18.09	62,62,62,62	0
55	MG	2A	3040	1/1	0.86	0.35	18.07	63,63,63,63	0
55	MG	1A	3155	1/1	0.93	0.59	17.92	27,27,27,27	0
55	MG	1A	3260	1/1	0.89	0.51	17.76	36,36,36,36	0
55	MG	17	101	1/1	0.92	0.42	17.56	35,35,35,35	0
55	MG	2P	201	1/1	0.94	0.56	17.55	51,51,51,51	0
55	MG	2A	3566	1/1	0.95	0.34	17.27	64,64,64,64	0
55	MG	18	3302	1/1	0.82	0.54	17.08	40,40,40,40	0
55	MG	2A	3412	1/1	0.90	0.52	16.55	70,70,70,70	0
55	MG	1N	8001	1/1	0.94	0.45	16.51	51,51,51,51	0
55	MG	2A	3538	1/1	0.87	0.59	16.16	62,62,62,62	0
55	MG	2A	3219	1/1	0.97	0.36	16.12	22,22,22,22	0
55	MG	1A	3641	1/1	0.87	0.46	16.10	35,35,35,35	0
55	MG	1A	3708	1/1	0.89	0.50	16.01	53,53,53,53	0
55	MG	1F	314	1/1	0.49	0.31	15.91	53,53,53,53	0
55	MG	2A	3810	1/1	0.89	0.32	15.89	51,51,51,51	0
55	MG	2A	3242	1/1	0.95	0.23	15.81	40,40,40,40	0
55	MG	2a	1753	1/1	0.93	0.49	15.68	69,69,69,69	0
55	MG	1A	3278	1/1	0.83	0.32	15.53	37,37,37,37	0
55	MG	15	103	1/1	0.96	0.32	15.45	34,34,34,34	0
55	MG	2U	202	1/1	0.93	0.62	15.25	46,46,46,46	0
55	MG	1a	3137	1/1	0.86	0.29	15.23	68,68,68,68	0
55	MG	2A	3750	1/1	0.91	0.33	15.19	63,63,63,63	0
55	MG	2A	3203	1/1	0.95	1.09	15.03	63,63,63,63	0
55	MG	1A	3285	1/1	0.92	0.28	15.03	47,47,47,47	0
55	MG	23	101	1/1	0.95	0.87	14.70	64,64,64,64	0
55	MG	1a	3016	1/1	0.86	0.42	14.70	80,80,80,80	0
55	MG	2A	3649	1/1	0.90	0.41	14.50	49,49,49,49	0
55	MG	2A	3455	1/1	0.40	0.58	14.40	59,59,59,59	0
55	MG	1A	3129	1/1	0.93	0.27	14.31	36,36,36,36	0
55	MG	2A	3676	1/1	0.92	0.41	14.06	73,73,73,73	0
55	MG	2A	3078	1/1	0.83	0.61	13.92	51,51,51,51	0
55	MG	1A	3878	1/1	0.78	0.28	13.67	46,46,46,46	0
55	MG	2A	3222	1/1	0.88	0.40	13.65	62,62,62,62	0
55	MG	2A	3160	1/1	0.98	0.39	13.64	46,46,46,46	0
55	MG	2A	3822	1/1	0.88	0.31	13.63	53,53,53,53	0
55	MG	2F	304	1/1	0.88	0.58	13.49	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3018	1/1	0.94	0.41	13.42	23,23,23,23	0
55	MG	1e	3002	1/1	0.85	0.50	13.41	58,58,58,58	0
55	MG	1A	3113	1/1	0.91	0.32	13.40	41,41,41,41	0
55	MG	1Q	201	1/1	0.90	0.50	13.27	44,44,44,44	0
55	MG	1A	3467	1/1	0.90	0.22	13.11	32,32,32,32	0
55	MG	1a	3088	1/1	0.97	0.37	12.82	63,63,63,63	0
55	MG	1A	3480	1/1	0.93	0.27	12.75	34,34,34,34	0
55	MG	1F	311	1/1	0.84	0.40	12.69	25,25,25,25	0
55	MG	1A	3904	1/1	0.92	0.31	12.35	17,17,17,17	0
55	MG	1A	3863	1/1	0.92	0.23	12.28	58,58,58,58	0
55	MG	2A	3567	1/1	0.96	0.44	12.14	51,51,51,51	0
55	MG	1a	3057	1/1	0.81	0.34	12.10	81,81,81,81	0
55	MG	2A	3083	1/1	0.96	0.31	12.03	57,57,57,57	0
55	MG	2A	3482	1/1	0.84	0.39	11.98	54,54,54,54	0
55	MG	1A	3228	1/1	0.74	0.35	11.98	28,28,28,28	0
55	MG	2V	204	1/1	0.97	0.39	11.97	77,77,77,77	0
55	MG	2A	3099	1/1	0.70	0.31	11.96	52,52,52,52	0
55	MG	1P	202	1/1	0.96	0.39	11.94	28,28,28,28	0
55	MG	1D	304	1/1	0.89	0.37	11.92	37,37,37,37	0
55	MG	1A	3655	1/1	0.97	0.32	11.90	41,41,41,41	0
55	MG	2A	3720	1/1	0.84	0.28	11.86	58,58,58,58	0
55	MG	2A	3164	1/1	0.92	0.40	11.61	56,56,56,56	0
55	MG	1A	3068	1/1	0.95	0.29	11.60	27,27,27,27	0
55	MG	2A	3032	1/1	0.88	0.61	11.35	66,66,66,66	0
55	MG	1a	3136	1/1	0.90	0.35	11.19	79,79,79,79	0
55	MG	2A	3630	1/1	0.94	0.31	10.81	58,58,58,58	0
55	MG	2A	3445	1/1	0.73	0.32	10.80	48,48,48,48	0
55	MG	1A	3201	1/1	0.86	0.34	10.64	41,41,41,41	0
55	MG	2A	3019	1/1	0.63	0.22	10.54	45,45,45,45	0
55	MG	1D	310	1/1	0.95	0.52	10.29	42,42,42,42	0
55	MG	2E	301	1/1	0.96	0.27	10.25	43,43,43,43	0
55	MG	2a	1621	1/1	0.86	0.29	10.24	58,58,58,58	0
55	MG	2A	3190	1/1	0.93	0.47	10.16	68,68,68,68	0
55	MG	2A	3807	1/1	0.96	0.38	10.07	48,48,48,48	0
55	MG	2A	3052	1/1	0.97	0.43	9.94	42,42,42,42	0
55	MG	2U	201	1/1	0.88	0.47	9.90	64,64,64,64	0
55	MG	2I	101	1/1	0.93	0.76	9.85	61,61,61,61	0
55	MG	2A	3228	1/1	0.84	0.21	9.67	51,51,51,51	0
55	MG	2A	3055	1/1	0.85	0.32	9.65	49,49,49,49	0
55	MG	1A	3315	1/1	0.81	0.28	9.63	45,45,45,45	0
55	MG	1A	3549	1/1	0.87	0.33	9.62	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3655	1/1	0.78	0.27	9.56	60,60,60,60	0
55	MG	1A	3589	1/1	0.77	0.27	9.52	36,36,36,36	0
55	MG	2B	3003	1/1	0.90	0.35	9.42	73,73,73,73	0
55	MG	2B	3006	1/1	0.90	0.41	9.36	80,80,80,80	0
55	MG	1A	3141	1/1	0.98	0.31	9.27	37,37,37,37	0
55	MG	1A	3027	1/1	0.90	0.32	9.26	31,31,31,31	0
55	MG	1A	3085	1/1	0.97	0.36	9.26	34,34,34,34	0
55	MG	2A	3502	1/1	0.51	0.31	9.14	70,70,70,70	0
55	MG	2a	1781	1/1	0.94	0.26	9.12	76,76,76,76	0
55	MG	2A	3527	1/1	0.95	0.31	9.02	73,73,73,73	0
55	MG	13	101	1/1	0.94	0.36	8.95	32,32,32,32	0
55	MG	28	102	1/1	0.77	0.70	8.93	59,59,59,59	0
55	MG	13	102	1/1	0.93	0.36	8.89	44,44,44,44	0
55	MG	1A	3808	1/1	0.75	0.24	8.84	38,38,38,38	0
55	MG	1A	3711	1/1	0.92	0.26	8.68	39,39,39,39	0
55	MG	2a	1634	1/1	0.95	0.54	8.51	81,81,81,81	0
55	MG	2A	3143	1/1	0.89	0.28	8.26	53,53,53,53	0
55	MG	2A	3523	1/1	0.84	0.26	8.22	61,61,61,61	0
55	MG	1A	3642	1/1	0.89	0.54	8.19	36,36,36,36	0
55	MG	1A	3261	1/1	0.95	0.36	7.89	28,28,28,28	0
55	MG	2a	1772	1/1	0.72	0.38	7.89	92,92,92,92	0
55	MG	25	102	1/1	0.94	0.35	7.85	62,62,62,62	0
55	MG	1a	3023	1/1	0.92	0.26	7.77	53,53,53,53	0
55	MG	1U	205	1/1	0.98	0.36	7.71	29,29,29,29	0
55	MG	27	101	1/1	0.95	0.21	7.38	55,55,55,55	0
55	MG	1A	3459	1/1	0.81	0.33	7.37	50,50,50,50	0
55	MG	2A	3448	1/1	0.91	0.25	7.19	51,51,51,51	0
55	MG	1F	306	1/1	0.87	0.24	7.17	39,39,39,39	0
55	MG	1A	3726	1/1	0.91	0.24	7.10	29,29,29,29	0
55	MG	2A	3066	1/1	0.94	0.40	7.04	58,58,58,58	0
55	MG	1A	3908	1/1	0.94	0.37	7.00	33,33,33,33	0
55	MG	1A	3127	1/1	0.95	0.20	6.86	14,14,14,14	0
55	MG	2a	1603	1/1	0.88	0.24	6.83	69,69,69,69	0
55	MG	2A	3165	1/1	0.85	0.29	6.67	58,58,58,58	0
55	MG	15	101	1/1	0.82	0.25	6.58	42,42,42,42	0
55	MG	1A	3124	1/1	0.78	0.24	6.56	63,63,63,63	0
55	MG	2A	3490	1/1	0.96	0.22	6.50	33,33,33,33	0
55	MG	1D	314	1/1	0.91	0.27	6.49	34,34,34,34	0
55	MG	2a	1639	1/1	0.95	0.54	6.49	50,50,50,50	0
55	MG	2A	3086	1/1	0.84	0.29	6.48	56,56,56,56	0
55	MG	2A	3158	1/1	0.87	0.29	6.42	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3221	1/1	0.84	0.25	6.32	52,52,52,52	0
55	MG	2H	201	1/1	0.77	0.81	6.28	108,108,108,108	0
55	MG	1A	3110	1/1	0.96	0.25	6.18	38,38,38,38	0
55	MG	2A	3801	1/1	0.98	0.26	6.06	21,21,21,21	0
55	MG	1A	3273	1/1	0.98	0.25	6.05	19,19,19,19	0
55	MG	1a	3211	1/1	0.94	0.23	6.02	59,59,59,59	0
55	MG	1A	3885	1/1	0.84	0.23	5.98	37,37,37,37	0
55	MG	2a	1682	1/1	0.85	0.43	5.96	88,88,88,88	0
55	MG	1V	202	1/1	0.97	0.25	5.96	25,25,25,25	0
55	MG	2A	3157	1/1	0.92	0.29	5.96	62,62,62,62	0
55	MG	1a	3052	1/1	0.88	0.22	5.88	51,51,51,51	0
55	MG	1U	206	1/1	0.93	0.27	5.70	28,28,28,28	0
55	MG	1a	3024	1/1	0.88	0.21	5.54	57,57,57,57	0
55	MG	2A	3721	1/1	0.88	0.26	5.48	42,42,42,42	0
55	MG	2B	3011	1/1	0.48	0.21	5.43	90,90,90,90	0
55	MG	2A	3432	1/1	0.88	0.21	5.28	74,74,74,74	0
55	MG	1A	3666	1/1	0.91	0.22	5.24	45,45,45,45	0
55	MG	1A	3276	1/1	0.94	0.24	5.21	3,3,3,3	0
55	MG	1D	303	1/1	0.91	0.29	5.10	52,52,52,52	0
55	MG	1A	3208	1/1	0.92	0.22	5.07	37,37,37,37	0
55	MG	2A	3759	1/1	0.91	0.31	5.04	88,88,88,88	0
55	MG	1F	301	1/1	0.93	0.31	5.00	28,28,28,28	0
55	MG	2a	1646	1/1	0.77	0.22	4.94	56,56,56,56	0
55	MG	2e	3002	1/1	0.63	0.35	4.90	83,83,83,83	0
55	MG	1A	3646	1/1	0.89	0.20	4.86	31,31,31,31	0
55	MG	2n	502	1/1	0.58	0.42	4.85	82,82,82,82	0
55	MG	2A	3216	1/1	0.98	0.23	4.84	41,41,41,41	0
55	MG	2a	1663	1/1	0.96	0.29	4.77	63,63,63,63	0
55	MG	2a	1719	1/1	0.72	0.22	4.75	75,75,75,75	0
55	MG	2d	503	1/1	0.85	0.43	4.72	79,79,79,79	0
55	MG	1a	3015	1/1	0.97	0.22	4.65	74,74,74,74	0
55	MG	1A	3553	1/1	0.95	0.24	4.59	37,37,37,37	0
55	MG	1a	3104	1/1	0.93	0.29	4.58	82,82,82,82	0
55	MG	1A	3265	1/1	0.94	0.18	4.56	44,44,44,44	0
55	MG	2A	3365	1/1	0.94	0.22	4.54	39,39,39,39	0
55	MG	2A	3277	1/1	0.90	0.24	4.50	36,36,36,36	0
55	MG	2d	505	1/1	0.83	0.38	4.44	101,101,101,101	0
55	MG	1A	3257	1/1	0.92	0.24	4.40	40,40,40,40	0
55	MG	1A	3147	1/1	0.82	0.19	4.39	40,40,40,40	0
55	MG	1A	3551	1/1	0.86	0.35	4.39	60,60,60,60	0
55	MG	1U	201	1/1	0.92	0.27	4.36	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2n	503	1/1	0.95	0.30	4.35	85,85,85,85	0
55	MG	1A	3005	1/1	0.92	0.20	4.17	22,22,22,22	0
55	MG	1D	313	1/1	0.84	0.20	4.11	51,51,51,51	0
55	MG	1A	3482	1/1	0.96	0.20	4.05	43,43,43,43	0
55	MG	1A	3773	1/1	0.97	0.17	3.96	44,44,44,44	0
55	MG	1a	3021	1/1	0.90	0.21	3.94	63,63,63,63	0
55	MG	1A	3494	1/1	0.92	0.18	3.92	59,59,59,59	0
55	MG	2A	3479	1/1	0.89	0.22	3.76	40,40,40,40	0
55	MG	2A	3123	1/1	0.94	0.24	3.73	43,43,43,43	0
55	MG	1A	3256	1/1	0.93	0.20	3.66	41,41,41,41	0
55	MG	2A	3095	1/1	0.86	0.17	3.64	64,64,64,64	0
55	MG	2A	3414	1/1	0.93	0.23	3.61	72,72,72,72	0
55	MG	1R	203	1/1	0.95	0.22	3.57	19,19,19,19	0
55	MG	1A	3372	1/1	0.96	0.18	3.51	29,29,29,29	0
55	MG	1F	302	1/1	0.81	0.23	3.33	35,35,35,35	0
55	MG	1A	3593	1/1	0.86	0.17	3.30	34,34,34,34	0
55	MG	2A	3034	1/1	0.82	0.20	3.30	54,54,54,54	0
55	MG	1D	301	1/1	0.97	0.22	3.26	32,32,32,32	0
55	MG	1A	3031	1/1	0.78	0.20	3.26	22,22,22,22	0
55	MG	1a	3208	1/1	0.88	0.23	3.25	75,75,75,75	0
55	MG	1n	502	1/1	0.66	0.29	3.19	63,63,63,63	0
55	MG	2A	3249	1/1	0.97	0.24	3.15	43,43,43,43	0
55	MG	2A	3777	1/1	0.76	0.23	3.14	83,83,83,83	0
55	MG	1F	305	1/1	0.88	0.24	3.10	29,29,29,29	0
55	MG	2A	3199	1/1	0.98	0.27	3.10	65,65,65,65	0
55	MG	1A	3877	1/1	0.89	0.20	3.10	63,63,63,63	0
55	MG	1B	3008	1/1	0.94	0.17	3.08	57,57,57,57	0
55	MG	2a	1666	1/1	0.89	0.20	3.03	79,79,79,79	0
55	MG	1D	311	1/1	0.91	0.22	3.03	38,38,38,38	0
55	MG	1A	3446	1/1	0.92	0.20	2.99	49,49,49,49	0
55	MG	1A	3202	1/1	0.82	0.23	2.99	63,63,63,63	0
55	MG	1a	3042	1/1	0.95	0.20	2.95	53,53,53,53	0
55	MG	1a	3020	1/1	0.87	0.20	2.86	58,58,58,58	0
55	MG	1B	3023	1/1	0.85	0.18	2.77	63,63,63,63	0
55	MG	2a	1722	1/1	0.72	0.17	2.77	82,82,82,82	0
55	MG	1D	312	1/1	0.95	0.23	2.76	15,15,15,15	0
55	MG	1A	3159	1/1	0.93	0.27	2.75	30,30,30,30	0
55	MG	1A	3040	1/1	0.96	0.17	2.65	37,37,37,37	0
55	MG	1A	3313	1/1	0.88	0.20	2.60	55,55,55,55	0
55	MG	2A	3252	1/1	0.78	0.20	2.58	69,69,69,69	0
55	MG	2A	3315	1/1	0.97	0.15	2.57	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3025	1/1	0.86	0.19	2.54	38,38,38,38	0
55	MG	2A	3001	1/1	0.89	0.18	2.50	55,55,55,55	0
55	MG	2a	1694	1/1	0.78	0.23	2.41	78,78,78,78	0
55	MG	2A	3124	1/1	0.99	0.22	2.40	47,47,47,47	0
55	MG	2A	3585	1/1	0.86	0.17	2.39	68,68,68,68	0
55	MG	1A	3021	1/1	0.87	0.16	2.34	42,42,42,42	0
55	MG	2A	3766	1/1	0.91	0.17	2.34	81,81,81,81	0
55	MG	1A	3709	1/1	0.88	0.18	2.28	49,49,49,49	0
55	MG	2A	3097	1/1	0.97	0.16	2.28	35,35,35,35	0
55	MG	2A	3107	1/1	0.90	0.17	2.25	57,57,57,57	0
55	MG	2A	3568	1/1	0.92	0.24	2.24	68,68,68,68	0
55	MG	2D	306	1/1	0.94	0.21	2.19	57,57,57,57	0
55	MG	1a	3075	1/1	0.85	0.18	2.10	48,48,48,48	0
55	MG	10	103	1/1	0.90	0.21	2.09	65,65,65,65	0
55	MG	2X	102	1/1	0.80	0.47	2.03	82,82,82,82	0
55	MG	1D	318	1/1	0.86	0.18	1.99	50,50,50,50	0
55	MG	1A	3012	1/1	0.92	0.17	1.99	22,22,22,22	0
55	MG	1A	3679	1/1	0.93	0.21	1.98	44,44,44,44	0
55	MG	1A	3034	1/1	0.86	0.16	1.87	57,57,57,57	0
55	MG	2A	3100	1/1	0.92	0.20	1.85	58,58,58,58	0
55	MG	1a	3065	1/1	0.86	0.31	1.79	65,65,65,65	0
55	MG	1a	3221	1/1	0.97	0.25	1.76	71,71,71,71	0
55	MG	2D	304	1/1	0.71	0.28	1.75	55,55,55,55	0
55	MG	2A	3352	1/1	0.95	0.17	1.74	59,59,59,59	0
55	MG	2A	3757	1/1	0.93	0.35	1.71	53,53,53,53	0
55	MG	1R	204	1/1	0.84	0.24	1.71	53,53,53,53	0
55	MG	2A	3079	1/1	0.99	0.27	1.71	50,50,50,50	0
55	MG	2A	3374	1/1	0.94	0.16	1.68	62,62,62,62	0
55	MG	2A	3775	1/1	0.94	0.16	1.66	57,57,57,57	0
55	MG	2A	3700	1/1	0.96	0.16	1.66	87,87,87,87	0
55	MG	2a	1652	1/1	0.75	0.35	1.65	90,90,90,90	0
55	MG	1a	3223	1/1	0.92	0.19	1.64	54,54,54,54	0
55	MG	2A	3447	1/1	0.92	0.17	1.63	73,73,73,73	0
55	MG	1A	3130	1/1	0.89	0.24	1.57	33,33,33,33	0
55	MG	2A	3321	1/1	0.92	0.18	1.52	34,34,34,34	0
55	MG	2b	3001	1/1	0.85	0.18	1.48	85,85,85,85	0
55	MG	1a	3150	1/1	0.73	0.32	1.46	99,99,99,99	0
55	MG	2a	1615	1/1	0.88	0.15	1.41	47,47,47,47	0
55	MG	2A	3201	1/1	0.83	0.23	1.41	48,48,48,48	0
55	MG	2G	3001	1/1	0.69	0.29	1.39	90,90,90,90	0
55	MG	2a	1783	1/1	0.96	0.17	1.38	53,53,53,53	0
55	MG	2A	3808	1/1	0.91	0.21	1.37	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2B	3004	1/1	0.83	0.19	1.33	76,76,76,76	0
55	MG	1A	3897	1/1	0.99	0.20	1.24	11,11,11,11	0
55	MG	1A	3058	1/1	0.74	0.16	1.23	65,65,65,65	0
55	MG	1A	3357	1/1	0.96	0.17	1.21	20,20,20,20	0
55	MG	1A	3800	1/1	0.94	0.16	1.19	64,64,64,64	0
55	MG	2A	3077	1/1	0.95	0.19	1.17	56,56,56,56	0
55	MG	1A	3335	1/1	0.95	0.18	1.17	19,19,19,19	0
55	MG	1A	3540	1/1	0.99	0.17	1.16	19,19,19,19	0
55	MG	1a	3210	1/1	0.93	0.15	1.15	78,78,78,78	0
55	MG	1a	3107	1/1	0.89	0.18	1.13	67,67,67,67	0
55	MG	1A	3478	1/1	0.88	0.16	1.12	44,44,44,44	0
55	MG	2A	3608	1/1	0.92	0.16	1.11	62,62,62,62	0
55	MG	1A	3399	1/1	0.96	0.20	1.08	15,15,15,15	0
55	MG	1A	3116	1/1	0.82	0.12	1.07	74,74,74,74	0
55	MG	1A	3250	1/1	0.97	0.17	1.05	11,11,11,11	0
55	MG	1a	3003	1/1	0.86	0.18	1.05	65,65,65,65	0
55	MG	1A	3065	1/1	0.99	0.19	1.05	32,32,32,32	0
55	MG	1A	3299	1/1	0.97	0.17	1.02	28,28,28,28	0
55	MG	1D	317	1/1	0.93	0.25	1.01	57,57,57,57	0
55	MG	1a	3047	1/1	0.83	0.20	1.00	68,68,68,68	0
55	MG	1a	3071	1/1	0.89	0.16	0.92	53,53,53,53	0
57	ZN	1Y	501	1/1	0.99	0.13	0.90	61,61,61,61	0
55	MG	2A	3481	1/1	0.91	0.23	0.83	67,67,67,67	0
55	MG	2A	3812	1/1	0.84	0.23	0.83	60,60,60,60	0
55	MG	1A	3672	1/1	0.86	0.17	0.81	49,49,49,49	0
55	MG	2A	3547	1/1	0.86	0.16	0.81	41,41,41,41	0
55	MG	2f	8001	1/1	0.87	0.17	0.80	56,56,56,56	0
55	MG	2A	3005	1/1	0.92	0.13	0.79	44,44,44,44	0
55	MG	1a	3103	1/1	0.91	0.17	0.75	72,72,72,72	0
55	MG	2A	3007	1/1	0.95	0.19	0.67	61,61,61,61	0
55	MG	2F	309	1/1	0.86	0.20	0.66	60,60,60,60	0
55	MG	1R	202	1/1	0.97	0.17	0.62	46,46,46,46	0
55	MG	2A	3528	1/1	0.91	0.17	0.61	34,34,34,34	0
55	MG	1E	307	1/1	0.97	0.19	0.59	33,33,33,33	0
55	MG	1A	3350	1/1	0.91	0.16	0.58	46,46,46,46	0
55	MG	1k	3001	1/1	0.96	0.16	0.58	48,48,48,48	0
55	MG	1A	3367	1/1	0.95	0.18	0.51	30,30,30,30	0
55	MG	1a	3076	1/1	0.78	0.22	0.49	74,74,74,74	0
55	MG	1A	3298	1/1	0.94	0.19	0.41	27,27,27,27	0
55	MG	11	103	1/1	0.82	0.18	0.37	50,50,50,50	0
55	MG	1a	3064	1/1	0.70	0.25	0.37	78,78,78,78	0
55	MG	2D	309	1/1	0.95	0.19	0.36	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3208	1/1	0.89	0.15	0.30	60,60,60,60	0
55	MG	1A	3637	1/1	0.95	0.17	0.25	38,38,38,38	0
55	MG	2a	1629	1/1	0.80	0.15	0.24	90,90,90,90	0
55	MG	2A	3012	1/1	0.96	0.17	0.23	38,38,38,38	0
55	MG	1A	3029	1/1	0.94	0.19	0.23	38,38,38,38	0
55	MG	1A	3845	1/1	0.94	0.18	0.18	43,43,43,43	0
55	MG	2A	3223	1/1	0.95	0.13	0.17	68,68,68,68	0
57	ZN	15	106	1/1	0.99	0.16	0.17	47,47,47,47	0
55	MG	1a	3098	1/1	0.96	0.17	0.15	61,61,61,61	0
55	MG	2a	1793	1/1	0.89	0.15	0.13	61,61,61,61	0
55	MG	2A	3046	1/1	0.84	0.16	0.11	51,51,51,51	0
55	MG	1a	3018	1/1	0.86	0.16	0.10	64,64,64,64	0
55	MG	2V	203	1/1	0.92	0.15	0.08	59,59,59,59	0
55	MG	1b	3001	1/1	0.81	0.13	0.07	81,81,81,81	0
55	MG	1a	3219	1/1	0.98	0.16	0.05	63,63,63,63	0
55	MG	2A	3316	1/1	0.98	0.17	0.04	43,43,43,43	0
55	MG	2a	1754	1/1	0.82	0.17	0.03	85,85,85,85	0
55	MG	1A	3543	1/1	0.95	0.16	0.01	63,63,63,63	0
55	MG	2a	1676	1/1	0.94	0.16	-0.02	55,55,55,55	0
55	MG	1B	3013	1/1	0.86	0.12	-0.03	58,58,58,58	0
55	MG	2A	3294	1/1	0.92	0.16	-0.09	55,55,55,55	0
55	MG	1A	3349	1/1	0.91	0.16	-0.09	25,25,25,25	0
55	MG	1A	3652	1/1	0.96	0.11	-0.10	34,34,34,34	0
55	MG	1a	3151	1/1	0.85	0.15	-0.12	76,76,76,76	0
55	MG	2a	1796	1/1	0.94	0.14	-0.18	60,60,60,60	0
55	MG	1A	3901	1/1	0.81	0.16	-0.19	42,42,42,42	0
55	MG	2a	1628	1/1	0.96	0.15	-0.20	54,54,54,54	0
55	MG	2a	1707	1/1	0.92	0.19	-0.21	92,92,92,92	0
55	MG	1a	3054	1/1	0.96	0.13	-0.27	82,82,82,82	0
55	MG	1A	3255	1/1	0.87	0.17	-0.27	34,34,34,34	0
55	MG	2a	1685	1/1	0.99	0.15	-0.33	56,56,56,56	0
55	MG	1m	201	1/1	0.95	0.16	-0.36	72,72,72,72	0
55	MG	1A	3338	1/1	0.90	0.16	-0.42	20,20,20,20	0
55	MG	1A	3333	1/1	0.97	0.17	-0.44	17,17,17,17	0
57	ZN	26	101	1/1	0.96	0.12	-0.44	64,64,64,64	0
55	MG	1A	3042	1/1	0.92	0.14	-0.45	25,25,25,25	0
55	MG	2A	3202	1/1	0.96	0.15	-0.48	56,56,56,56	0
55	MG	1a	3050	1/1	0.93	0.15	-0.50	45,45,45,45	0
55	MG	1A	3138	1/1	0.90	0.12	-0.54	52,52,52,52	0
55	MG	1a	3007	1/1	0.90	0.17	-0.54	74,74,74,74	0
55	MG	1A	3436	1/1	0.93	0.16	-0.55	49,49,49,49	0
55	MG	1A	3674	1/1	0.94	0.15	-0.62	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1E	308	1/1	0.97	0.15	-0.64	49,49,49,49	0
55	MG	1A	3615	1/1	0.95	0.14	-0.66	19,19,19,19	0
55	MG	1A	3339	1/1	0.94	0.14	-0.69	18,18,18,18	0
55	MG	2A	3070	1/1	0.97	0.17	-0.69	35,35,35,35	0
55	MG	1A	3484	1/1	0.90	0.12	-0.72	47,47,47,47	0
55	MG	2A	3393	1/1	0.78	0.14	-0.73	52,52,52,52	0
57	ZN	25	104	1/1	0.99	0.11	-0.74	54,54,54,54	0
55	MG	1A	3529	1/1	0.97	0.14	-0.75	58,58,58,58	0
55	MG	2A	3385	1/1	0.93	0.17	-0.77	32,32,32,32	0
57	ZN	1n	501	1/1	0.95	0.15	-0.80	88,88,88,88	0
55	MG	1d	506	1/1	0.94	0.09	-0.81	91,91,91,91	0
55	MG	1F	313	1/1	0.95	0.15	-0.81	32,32,32,32	0
55	MG	2A	3354	1/1	0.97	0.17	-0.81	26,26,26,26	0
58	SF4	1d	501	8/8	0.99	0.14	-0.82	65,70,75,78	0
55	MG	2A	3265	1/1	0.93	0.15	-0.86	59,59,59,59	0
55	MG	1B	3004	1/1	0.97	0.11	-0.87	44,44,44,44	0
55	MG	2A	3371	1/1	0.94	0.17	-0.95	36,36,36,36	0
55	MG	1a	3044	1/1	0.93	0.11	-0.97	66,66,66,66	0
57	ZN	19	102	1/1	1.00	0.12	-0.97	43,43,43,43	0
55	MG	1A	3858	1/1	0.94	0.11	-0.97	56,56,56,56	0
55	MG	2m	201	1/1	0.76	0.11	-1.01	79,79,79,79	0
55	MG	2a	1651	1/1	0.71	0.12	-1.02	69,69,69,69	0
58	SF4	2d	501	8/8	0.99	0.12	-1.02	65,69,77,88	0
55	MG	2G	3003	1/1	0.66	0.12	-1.05	81,81,81,81	0
57	ZN	16	101	1/1	0.99	0.12	-1.05	44,44,44,44	0
55	MG	1a	3011	1/1	0.94	0.14	-1.09	32,32,32,32	0
57	ZN	29	501	1/1	0.98	0.10	-1.16	75,75,75,75	0
55	MG	2A	3577	1/1	0.93	0.10	-1.18	56,56,56,56	0
55	MG	2d	502	1/1	0.99	0.13	-1.20	74,74,74,74	0
55	MG	1A	3809	1/1	0.94	0.15	-1.23	13,13,13,13	0
55	MG	2A	3420	1/1	0.86	0.09	-1.24	60,60,60,60	0
55	MG	2A	3291	1/1	0.94	0.15	-1.24	34,34,34,34	0
55	MG	1Q	205	1/1	0.96	0.12	-1.27	43,43,43,43	0
55	MG	2A	3367	1/1	0.96	0.15	-1.27	37,37,37,37	0
55	MG	2A	3776	1/1	0.88	0.15	-1.27	43,43,43,43	0
55	MG	1a	3148	1/1	0.84	0.13	-1.27	82,82,82,82	0
55	MG	2A	3198	1/1	0.92	0.17	-1.31	27,27,27,27	0
55	MG	1A	3126	1/1	0.90	0.15	-1.32	34,34,34,34	0
55	MG	2A	3358	1/1	0.99	0.16	-1.39	45,45,45,45	0
55	MG	2X	103	1/1	0.90	0.11	-1.40	58,58,58,58	0
55	MG	2a	1752	1/1	0.87	0.09	-1.42	86,86,86,86	0
55	MG	2A	3214	1/1	0.95	0.14	-1.43	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3356	1/1	0.97	0.15	-1.45	25,25,25,25	0
55	MG	1A	3412	1/1	0.97	0.16	-1.45	12,12,12,12	0
55	MG	2F	305	1/1	0.91	0.13	-1.47	46,46,46,46	0
55	MG	1A	3514	1/1	0.89	0.12	-1.53	35,35,35,35	0
55	MG	2A	3044	1/1	0.80	0.10	-1.55	79,79,79,79	0
57	ZN	2Y	501	1/1	0.97	0.06	-1.56	95,95,95,95	0
55	MG	2A	3787	1/1	0.96	0.13	-1.59	61,61,61,61	0
55	MG	2A	3089	1/1	0.89	0.10	-1.59	56,56,56,56	0
55	MG	1A	3738	1/1	0.95	0.13	-1.62	14,14,14,14	0
55	MG	1A	3418	1/1	0.96	0.14	-1.62	26,26,26,26	0
55	MG	2a	1720	1/1	0.91	0.09	-1.66	73,73,73,73	0
55	MG	2A	3688	1/1	0.93	0.14	-1.67	66,66,66,66	0
55	MG	2A	3395	1/1	0.95	0.14	-1.68	35,35,35,35	0
55	MG	2A	3226	1/1	0.96	0.12	-1.68	44,44,44,44	0
55	MG	2A	3301	1/1	0.91	0.14	-1.74	49,49,49,49	0
55	MG	2B	3012	1/1	0.48	0.10	-1.75	87,87,87,87	0
55	MG	2D	311	1/1	0.94	0.16	-1.76	53,53,53,53	0
55	MG	2A	3296	1/1	0.97	0.15	-1.77	42,42,42,42	0
55	MG	2A	3273	1/1	0.83	0.11	-1.78	60,60,60,60	0
55	MG	1A	3007	1/1	0.91	0.12	-1.78	38,38,38,38	0
55	MG	1X	8001	1/1	0.96	0.10	-1.78	31,31,31,31	0
55	MG	1A	3730	1/1	0.86	0.12	-1.80	65,65,65,65	0
55	MG	1A	3197	1/1	0.99	0.13	-1.84	25,25,25,25	0
55	MG	1A	3425	1/1	0.95	0.14	-1.85	20,20,20,20	0
55	MG	1A	3023	1/1	0.91	0.14	-1.87	21,21,21,21	0
55	MG	2D	310	1/1	0.95	0.10	-1.88	55,55,55,55	0
57	ZN	2n	501	1/1	0.95	0.08	-1.90	108,108,108,108	0
55	MG	1A	3448	1/1	0.96	0.15	-1.91	23,23,23,23	0
57	ZN	14	501	1/1	0.97	0.04	-1.93	109,109,109,109	0
55	MG	2a	1626	1/1	0.92	0.12	-1.94	60,60,60,60	0
55	MG	1G	3001	1/1	0.98	0.10	-1.95	67,67,67,67	0
55	MG	1a	3032	1/1	0.92	0.14	-1.96	45,45,45,45	0
55	MG	1a	3191	1/1	0.90	0.13	-1.97	47,47,47,47	0
57	ZN	24	501	1/1	0.96	0.03	-1.98	129,129,129,129	0
55	MG	2A	3276	1/1	0.92	0.14	-2.00	48,48,48,48	0
55	MG	1A	3609	1/1	0.95	0.09	-2.00	62,62,62,62	0
55	MG	1A	3770	1/1	0.97	0.13	-2.01	34,34,34,34	0
55	MG	1G	3003	1/1	0.97	0.07	-2.02	47,47,47,47	0
55	MG	2E	306	1/1	0.96	0.13	-2.03	49,49,49,49	0
55	MG	2Q	8005	1/1	0.97	0.09	-2.04	62,62,62,62	0
55	MG	2A	3088	1/1	0.82	0.07	-2.11	81,81,81,81	0
55	MG	1a	3146	1/1	0.88	0.07	-2.12	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3138	1/1	0.92	0.12	-2.15	58,58,58,58	0
55	MG	1a	3036	1/1	0.91	0.12	-2.16	49,49,49,49	0
55	MG	2A	3271	1/1	0.94	0.15	-2.23	36,36,36,36	0
55	MG	1A	3443	1/1	0.87	0.14	-2.24	22,22,22,22	0
55	MG	2A	3616	1/1	0.95	0.12	-2.28	53,53,53,53	0
55	MG	2A	3189	1/1	0.97	0.16	-2.31	43,43,43,43	0
55	MG	2A	3389	1/1	0.84	0.16	-2.32	46,46,46,46	0
55	MG	1A	3460	1/1	0.99	0.13	-2.33	20,20,20,20	0
55	MG	2A	3805	1/1	0.82	0.14	-2.33	74,74,74,74	0
55	MG	1A	3283	1/1	0.94	0.11	-2.35	25,25,25,25	0
55	MG	2A	3669	1/1	0.97	0.13	-2.35	40,40,40,40	0
55	MG	1a	3207	1/1	0.91	0.12	-2.37	76,76,76,76	0
55	MG	2I	102	1/1	0.98	0.07	-2.44	60,60,60,60	0
55	MG	1A	3786	1/1	0.94	0.13	-2.45	23,23,23,23	0
55	MG	2A	3699	1/1	0.97	0.12	-2.47	38,38,38,38	0
55	MG	2A	3698	1/1	0.97	0.13	-2.47	42,42,42,42	0
55	MG	1B	3005	1/1	0.94	0.10	-2.47	54,54,54,54	0
55	MG	2A	3279	1/1	0.94	0.15	-2.51	45,45,45,45	0
55	MG	2a	1680	1/1	0.97	0.09	-2.52	55,55,55,55	0
55	MG	2A	3293	1/1	0.96	0.12	-2.53	40,40,40,40	0
55	MG	1A	3391	1/1	0.97	0.15	-2.54	18,18,18,18	0
55	MG	1A	3334	1/1	0.99	0.13	-2.56	20,20,20,20	0
55	MG	2a	1794	1/1	0.98	0.07	-2.57	70,70,70,70	0
55	MG	1A	3626	1/1	0.97	0.12	-2.57	44,44,44,44	0
55	MG	2a	1725	1/1	0.94	0.12	-2.59	86,86,86,86	0
55	MG	2A	3353	1/1	0.95	0.07	-2.61	72,72,72,72	0
55	MG	2A	3020	1/1	0.89	0.10	-2.64	42,42,42,42	0
55	MG	2Q	8002	1/1	0.92	0.08	-2.66	62,62,62,62	0
55	MG	2a	1766	1/1	0.81	0.10	-2.67	91,91,91,91	0
55	MG	28	103	1/1	0.90	0.10	-2.67	77,77,77,77	0
55	MG	2a	1612	1/1	0.97	0.12	-2.67	51,51,51,51	0
55	MG	2A	3696	1/1	0.94	0.09	-2.68	62,62,62,62	0
55	MG	1A	3416	1/1	0.97	0.13	-2.68	26,26,26,26	0
55	MG	1A	3378	1/1	0.93	0.12	-2.69	20,20,20,20	0
55	MG	2A	3153	1/1	0.98	0.10	-2.70	52,52,52,52	0
55	MG	1A	3556	1/1	0.90	0.15	-2.73	14,14,14,14	0
55	MG	2A	3033	1/1	0.97	0.09	-2.73	59,59,59,59	0
55	MG	2A	3498	1/1	0.96	0.10	-2.80	39,39,39,39	0
55	MG	20	105	1/1	0.97	0.12	-2.82	81,81,81,81	0
55	MG	1A	3340	1/1	0.96	0.12	-2.82	22,22,22,22	0
55	MG	1A	3280	1/1	0.98	0.09	-2.82	29,29,29,29	0
55	MG	1A	3453	1/1	0.99	0.13	-2.83	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3466	1/1	0.99	0.10	-2.87	37,37,37,37	0
55	MG	2A	3620	1/1	0.96	0.10	-2.87	45,45,45,45	0
55	MG	2A	3409	1/1	0.94	0.12	-2.89	48,48,48,48	0
55	MG	1A	3332	1/1	0.96	0.14	-2.91	28,28,28,28	0
55	MG	1A	3117	1/1	0.92	0.11	-2.94	44,44,44,44	0
55	MG	1A	3347	1/1	0.95	0.11	-2.97	18,18,18,18	0
55	MG	2A	3278	1/1	0.92	0.10	-3.00	56,56,56,56	0
55	MG	2A	3603	1/1	0.96	0.11	-3.03	61,61,61,61	0
55	MG	2A	3572	1/1	0.97	0.13	-3.06	55,55,55,55	0
55	MG	2A	3499	1/1	0.92	0.08	-3.08	65,65,65,65	0
55	MG	1a	3199	1/1	0.83	0.07	-3.10	68,68,68,68	0
55	MG	1A	3513	1/1	0.91	0.09	-3.14	27,27,27,27	0
55	MG	2A	3379	1/1	0.94	0.09	-3.16	61,61,61,61	0
55	MG	1A	3330	1/1	0.97	0.10	-3.17	37,37,37,37	0
55	MG	2A	3595	1/1	0.91	0.11	-3.19	52,52,52,52	0
55	MG	1A	3296	1/1	0.97	0.15	-3.27	20,20,20,20	0
55	MG	2A	3725	1/1	0.90	0.05	-3.29	64,64,64,64	0
55	MG	2A	3360	1/1	0.92	0.10	-3.31	64,64,64,64	0
55	MG	1A	3728	1/1	0.91	0.10	-3.32	54,54,54,54	0
55	MG	1a	3033	1/1	0.97	0.10	-3.32	50,50,50,50	0
55	MG	2A	3269	1/1	0.96	0.08	-3.35	45,45,45,45	0
55	MG	1A	3477	1/1	0.92	0.12	-3.36	20,20,20,20	0
55	MG	2A	3241	1/1	0.89	0.15	-3.39	49,49,49,49	0
55	MG	1A	3779	1/1	0.98	0.09	-3.41	24,24,24,24	0
55	MG	1A	3686	1/1	0.94	0.08	-3.42	35,35,35,35	0
55	MG	1A	3700	1/1	0.94	0.12	-3.42	24,24,24,24	0
55	MG	1a	3194	1/1	0.84	0.10	-3.42	83,83,83,83	0
55	MG	1a	3203	1/1	0.90	0.12	-3.45	67,67,67,67	0
55	MG	2A	3680	1/1	0.96	0.10	-3.45	66,66,66,66	0
55	MG	1A	3271	1/1	0.96	0.10	-3.47	22,22,22,22	0
55	MG	1a	3209	1/1	0.94	0.12	-3.50	52,52,52,52	0
55	MG	1P	204	1/1	0.84	0.12	-3.55	35,35,35,35	0
55	MG	2A	3300	1/1	0.98	0.11	-3.56	36,36,36,36	0
55	MG	2A	3691	1/1	0.93	0.12	-3.59	70,70,70,70	0
55	MG	2a	1611	1/1	0.91	0.10	-3.60	58,58,58,58	0
55	MG	1A	3527	1/1	0.96	0.08	-3.61	35,35,35,35	0
55	MG	1A	3308	1/1	0.94	0.08	-3.63	42,42,42,42	0
55	MG	1A	3565	1/1	0.97	0.13	-3.66	20,20,20,20	0
55	MG	1A	3060	1/1	0.89	0.11	-3.69	36,36,36,36	0
55	MG	1E	301	1/1	0.96	0.12	-3.71	15,15,15,15	0
55	MG	1A	3430	1/1	0.98	0.12	-3.72	16,16,16,16	0
55	MG	1A	3558	1/1	0.97	0.11	-3.73	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3390	1/1	0.98	0.14	-3.73	49,49,49,49	0
55	MG	1A	3383	1/1	0.94	0.12	-3.73	20,20,20,20	0
55	MG	2A	3400	1/1	0.95	0.12	-3.73	43,43,43,43	0
55	MG	2a	1608	1/1	0.92	0.09	-3.75	51,51,51,51	0
55	MG	2A	3284	1/1	0.96	0.10	-3.79	37,37,37,37	0
55	MG	1a	3174	1/1	0.97	0.11	-3.84	70,70,70,70	0
55	MG	2A	3541	1/1	0.89	0.07	-3.85	78,78,78,78	0
55	MG	1A	3530	1/1	0.89	0.12	-3.86	44,44,44,44	0
55	MG	2A	3347	1/1	0.90	0.09	-3.98	80,80,80,80	0
55	MG	1A	3696	1/1	0.91	0.10	-3.98	29,29,29,29	0
55	MG	2A	3728	1/1	0.93	0.11	-3.99	34,34,34,34	0
55	MG	1A	3344	1/1	0.95	0.08	-4.00	25,25,25,25	0
55	MG	1A	3423	1/1	0.97	0.13	-4.01	20,20,20,20	0
55	MG	1E	304	1/1	0.86	0.11	-4.01	46,46,46,46	0
55	MG	2a	1672	1/1	0.94	0.13	-4.03	57,57,57,57	0
55	MG	2A	3402	1/1	0.99	0.10	-4.04	37,37,37,37	0
55	MG	2A	3313	1/1	0.94	0.08	-4.05	40,40,40,40	0
55	MG	11	102	1/1	0.99	0.05	-4.11	56,56,56,56	0
55	MG	2A	3282	1/1	0.94	0.12	-4.13	34,34,34,34	0
55	MG	1A	3868	1/1	0.95	0.10	-4.18	29,29,29,29	0
55	MG	2A	3341	1/1	0.95	0.17	-4.18	34,34,34,34	0
55	MG	1A	3776	1/1	0.97	0.10	-4.19	43,43,43,43	0
55	MG	2A	3274	1/1	0.96	0.05	-4.20	61,61,61,61	0
55	MG	1a	3220	1/1	0.93	0.08	-4.20	65,65,65,65	0
55	MG	1A	3639	1/1	0.96	0.10	-4.22	47,47,47,47	0
55	MG	2A	3288	1/1	0.99	0.07	-4.23	30,30,30,30	0
55	MG	1A	3884	1/1	0.94	0.07	-4.23	18,18,18,18	0
55	MG	2A	3684	1/1	0.90	0.12	-4.26	57,57,57,57	0
55	MG	1A	3813	1/1	0.95	0.08	-4.28	25,25,25,25	0
55	MG	18	3303	1/1	0.96	0.07	-4.32	52,52,52,52	0
55	MG	1A	3352	1/1	0.94	0.09	-4.36	22,22,22,22	0
55	MG	2A	3722	1/1	0.91	0.08	-4.37	67,67,67,67	0
55	MG	1A	3417	1/1	0.97	0.10	-4.50	22,22,22,22	0
55	MG	1A	3661	1/1	0.98	0.07	-4.51	33,33,33,33	0
55	MG	2A	3384	1/1	0.98	0.09	-4.53	68,68,68,68	0
55	MG	1A	3001	1/1	0.90	0.10	-4.54	32,32,32,32	0
55	MG	1A	3329	1/1	0.98	0.11	-4.54	40,40,40,40	0
55	MG	2A	3467	1/1	0.96	0.08	-4.60	57,57,57,57	0
55	MG	1a	3110	1/1	0.98	0.07	-4.69	52,52,52,52	0
55	MG	2A	3361	1/1	0.94	0.07	-4.69	64,64,64,64	0
55	MG	1A	3447	1/1	0.99	0.15	-4.71	17,17,17,17	0
55	MG	2A	3657	1/1	0.93	0.08	-4.73	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3452	1/1	0.98	0.07	-4.75	51,51,51,51	0
55	MG	2A	3597	1/1	0.92	0.10	-4.78	51,51,51,51	0
55	MG	2A	3709	1/1	0.99	0.09	-4.79	45,45,45,45	0
55	MG	1a	3094	1/1	0.91	0.09	-4.86	46,46,46,46	0
55	MG	1a	3171	1/1	0.98	0.10	-4.89	50,50,50,50	0
55	MG	2a	1786	1/1	0.92	0.07	-4.97	90,90,90,90	0
55	MG	2A	3238	1/1	0.98	0.09	-4.98	38,38,38,38	0
55	MG	1a	3013	1/1	0.96	0.05	-5.18	72,72,72,72	0
55	MG	2A	3730	1/1	0.97	0.12	-5.20	56,56,56,56	0
55	MG	2a	1743	1/1	0.97	0.04	-5.22	55,55,55,55	0
55	MG	1A	3724	1/1	0.93	0.06	-5.26	71,71,71,71	0
55	MG	2A	3359	1/1	0.92	0.07	-5.29	51,51,51,51	0
55	MG	2A	3304	1/1	0.83	0.09	-5.29	48,48,48,48	0
55	MG	1Q	202	1/1	0.97	0.07	-5.30	39,39,39,39	0
55	MG	2a	1771	1/1	0.98	0.07	-5.33	55,55,55,55	0
55	MG	2a	1763	1/1	0.96	0.09	-5.37	55,55,55,55	0
55	MG	2A	3311	1/1	0.94	0.14	-5.38	42,42,42,42	0
55	MG	1B	3016	1/1	0.90	0.07	-5.42	51,51,51,51	0
55	MG	2A	3422	1/1	0.95	0.08	-5.44	52,52,52,52	0
55	MG	2A	3617	1/1	0.94	0.09	-5.44	33,33,33,33	0
55	MG	2A	3780	1/1	0.94	0.11	-5.47	40,40,40,40	0
55	MG	1a	3029	1/1	0.84	0.09	-5.48	55,55,55,55	0
55	MG	2A	3726	1/1	0.85	0.09	-5.53	41,41,41,41	0
55	MG	2A	3006	1/1	0.95	0.12	-5.54	36,36,36,36	0
55	MG	2A	3525	1/1	0.85	0.07	-5.56	50,50,50,50	0
55	MG	2A	3763	1/1	0.95	0.12	-5.57	41,41,41,41	0
55	MG	1A	3844	1/1	0.97	0.07	-5.64	27,27,27,27	0
55	MG	1A	3572	1/1	0.95	0.11	-5.74	41,41,41,41	0
55	MG	1A	3437	1/1	0.98	0.07	-5.74	34,34,34,34	0
55	MG	2A	3713	1/1	0.96	0.03	-5.76	79,79,79,79	0
55	MG	1A	3327	1/1	0.93	0.13	-5.81	18,18,18,18	0
55	MG	2A	3587	1/1	0.88	0.08	-5.82	68,68,68,68	0
55	MG	1A	3305	1/1	0.96	0.14	-5.83	16,16,16,16	0
55	MG	2A	3519	1/1	0.95	0.10	-5.85	73,73,73,73	0
55	MG	2A	3239	1/1	0.98	0.09	-5.95	38,38,38,38	0
55	MG	1A	3481	1/1	0.93	0.10	-6.00	23,23,23,23	0
55	MG	2A	3419	1/1	0.96	0.08	-6.05	33,33,33,33	0
55	MG	2A	3645	1/1	0.98	0.08	-6.08	62,62,62,62	0
55	MG	1A	3644	1/1	0.95	0.12	-6.12	18,18,18,18	0
55	MG	2A	3492	1/1	0.98	0.07	-6.12	52,52,52,52	0
55	MG	2a	1669	1/1	0.96	0.10	-6.13	46,46,46,46	0
55	MG	2A	3286	1/1	0.94	0.11	-6.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3693	1/1	0.86	0.07	-6.27	42,42,42,42	0
55	MG	1A	3454	1/1	0.90	0.08	-6.32	56,56,56,56	0
55	MG	1A	3752	1/1	0.98	0.07	-6.38	22,22,22,22	0
55	MG	1A	3422	1/1	0.97	0.10	-6.61	30,30,30,30	0
55	MG	1A	3325	1/1	0.98	0.06	-6.71	28,28,28,28	0
55	MG	2A	3235	1/1	0.96	0.08	-6.74	69,69,69,69	0
55	MG	1A	3768	1/1	0.95	0.11	-6.81	46,46,46,46	0
55	MG	2E	302	1/1	0.97	0.06	-6.81	35,35,35,35	0
55	MG	2A	3469	1/1	0.84	0.13	-6.87	68,68,68,68	0
55	MG	1A	3451	1/1	0.92	0.06	-7.15	43,43,43,43	0
55	MG	1A	3663	1/1	0.95	0.08	-7.19	26,26,26,26	0
55	MG	2A	3694	1/1	0.94	0.04	-7.21	65,65,65,65	0
55	MG	1A	3284	1/1	0.98	0.12	-7.27	43,43,43,43	0
55	MG	1A	3793	1/1	0.97	0.06	-7.33	52,52,52,52	0
55	MG	1A	3342	1/1	0.97	0.09	-7.42	21,21,21,21	0
55	MG	2A	3601	1/1	0.94	0.10	-7.44	58,58,58,58	0
55	MG	1A	3470	1/1	0.92	0.10	-7.46	28,28,28,28	0
55	MG	2A	3333	1/1	0.96	0.13	-7.60	42,42,42,42	0
55	MG	1A	3681	1/1	0.85	0.06	-7.61	38,38,38,38	0
55	MG	1A	3306	1/1	0.98	0.12	-7.70	14,14,14,14	0
55	MG	2A	3250	1/1	0.84	0.09	-7.77	31,31,31,31	0
55	MG	1A	3785	1/1	0.98	0.08	-7.79	25,25,25,25	0
55	MG	1A	3369	1/1	0.97	0.07	-7.83	14,14,14,14	0
55	MG	2A	3571	1/1	0.90	0.12	-7.87	41,41,41,41	0
55	MG	2A	3326	1/1	0.97	0.10	-8.07	35,35,35,35	0
55	MG	1A	3282	1/1	0.95	0.09	-8.07	26,26,26,26	0
55	MG	1a	3091	1/1	0.98	0.08	-8.26	37,37,37,37	0
55	MG	2A	3225	1/1	0.88	0.09	-8.59	51,51,51,51	0
55	MG	2a	1776	1/1	0.84	0.10	-8.63	80,80,80,80	0
55	MG	1A	3432	1/1	0.90	0.08	-8.71	49,49,49,49	0
55	MG	1A	3462	1/1	0.95	0.04	-8.87	40,40,40,40	0
55	MG	1a	3198	1/1	0.96	0.05	-8.96	47,47,47,47	0
55	MG	1A	3442	1/1	0.95	0.07	-9.06	49,49,49,49	0
55	MG	1A	3740	1/1	0.98	0.04	-9.17	26,26,26,26	0
55	MG	1a	3072	1/1	0.96	0.06	-9.29	65,65,65,65	0
55	MG	2A	3614	1/1	0.86	0.06	-9.32	58,58,58,58	0
55	MG	1A	3871	1/1	0.95	0.09	-9.34	21,21,21,21	0
55	MG	1A	3405	1/1	0.98	0.09	-10.04	42,42,42,42	0
55	MG	1A	3766	1/1	0.95	0.07	-10.09	39,39,39,39	0
55	MG	2A	3364	1/1	0.96	0.07	-10.45	60,60,60,60	0
55	MG	1A	3782	1/1	0.98	0.06	-11.06	33,33,33,33	0
55	MG	2A	3206	1/1	0.98	0.09	-12.76	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3879	1/1	0.96	0.10	-13.79	41,41,41,41	0
55	MG	1A	3818	1/1	0.96	0.05	-14.65	24,24,24,24	0
55	MG	2A	3648	1/1	0.97	0.06	-15.71	34,34,34,34	0
55	MG	2A	3283	1/1	0.96	0.09	-19.63	37,37,37,37	0
55	MG	2a	1688	1/1	0.92	0.09	-21.52	56,56,56,56	0
55	MG	1A	3429	1/1	0.99	0.10	-21.64	26,26,26,26	0
55	MG	2A	3220	1/1	0.98	0.10	-	66,66,66,66	0
55	MG	2a	1748	1/1	0.92	0.05	-	79,79,79,79	0
55	MG	2a	1746	1/1	0.97	0.06	-	69,69,69,69	0
55	MG	2A	3471	1/1	0.75	0.16	-	79,79,79,79	0
55	MG	2a	1631	1/1	0.68	0.55	-	85,85,85,85	0
55	MG	2a	1635	1/1	0.87	0.48	-	77,77,77,77	0
55	MG	2A	3629	1/1	0.78	0.10	-	74,74,74,74	0
55	MG	1A	3172	1/1	0.87	0.38	-	50,50,50,50	0
55	MG	2A	3418	1/1	0.92	0.11	-	55,55,55,55	0
55	MG	1A	3047	1/1	0.96	0.15	-	24,24,24,24	0
55	MG	2A	3267	1/1	0.97	0.25	-	61,61,61,61	0
55	MG	1A	3214	1/1	0.89	0.21	-	40,40,40,40	0
55	MG	2B	3007	1/1	0.87	0.12	-	81,81,81,81	0
55	MG	2a	1733	1/1	0.92	0.16	-	67,67,67,67	0
55	MG	1A	3678	1/1	0.82	0.37	-	37,37,37,37	0
55	MG	1a	3006	1/1	0.88	0.48	-	74,74,74,74	0
55	MG	1B	3015	1/1	0.71	0.16	-	66,66,66,66	0
55	MG	2A	3607	1/1	0.94	0.12	-	80,80,80,80	0
55	MG	2A	3707	1/1	0.81	0.46	-	75,75,75,75	0
55	MG	1A	3559	1/1	0.96	0.18	-	26,26,26,26	0
55	MG	1A	3729	1/1	0.90	0.21	-	47,47,47,47	0
55	MG	1A	3004	1/1	0.83	0.28	-	41,41,41,41	0
55	MG	1A	3461	1/1	0.96	0.09	-	63,63,63,63	0
55	MG	2A	3450	1/1	0.95	0.16	-	40,40,40,40	0
55	MG	2A	3429	1/1	0.90	0.10	-	64,64,64,64	0
55	MG	2A	3551	1/1	0.97	0.06	-	71,71,71,71	0
55	MG	2A	3532	1/1	0.95	0.06	-	84,84,84,84	0
55	MG	1A	3180	1/1	0.84	0.37	-	48,48,48,48	0
55	MG	1a	3069	1/1	0.86	0.19	-	62,62,62,62	0
55	MG	2A	3778	1/1	0.97	0.21	-	50,50,50,50	0
55	MG	1A	3769	1/1	0.99	0.06	-	61,61,61,61	0
55	MG	2A	3627	1/1	0.72	0.24	-	66,66,66,66	0
55	MG	1a	3010	1/1	0.93	0.14	-	78,78,78,78	0
55	MG	2A	3319	1/1	0.89	0.06	-	78,78,78,78	0
55	MG	1A	3538	1/1	0.78	0.26	-	60,60,60,60	0
55	MG	1A	3346	1/1	0.93	0.09	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3236	1/1	0.94	0.08	-	80,80,80,80	0
55	MG	2a	1624	1/1	0.99	0.19	-	53,53,53,53	0
55	MG	2A	3136	1/1	0.79	0.48	-	55,55,55,55	0
55	MG	2A	3232	1/1	0.90	0.08	-	67,67,67,67	0
55	MG	1A	3431	1/1	0.94	0.12	-	40,40,40,40	0
55	MG	1A	3384	1/1	0.92	0.45	-	58,58,58,58	0
55	MG	1A	3761	1/1	0.87	0.12	-	64,64,64,64	0
55	MG	2A	3773	1/1	0.75	0.12	-	85,85,85,85	0
55	MG	2A	3558	1/1	0.94	0.08	-	59,59,59,59	0
55	MG	1A	3003	1/1	0.98	0.09	-	20,20,20,20	0
55	MG	2A	3444	1/1	0.95	0.14	-	31,31,31,31	0
55	MG	2a	1655	1/1	0.97	0.06	-	84,84,84,84	0
55	MG	2A	3309	1/1	0.96	0.09	-	65,65,65,65	0
55	MG	1A	3055	1/1	0.93	0.23	-	53,53,53,53	0
55	MG	1a	3134	1/1	0.87	0.25	-	78,78,78,78	0
55	MG	1A	3676	1/1	0.82	0.22	-	70,70,70,70	0
55	MG	1A	3499	1/1	0.92	0.12	-	59,59,59,59	0
55	MG	2A	3363	1/1	0.91	0.14	-	50,50,50,50	0
55	MG	1A	3554	1/1	0.76	0.23	-	69,69,69,69	0
55	MG	1A	3823	1/1	0.94	0.12	-	28,28,28,28	0
55	MG	1A	3697	1/1	0.98	0.13	-	19,19,19,19	0
55	MG	2a	1728	1/1	0.93	0.13	-	86,86,86,86	0
55	MG	2A	3768	1/1	0.24	0.35	-	95,95,95,95	0
55	MG	2A	3437	1/1	0.96	0.19	-	78,78,78,78	0
55	MG	2A	3254	1/1	0.96	0.26	-	54,54,54,54	0
55	MG	1A	3668	1/1	0.85	0.08	-	85,85,85,85	0
55	MG	2A	3537	1/1	0.90	0.16	-	61,61,61,61	0
55	MG	1A	3911	1/1	0.84	0.29	-	39,39,39,39	0
55	MG	2A	3744	1/1	0.96	0.21	-	64,64,64,64	0
55	MG	2A	3612	1/1	0.82	0.16	-	38,38,38,38	0
55	MG	1A	3288	1/1	0.98	0.14	-	26,26,26,26	0
55	MG	1A	3038	1/1	0.89	0.49	-	66,66,66,66	0
55	MG	2A	3712	1/1	0.92	0.15	-	63,63,63,63	0
55	MG	2A	3320	1/1	0.65	0.13	-	79,79,79,79	0
55	MG	2a	1661	1/1	0.97	0.26	-	63,63,63,63	0
55	MG	2a	1668	1/1	0.92	0.08	-	51,51,51,51	0
55	MG	1A	3101	1/1	0.85	0.66	-	63,63,63,63	0
55	MG	1A	3583	1/1	0.96	0.22	-	37,37,37,37	0
55	MG	1A	3772	1/1	0.91	0.16	-	37,37,37,37	0
55	MG	1A	3157	1/1	0.89	0.15	-	57,57,57,57	0
55	MG	2a	1674	1/1	0.67	0.19	-	89,89,89,89	0
55	MG	1A	3895	1/1	0.72	0.46	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1604	1/1	0.98	0.15	-	53,53,53,53	0
55	MG	1a	3127	1/1	0.96	0.10	-	53,53,53,53	0
55	MG	1a	3155	1/1	0.95	0.11	-	78,78,78,78	0
55	MG	1A	3272	1/1	0.90	0.26	-	56,56,56,56	0
55	MG	2A	3604	1/1	0.95	0.34	-	65,65,65,65	0
55	MG	2A	3711	1/1	0.97	0.08	-	70,70,70,70	0
55	MG	1a	3009	1/1	0.91	0.30	-	69,69,69,69	0
55	MG	2A	3350	1/1	0.91	0.09	-	49,49,49,49	0
55	MG	1A	3375	1/1	0.94	0.14	-	51,51,51,51	0
55	MG	10	101	1/1	0.84	0.66	-	52,52,52,52	0
55	MG	1A	3420	1/1	0.93	0.13	-	27,27,27,27	0
55	MG	1A	3009	1/1	0.88	0.24	-	28,28,28,28	0
55	MG	1A	3614	1/1	0.98	0.15	-	70,70,70,70	0
55	MG	2A	3820	1/1	0.95	0.11	-	69,69,69,69	0
55	MG	2A	3378	1/1	0.96	0.15	-	51,51,51,51	0
55	MG	1A	3569	1/1	0.83	0.16	-	43,43,43,43	0
55	MG	2A	3405	1/1	0.98	0.08	-	43,43,43,43	0
55	MG	1A	3533	1/1	0.81	0.14	-	60,60,60,60	0
55	MG	1a	3083	1/1	0.97	0.25	-	67,67,67,67	0
55	MG	1a	3059	1/1	0.95	0.16	-	80,80,80,80	0
55	MG	10	106	1/1	0.94	0.07	-	58,58,58,58	0
55	MG	2A	3813	1/1	0.67	0.44	-	57,57,57,57	0
55	MG	1A	3205	1/1	0.84	0.50	-	44,44,44,44	0
55	MG	1a	3204	1/1	0.94	0.06	-	72,72,72,72	0
55	MG	1A	3395	1/1	0.94	0.10	-	44,44,44,44	0
55	MG	2A	3253	1/1	0.94	0.15	-	56,56,56,56	0
55	MG	15	105	1/1	0.90	0.30	-	43,43,43,43	0
55	MG	1A	3267	1/1	0.84	0.12	-	79,79,79,79	0
55	MG	1A	3737	1/1	0.94	0.11	-	14,14,14,14	0
55	MG	1A	3196	1/1	0.78	0.24	-	36,36,36,36	0
55	MG	1A	3790	1/1	0.73	0.21	-	84,84,84,84	0
55	MG	2A	3682	1/1	0.96	0.17	-	67,67,67,67	0
55	MG	28	101	1/1	0.78	1.05	-	64,64,64,64	0
55	MG	2A	3028	1/1	0.93	0.29	-	64,64,64,64	0
55	MG	1A	3207	1/1	0.94	0.34	-	45,45,45,45	0
55	MG	2A	3042	1/1	0.94	0.17	-	27,27,27,27	0
55	MG	2A	3317	1/1	0.92	0.15	-	55,55,55,55	0
55	MG	1h	3001	1/1	0.80	0.64	-	63,63,63,63	0
55	MG	1A	3164	1/1	0.81	0.30	-	59,59,59,59	0
55	MG	2A	3789	1/1	0.90	0.21	-	62,62,62,62	0
55	MG	1E	305	1/1	0.94	0.16	-	26,26,26,26	0
55	MG	1A	3348	1/1	0.90	0.08	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3849	1/1	0.92	0.27	-	89,89,89,89	0
55	MG	2a	1795	1/1	0.91	0.16	-	57,57,57,57	0
55	MG	1A	3134	1/1	0.80	0.23	-	65,65,65,65	0
55	MG	1A	3368	1/1	0.94	0.19	-	29,29,29,29	0
55	MG	1A	3227	1/1	0.85	0.40	-	34,34,34,34	0
55	MG	1A	3801	1/1	0.94	0.04	-	56,56,56,56	0
55	MG	2A	3675	1/1	0.82	0.15	-	70,70,70,70	0
55	MG	1A	3006	1/1	0.95	0.11	-	21,21,21,21	0
55	MG	2A	3002	1/1	0.93	0.12	-	63,63,63,63	0
55	MG	2a	1749	1/1	0.95	0.05	-	80,80,80,80	0
55	MG	1A	3542	1/1	0.98	0.11	-	77,77,77,77	0
55	MG	2A	3792	1/1	0.41	1.03	-	79,79,79,79	0
55	MG	1a	3145	1/1	0.88	0.23	-	77,77,77,77	0
55	MG	1A	3311	1/1	0.94	0.06	-	34,34,34,34	0
55	MG	2A	3803	1/1	0.81	0.52	-	69,69,69,69	0
55	MG	2A	3045	1/1	0.89	0.25	-	46,46,46,46	0
55	MG	2A	3733	1/1	0.93	0.07	-	60,60,60,60	0
55	MG	2A	3209	1/1	0.97	0.10	-	81,81,81,81	0
55	MG	2A	3560	1/1	0.91	0.19	-	53,53,53,53	0
55	MG	1A	3057	1/1	0.88	0.07	-	54,54,54,54	0
55	MG	1A	3596	1/1	0.92	0.23	-	58,58,58,58	0
55	MG	2A	3636	1/1	0.81	0.08	-	73,73,73,73	0
55	MG	1A	3758	1/1	0.80	0.64	-	53,53,53,53	0
55	MG	2a	1717	1/1	0.71	0.17	-	73,73,73,73	0
55	MG	1A	3656	1/1	0.90	0.25	-	79,79,79,79	0
55	MG	1a	3181	1/1	0.83	0.08	-	74,74,74,74	0
55	MG	1A	3111	1/1	0.83	0.41	-	42,42,42,42	0
55	MG	2A	3476	1/1	0.64	0.48	-	78,78,78,78	0
55	MG	1A	3084	1/1	0.66	0.70	-	47,47,47,47	0
55	MG	2A	3563	1/1	0.59	0.65	-	77,77,77,77	0
55	MG	1A	3090	1/1	0.81	0.45	-	37,37,37,37	0
55	MG	1A	3136	1/1	0.89	0.10	-	68,68,68,68	0
55	MG	2a	1695	1/1	0.98	0.24	-	58,58,58,58	0
55	MG	1A	3653	1/1	0.94	0.14	-	62,62,62,62	0
55	MG	2A	3431	1/1	0.79	0.31	-	77,77,77,77	0
55	MG	1A	3022	1/1	0.93	0.42	-	31,31,31,31	0
55	MG	1A	3526	1/1	0.78	0.14	-	64,64,64,64	0
55	MG	1A	3837	1/1	0.74	0.08	-	84,84,84,84	0
55	MG	1A	3907	1/1	0.90	0.28	-	46,46,46,46	0
55	MG	1S	201	1/1	0.88	0.36	-	55,55,55,55	0
55	MG	2a	1740	1/1	0.98	0.05	-	70,70,70,70	0
55	MG	2a	1648	1/1	0.87	0.13	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3719	1/1	0.73	0.18	-	70,70,70,70	0
55	MG	2A	3811	1/1	0.91	0.17	-	67,67,67,67	0
55	MG	2a	1788	1/1	0.89	0.04	-	86,86,86,86	0
55	MG	2A	3058	1/1	0.78	1.07	-	53,53,53,53	0
55	MG	1a	3201	1/1	0.95	0.14	-	92,92,92,92	0
55	MG	1A	3512	1/1	0.93	0.27	-	46,46,46,46	0
55	MG	1A	3806	1/1	0.82	0.12	-	65,65,65,65	0
55	MG	2A	3337	1/1	0.87	0.14	-	79,79,79,79	0
55	MG	1A	3011	1/1	0.84	0.35	-	41,41,41,41	0
55	MG	2A	3193	1/1	0.78	0.10	-	76,76,76,76	0
55	MG	2a	1645	1/1	0.81	0.31	-	63,63,63,63	0
55	MG	1A	3804	1/1	0.88	0.09	-	87,87,87,87	0
55	MG	1A	3078	1/1	0.92	0.56	-	39,39,39,39	0
55	MG	1A	3221	1/1	0.83	0.14	-	56,56,56,56	0
55	MG	2A	3771	1/1	0.78	0.13	-	68,68,68,68	0
55	MG	2A	3817	1/1	0.98	0.13	-	65,65,65,65	0
55	MG	2A	3754	1/1	0.83	0.24	-	101,101,101,101	0
55	MG	1A	3374	1/1	0.98	0.09	-	62,62,62,62	0
55	MG	2A	3761	1/1	0.89	0.12	-	38,38,38,38	0
55	MG	2A	3738	1/1	0.95	0.10	-	86,86,86,86	0
55	MG	1A	3281	1/1	0.88	0.10	-	54,54,54,54	0
55	MG	2A	3053	1/1	0.89	0.17	-	57,57,57,57	0
55	MG	2A	3515	1/1	0.94	0.22	-	52,52,52,52	0
55	MG	1A	3317	1/1	0.89	0.11	-	73,73,73,73	0
55	MG	1A	3827	1/1	0.96	0.13	-	64,64,64,64	0
55	MG	1a	3121	1/1	0.97	0.49	-	62,62,62,62	0
55	MG	1d	503	1/1	0.73	0.33	-	63,63,63,63	0
55	MG	1A	3567	1/1	0.94	0.23	-	30,30,30,30	0
55	MG	1a	3055	1/1	0.88	0.58	-	47,47,47,47	0
55	MG	2a	1653	1/1	0.67	0.44	-	85,85,85,85	0
55	MG	2A	3661	1/1	0.85	0.07	-	85,85,85,85	0
55	MG	2A	3593	1/1	0.86	0.19	-	68,68,68,68	0
55	MG	1A	3810	1/1	0.95	0.11	-	27,27,27,27	0
55	MG	1D	315	1/1	0.83	0.36	-	68,68,68,68	0
55	MG	1A	3093	1/1	0.88	0.33	-	43,43,43,43	0
55	MG	1A	3764	1/1	0.81	0.09	-	67,67,67,67	0
55	MG	1A	3407	1/1	0.92	0.05	-	48,48,48,48	0
55	MG	1U	202	1/1	0.95	0.18	-	43,43,43,43	0
55	MG	2A	3625	1/1	0.88	0.09	-	74,74,74,74	0
55	MG	2A	3113	1/1	0.78	0.20	-	66,66,66,66	0
55	MG	1A	3658	1/1	0.84	0.51	-	38,38,38,38	0
55	MG	2A	3108	1/1	0.78	0.29	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3745	1/1	0.80	0.07	-	54,54,54,54	0
55	MG	1A	3105	1/1	0.68	0.30	-	46,46,46,46	0
55	MG	1A	3076	1/1	0.91	0.23	-	63,63,63,63	0
55	MG	1A	3161	1/1	0.85	0.41	-	55,55,55,55	0
55	MG	1A	3435	1/1	0.94	0.08	-	69,69,69,69	0
55	MG	2A	3806	1/1	0.94	0.19	-	73,73,73,73	0
55	MG	1A	3502	1/1	0.98	0.11	-	62,62,62,62	0
55	MG	1a	3080	1/1	0.97	0.11	-	69,69,69,69	0
55	MG	1A	3323	1/1	0.93	0.19	-	46,46,46,46	0
55	MG	1A	3587	1/1	0.98	0.06	-	50,50,50,50	0
55	MG	2a	1623	1/1	0.81	0.25	-	78,78,78,78	0
55	MG	2A	3819	1/1	0.73	0.17	-	90,90,90,90	0
55	MG	1A	3591	1/1	0.93	0.08	-	30,30,30,30	0
55	MG	2a	1689	1/1	0.92	0.09	-	58,58,58,58	0
55	MG	2B	3009	1/1	0.95	0.09	-	71,71,71,71	0
55	MG	2D	301	1/1	0.91	0.78	-	47,47,47,47	0
55	MG	2A	3664	1/1	0.86	0.11	-	75,75,75,75	0
55	MG	2A	3098	1/1	0.94	0.19	-	53,53,53,53	0
55	MG	2a	1787	1/1	0.70	0.18	-	80,80,80,80	0
55	MG	2A	3791	1/1	0.96	0.08	-	45,45,45,45	0
55	MG	1a	3217	1/1	0.88	0.14	-	87,87,87,87	0
55	MG	2A	3421	1/1	0.88	0.30	-	58,58,58,58	0
55	MG	2A	3666	1/1	0.91	0.05	-	70,70,70,70	0
55	MG	2A	3348	1/1	0.88	0.10	-	76,76,76,76	0
55	MG	1A	3797	1/1	0.98	0.06	-	28,28,28,28	0
55	MG	2A	3570	1/1	0.91	0.13	-	57,57,57,57	0
55	MG	1A	3394	1/1	0.95	0.19	-	50,50,50,50	0
55	MG	1a	3074	1/1	0.70	0.34	-	65,65,65,65	0
55	MG	1a	3043	1/1	0.91	0.42	-	68,68,68,68	0
55	MG	2A	3752	1/1	0.51	0.35	-	77,77,77,77	0
55	MG	1t	3001	1/1	0.90	0.33	-	76,76,76,76	0
55	MG	1A	3052	1/1	0.91	0.80	-	36,36,36,36	0
55	MG	1a	3048	1/1	0.78	0.14	-	66,66,66,66	0
55	MG	1a	3108	1/1	0.72	0.06	-	81,81,81,81	0
55	MG	1A	3654	1/1	0.74	0.12	-	41,41,41,41	0
55	MG	1A	3137	1/1	0.93	0.95	-	46,46,46,46	0
55	MG	2A	3652	1/1	0.88	0.63	-	53,53,53,53	0
55	MG	2A	3449	1/1	0.86	0.21	-	84,84,84,84	0
55	MG	1A	3718	1/1	0.93	0.22	-	67,67,67,67	0
55	MG	1A	3794	1/1	0.81	0.22	-	59,59,59,59	0
55	MG	2a	1633	1/1	0.86	0.27	-	79,79,79,79	0
55	MG	1A	3580	1/1	0.89	0.14	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3160	1/1	0.82	0.25	-	84,84,84,84	0
55	MG	1A	3259	1/1	0.71	0.19	-	52,52,52,52	0
55	MG	2A	3131	1/1	0.78	0.30	-	65,65,65,65	0
55	MG	1A	3886	1/1	0.93	0.16	-	61,61,61,61	0
55	MG	2A	3477	1/1	0.83	0.29	-	68,68,68,68	0
55	MG	1A	3441	1/1	0.98	0.13	-	40,40,40,40	0
55	MG	1a	3124	1/1	0.84	0.30	-	77,77,77,77	0
55	MG	1A	3913	1/1	0.75	0.42	-	63,63,63,63	0
55	MG	1a	3063	1/1	0.74	0.94	-	64,64,64,64	0
55	MG	1D	316	1/1	0.91	0.10	-	73,73,73,73	0
55	MG	2A	3501	1/1	0.97	0.11	-	76,76,76,76	0
55	MG	2A	3545	1/1	0.95	0.18	-	97,97,97,97	0
55	MG	1A	3880	1/1	0.94	0.10	-	66,66,66,66	0
55	MG	1A	3602	1/1	0.74	0.23	-	76,76,76,76	0
55	MG	2A	3673	1/1	0.75	0.35	-	65,65,65,65	0
55	MG	1a	3123	1/1	0.76	0.17	-	86,86,86,86	0
55	MG	2A	3681	1/1	0.85	0.10	-	71,71,71,71	0
55	MG	2A	3737	1/1	0.94	0.07	-	80,80,80,80	0
55	MG	2A	3740	1/1	0.92	0.24	-	68,68,68,68	0
55	MG	1a	3102	1/1	0.95	0.08	-	48,48,48,48	0
55	MG	1A	3341	1/1	0.92	0.12	-	20,20,20,20	0
55	MG	2A	3016	1/1	0.96	0.74	-	46,46,46,46	0
55	MG	2A	3524	1/1	0.94	0.09	-	67,67,67,67	0
55	MG	2a	1637	1/1	0.66	1.02	-	71,71,71,71	0
55	MG	2Q	8001	1/1	0.97	0.03	-	79,79,79,79	0
55	MG	1A	3534	1/1	0.85	0.12	-	52,52,52,52	0
55	MG	1a	3166	1/1	0.92	0.09	-	80,80,80,80	0
55	MG	2a	1782	1/1	0.96	0.20	-	70,70,70,70	0
55	MG	2B	3002	1/1	0.86	0.11	-	78,78,78,78	0
55	MG	1A	3421	1/1	0.97	0.11	-	28,28,28,28	0
55	MG	1A	3778	1/1	0.91	0.07	-	83,83,83,83	0
55	MG	2A	3215	1/1	0.88	0.24	-	80,80,80,80	0
55	MG	1a	3008	1/1	0.92	0.42	-	60,60,60,60	0
55	MG	1A	3128	1/1	0.89	0.16	-	31,31,31,31	0
55	MG	1A	3659	1/1	0.73	0.12	-	57,57,57,57	0
55	MG	1A	3169	1/1	0.85	0.19	-	62,62,62,62	0
55	MG	1A	3784	1/1	0.94	0.07	-	42,42,42,42	0
55	MG	2A	3613	1/1	0.98	0.08	-	55,55,55,55	0
55	MG	1a	3205	1/1	0.97	0.07	-	77,77,77,77	0
55	MG	1A	3836	1/1	0.91	0.12	-	54,54,54,54	0
55	MG	1A	3792	1/1	0.90	0.21	-	55,55,55,55	0
55	MG	1a	3025	1/1	0.96	0.10	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3586	1/1	0.73	0.17	-	101,101,101,101	0
55	MG	2A	3727	1/1	0.89	0.51	-	65,65,65,65	0
55	MG	2A	3628	1/1	0.94	0.31	-	63,63,63,63	0
55	MG	2A	3426	1/1	0.91	0.19	-	70,70,70,70	0
55	MG	2A	3061	1/1	0.89	0.21	-	62,62,62,62	0
55	MG	1a	3002	1/1	0.97	0.15	-	82,82,82,82	0
55	MG	1a	3022	1/1	0.65	0.66	-	66,66,66,66	0
55	MG	2a	1662	1/1	0.93	0.09	-	74,74,74,74	0
55	MG	2a	1690	1/1	0.93	0.24	-	83,83,83,83	0
55	MG	2A	3260	1/1	0.91	0.12	-	66,66,66,66	0
55	MG	1A	3264	1/1	0.88	0.14	-	37,37,37,37	0
55	MG	1A	3798	1/1	0.98	0.09	-	48,48,48,48	0
55	MG	2a	1605	1/1	0.93	0.30	-	56,56,56,56	0
55	MG	2a	1675	1/1	0.96	0.09	-	51,51,51,51	0
55	MG	1A	3046	1/1	0.86	0.27	-	38,38,38,38	0
55	MG	2A	3334	1/1	0.93	0.16	-	45,45,45,45	0
55	MG	1A	3619	1/1	0.97	0.16	-	44,44,44,44	0
55	MG	2A	3183	1/1	0.95	0.20	-	75,75,75,75	0
55	MG	1A	3688	1/1	0.95	0.09	-	26,26,26,26	0
55	MG	1a	3004	1/1	0.64	0.19	-	69,69,69,69	0
55	MG	1A	3617	1/1	0.98	0.05	-	38,38,38,38	0
55	MG	2A	3135	1/1	0.87	0.93	-	71,71,71,71	0
55	MG	2A	3794	1/1	0.79	0.13	-	75,75,75,75	0
55	MG	2A	3619	1/1	0.94	0.11	-	50,50,50,50	0
55	MG	2a	1683	1/1	0.85	0.16	-	67,67,67,67	0
55	MG	1B	3020	1/1	0.95	0.27	-	73,73,73,73	0
55	MG	2A	3463	1/1	0.85	0.32	-	76,76,76,76	0
55	MG	1A	3351	1/1	0.97	0.29	-	54,54,54,54	0
55	MG	2A	3425	1/1	0.69	0.22	-	71,71,71,71	0
55	MG	1A	3099	1/1	0.91	0.30	-	62,62,62,62	0
55	MG	1a	3185	1/1	0.82	0.17	-	68,68,68,68	0
55	MG	2A	3637	1/1	0.67	0.07	-	61,61,61,61	0
55	MG	1A	3616	1/1	0.95	0.04	-	48,48,48,48	0
55	MG	2A	3212	1/1	0.91	0.15	-	60,60,60,60	0
55	MG	1A	3632	1/1	0.97	0.11	-	49,49,49,49	0
55	MG	2A	3755	1/1	0.92	0.11	-	63,63,63,63	0
55	MG	1A	3081	1/1	0.97	0.50	-	33,33,33,33	0
55	MG	1A	3075	1/1	0.94	0.76	-	41,41,41,41	0
55	MG	1a	3092	1/1	0.88	0.07	-	85,85,85,85	0
55	MG	1A	3564	1/1	0.96	0.16	-	43,43,43,43	0
55	MG	2A	3210	1/1	0.94	0.09	-	95,95,95,95	0
55	MG	2A	3692	1/1	0.89	0.07	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1620	1/1	0.84	0.26	-	77,77,77,77	0
55	MG	19	101	1/1	0.87	0.30	-	41,41,41,41	0
55	MG	1A	3630	1/1	0.79	0.21	-	55,55,55,55	0
55	MG	1A	3550	1/1	0.89	0.27	-	44,44,44,44	0
55	MG	2A	3013	1/1	0.93	0.10	-	60,60,60,60	0
55	MG	2a	1622	1/1	0.94	0.43	-	50,50,50,50	0
55	MG	2A	3430	1/1	0.92	0.20	-	74,74,74,74	0
55	MG	1A	3715	1/1	0.90	0.04	-	85,85,85,85	0
55	MG	2a	1650	1/1	0.88	0.66	-	55,55,55,55	0
55	MG	1A	3450	1/1	0.94	0.13	-	19,19,19,19	0
55	MG	1A	3106	1/1	0.79	0.43	-	42,42,42,42	0
55	MG	1A	3219	1/1	0.85	0.19	-	49,49,49,49	0
55	MG	2a	1773	1/1	0.88	0.25	-	89,89,89,89	0
55	MG	2A	3067	1/1	0.99	0.10	-	62,62,62,62	0
55	MG	1A	3150	1/1	0.84	0.15	-	39,39,39,39	0
55	MG	1A	3675	1/1	0.82	0.56	-	47,47,47,47	0
55	MG	2A	3758	1/1	0.91	0.14	-	77,77,77,77	0
55	MG	1F	307	1/1	0.88	0.76	-	29,29,29,29	0
55	MG	1A	3734	1/1	0.72	0.41	-	45,45,45,45	0
55	MG	2A	3015	1/1	0.87	0.69	-	50,50,50,50	0
55	MG	2A	3600	1/1	0.91	0.49	-	54,54,54,54	0
55	MG	2A	3428	1/1	0.91	0.27	-	71,71,71,71	0
55	MG	2A	3366	1/1	0.90	0.05	-	92,92,92,92	0
55	MG	1a	3014	1/1	0.97	0.32	-	81,81,81,81	0
55	MG	1A	3544	1/1	0.98	0.29	-	34,34,34,34	0
55	MG	1a	3190	1/1	0.99	0.04	-	79,79,79,79	0
55	MG	1A	3683	1/1	0.97	0.28	-	51,51,51,51	0
55	MG	2A	3147	1/1	0.88	0.11	-	78,78,78,78	0
55	MG	1A	3324	1/1	0.82	0.13	-	40,40,40,40	0
55	MG	2A	3331	1/1	0.89	0.09	-	61,61,61,61	0
55	MG	1A	3821	1/1	0.95	0.10	-	54,54,54,54	0
55	MG	1A	3343	1/1	0.97	0.09	-	26,26,26,26	0
55	MG	2a	1697	1/1	0.82	0.08	-	80,80,80,80	0
55	MG	1A	3860	1/1	0.94	0.14	-	53,53,53,53	0
55	MG	1A	3492	1/1	0.98	0.16	-	50,50,50,50	0
55	MG	20	106	1/1	0.86	0.48	-	78,78,78,78	0
55	MG	1A	3235	1/1	0.93	0.36	-	38,38,38,38	0
55	MG	2A	3258	1/1	0.88	0.08	-	59,59,59,59	0
55	MG	2A	3514	1/1	0.97	0.47	-	53,53,53,53	0
55	MG	1a	3066	1/1	0.90	0.11	-	68,68,68,68	0
55	MG	2A	3192	1/1	0.79	1.03	-	64,64,64,64	0
55	MG	1A	3744	1/1	0.98	0.06	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3644	1/1	0.96	0.14	-	63,63,63,63	0
55	MG	2A	3194	1/1	0.68	0.09	-	84,84,84,84	0
55	MG	2A	3391	1/1	0.95	0.07	-	43,43,43,43	0
55	MG	2A	3799	1/1	0.86	0.31	-	83,83,83,83	0
55	MG	2A	3741	1/1	0.94	0.04	-	70,70,70,70	0
55	MG	2A	3687	1/1	0.95	0.17	-	49,49,49,49	0
55	MG	1a	3093	1/1	0.96	0.06	-	73,73,73,73	0
55	MG	1A	3120	1/1	0.82	0.61	-	34,34,34,34	0
55	MG	2A	3749	1/1	0.93	0.05	-	85,85,85,85	0
55	MG	1a	3079	1/1	0.95	0.17	-	55,55,55,55	0
55	MG	1A	3874	1/1	0.97	0.16	-	59,59,59,59	0
55	MG	2A	3172	1/1	0.53	0.34	-	69,69,69,69	0
55	MG	2A	3039	1/1	0.87	0.81	-	60,60,60,60	0
55	MG	2a	1742	1/1	0.62	0.59	-	113,113,113,113	0
55	MG	1A	3815	1/1	0.85	0.58	-	51,51,51,51	0
55	MG	2A	3159	1/1	0.84	0.78	-	58,58,58,58	0
55	MG	1A	3618	1/1	0.91	0.24	-	72,72,72,72	0
55	MG	1A	3829	1/1	0.94	0.19	-	60,60,60,60	0
55	MG	1H	8001	1/1	0.85	0.11	-	76,76,76,76	0
55	MG	2A	3690	1/1	0.90	0.19	-	84,84,84,84	0
55	MG	1A	3331	1/1	0.86	0.09	-	22,22,22,22	0
55	MG	1A	3304	1/1	0.98	0.08	-	45,45,45,45	0
55	MG	2A	3047	1/1	0.74	0.86	-	63,63,63,63	0
55	MG	1A	3702	1/1	0.48	0.73	-	55,55,55,55	0
55	MG	2a	1737	1/1	0.93	0.23	-	69,69,69,69	0
55	MG	1A	3144	1/1	0.77	0.37	-	64,64,64,64	0
55	MG	1A	3490	1/1	0.83	0.18	-	62,62,62,62	0
55	MG	2a	1670	1/1	0.82	0.13	-	84,84,84,84	0
55	MG	1A	3363	1/1	0.91	0.08	-	26,26,26,26	0
55	MG	1A	3833	1/1	0.91	0.21	-	69,69,69,69	0
55	MG	2A	3096	1/1	0.91	0.14	-	46,46,46,46	0
55	MG	1A	3504	1/1	0.96	0.19	-	19,19,19,19	0
55	MG	2A	3082	1/1	0.93	0.14	-	56,56,56,56	0
55	MG	1A	3457	1/1	0.78	0.10	-	24,24,24,24	0
55	MG	2A	3122	1/1	0.96	0.38	-	46,46,46,46	0
55	MG	1a	3197	1/1	0.86	0.15	-	82,82,82,82	0
55	MG	1a	3200	1/1	0.93	0.08	-	93,93,93,93	0
55	MG	1A	3094	1/1	0.90	0.71	-	30,30,30,30	0
55	MG	1a	3152	1/1	0.84	0.16	-	91,91,91,91	0
55	MG	2A	3739	1/1	0.97	0.07	-	69,69,69,69	0
55	MG	1A	3037	1/1	0.92	0.08	-	56,56,56,56	0
55	MG	2a	1701	1/1	0.91	0.22	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1h	3002	1/1	0.96	0.08	-	76,76,76,76	0
55	MG	1A	3506	1/1	0.77	0.16	-	71,71,71,71	0
55	MG	1W	3003	1/1	0.81	0.47	-	41,41,41,41	0
55	MG	1A	3864	1/1	0.97	0.11	-	49,49,49,49	0
55	MG	1A	3035	1/1	0.94	0.14	-	37,37,37,37	0
55	MG	2a	1714	1/1	0.97	0.12	-	71,71,71,71	0
55	MG	1A	3622	1/1	0.95	0.09	-	76,76,76,76	0
55	MG	1A	3716	1/1	0.95	0.08	-	46,46,46,46	0
55	MG	2A	3338	1/1	0.84	0.70	-	70,70,70,70	0
55	MG	2A	3695	1/1	0.96	0.10	-	97,97,97,97	0
55	MG	2A	3196	1/1	0.92	0.17	-	77,77,77,77	0
55	MG	1A	3625	1/1	0.90	0.46	-	35,35,35,35	0
55	MG	2a	1708	1/1	0.85	0.12	-	83,83,83,83	0
55	MG	2A	3186	1/1	0.87	0.87	-	61,61,61,61	0
55	MG	1B	3003	1/1	0.81	0.13	-	64,64,64,64	0
55	MG	1A	3153	1/1	0.96	0.19	-	49,49,49,49	0
55	MG	1A	3671	1/1	0.92	0.19	-	46,46,46,46	0
55	MG	1A	3181	1/1	0.58	0.24	-	51,51,51,51	0
55	MG	1a	3115	1/1	0.94	0.39	-	66,66,66,66	0
55	MG	2a	1739	1/1	0.91	0.08	-	86,86,86,86	0
55	MG	2A	3423	1/1	0.77	0.10	-	79,79,79,79	0
55	MG	2a	1751	1/1	0.91	0.18	-	107,107,107,107	0
55	MG	2A	3084	1/1	0.98	0.27	-	45,45,45,45	0
55	MG	1A	3166	1/1	0.95	0.43	-	46,46,46,46	0
55	MG	1A	3487	1/1	0.91	0.32	-	57,57,57,57	0
55	MG	2A	3631	1/1	0.81	0.32	-	86,86,86,86	0
55	MG	1A	3388	1/1	0.96	0.19	-	48,48,48,48	0
55	MG	2A	3101	1/1	0.49	0.22	-	74,74,74,74	0
55	MG	1A	3115	1/1	0.92	0.07	-	54,54,54,54	0
55	MG	2A	3453	1/1	0.97	0.18	-	81,81,81,81	0
55	MG	1a	3147	1/1	0.97	0.12	-	85,85,85,85	0
55	MG	2A	3765	1/1	0.79	0.55	-	59,59,59,59	0
55	MG	1a	3067	1/1	0.87	0.14	-	65,65,65,65	0
55	MG	1A	3404	1/1	0.82	0.09	-	60,60,60,60	0
55	MG	2A	3185	1/1	0.89	0.79	-	62,62,62,62	0
55	MG	1a	3178	1/1	0.91	0.15	-	75,75,75,75	0
55	MG	2A	3343	1/1	0.93	0.04	-	73,73,73,73	0
55	MG	1A	3623	1/1	0.71	0.30	-	56,56,56,56	0
55	MG	1A	3322	1/1	0.97	0.23	-	48,48,48,48	0
55	MG	1A	3194	1/1	0.86	0.49	-	34,34,34,34	0
55	MG	1A	3748	1/1	0.93	0.09	-	50,50,50,50	0
55	MG	1A	3013	1/1	0.96	0.07	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3449	1/1	0.91	0.16	-	21,21,21,21	0
55	MG	1A	3819	1/1	0.95	0.13	-	58,58,58,58	0
55	MG	1A	3289	1/1	0.94	0.13	-	53,53,53,53	0
55	MG	2B	3015	1/1	0.75	0.15	-	85,85,85,85	0
55	MG	2a	1726	1/1	0.90	0.09	-	78,78,78,78	0
55	MG	1A	3870	1/1	0.92	0.24	-	54,54,54,54	0
55	MG	2a	1692	1/1	0.86	0.29	-	85,85,85,85	0
55	MG	1A	3179	1/1	0.89	0.60	-	38,38,38,38	0
55	MG	1A	3297	1/1	0.95	0.16	-	15,15,15,15	0
55	MG	2A	3229	1/1	0.92	0.16	-	82,82,82,82	0
55	MG	2A	3654	1/1	0.91	0.09	-	34,34,34,34	0
55	MG	20	104	1/1	0.87	0.24	-	81,81,81,81	0
55	MG	1a	3163	1/1	0.93	0.10	-	74,74,74,74	0
55	MG	1A	3796	1/1	0.96	0.11	-	43,43,43,43	0
55	MG	1A	3694	1/1	0.91	0.10	-	35,35,35,35	0
55	MG	2l	201	1/1	0.80	0.15	-	79,79,79,79	0
55	MG	1A	3855	1/1	0.82	0.28	-	48,48,48,48	0
55	MG	2A	3373	1/1	0.97	0.11	-	48,48,48,48	0
55	MG	20	103	1/1	0.90	0.30	-	59,59,59,59	0
55	MG	1A	3713	1/1	0.83	0.20	-	98,98,98,98	0
55	MG	1A	3365	1/1	0.98	0.11	-	40,40,40,40	0
55	MG	2A	3767	1/1	0.98	0.06	-	65,65,65,65	0
55	MG	2A	3599	1/1	0.92	0.12	-	75,75,75,75	0
55	MG	2A	3491	1/1	0.96	0.10	-	51,51,51,51	0
55	MG	1A	3834	1/1	0.87	0.11	-	61,61,61,61	0
55	MG	1A	3707	1/1	0.91	0.22	-	72,72,72,72	0
55	MG	2A	3454	1/1	0.87	0.13	-	81,81,81,81	0
55	MG	2a	1673	1/1	0.91	0.15	-	63,63,63,63	0
55	MG	2A	3073	1/1	0.94	0.55	-	48,48,48,48	0
55	MG	1A	3220	1/1	0.74	0.68	-	77,77,77,77	0
55	MG	1A	3750	1/1	0.91	0.09	-	52,52,52,52	0
55	MG	2B	3001	1/1	0.97	0.12	-	64,64,64,64	0
55	MG	1A	3811	1/1	0.98	0.05	-	56,56,56,56	0
55	MG	1A	3086	1/1	0.97	0.06	-	50,50,50,50	0
55	MG	2A	3800	1/1	0.43	0.27	-	112,112,112,112	0
55	MG	1A	3191	1/1	0.96	0.19	-	66,66,66,66	0
55	MG	1A	3030	1/1	0.94	0.12	-	30,30,30,30	0
55	MG	1A	3406	1/1	0.93	0.18	-	46,46,46,46	0
55	MG	2A	3641	1/1	0.75	0.13	-	77,77,77,77	0
55	MG	1F	312	1/1	0.87	0.29	-	44,44,44,44	0
55	MG	1A	3839	1/1	0.82	0.15	-	59,59,59,59	0
55	MG	2F	310	1/1	0.95	0.15	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3523	1/1	0.88	0.19	-	56,56,56,56	0
55	MG	2A	3127	1/1	0.96	0.37	-	60,60,60,60	0
55	MG	2A	3735	1/1	0.97	0.17	-	49,49,49,49	0
55	MG	2A	3529	1/1	0.94	0.13	-	75,75,75,75	0
55	MG	2A	3462	1/1	0.82	0.18	-	62,62,62,62	0
55	MG	1a	3157	1/1	0.95	0.07	-	82,82,82,82	0
55	MG	2a	1686	1/1	0.51	0.25	-	108,108,108,108	0
55	MG	1V	203	1/1	0.97	0.12	-	60,60,60,60	0
55	MG	1A	3355	1/1	0.96	0.12	-	53,53,53,53	0
55	MG	1A	3720	1/1	0.95	0.06	-	65,65,65,65	0
55	MG	2A	3489	1/1	0.70	0.16	-	81,81,81,81	0
55	MG	2A	3442	1/1	0.89	0.23	-	81,81,81,81	0
55	MG	2A	3484	1/1	0.93	0.48	-	46,46,46,46	0
55	MG	1B	3012	1/1	0.89	0.07	-	44,44,44,44	0
55	MG	1A	3100	1/1	0.95	0.26	-	25,25,25,25	0
55	MG	2A	3237	1/1	0.92	0.17	-	67,67,67,67	0
55	MG	1A	3866	1/1	0.90	0.20	-	61,61,61,61	0
55	MG	1a	3165	1/1	0.92	0.59	-	75,75,75,75	0
55	MG	2A	3275	1/1	0.97	0.09	-	47,47,47,47	0
55	MG	2A	3245	1/1	0.90	0.31	-	78,78,78,78	0
55	MG	1A	3010	1/1	0.95	0.40	-	37,37,37,37	0
55	MG	2d	504	1/1	0.56	0.15	-	90,90,90,90	0
55	MG	1A	3805	1/1	0.93	0.07	-	65,65,65,65	0
55	MG	19	103	1/1	0.96	0.08	-	61,61,61,61	0
55	MG	1A	3316	1/1	0.92	0.11	-	58,58,58,58	0
55	MG	1A	3701	1/1	0.92	0.49	-	40,40,40,40	0
55	MG	2A	3715	1/1	0.94	0.08	-	66,66,66,66	0
55	MG	2A	3129	1/1	0.45	0.61	-	75,75,75,75	0
55	MG	1A	3643	1/1	0.93	0.11	-	34,34,34,34	0
55	MG	2A	3049	1/1	0.93	0.20	-	38,38,38,38	0
55	MG	1A	3438	1/1	0.96	0.08	-	57,57,57,57	0
55	MG	1A	3789	1/1	0.95	0.10	-	31,31,31,31	0
55	MG	1a	3168	1/1	0.70	0.10	-	79,79,79,79	0
55	MG	1A	3906	1/1	0.96	0.09	-	59,59,59,59	0
55	MG	2A	3724	1/1	0.91	0.11	-	45,45,45,45	0
55	MG	1A	3091	1/1	0.97	0.29	-	16,16,16,16	0
55	MG	2A	3142	1/1	0.56	0.98	-	60,60,60,60	0
55	MG	1A	3409	1/1	0.97	0.07	-	49,49,49,49	0
55	MG	2a	1606	1/1	0.85	0.63	-	69,69,69,69	0
55	MG	1a	3111	1/1	0.99	0.13	-	56,56,56,56	0
55	MG	2A	3705	1/1	0.86	0.20	-	75,75,75,75	0
55	MG	2A	3746	1/1	0.84	0.18	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3525	1/1	0.92	0.18	-	57,57,57,57	0
55	MG	1a	3120	1/1	0.91	0.10	-	65,65,65,65	0
55	MG	1A	3889	1/1	0.70	0.40	-	46,46,46,46	0
55	MG	1A	3294	1/1	0.92	0.06	-	33,33,33,33	0
55	MG	1A	3684	1/1	0.65	0.26	-	49,49,49,49	0
55	MG	1A	3508	1/1	0.97	0.13	-	51,51,51,51	0
55	MG	1A	3002	1/1	0.90	0.22	-	48,48,48,48	0
55	MG	1A	3234	1/1	0.96	0.12	-	48,48,48,48	0
55	MG	2A	3710	1/1	0.97	0.10	-	60,60,60,60	0
55	MG	1A	3092	1/1	0.84	0.28	-	37,37,37,37	0
55	MG	2a	1768	1/1	0.73	0.10	-	80,80,80,80	0
55	MG	1a	3153	1/1	0.88	0.14	-	57,57,57,57	0
55	MG	2A	3510	1/1	0.61	0.21	-	103,103,103,103	0
55	MG	1B	3007	1/1	0.90	0.12	-	51,51,51,51	0
55	MG	2A	3494	1/1	0.93	0.10	-	77,77,77,77	0
55	MG	1A	3519	1/1	0.75	0.12	-	46,46,46,46	0
55	MG	1A	3887	1/1	0.89	0.27	-	44,44,44,44	0
55	MG	1A	3336	1/1	0.95	0.10	-	21,21,21,21	0
55	MG	1A	3739	1/1	0.98	0.16	-	22,22,22,22	0
55	MG	2A	3589	1/1	0.87	0.25	-	82,82,82,82	0
55	MG	2A	3475	1/1	0.85	0.13	-	76,76,76,76	0
55	MG	1A	3854	1/1	0.81	0.12	-	72,72,72,72	0
55	MG	1a	3012	1/1	0.83	0.15	-	68,68,68,68	0
55	MG	1A	3275	1/1	0.96	0.16	-	27,27,27,27	0
55	MG	1A	3505	1/1	0.96	0.18	-	31,31,31,31	0
55	MG	2A	3128	1/1	0.88	0.11	-	61,61,61,61	0
55	MG	1E	306	1/1	0.79	0.18	-	52,52,52,52	0
55	MG	1A	3610	1/1	0.81	0.20	-	70,70,70,70	0
55	MG	2a	1715	1/1	0.93	0.14	-	82,82,82,82	0
55	MG	2A	3312	1/1	0.97	0.15	-	53,53,53,53	0
55	MG	1A	3373	1/1	0.94	0.11	-	58,58,58,58	0
55	MG	1A	3822	1/1	0.94	0.09	-	58,58,58,58	0
55	MG	2a	1755	1/1	0.97	0.71	-	81,81,81,81	0
55	MG	2A	3679	1/1	0.98	0.08	-	52,52,52,52	0
55	MG	1A	3563	1/1	0.75	0.22	-	59,59,59,59	0
55	MG	10	104	1/1	0.83	0.11	-	50,50,50,50	0
55	MG	1A	3209	1/1	0.94	0.17	-	72,72,72,72	0
55	MG	2a	1779	1/1	0.86	0.49	-	75,75,75,75	0
55	MG	2A	3149	1/1	0.86	0.25	-	63,63,63,63	0
55	MG	1a	3019	1/1	0.87	0.21	-	54,54,54,54	0
55	MG	2A	3424	1/1	0.95	0.20	-	50,50,50,50	0
55	MG	2A	3139	1/1	0.94	0.51	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3156	1/1	0.95	0.17	-	69,69,69,69	0
55	MG	2Q	8003	1/1	0.95	0.17	-	57,57,57,57	0
55	MG	2A	3464	1/1	0.85	0.32	-	90,90,90,90	0
55	MG	2A	3706	1/1	0.59	0.12	-	90,90,90,90	0
55	MG	2a	1791	1/1	0.91	0.21	-	71,71,71,71	0
55	MG	2A	3638	1/1	0.92	0.17	-	86,86,86,86	0
55	MG	1A	3149	1/1	0.87	0.68	-	43,43,43,43	0
55	MG	2A	3772	1/1	0.93	0.08	-	63,63,63,63	0
55	MG	1A	3064	1/1	0.91	0.32	-	29,29,29,29	0
55	MG	1A	3376	1/1	0.92	0.06	-	72,72,72,72	0
55	MG	2A	3117	1/1	0.81	0.24	-	58,58,58,58	0
55	MG	1a	3141	1/1	0.94	0.10	-	75,75,75,75	0
55	MG	2A	3355	1/1	0.98	0.03	-	76,76,76,76	0
55	MG	2A	3504	1/1	0.89	0.21	-	55,55,55,55	0
55	MG	1A	3607	1/1	0.90	0.07	-	60,60,60,60	0
55	MG	2A	3651	1/1	0.94	0.22	-	56,56,56,56	0
55	MG	1A	3066	1/1	0.83	0.60	-	45,45,45,45	0
55	MG	2A	3404	1/1	0.91	0.05	-	63,63,63,63	0
55	MG	2a	1647	1/1	0.86	0.14	-	81,81,81,81	0
55	MG	1A	3850	1/1	0.96	0.08	-	21,21,21,21	0
55	MG	2A	3380	1/1	0.87	0.21	-	81,81,81,81	0
55	MG	1a	3030	1/1	0.95	0.90	-	61,61,61,61	0
55	MG	1A	3054	1/1	0.89	0.31	-	49,49,49,49	0
55	MG	2X	101	1/1	0.87	0.20	-	61,61,61,61	0
55	MG	2B	3016	1/1	0.80	0.16	-	90,90,90,90	0
55	MG	1A	3574	1/1	0.79	0.29	-	64,64,64,64	0
55	MG	2A	3246	1/1	0.67	0.09	-	92,92,92,92	0
55	MG	1A	3717	1/1	0.97	0.09	-	35,35,35,35	0
55	MG	1A	3803	1/1	0.94	0.06	-	39,39,39,39	0
55	MG	1A	3210	1/1	0.77	0.25	-	45,45,45,45	0
55	MG	1B	3001	1/1	0.98	0.22	-	55,55,55,55	0
55	MG	2A	3118	1/1	0.94	0.32	-	52,52,52,52	0
55	MG	1A	3703	1/1	0.81	0.51	-	30,30,30,30	0
55	MG	2A	3472	1/1	0.89	0.37	-	88,88,88,88	0
55	MG	1A	3109	1/1	0.97	0.12	-	30,30,30,30	0
55	MG	2A	3218	1/1	0.89	0.07	-	52,52,52,52	0
55	MG	18	3301	1/1	0.70	0.59	-	70,70,70,70	0
55	MG	1A	3263	1/1	0.96	0.18	-	17,17,17,17	0
55	MG	1A	3156	1/1	0.87	0.75	-	54,54,54,54	0
55	MG	2A	3145	1/1	0.94	0.16	-	79,79,79,79	0
55	MG	1A	3277	1/1	0.95	0.16	-	30,30,30,30	0
55	MG	2R	203	1/1	0.95	0.18	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3230	1/1	0.70	0.35	-	50,50,50,50	0
55	MG	2A	3605	1/1	0.87	0.24	-	63,63,63,63	0
55	MG	2a	1765	1/1	0.97	0.10	-	71,71,71,71	0
55	MG	1a	3122	1/1	0.96	0.31	-	71,71,71,71	0
55	MG	1A	3402	1/1	0.92	0.29	-	43,43,43,43	0
55	MG	1A	3083	1/1	0.95	0.06	-	57,57,57,57	0
55	MG	2A	3080	1/1	0.60	0.41	-	69,69,69,69	0
55	MG	1a	3188	1/1	0.94	0.18	-	64,64,64,64	0
55	MG	1a	3028	1/1	0.79	0.23	-	55,55,55,55	0
55	MG	2A	3041	1/1	0.92	0.09	-	73,73,73,73	0
55	MG	1A	3204	1/1	0.77	0.64	-	39,39,39,39	0
55	MG	2A	3433	1/1	0.97	0.11	-	66,66,66,66	0
55	MG	2A	3624	1/1	0.90	0.83	-	62,62,62,62	0
55	MG	1A	3121	1/1	0.94	0.15	-	43,43,43,43	0
55	MG	1A	3899	1/1	0.63	0.38	-	51,51,51,51	0
55	MG	1A	3292	1/1	0.95	0.17	-	52,52,52,52	0
55	MG	2a	1710	1/1	0.75	0.41	-	86,86,86,86	0
55	MG	2A	3470	1/1	0.90	0.13	-	63,63,63,63	0
55	MG	2A	3677	1/1	0.81	0.19	-	56,56,56,56	0
55	MG	2E	307	1/1	0.90	0.07	-	73,73,73,73	0
55	MG	1A	3455	1/1	0.87	0.10	-	49,49,49,49	0
55	MG	2A	3465	1/1	0.86	0.20	-	71,71,71,71	0
55	MG	1A	3053	1/1	0.84	0.29	-	58,58,58,58	0
55	MG	1a	3037	1/1	0.99	0.17	-	68,68,68,68	0
55	MG	1A	3270	1/1	0.93	0.17	-	18,18,18,18	0
55	MG	1A	3848	1/1	0.59	0.64	-	68,68,68,68	0
55	MG	1A	3846	1/1	0.96	0.12	-	53,53,53,53	0
55	MG	1A	3552	1/1	0.71	0.39	-	45,45,45,45	0
55	MG	1A	3269	1/1	0.95	0.07	-	62,62,62,62	0
55	MG	2A	3064	1/1	0.56	0.10	-	72,72,72,72	0
55	MG	1A	3426	1/1	0.99	0.06	-	18,18,18,18	0
55	MG	2A	3487	1/1	0.80	0.39	-	68,68,68,68	0
55	MG	1A	3594	1/1	0.96	0.16	-	24,24,24,24	0
55	MG	2A	3647	1/1	0.85	0.24	-	88,88,88,88	0
55	MG	2A	3565	1/1	0.93	0.07	-	56,56,56,56	0
55	MG	2a	1706	1/1	0.93	0.27	-	63,63,63,63	0
55	MG	1A	3132	1/1	0.92	0.17	-	35,35,35,35	0
55	MG	2A	3446	1/1	0.88	0.29	-	62,62,62,62	0
55	MG	2A	3451	1/1	0.89	0.29	-	67,67,67,67	0
55	MG	1A	3859	1/1	0.85	0.35	-	87,87,87,87	0
55	MG	1a	3045	1/1	0.97	0.26	-	57,57,57,57	0
55	MG	1A	3245	1/1	0.88	0.51	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3543	1/1	0.78	0.40	-	82,82,82,82	0
55	MG	1A	3873	1/1	0.94	0.10	-	49,49,49,49	0
55	MG	2A	3535	1/1	0.83	0.27	-	86,86,86,86	0
55	MG	1A	3742	1/1	0.90	0.87	-	71,71,71,71	0
55	MG	1A	3183	1/1	0.64	0.63	-	46,46,46,46	0
55	MG	2A	3723	1/1	0.96	0.05	-	73,73,73,73	0
55	MG	2A	3289	1/1	0.98	0.12	-	46,46,46,46	0
55	MG	2a	1636	1/1	0.71	0.60	-	83,83,83,83	0
55	MG	1A	3279	1/1	0.93	0.11	-	56,56,56,56	0
55	MG	1A	3361	1/1	0.74	0.10	-	75,75,75,75	0
55	MG	2a	1738	1/1	0.95	0.79	-	85,85,85,85	0
55	MG	2A	3036	1/1	0.91	0.52	-	48,48,48,48	0
55	MG	1A	3428	1/1	0.95	0.10	-	68,68,68,68	0
55	MG	2A	3456	1/1	0.82	0.35	-	70,70,70,70	0
55	MG	1A	3507	1/1	0.87	0.28	-	48,48,48,48	0
55	MG	2a	1618	1/1	0.95	0.43	-	81,81,81,81	0
55	MG	1A	3817	1/1	0.90	0.36	-	72,72,72,72	0
55	MG	2A	3544	1/1	0.93	0.06	-	90,90,90,90	0
55	MG	1g	3001	1/1	0.94	0.20	-	66,66,66,66	0
55	MG	2A	3030	1/1	0.75	0.21	-	69,69,69,69	0
55	MG	1A	3578	1/1	0.72	0.15	-	86,86,86,86	0
55	MG	2A	3211	1/1	0.83	0.13	-	45,45,45,45	0
55	MG	2A	3057	1/1	0.90	1.07	-	49,49,49,49	0
55	MG	1A	3246	1/1	0.45	0.19	-	78,78,78,78	0
55	MG	2A	3540	1/1	0.94	0.17	-	64,64,64,64	0
55	MG	2A	3162	1/1	0.58	0.36	-	82,82,82,82	0
55	MG	1a	3106	1/1	0.93	0.06	-	60,60,60,60	0
55	MG	2e	3001	1/1	0.87	0.28	-	67,67,67,67	0
55	MG	2A	3105	1/1	0.71	0.25	-	82,82,82,82	0
55	MG	1A	3203	1/1	0.96	0.30	-	35,35,35,35	0
55	MG	1a	3089	1/1	0.98	0.06	-	52,52,52,52	0
55	MG	1A	3473	1/1	0.95	0.06	-	63,63,63,63	0
55	MG	2A	3344	1/1	0.95	0.11	-	55,55,55,55	0
55	MG	1A	3485	1/1	0.87	0.20	-	47,47,47,47	0
55	MG	1A	3133	1/1	0.90	0.56	-	35,35,35,35	0
55	MG	1A	3195	1/1	0.89	0.33	-	46,46,46,46	0
55	MG	2a	1601	1/1	0.95	0.32	-	79,79,79,79	0
55	MG	1a	3132	1/1	0.71	0.24	-	91,91,91,91	0
55	MG	1W	3001	1/1	0.90	0.22	-	38,38,38,38	0
55	MG	1A	3662	1/1	0.88	0.09	-	52,52,52,52	0
55	MG	1A	3601	1/1	0.96	0.34	-	37,37,37,37	0
55	MG	2A	3716	1/1	0.89	0.15	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3561	1/1	0.94	0.08	-	47,47,47,47	0
55	MG	2A	3280	1/1	0.97	0.07	-	51,51,51,51	0
55	MG	2A	3182	1/1	0.93	0.25	-	72,72,72,72	0
55	MG	2A	3734	1/1	0.98	0.04	-	67,67,67,67	0
55	MG	1A	3791	1/1	0.98	0.06	-	33,33,33,33	0
55	MG	1A	3795	1/1	0.97	0.36	-	46,46,46,46	0
55	MG	1a	3073	1/1	0.72	0.19	-	74,74,74,74	0
55	MG	1A	3835	1/1	0.80	0.07	-	48,48,48,48	0
55	MG	1A	3400	1/1	0.81	0.23	-	63,63,63,63	0
55	MG	2A	3130	1/1	0.86	0.19	-	58,58,58,58	0
55	MG	1A	3089	1/1	0.84	0.37	-	37,37,37,37	0
55	MG	1A	3039	1/1	0.92	0.30	-	55,55,55,55	0
55	MG	2A	3115	1/1	0.88	0.17	-	66,66,66,66	0
55	MG	1A	3174	1/1	0.87	0.15	-	44,44,44,44	0
55	MG	1A	3495	1/1	0.95	0.14	-	49,49,49,49	0
55	MG	1A	3041	1/1	0.81	0.37	-	62,62,62,62	0
55	MG	2A	3074	1/1	0.64	0.44	-	48,48,48,48	0
55	MG	2A	3285	1/1	0.85	0.11	-	47,47,47,47	0
55	MG	1A	3244	1/1	0.65	0.82	-	72,72,72,72	0
55	MG	1a	3058	1/1	0.62	0.67	-	82,82,82,82	0
55	MG	1a	3001	1/1	0.84	0.05	-	76,76,76,76	0
55	MG	1A	3517	1/1	0.82	0.19	-	68,68,68,68	0
55	MG	2A	3029	1/1	0.97	0.23	-	61,61,61,61	0
55	MG	1A	3712	1/1	0.96	0.16	-	52,52,52,52	0
55	MG	2A	3287	1/1	0.93	0.09	-	39,39,39,39	0
55	MG	2P	202	1/1	0.76	0.56	-	73,73,73,73	0
55	MG	2A	3292	1/1	0.97	0.28	-	77,77,77,77	0
55	MG	2A	3035	1/1	0.89	0.40	-	32,32,32,32	0
55	MG	1A	3521	1/1	0.94	0.19	-	45,45,45,45	0
55	MG	2B	3005	1/1	0.79	0.10	-	69,69,69,69	0
55	MG	2A	3351	1/1	0.96	0.11	-	68,68,68,68	0
55	MG	1A	3069	1/1	0.93	0.17	-	38,38,38,38	0
55	MG	2A	3207	1/1	0.89	0.12	-	70,70,70,70	0
55	MG	1a	3172	1/1	0.93	0.17	-	77,77,77,77	0
55	MG	1A	3832	1/1	0.96	0.11	-	55,55,55,55	0
55	MG	1a	3162	1/1	0.95	0.06	-	77,77,77,77	0
55	MG	1A	3882	1/1	0.91	0.13	-	62,62,62,62	0
55	MG	1A	3237	1/1	0.92	0.15	-	53,53,53,53	0
55	MG	2A	3325	1/1	0.98	0.07	-	51,51,51,51	0
55	MG	1A	3291	1/1	0.95	0.15	-	30,30,30,30	0
55	MG	2A	3382	1/1	0.94	0.19	-	65,65,65,65	0
55	MG	2A	3440	1/1	0.95	0.16	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3241	1/1	0.95	0.23	-	30,30,30,30	0
55	MG	2A	3381	1/1	0.88	0.08	-	77,77,77,77	0
55	MG	1A	3307	1/1	0.97	0.06	-	63,63,63,63	0
55	MG	2A	3383	1/1	0.92	0.17	-	57,57,57,57	0
55	MG	2A	3536	1/1	0.95	0.06	-	64,64,64,64	0
55	MG	2U	204	1/1	0.95	0.17	-	55,55,55,55	0
55	MG	1a	3112	1/1	0.93	0.17	-	86,86,86,86	0
55	MG	1A	3690	1/1	0.89	0.11	-	67,67,67,67	0
55	MG	2a	1699	1/1	0.80	0.12	-	74,74,74,74	0
55	MG	1A	3698	1/1	0.94	0.13	-	48,48,48,48	0
55	MG	2a	1614	1/1	0.76	1.37	-	75,75,75,75	0
55	MG	1B	3021	1/1	0.80	0.12	-	66,66,66,66	0
55	MG	1a	3129	1/1	0.89	0.08	-	66,66,66,66	0
55	MG	2A	3770	1/1	0.95	0.04	-	79,79,79,79	0
55	MG	2A	3413	1/1	0.91	0.12	-	70,70,70,70	0
55	MG	1A	3486	1/1	0.96	0.13	-	63,63,63,63	0
55	MG	2A	3217	1/1	0.96	0.14	-	32,32,32,32	0
55	MG	2A	3168	1/1	0.92	0.29	-	53,53,53,53	0
55	MG	2A	3701	1/1	0.98	0.06	-	60,60,60,60	0
55	MG	1A	3386	1/1	0.93	0.08	-	61,61,61,61	0
55	MG	1A	3548	1/1	0.79	0.25	-	39,39,39,39	0
55	MG	2a	1641	1/1	0.83	0.22	-	77,77,77,77	0
55	MG	2A	3091	1/1	0.75	0.44	-	54,54,54,54	0
55	MG	2A	3011	1/1	0.90	0.42	-	58,58,58,58	0
55	MG	1a	3196	1/1	0.92	0.09	-	77,77,77,77	0
55	MG	17	105	1/1	0.85	0.25	-	52,52,52,52	0
55	MG	2a	1678	1/1	0.98	0.46	-	65,65,65,65	0
55	MG	1a	3061	1/1	0.95	0.17	-	74,74,74,74	0
55	MG	1A	3541	1/1	0.96	0.61	-	34,34,34,34	0
55	MG	1A	3722	1/1	0.83	0.14	-	62,62,62,62	0
55	MG	2A	3167	1/1	0.89	0.25	-	56,56,56,56	0
55	MG	1A	3165	1/1	0.64	0.30	-	80,80,80,80	0
55	MG	2A	3788	1/1	0.90	0.17	-	88,88,88,88	0
55	MG	2A	3204	1/1	0.93	0.31	-	54,54,54,54	0
55	MG	1A	3840	1/1	0.81	0.28	-	61,61,61,61	0
55	MG	2A	3213	1/1	0.93	0.16	-	33,33,33,33	0
55	MG	2A	3401	1/1	0.91	0.18	-	66,66,66,66	0
55	MG	1A	3670	1/1	0.87	0.24	-	53,53,53,53	0
55	MG	2a	1730	1/1	0.72	0.26	-	92,92,92,92	0
55	MG	1A	3218	1/1	0.92	0.42	-	35,35,35,35	0
55	MG	1A	3891	1/1	0.91	0.18	-	64,64,64,64	0
55	MG	1A	3682	1/1	0.94	0.27	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3096	1/1	0.95	0.17	-	78,78,78,78	0
55	MG	1A	3645	1/1	0.91	0.30	-	54,54,54,54	0
55	MG	2a	1727	1/1	0.76	0.39	-	91,91,91,91	0
55	MG	1a	3175	1/1	0.89	0.14	-	85,85,85,85	0
55	MG	1A	3515	1/1	0.93	0.19	-	54,54,54,54	0
55	MG	2A	3257	1/1	0.75	0.49	-	68,68,68,68	0
55	MG	1a	3100	1/1	0.97	0.30	-	60,60,60,60	0
55	MG	1a	3169	1/1	0.82	0.36	-	95,95,95,95	0
55	MG	2a	1638	1/1	0.97	0.16	-	73,73,73,73	0
55	MG	2a	1660	1/1	0.87	0.15	-	79,79,79,79	0
55	MG	1A	3112	1/1	0.96	0.17	-	42,42,42,42	0
55	MG	2A	3511	1/1	0.55	0.15	-	90,90,90,90	0
55	MG	2A	3169	1/1	0.93	0.81	-	50,50,50,50	0
55	MG	2A	3056	1/1	0.87	0.16	-	59,59,59,59	0
55	MG	2A	3231	1/1	0.97	0.19	-	48,48,48,48	0
55	MG	2E	305	1/1	0.97	0.11	-	34,34,34,34	0
55	MG	2A	3038	1/1	0.89	0.10	-	49,49,49,49	0
55	MG	2A	3063	1/1	0.95	1.27	-	49,49,49,49	0
55	MG	2A	3410	1/1	0.93	0.10	-	83,83,83,83	0
55	MG	1A	3408	1/1	0.89	0.20	-	43,43,43,43	0
55	MG	1a	3213	1/1	0.86	0.30	-	64,64,64,64	0
55	MG	2A	3037	1/1	0.95	0.17	-	24,24,24,24	0
55	MG	2A	3346	1/1	0.90	0.06	-	77,77,77,77	0
55	MG	2A	3322	1/1	0.95	0.07	-	62,62,62,62	0
55	MG	1A	3582	1/1	0.92	0.29	-	69,69,69,69	0
55	MG	2B	3017	1/1	0.86	0.13	-	84,84,84,84	0
55	MG	2A	3332	1/1	0.95	0.08	-	46,46,46,46	0
55	MG	2A	3672	1/1	0.61	0.27	-	59,59,59,59	0
55	MG	2A	3081	1/1	0.86	0.16	-	46,46,46,46	0
55	MG	2a	1659	1/1	0.90	0.11	-	71,71,71,71	0
55	MG	1W	3002	1/1	0.92	0.19	-	49,49,49,49	0
55	MG	1A	3044	1/1	0.93	0.31	-	33,33,33,33	0
55	MG	2A	3255	1/1	0.95	0.18	-	62,62,62,62	0
55	MG	2A	3683	1/1	0.99	0.06	-	60,60,60,60	0
55	MG	1A	3660	1/1	0.82	0.36	-	56,56,56,56	0
55	MG	2A	3187	1/1	0.93	0.60	-	73,73,73,73	0
55	MG	2a	1664	1/1	0.95	0.34	-	69,69,69,69	0
55	MG	1a	3062	1/1	0.91	0.36	-	79,79,79,79	0
55	MG	1a	3133	1/1	0.90	0.33	-	74,74,74,74	0
55	MG	1A	3765	1/1	0.94	0.10	-	39,39,39,39	0
55	MG	2A	3163	1/1	0.77	0.49	-	78,78,78,78	0
55	MG	1A	3731	1/1	0.88	0.12	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3916	1/1	0.92	0.42	-	29,29,29,29	0
55	MG	1A	3633	1/1	0.91	0.25	-	79,79,79,79	0
55	MG	1a	3135	1/1	0.92	0.12	-	77,77,77,77	0
55	MG	2A	3407	1/1	0.97	0.31	-	74,74,74,74	0
55	MG	1A	3145	1/1	0.89	0.39	-	29,29,29,29	0
55	MG	2A	3133	1/1	0.92	0.37	-	60,60,60,60	0
55	MG	2a	1785	1/1	0.86	0.07	-	68,68,68,68	0
55	MG	2A	3662	1/1	0.96	0.07	-	68,68,68,68	0
55	MG	2A	3141	1/1	0.83	0.56	-	51,51,51,51	0
55	MG	2a	1616	1/1	0.92	0.13	-	68,68,68,68	0
55	MG	1A	3751	1/1	0.96	0.20	-	39,39,39,39	0
55	MG	1a	3173	1/1	0.86	0.23	-	71,71,71,71	0
55	MG	1A	3397	1/1	0.98	0.03	-	64,64,64,64	0
55	MG	1A	3302	1/1	0.89	0.10	-	42,42,42,42	0
55	MG	1A	3903	1/1	0.92	0.24	-	59,59,59,59	0
55	MG	2A	3554	1/1	0.94	0.23	-	58,58,58,58	0
55	MG	2A	3634	1/1	0.88	0.19	-	83,83,83,83	0
55	MG	1A	3310	1/1	0.95	0.25	-	41,41,41,41	0
55	MG	1a	3202	1/1	0.99	0.07	-	47,47,47,47	0
55	MG	1A	3704	1/1	0.94	0.06	-	42,42,42,42	0
55	MG	1A	3476	1/1	0.93	0.21	-	45,45,45,45	0
55	MG	2A	3729	1/1	0.92	0.14	-	70,70,70,70	0
55	MG	1A	3469	1/1	0.94	0.17	-	39,39,39,39	0
55	MG	1A	3059	1/1	0.98	0.18	-	35,35,35,35	0
55	MG	2A	3043	1/1	0.97	0.12	-	72,72,72,72	0
55	MG	1a	3142	1/1	0.98	0.09	-	85,85,85,85	0
55	MG	1A	3073	1/1	0.89	0.72	-	43,43,43,43	0
55	MG	2A	3323	1/1	0.99	0.22	-	66,66,66,66	0
55	MG	1a	3125	1/1	0.98	0.29	-	74,74,74,74	0
55	MG	1A	3760	1/1	0.80	0.26	-	65,65,65,65	0
55	MG	1A	3747	1/1	0.88	0.07	-	45,45,45,45	0
55	MG	1A	3301	1/1	0.90	0.21	-	41,41,41,41	0
55	MG	2A	3561	1/1	0.95	0.08	-	59,59,59,59	0
55	MG	1A	3816	1/1	0.97	0.11	-	19,19,19,19	0
55	MG	1A	3182	1/1	0.88	0.83	-	46,46,46,46	0
55	MG	2A	3533	1/1	0.04	0.39	-	99,99,99,99	0
55	MG	2a	1724	1/1	0.68	0.29	-	93,93,93,93	0
55	MG	1a	3193	1/1	0.93	0.20	-	74,74,74,74	0
55	MG	1a	3139	1/1	0.81	0.18	-	69,69,69,69	0
55	MG	2A	3802	1/1	0.87	0.27	-	97,97,97,97	0
55	MG	1A	3579	1/1	0.88	0.14	-	64,64,64,64	0
55	MG	1B	3022	1/1	0.96	0.38	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3034	1/1	0.69	0.22	-	84,84,84,84	0
55	MG	1A	3143	1/1	0.75	0.50	-	45,45,45,45	0
55	MG	2a	1721	1/1	0.91	0.16	-	84,84,84,84	0
55	MG	1A	3017	1/1	0.91	0.40	-	31,31,31,31	0
55	MG	2A	3797	1/1	0.91	0.14	-	75,75,75,75	0
55	MG	2a	1610	1/1	0.93	0.56	-	74,74,74,74	0
55	MG	1a	3038	1/1	0.74	0.75	-	79,79,79,79	0
55	MG	1A	3345	1/1	0.96	0.17	-	45,45,45,45	0
55	MG	1A	3439	1/1	0.98	0.07	-	54,54,54,54	0
55	MG	2A	3161	1/1	0.80	0.61	-	54,54,54,54	0
55	MG	1A	3862	1/1	0.95	0.11	-	59,59,59,59	0
55	MG	1A	3097	1/1	0.88	0.52	-	48,48,48,48	0
55	MG	2A	3290	1/1	0.80	0.17	-	64,64,64,64	0
55	MG	1a	3180	1/1	0.85	0.21	-	102,102,102,102	0
55	MG	2A	3574	1/1	0.65	0.23	-	98,98,98,98	0
55	MG	2A	3314	1/1	0.99	0.13	-	60,60,60,60	0
55	MG	2a	1703	1/1	0.94	0.08	-	61,61,61,61	0
55	MG	2A	3591	1/1	0.97	0.19	-	53,53,53,53	0
55	MG	1A	3759	1/1	0.88	0.24	-	61,61,61,61	0
55	MG	2A	3460	1/1	0.96	0.10	-	55,55,55,55	0
55	MG	1A	3824	1/1	0.91	0.16	-	47,47,47,47	0
55	MG	2A	3670	1/1	0.91	0.08	-	84,84,84,84	0
55	MG	1A	3847	1/1	0.89	0.12	-	58,58,58,58	0
55	MG	2A	3485	1/1	0.75	0.45	-	73,73,73,73	0
55	MG	1A	3268	1/1	0.94	0.17	-	35,35,35,35	0
55	MG	1a	3081	1/1	0.97	0.23	-	69,69,69,69	0
55	MG	2A	3181	1/1	0.92	0.23	-	79,79,79,79	0
55	MG	1A	3695	1/1	0.83	0.29	-	60,60,60,60	0
55	MG	1A	3222	1/1	0.89	0.56	-	36,36,36,36	0
55	MG	1A	3151	1/1	0.84	0.16	-	46,46,46,46	0
55	MG	2A	3459	1/1	0.89	0.31	-	71,71,71,71	0
55	MG	1a	3206	1/1	0.97	0.04	-	68,68,68,68	0
55	MG	1A	3131	1/1	0.64	0.22	-	62,62,62,62	0
55	MG	2A	3642	1/1	0.71	0.12	-	82,82,82,82	0
55	MG	1Y	502	1/1	0.97	0.11	-	74,74,74,74	0
55	MG	2A	3184	1/1	0.67	0.38	-	73,73,73,73	0
55	MG	1A	3381	1/1	0.92	0.10	-	62,62,62,62	0
55	MG	1A	3600	1/1	0.82	0.09	-	67,67,67,67	0
55	MG	1A	3396	1/1	0.64	0.46	-	66,66,66,66	0
55	MG	2a	1789	1/1	0.93	0.11	-	86,86,86,86	0
55	MG	1A	3190	1/1	0.80	0.12	-	72,72,72,72	0
55	MG	2A	3262	1/1	0.95	0.23	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3465	1/1	0.85	0.23	-	54,54,54,54	0
55	MG	2A	3622	1/1	0.89	0.37	-	49,49,49,49	0
55	MG	2A	3480	1/1	0.70	0.23	-	81,81,81,81	0
55	MG	1A	3820	1/1	0.94	0.60	-	41,41,41,41	0
55	MG	1A	3217	1/1	0.95	0.43	-	45,45,45,45	0
55	MG	1A	3757	1/1	0.88	0.19	-	37,37,37,37	0
55	MG	2A	3689	1/1	0.90	0.20	-	67,67,67,67	0
55	MG	1A	3427	1/1	0.95	0.08	-	42,42,42,42	0
55	MG	1D	308	1/1	0.82	0.09	-	58,58,58,58	0
55	MG	2A	3704	1/1	0.88	0.06	-	62,62,62,62	0
55	MG	1A	3043	1/1	0.98	0.29	-	10,10,10,10	0
55	MG	2A	3010	1/1	0.43	0.32	-	63,63,63,63	0
55	MG	1A	3546	1/1	0.97	0.33	-	25,25,25,25	0
55	MG	2A	3415	1/1	0.84	0.07	-	80,80,80,80	0
55	MG	2a	1774	1/1	0.82	0.11	-	91,91,91,91	0
55	MG	2A	3443	1/1	0.95	0.18	-	63,63,63,63	0
55	MG	2A	3594	1/1	0.93	0.10	-	56,56,56,56	0
55	MG	1A	3620	1/1	0.94	0.05	-	50,50,50,50	0
55	MG	1a	3218	1/1	0.68	0.29	-	72,72,72,72	0
55	MG	1A	3787	1/1	0.88	0.16	-	59,59,59,59	0
55	MG	1A	3667	1/1	0.98	0.19	-	46,46,46,46	0
55	MG	2a	1732	1/1	0.93	0.09	-	74,74,74,74	0
55	MG	1B	3002	1/1	0.62	0.28	-	69,69,69,69	0
55	MG	1A	3328	1/1	0.98	0.12	-	22,22,22,22	0
55	MG	2a	1780	1/1	0.97	0.06	-	68,68,68,68	0
55	MG	2A	3762	1/1	0.79	0.61	-	60,60,60,60	0
55	MG	1A	3295	1/1	0.99	0.12	-	13,13,13,13	0
55	MG	2A	3611	1/1	0.95	0.42	-	83,83,83,83	0
55	MG	1A	3411	1/1	0.93	0.17	-	52,52,52,52	0
55	MG	2A	3615	1/1	0.89	0.20	-	56,56,56,56	0
55	MG	1A	3488	1/1	0.91	0.47	-	43,43,43,43	0
55	MG	2A	3606	1/1	0.33	0.27	-	68,68,68,68	0
55	MG	1A	3754	1/1	0.97	0.05	-	39,39,39,39	0
55	MG	2a	1713	1/1	0.93	0.06	-	69,69,69,69	0
55	MG	2g	3001	1/1	0.82	0.17	-	72,72,72,72	0
55	MG	1A	3568	1/1	0.87	0.20	-	63,63,63,63	0
55	MG	2A	3112	1/1	0.94	0.59	-	77,77,77,77	0
55	MG	1A	3598	1/1	0.91	0.12	-	83,83,83,83	0
55	MG	1A	3146	1/1	0.85	0.12	-	54,54,54,54	0
55	MG	2A	3439	1/1	0.94	0.38	-	64,64,64,64	0
55	MG	1A	3532	1/1	0.87	0.23	-	69,69,69,69	0
55	MG	1A	3063	1/1	0.88	0.23	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3328	1/1	0.86	0.26	-	72,72,72,72	0
55	MG	1A	3825	1/1	0.88	0.10	-	68,68,68,68	0
55	MG	1B	3009	1/1	0.86	0.25	-	60,60,60,60	0
55	MG	2A	3175	1/1	0.84	0.99	-	69,69,69,69	0
55	MG	10	108	1/1	0.93	0.68	-	43,43,43,43	0
55	MG	1A	3216	1/1	0.89	0.24	-	52,52,52,52	0
55	MG	2A	3003	1/1	0.99	0.11	-	31,31,31,31	0
55	MG	2A	3299	1/1	0.84	0.21	-	75,75,75,75	0
55	MG	1A	3032	1/1	0.81	0.29	-	45,45,45,45	0
55	MG	1A	3802	1/1	0.90	0.16	-	39,39,39,39	0
55	MG	1A	3608	1/1	0.83	0.23	-	74,74,74,74	0
55	MG	1A	3767	1/1	0.87	0.06	-	51,51,51,51	0
55	MG	2A	3060	1/1	0.86	0.80	-	52,52,52,52	0
55	MG	2a	1617	1/1	0.91	0.36	-	65,65,65,65	0
55	MG	1A	3380	1/1	0.96	0.18	-	52,52,52,52	0
55	MG	2A	3517	1/1	0.94	0.12	-	64,64,64,64	0
55	MG	1A	3314	1/1	0.91	0.12	-	52,52,52,52	0
55	MG	2a	1757	1/1	0.90	0.11	-	71,71,71,71	0
55	MG	1A	3015	1/1	0.97	0.41	-	23,23,23,23	0
55	MG	2A	3180	1/1	0.82	0.22	-	63,63,63,63	0
55	MG	1A	3434	1/1	0.97	0.21	-	16,16,16,16	0
55	MG	2A	3522	1/1	0.77	0.17	-	82,82,82,82	0
55	MG	2A	3731	1/1	0.89	0.16	-	70,70,70,70	0
55	MG	1U	207	1/1	0.88	0.23	-	47,47,47,47	0
55	MG	1A	3909	1/1	0.98	0.15	-	32,32,32,32	0
55	MG	2A	3008	1/1	0.78	0.33	-	69,69,69,69	0
55	MG	2A	3497	1/1	0.79	0.14	-	89,89,89,89	0
55	MG	1A	3636	1/1	0.91	0.11	-	38,38,38,38	0
55	MG	1A	3489	1/1	0.95	0.08	-	33,33,33,33	0
55	MG	1A	3095	1/1	0.59	0.78	-	61,61,61,61	0
55	MG	2a	1735	1/1	0.92	0.08	-	81,81,81,81	0
55	MG	2a	1784	1/1	0.93	0.09	-	80,80,80,80	0
55	MG	2A	3408	1/1	0.94	0.14	-	67,67,67,67	0
55	MG	1A	3176	1/1	0.97	0.28	-	52,52,52,52	0
55	MG	1A	3056	1/1	0.95	0.19	-	28,28,28,28	0
55	MG	1A	3225	1/1	0.98	0.10	-	34,34,34,34	0
55	MG	2A	3717	1/1	0.74	0.19	-	92,92,92,92	0
55	MG	1A	3050	1/1	0.95	0.37	-	29,29,29,29	0
55	MG	2A	3126	1/1	0.93	0.13	-	55,55,55,55	0
55	MG	2a	1741	1/1	0.75	0.07	-	75,75,75,75	0
55	MG	2A	3065	1/1	0.84	0.13	-	56,56,56,56	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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3534	1/1	0.87	0.67	-	80,80,80,80	0
55	MG	2A	3436	1/1	0.91	0.12	-	72,72,72,72	0
55	MG	1A	3062	1/1	0.95	0.21	-	37,37,37,37	0
55	MG	1A	3566	1/1	0.95	0.11	-	23,23,23,23	0
55	MG	2A	3230	1/1	0.92	0.35	-	51,51,51,51	0
55	MG	1A	3379	1/1	0.97	0.14	-	43,43,43,43	0
55	MG	1A	3852	1/1	0.95	0.22	-	24,24,24,24	0
55	MG	1A	3135	1/1	0.84	0.20	-	37,37,37,37	0
55	MG	1A	3497	1/1	0.96	0.14	-	66,66,66,66	0
55	MG	1a	3130	1/1	0.91	0.29	-	62,62,62,62	0
55	MG	17	104	1/1	0.95	0.32	-	61,61,61,61	0
55	MG	2A	3102	1/1	0.88	0.41	-	56,56,56,56	0
55	MG	1A	3584	1/1	0.96	0.07	-	37,37,37,37	0
55	MG	2A	3179	1/1	0.94	0.99	-	48,48,48,48	0
55	MG	1A	3876	1/1	0.84	0.06	-	64,64,64,64	0
55	MG	1B	3006	1/1	0.60	0.21	-	59,59,59,59	0
55	MG	1a	3215	1/1	0.52	0.25	-	86,86,86,86	0
55	MG	2a	1687	1/1	0.97	0.23	-	55,55,55,55	0
55	MG	2A	3085	1/1	0.97	0.25	-	62,62,62,62	0
55	MG	2a	1696	1/1	0.89	0.09	-	77,77,77,77	0
55	MG	2A	3104	1/1	0.73	0.16	-	56,56,56,56	0
55	MG	1a	3189	1/1	0.92	0.25	-	84,84,84,84	0
55	MG	2A	3505	1/1	0.96	0.17	-	44,44,44,44	0
55	MG	1a	3040	1/1	0.81	0.24	-	75,75,75,75	0
55	MG	2A	3553	1/1	0.47	1.12	-	89,89,89,89	0
55	MG	1A	3290	1/1	0.98	0.04	-	49,49,49,49	0
55	MG	1A	3869	1/1	0.83	0.18	-	39,39,39,39	0
55	MG	1A	3647	1/1	0.96	0.11	-	39,39,39,39	0
55	MG	2A	3174	1/1	0.89	0.17	-	58,58,58,58	0
55	MG	2A	3582	1/1	0.65	0.61	-	64,64,64,64	0
55	MG	1A	3286	1/1	0.97	0.11	-	64,64,64,64	0
55	MG	1A	3687	1/1	0.95	0.17	-	56,56,56,56	0
55	MG	1a	3090	1/1	0.94	0.06	-	40,40,40,40	0
55	MG	1A	3634	1/1	0.78	0.22	-	38,38,38,38	0
55	MG	2A	3109	1/1	0.72	0.58	-	64,64,64,64	0
55	MG	2A	3240	1/1	0.88	0.16	-	34,34,34,34	0
55	MG	1a	3212	1/1	0.94	0.05	-	51,51,51,51	0
55	MG	1a	3078	1/1	0.87	0.66	-	78,78,78,78	0
55	MG	1A	3321	1/1	0.83	0.16	-	55,55,55,55	0
55	MG	1A	3463	1/1	0.95	0.10	-	28,28,28,28	0
55	MG	1A	3008	1/1	0.92	0.25	-	46,46,46,46	0
55	MG	2A	3796	1/1	0.87	0.67	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2R	202	1/1	0.80	0.35	-	74,74,74,74	0
55	MG	1A	3689	1/1	0.94	0.10	-	68,68,68,68	0
55	MG	2A	3473	1/1	0.97	0.09	-	61,61,61,61	0
55	MG	1A	3239	1/1	0.89	0.24	-	35,35,35,35	0
55	MG	1U	203	1/1	0.95	0.51	-	42,42,42,42	0
55	MG	2A	3753	1/1	0.89	0.15	-	71,71,71,71	0
55	MG	1a	3070	1/1	0.94	0.17	-	62,62,62,62	0
55	MG	2A	3076	1/1	0.94	0.28	-	55,55,55,55	0
55	MG	1A	3902	1/1	0.96	0.13	-	56,56,56,56	0
55	MG	1A	3048	1/1	0.89	0.71	-	33,33,33,33	0
55	MG	2a	1736	1/1	0.81	0.35	-	78,78,78,78	0
55	MG	2a	1729	1/1	0.90	0.14	-	60,60,60,60	0
55	MG	2A	3372	1/1	0.99	0.12	-	38,38,38,38	0
55	MG	1A	3410	1/1	0.97	0.19	-	42,42,42,42	0
55	MG	1A	3163	1/1	0.88	0.21	-	65,65,65,65	0
55	MG	2A	3552	1/1	0.98	0.33	-	52,52,52,52	0
55	MG	2A	3310	1/1	0.92	0.11	-	57,57,57,57	0
55	MG	2A	3195	1/1	0.82	0.13	-	55,55,55,55	0
55	MG	1A	3312	1/1	0.94	0.07	-	64,64,64,64	0
55	MG	2A	3702	1/1	0.95	0.16	-	34,34,34,34	0
55	MG	1A	3518	1/1	0.96	0.12	-	77,77,77,77	0
55	MG	1A	3125	1/1	0.96	0.17	-	45,45,45,45	0
55	MG	2A	3748	1/1	0.88	0.14	-	68,68,68,68	0
55	MG	1d	505	1/1	0.94	0.05	-	74,74,74,74	0
55	MG	2a	1684	1/1	0.91	0.07	-	76,76,76,76	0
55	MG	1a	3039	1/1	0.84	0.36	-	62,62,62,62	0
55	MG	1A	3500	1/1	0.97	0.36	-	65,65,65,65	0
55	MG	2A	3050	1/1	0.85	0.42	-	64,64,64,64	0
55	MG	1A	3358	1/1	0.92	0.13	-	19,19,19,19	0
55	MG	1A	3522	1/1	0.95	0.13	-	26,26,26,26	0
55	MG	2a	1658	1/1	0.89	0.08	-	74,74,74,74	0
55	MG	2A	3783	1/1	0.93	0.12	-	78,78,78,78	0
55	MG	2A	3308	1/1	0.97	0.22	-	52,52,52,52	0
55	MG	2A	3503	1/1	0.98	0.22	-	53,53,53,53	0
55	MG	2A	3816	1/1	0.69	0.32	-	51,51,51,51	0
55	MG	2a	1681	1/1	0.93	0.12	-	84,84,84,84	0
55	MG	1A	3780	1/1	0.94	0.04	-	58,58,58,58	0
55	MG	1A	3223	1/1	0.98	0.09	-	42,42,42,42	0
55	MG	1A	3458	1/1	0.95	0.10	-	46,46,46,46	0
55	MG	2A	3397	1/1	0.94	0.10	-	76,76,76,76	0
55	MG	2A	3640	1/1	0.92	0.22	-	78,78,78,78	0
55	MG	1A	3562	1/1	0.98	0.23	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3307	1/1	0.73	0.10	-	54,54,54,54	0
55	MG	2A	3635	1/1	0.92	0.05	-	92,92,92,92	0
55	MG	1A	3479	1/1	0.92	0.13	-	39,39,39,39	0
55	MG	2A	3496	1/1	0.95	0.15	-	43,43,43,43	0
55	MG	2S	201	1/1	0.80	0.35	-	67,67,67,67	0
55	MG	2A	3375	1/1	0.79	0.47	-	49,49,49,49	0
55	MG	2a	1792	1/1	0.86	0.31	-	52,52,52,52	0
55	MG	1a	3087	1/1	0.92	0.06	-	57,57,57,57	0
55	MG	1A	3362	1/1	0.96	0.14	-	20,20,20,20	0
55	MG	1a	3117	1/1	0.87	0.22	-	61,61,61,61	0
55	MG	1A	3108	1/1	0.96	0.19	-	24,24,24,24	0
55	MG	2A	3386	1/1	0.72	0.28	-	102,102,102,102	0
55	MG	1A	3699	1/1	0.96	0.08	-	38,38,38,38	0
55	MG	1a	3179	1/1	0.76	0.07	-	78,78,78,78	0
55	MG	1a	3159	1/1	0.88	0.12	-	65,65,65,65	0
55	MG	1B	3024	1/1	0.86	0.12	-	62,62,62,62	0
55	MG	1N	8003	1/1	0.87	0.18	-	69,69,69,69	0
55	MG	2A	3259	1/1	0.89	0.12	-	34,34,34,34	0
55	MG	2A	3685	1/1	0.76	0.30	-	54,54,54,54	0
55	MG	1A	3456	1/1	0.65	0.22	-	59,59,59,59	0
55	MG	1A	3389	1/1	0.96	0.16	-	48,48,48,48	0
55	MG	2A	3531	1/1	0.93	0.09	-	83,83,83,83	0
55	MG	2a	1642	1/1	0.75	0.14	-	68,68,68,68	0
55	MG	1A	3721	1/1	0.91	0.17	-	50,50,50,50	0
55	MG	2a	1705	1/1	0.95	0.21	-	69,69,69,69	0
55	MG	2A	3434	1/1	0.94	0.10	-	65,65,65,65	0
55	MG	2A	3708	1/1	0.93	0.15	-	66,66,66,66	0
55	MG	2a	1764	1/1	0.86	0.08	-	59,59,59,59	0
55	MG	1A	3249	1/1	0.96	0.14	-	21,21,21,21	0
55	MG	2h	8001	1/1	0.80	0.29	-	77,77,77,77	0
55	MG	1A	3496	1/1	0.97	0.07	-	51,51,51,51	0
55	MG	1a	3027	1/1	0.90	0.45	-	70,70,70,70	0
55	MG	1a	3187	1/1	0.93	0.07	-	89,89,89,89	0
55	MG	2A	3736	1/1	0.78	0.12	-	95,95,95,95	0
55	MG	1a	3099	1/1	0.99	0.14	-	61,61,61,61	0
55	MG	2A	3507	1/1	0.65	0.58	-	69,69,69,69	0
55	MG	1A	3096	1/1	0.97	0.54	-	34,34,34,34	0
55	MG	1A	3775	1/1	0.92	0.15	-	72,72,72,72	0
55	MG	1A	3440	1/1	0.91	0.14	-	47,47,47,47	0
55	MG	2A	3075	1/1	0.90	0.26	-	53,53,53,53	0
55	MG	2A	3340	1/1	0.90	0.27	-	52,52,52,52	0
55	MG	1A	3071	1/1	0.77	0.51	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3082	1/1	0.94	0.19	-	62,62,62,62	0
55	MG	2A	3441	1/1	0.67	0.21	-	90,90,90,90	0
55	MG	2A	3815	1/1	0.82	0.46	-	67,67,67,67	0
55	MG	1A	3531	1/1	0.95	0.05	-	46,46,46,46	0
55	MG	1A	3186	1/1	0.72	0.23	-	72,72,72,72	0
55	MG	1a	3017	1/1	0.84	0.31	-	65,65,65,65	0
55	MG	2A	3703	1/1	0.90	0.26	-	93,93,93,93	0
55	MG	1A	3320	1/1	0.95	0.15	-	62,62,62,62	0
55	MG	1a	3035	1/1	0.89	1.12	-	64,64,64,64	0
55	MG	2A	3697	1/1	0.91	0.07	-	57,57,57,57	0
55	MG	2a	1778	1/1	0.93	0.06	-	79,79,79,79	0
55	MG	1A	3016	1/1	0.95	0.50	-	19,19,19,19	0
55	MG	1A	3498	1/1	0.65	0.10	-	70,70,70,70	0
55	MG	1a	3060	1/1	0.94	0.20	-	69,69,69,69	0
55	MG	2A	3678	1/1	0.88	0.09	-	92,92,92,92	0
55	MG	1a	3005	1/1	0.42	0.18	-	81,81,81,81	0
55	MG	2a	1744	1/1	0.90	0.15	-	76,76,76,76	0
55	MG	1A	3014	1/1	0.91	0.63	-	41,41,41,41	0
55	MG	2A	3022	1/1	0.80	0.13	-	68,68,68,68	0
55	MG	1a	3126	1/1	0.97	0.14	-	74,74,74,74	0
55	MG	1a	3077	1/1	0.81	0.41	-	81,81,81,81	0
55	MG	1a	3177	1/1	0.95	0.08	-	74,74,74,74	0
55	MG	1A	3783	1/1	0.84	0.10	-	55,55,55,55	0
55	MG	2A	3329	1/1	0.74	0.11	-	88,88,88,88	0
55	MG	1D	306	1/1	0.92	0.27	-	35,35,35,35	0
55	MG	1a	3105	1/1	0.94	0.14	-	58,58,58,58	0
55	MG	1a	3128	1/1	0.93	0.17	-	71,71,71,71	0
55	MG	1d	502	1/1	0.87	0.10	-	80,80,80,80	0
55	MG	2A	3550	1/1	0.96	0.10	-	48,48,48,48	0
55	MG	2A	3668	1/1	0.93	0.13	-	66,66,66,66	0
55	MG	1A	3236	1/1	0.71	0.23	-	79,79,79,79	0
55	MG	1A	3254	1/1	0.89	0.31	-	50,50,50,50	0
55	MG	1Q	203	1/1	0.93	0.20	-	38,38,38,38	0
55	MG	2A	3151	1/1	0.82	1.44	-	62,62,62,62	0
55	MG	2A	3785	1/1	0.93	0.09	-	60,60,60,60	0
55	MG	2A	3663	1/1	0.97	0.08	-	50,50,50,50	0
55	MG	2A	3349	1/1	0.97	0.06	-	77,77,77,77	0
55	MG	2A	3546	1/1	0.96	0.06	-	87,87,87,87	0
55	MG	1A	3483	1/1	0.96	0.20	-	38,38,38,38	0
55	MG	2a	1665	1/1	0.98	0.08	-	74,74,74,74	0
55	MG	2A	3653	1/1	0.88	0.22	-	77,77,77,77	0
55	MG	2a	1745	1/1	0.88	0.28	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1758	1/1	0.88	0.23	-	70,70,70,70	0
55	MG	2A	3665	1/1	0.94	0.09	-	59,59,59,59	0
55	MG	1A	3624	1/1	0.77	0.30	-	68,68,68,68	0
55	MG	2A	3339	1/1	0.93	0.05	-	71,71,71,71	0
55	MG	1a	3049	1/1	0.91	0.44	-	69,69,69,69	0
55	MG	2A	3548	1/1	0.94	0.06	-	65,65,65,65	0
55	MG	2a	1731	1/1	0.65	0.11	-	90,90,90,90	0
55	MG	2a	1775	1/1	0.98	0.08	-	63,63,63,63	0
55	MG	2A	3177	1/1	0.93	0.15	-	62,62,62,62	0
55	MG	2B	3013	1/1	0.64	0.12	-	84,84,84,84	0
55	MG	1A	3875	1/1	0.83	0.25	-	44,44,44,44	0
55	MG	1A	3200	1/1	0.88	0.90	-	37,37,37,37	0
55	MG	1a	3056	1/1	0.88	0.10	-	69,69,69,69	0
55	MG	1A	3491	1/1	0.91	0.29	-	55,55,55,55	0
55	MG	2A	3144	1/1	0.88	0.14	-	73,73,73,73	0
55	MG	2A	3059	1/1	0.80	0.54	-	64,64,64,64	0
55	MG	1A	3319	1/1	0.98	0.19	-	34,34,34,34	0
55	MG	1A	3881	1/1	0.95	0.26	-	43,43,43,43	0
55	MG	1A	3139	1/1	0.90	0.21	-	59,59,59,59	0
55	MG	1A	3377	1/1	0.85	0.07	-	70,70,70,70	0
55	MG	1A	3539	1/1	0.90	0.16	-	62,62,62,62	0
55	MG	1A	3392	1/1	0.94	0.13	-	35,35,35,35	0
55	MG	1A	3511	1/1	0.91	0.15	-	26,26,26,26	0
55	MG	2A	3188	1/1	0.94	0.17	-	45,45,45,45	0
55	MG	1A	3433	1/1	0.81	0.31	-	51,51,51,51	0
55	MG	1A	3673	1/1	0.98	0.13	-	35,35,35,35	0
55	MG	1A	3571	1/1	0.98	0.29	-	54,54,54,54	0
55	MG	1A	3912	1/1	0.94	0.14	-	43,43,43,43	0
55	MG	1A	3732	1/1	0.99	0.09	-	21,21,21,21	0
55	MG	1A	3664	1/1	0.94	0.12	-	59,59,59,59	0
55	MG	2A	3335	1/1	0.94	0.07	-	71,71,71,71	0
55	MG	1A	3026	1/1	0.88	0.14	-	63,63,63,63	0
55	MG	2A	3458	1/1	0.91	0.10	-	78,78,78,78	0
55	MG	2A	3576	1/1	0.97	0.39	-	52,52,52,52	0
55	MG	20	102	1/1	0.93	0.17	-	75,75,75,75	0
55	MG	2A	3798	1/1	0.89	0.18	-	93,93,93,93	0
55	MG	1A	3892	1/1	0.92	0.23	-	62,62,62,62	0
55	MG	1A	3387	1/1	0.93	0.13	-	70,70,70,70	0
55	MG	1A	3590	1/1	0.86	0.11	-	48,48,48,48	0
55	MG	1a	3118	1/1	0.91	0.08	-	70,70,70,70	0
55	MG	1A	3192	1/1	0.68	0.32	-	42,42,42,42	0
55	MG	2A	3650	1/1	0.77	0.34	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1H	8002	1/1	0.93	0.10	-	46,46,46,46	0
55	MG	2a	1613	1/1	0.94	0.41	-	61,61,61,61	0
55	MG	1A	3592	1/1	0.67	0.39	-	70,70,70,70	0
55	MG	2A	3295	1/1	0.90	0.26	-	71,71,71,71	0
55	MG	2A	3270	1/1	0.81	0.18	-	58,58,58,58	0
55	MG	2A	3584	1/1	0.91	0.23	-	62,62,62,62	0
55	MG	1A	3118	1/1	0.70	0.28	-	63,63,63,63	0
55	MG	2a	1693	1/1	0.98	0.21	-	54,54,54,54	0
55	MG	2A	3021	1/1	0.87	0.43	-	43,43,43,43	0
55	MG	1A	3692	1/1	0.96	0.07	-	43,43,43,43	0
55	MG	1A	3570	1/1	0.84	0.28	-	48,48,48,48	0
55	MG	2B	3008	1/1	0.90	0.12	-	83,83,83,83	0
55	MG	1a	3026	1/1	0.87	0.23	-	58,58,58,58	0
55	MG	1A	3853	1/1	0.79	0.10	-	25,25,25,25	0
55	MG	1a	3131	1/1	0.95	0.15	-	76,76,76,76	0
55	MG	1A	3419	1/1	0.96	0.14	-	37,37,37,37	0
55	MG	2A	3786	1/1	0.89	0.11	-	49,49,49,49	0
55	MG	2A	3227	1/1	0.95	0.14	-	65,65,65,65	0
55	MG	2A	3244	1/1	0.85	0.52	-	53,53,53,53	0
55	MG	2A	3809	1/1	0.73	0.27	-	75,75,75,75	0
55	MG	1A	3807	1/1	0.89	0.25	-	48,48,48,48	0
55	MG	1A	3167	1/1	0.80	0.30	-	52,52,52,52	0
55	MG	2A	3671	1/1	0.98	0.23	-	73,73,73,73	0
55	MG	1A	3364	1/1	0.98	0.25	-	36,36,36,36	0
55	MG	1A	3535	1/1	0.96	0.13	-	38,38,38,38	0
55	MG	1A	3413	1/1	0.96	0.08	-	43,43,43,43	0
55	MG	2A	3156	1/1	0.97	0.52	-	39,39,39,39	0
55	MG	1A	3741	1/1	0.92	0.10	-	56,56,56,56	0
55	MG	1A	3036	1/1	0.92	0.14	-	28,28,28,28	0
55	MG	2A	3549	1/1	0.92	0.05	-	74,74,74,74	0
55	MG	1a	3031	1/1	0.93	0.08	-	61,61,61,61	0
55	MG	1A	3213	1/1	0.95	0.85	-	32,32,32,32	0
55	MG	1A	3914	1/1	0.75	0.46	-	62,62,62,62	0
55	MG	2A	3578	1/1	0.98	0.06	-	61,61,61,61	0
55	MG	2A	3170	1/1	0.97	0.23	-	73,73,73,73	0
55	MG	1A	3650	1/1	0.94	0.36	-	49,49,49,49	0
55	MG	2A	3562	1/1	0.96	0.17	-	74,74,74,74	0
55	MG	1A	3771	1/1	0.88	0.06	-	71,71,71,71	0
55	MG	1a	3214	1/1	0.98	0.04	-	71,71,71,71	0
55	MG	1A	3865	1/1	0.93	0.14	-	75,75,75,75	0
55	MG	2A	3251	1/1	0.98	0.04	-	79,79,79,79	0
55	MG	2A	3048	1/1	0.91	0.24	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3680	1/1	0.95	0.10	-	59,59,59,59	0
55	MG	1A	3651	1/1	0.95	0.14	-	40,40,40,40	0
55	MG	1a	3084	1/1	0.94	0.29	-	64,64,64,64	0
55	MG	1A	3648	1/1	0.79	0.13	-	90,90,90,90	0
55	MG	2A	3342	1/1	0.68	0.21	-	76,76,76,76	0
55	MG	1A	3763	1/1	0.96	0.16	-	22,22,22,22	0
55	MG	1A	3229	1/1	0.97	0.23	-	62,62,62,62	0
55	MG	1A	3756	1/1	0.89	0.19	-	40,40,40,40	0
55	MG	1A	3238	1/1	0.94	0.39	-	38,38,38,38	0
55	MG	1B	3017	1/1	0.86	0.08	-	39,39,39,39	0
55	MG	1A	3727	1/1	0.92	0.22	-	40,40,40,40	0
55	MG	2A	3069	1/1	0.90	0.83	-	52,52,52,52	0
55	MG	1A	3621	1/1	0.95	0.12	-	40,40,40,40	0
55	MG	1A	3262	1/1	0.85	0.20	-	84,84,84,84	0
55	MG	1A	3287	1/1	0.89	0.22	-	45,45,45,45	0
55	MG	2A	3667	1/1	0.97	0.12	-	57,57,57,57	0
55	MG	1A	3669	1/1	0.95	0.24	-	56,56,56,56	0
55	MG	2A	3399	1/1	0.94	0.16	-	45,45,45,45	0
55	MG	2a	1654	1/1	0.85	0.54	-	70,70,70,70	0
55	MG	1A	3628	1/1	0.94	0.07	-	50,50,50,50	0
55	MG	1a	3195	1/1	0.95	0.11	-	62,62,62,62	0
55	MG	1A	3842	1/1	0.93	0.08	-	84,84,84,84	0
55	MG	2V	205	1/1	0.95	0.31	-	73,73,73,73	0
55	MG	1a	3176	1/1	0.94	0.15	-	92,92,92,92	0
55	MG	1a	3192	1/1	0.95	0.11	-	49,49,49,49	0
55	MG	1A	3168	1/1	0.86	0.35	-	53,53,53,53	0
55	MG	27	104	1/1	0.82	0.18	-	67,67,67,67	0
55	MG	1A	3560	1/1	0.93	0.06	-	72,72,72,72	0
55	MG	2B	3014	1/1	0.84	0.12	-	76,76,76,76	0
55	MG	2A	3362	1/1	0.93	0.18	-	61,61,61,61	0
55	MG	1A	3098	1/1	0.80	0.38	-	38,38,38,38	0
55	MG	2a	1643	1/1	0.74	0.31	-	73,73,73,73	0
55	MG	1a	3183	1/1	0.88	0.19	-	84,84,84,84	0
55	MG	1a	3154	1/1	0.86	0.11	-	100,100,100,100	0
55	MG	1A	3714	1/1	0.94	0.10	-	68,68,68,68	0
55	MG	1A	3743	1/1	0.95	0.10	-	45,45,45,45	0
55	MG	2U	203	1/1	0.90	0.10	-	71,71,71,71	0
55	MG	1A	3393	1/1	0.95	0.10	-	53,53,53,53	0
55	MG	2A	3583	1/1	0.88	0.23	-	72,72,72,72	0
55	MG	15	107	1/1	0.87	0.12	-	52,52,52,52	0
55	MG	1A	3303	1/1	0.95	0.15	-	13,13,13,13	0
55	MG	1A	3649	1/1	0.95	0.12	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3324	1/1	0.93	0.16	-	61,61,61,61	0
55	MG	1A	3851	1/1	0.97	0.06	-	21,21,21,21	0
55	MG	2A	3051	1/1	0.94	0.84	-	61,61,61,61	0
55	MG	2A	3468	1/1	0.88	0.11	-	80,80,80,80	0
55	MG	2a	1649	1/1	0.88	0.24	-	83,83,83,83	0
55	MG	1A	3212	1/1	0.87	0.41	-	43,43,43,43	0
55	MG	1A	3706	1/1	0.92	0.16	-	54,54,54,54	0
55	MG	2A	3137	1/1	0.97	0.84	-	60,60,60,60	0
55	MG	1A	3370	1/1	0.94	0.16	-	41,41,41,41	0
55	MG	2A	3526	1/1	0.94	0.13	-	73,73,73,73	0
55	MG	1A	3510	1/1	0.90	0.11	-	70,70,70,70	0
55	MG	2A	3087	1/1	0.96	0.18	-	62,62,62,62	0
55	MG	1A	3403	1/1	0.95	0.09	-	53,53,53,53	0
55	MG	2A	3377	1/1	0.81	0.11	-	94,94,94,94	0
55	MG	2A	3306	1/1	0.96	0.20	-	39,39,39,39	0
55	MG	2A	3693	1/1	0.96	0.06	-	95,95,95,95	0
55	MG	1A	3251	1/1	0.96	0.54	-	34,34,34,34	0
55	MG	1A	3547	1/1	0.92	0.45	-	35,35,35,35	0
55	MG	1A	3812	1/1	0.89	0.11	-	28,28,28,28	0
55	MG	2a	1609	1/1	0.70	1.42	-	77,77,77,77	0
55	MG	1A	3830	1/1	0.96	0.04	-	47,47,47,47	0
55	MG	1A	3883	1/1	0.85	0.07	-	58,58,58,58	0
55	MG	1A	3162	1/1	0.95	0.64	-	37,37,37,37	0
55	MG	1a	3085	1/1	0.95	0.27	-	64,64,64,64	0
55	MG	1A	3576	1/1	0.97	0.49	-	47,47,47,47	0
55	MG	2a	1656	1/1	0.73	0.41	-	72,72,72,72	0
55	MG	2A	3512	1/1	0.94	0.18	-	61,61,61,61	0
55	MG	1A	3872	1/1	0.97	0.08	-	29,29,29,29	0
55	MG	27	103	1/1	0.61	0.60	-	70,70,70,70	0
55	MG	2a	1677	1/1	0.88	0.22	-	71,71,71,71	0
55	MG	1A	3240	1/1	0.98	0.18	-	58,58,58,58	0
55	MG	1A	3079	1/1	0.85	0.21	-	40,40,40,40	0
55	MG	2A	3618	1/1	0.91	0.20	-	55,55,55,55	0
55	MG	2A	3478	1/1	0.76	0.18	-	94,94,94,94	0
55	MG	2a	1767	1/1	0.91	0.17	-	79,79,79,79	0
55	MG	2A	3764	1/1	0.94	0.12	-	72,72,72,72	0
55	MG	2A	3609	1/1	0.94	0.12	-	38,38,38,38	0
55	MG	1A	3187	1/1	0.95	0.09	-	52,52,52,52	0
55	MG	2a	1671	1/1	0.97	0.08	-	80,80,80,80	0
55	MG	1a	3119	1/1	0.94	0.09	-	81,81,81,81	0
55	MG	2a	1630	1/1	0.93	0.49	-	50,50,50,50	0
55	MG	1A	3604	1/1	0.77	0.13	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3178	1/1	0.89	0.28	-	39,39,39,39	0
55	MG	2A	3539	1/1	0.84	0.10	-	74,74,74,74	0
55	MG	1A	3799	1/1	0.98	0.10	-	49,49,49,49	0
55	MG	1A	3472	1/1	0.95	0.17	-	58,58,58,58	0
55	MG	1A	3555	1/1	0.88	0.10	-	61,61,61,61	0
55	MG	1A	3300	1/1	0.98	0.06	-	44,44,44,44	0
55	MG	2a	1716	1/1	0.89	0.16	-	73,73,73,73	0
55	MG	2A	3474	1/1	0.93	0.10	-	70,70,70,70	0
55	MG	2A	3520	1/1	0.81	0.61	-	65,65,65,65	0
55	MG	1A	3415	1/1	0.97	0.07	-	20,20,20,20	0
55	MG	2A	3804	1/1	0.81	0.20	-	35,35,35,35	0
55	MG	1A	3603	1/1	0.96	0.08	-	49,49,49,49	0
55	MG	1A	3326	1/1	0.96	0.12	-	24,24,24,24	0
55	MG	1a	3149	1/1	0.48	0.23	-	104,104,104,104	0
55	MG	1A	3049	1/1	0.94	0.53	-	45,45,45,45	0
55	MG	2A	3171	1/1	0.88	0.21	-	74,74,74,74	0
55	MG	2a	1750	1/1	0.91	0.12	-	83,83,83,83	0
55	MG	1A	3890	1/1	0.78	0.21	-	73,73,73,73	0
55	MG	2A	3745	1/1	0.96	0.19	-	70,70,70,70	0
55	MG	1A	3781	1/1	0.88	0.63	-	28,28,28,28	0
55	MG	2A	3633	1/1	0.91	0.11	-	82,82,82,82	0
55	MG	1A	3414	1/1	0.95	0.15	-	19,19,19,19	0
55	MG	1A	3710	1/1	0.92	0.10	-	42,42,42,42	0
55	MG	1A	3611	1/1	0.69	0.45	-	65,65,65,65	0
55	MG	1A	3074	1/1	0.84	0.68	-	29,29,29,29	0
55	MG	1A	3814	1/1	0.98	0.10	-	18,18,18,18	0
55	MG	1A	3501	1/1	0.69	0.18	-	64,64,64,64	0
55	MG	2A	3318	1/1	0.93	0.21	-	67,67,67,67	0
55	MG	1A	3337	1/1	0.98	0.10	-	39,39,39,39	0
55	MG	1A	3232	1/1	0.97	0.99	-	35,35,35,35	0
55	MG	2A	3493	1/1	0.94	0.27	-	51,51,51,51	0
55	MG	1A	3366	1/1	0.97	0.12	-	26,26,26,26	0
55	MG	2A	3461	1/1	0.95	0.11	-	34,34,34,34	0
55	MG	2B	3018	1/1	0.81	0.39	-	92,92,92,92	0
55	MG	1A	3631	1/1	0.82	0.18	-	59,59,59,59	0
55	MG	1A	3677	1/1	0.95	0.08	-	56,56,56,56	0
55	MG	1A	3466	1/1	0.98	0.08	-	46,46,46,46	0
55	MG	2A	3132	1/1	0.83	0.40	-	63,63,63,63	0
55	MG	2A	3495	1/1	0.96	0.09	-	59,59,59,59	0
55	MG	2A	3658	1/1	0.94	0.17	-	76,76,76,76	0
55	MG	2A	3116	1/1	0.96	0.13	-	43,43,43,43	0
55	MG	1A	3599	1/1	0.78	0.07	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2a	1723	1/1	0.93	0.23	-	110,110,110,110	0
55	MG	2A	3592	1/1	0.93	0.17	-	89,89,89,89	0
55	MG	2A	3596	1/1	0.86	0.13	-	65,65,65,65	0
55	MG	1A	3067	1/1	0.94	1.04	-	37,37,37,37	0
55	MG	2A	3303	1/1	0.93	0.12	-	88,88,88,88	0
55	MG	1A	3468	1/1	0.98	0.06	-	49,49,49,49	0
55	MG	2A	3121	1/1	0.90	0.15	-	81,81,81,81	0
55	MG	2A	3297	1/1	0.92	0.14	-	78,78,78,78	0
55	MG	1A	3309	1/1	0.93	0.16	-	32,32,32,32	0
55	MG	2a	1698	1/1	0.96	0.64	-	58,58,58,58	0
55	MG	1A	3152	1/1	0.99	0.07	-	53,53,53,53	0
55	MG	1a	3216	1/1	0.84	0.08	-	100,100,100,100	0
55	MG	1A	3629	1/1	0.96	0.22	-	42,42,42,42	0
55	MG	2D	303	1/1	0.87	0.57	-	50,50,50,50	0
55	MG	1a	3167	1/1	0.94	0.12	-	86,86,86,86	0
55	MG	2A	3233	1/1	0.95	0.17	-	73,73,73,73	0
55	MG	1A	3215	1/1	0.93	0.43	-	38,38,38,38	0
55	MG	1P	203	1/1	0.34	0.20	-	90,90,90,90	0
55	MG	2A	3368	1/1	0.98	0.05	-	42,42,42,42	0
55	MG	1A	3045	1/1	0.94	0.17	-	12,12,12,12	0
55	MG	1A	3171	1/1	0.86	0.65	-	44,44,44,44	0
55	MG	2A	3557	1/1	0.91	0.14	-	67,67,67,67	0
55	MG	1A	3452	1/1	0.86	0.46	-	76,76,76,76	0
55	MG	1A	3247	1/1	0.86	0.11	-	86,86,86,86	0
55	MG	1A	3528	1/1	0.94	0.15	-	57,57,57,57	0
55	MG	2A	3457	1/1	0.83	0.33	-	90,90,90,90	0
55	MG	1e	3001	1/1	0.88	0.19	-	55,55,55,55	0
55	MG	1A	3444	1/1	0.93	0.10	-	75,75,75,75	0
55	MG	2N	201	1/1	0.91	0.63	-	82,82,82,82	0
55	MG	2a	1679	1/1	0.95	0.09	-	63,63,63,63	0
55	MG	1A	3613	1/1	0.97	0.03	-	82,82,82,82	0
55	MG	2A	3427	1/1	0.91	0.13	-	61,61,61,61	0
55	MG	2A	3639	1/1	0.90	0.19	-	76,76,76,76	0
55	MG	2A	3403	1/1	0.89	0.26	-	79,79,79,79	0
55	MG	2A	3031	1/1	0.90	0.34	-	59,59,59,59	0
55	MG	1A	3353	1/1	0.98	0.12	-	67,67,67,67	0
55	MG	1Q	204	1/1	0.56	0.47	-	52,52,52,52	0
55	MG	2A	3176	1/1	0.88	0.46	-	51,51,51,51	0
55	MG	2A	3166	1/1	0.95	0.42	-	44,44,44,44	0
55	MG	2A	3266	1/1	0.97	0.14	-	65,65,65,65	0
55	MG	2A	3411	1/1	0.97	0.11	-	63,63,63,63	0
55	MG	2A	3559	1/1	0.73	0.40	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3602	1/1	0.90	0.06	-	73,73,73,73	0
55	MG	1A	3148	1/1	0.75	0.26	-	58,58,58,58	0
55	MG	1A	3635	1/1	0.91	0.27	-	39,39,39,39	0
55	MG	2a	1702	1/1	0.96	0.06	-	67,67,67,67	0
55	MG	2A	3516	1/1	0.98	0.08	-	45,45,45,45	0
55	MG	1A	3861	1/1	0.44	0.08	-	82,82,82,82	0
55	MG	2A	3261	1/1	0.94	0.11	-	88,88,88,88	0
55	MG	1A	3024	1/1	0.97	0.36	-	30,30,30,30	0
55	MG	1A	3736	1/1	0.96	0.16	-	55,55,55,55	0
55	MG	2A	3743	1/1	0.92	0.27	-	59,59,59,59	0
55	MG	1A	3585	1/1	0.98	0.27	-	59,59,59,59	0
55	MG	2A	3438	1/1	0.79	0.09	-	81,81,81,81	0
55	MG	2A	3024	1/1	0.77	0.24	-	58,58,58,58	0
55	MG	1A	3471	1/1	0.92	0.12	-	65,65,65,65	0
55	MG	1a	3041	1/1	0.82	0.18	-	72,72,72,72	0
55	MG	2A	3106	1/1	0.89	0.54	-	60,60,60,60	0
55	MG	1N	8002	1/1	0.91	0.15	-	64,64,64,64	0
55	MG	2a	1760	1/1	0.90	0.06	-	90,90,90,90	0
55	MG	2A	3714	1/1	0.97	0.10	-	49,49,49,49	0
55	MG	2a	1718	1/1	0.87	0.13	-	88,88,88,88	0
55	MG	1a	3068	1/1	0.96	0.30	-	73,73,73,73	0
55	MG	2a	1762	1/1	0.97	0.10	-	74,74,74,74	0
55	MG	1B	3019	1/1	0.83	0.14	-	60,60,60,60	0
55	MG	1A	3266	1/1	0.94	0.16	-	70,70,70,70	0
55	MG	2A	3760	1/1	0.96	0.08	-	40,40,40,40	0
55	MG	1F	309	1/1	0.92	0.11	-	28,28,28,28	0
55	MG	1A	3354	1/1	0.97	0.09	-	36,36,36,36	0
55	MG	1a	3158	1/1	0.92	0.07	-	88,88,88,88	0
55	MG	2A	3416	1/1	0.92	0.16	-	56,56,56,56	0
55	MG	1B	3014	1/1	0.98	0.07	-	41,41,41,41	0
55	MG	1o	3001	1/1	0.81	0.25	-	52,52,52,52	0
55	MG	1A	3382	1/1	0.96	0.16	-	52,52,52,52	0
55	MG	2A	3784	1/1	0.83	0.15	-	94,94,94,94	0
55	MG	1A	3293	1/1	0.88	0.09	-	75,75,75,75	0
55	MG	2A	3521	1/1	0.90	0.19	-	68,68,68,68	0
55	MG	1A	3401	1/1	0.95	0.06	-	62,62,62,62	0
55	MG	2A	3191	1/1	0.93	0.16	-	61,61,61,61	0
55	MG	1A	3359	1/1	0.89	0.10	-	64,64,64,64	0
55	MG	1a	3113	1/1	0.95	0.28	-	66,66,66,66	0
55	MG	2A	3518	1/1	0.99	0.14	-	71,71,71,71	0
55	MG	2A	3646	1/1	0.83	0.39	-	53,53,53,53	0
55	MG	2A	3398	1/1	0.92	0.18	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3068	1/1	0.82	0.34	-	56,56,56,56	0
55	MG	2a	1691	1/1	0.96	0.14	-	56,56,56,56	0
55	MG	1A	3140	1/1	0.93	0.17	-	37,37,37,37	0
55	MG	10	105	1/1	0.92	0.09	-	57,57,57,57	0
55	MG	2A	3263	1/1	0.96	0.18	-	46,46,46,46	0
55	MG	1A	3173	1/1	0.78	1.05	-	63,63,63,63	0
55	MG	1A	3493	1/1	0.97	0.12	-	30,30,30,30	0
55	MG	2a	1657	1/1	0.96	0.12	-	65,65,65,65	0
55	MG	2a	1667	1/1	0.97	0.10	-	64,64,64,64	0
55	MG	2A	3009	1/1	0.93	0.48	-	59,59,59,59	0
55	MG	2A	3026	1/1	0.90	0.33	-	73,73,73,73	0
55	MG	2A	3014	1/1	0.97	0.26	-	66,66,66,66	0
55	MG	2F	308	1/1	0.93	0.39	-	59,59,59,59	0
55	MG	2A	3387	1/1	0.91	0.15	-	68,68,68,68	0
55	MG	2a	1734	1/1	0.69	0.38	-	57,57,57,57	0
55	MG	2A	3330	1/1	0.95	0.14	-	57,57,57,57	0
55	MG	2A	3396	1/1	0.94	0.19	-	71,71,71,71	0
55	MG	1A	3723	1/1	0.97	0.10	-	47,47,47,47	0
55	MG	1A	3114	1/1	0.95	0.26	-	37,37,37,37	0
55	MG	2T	201	1/1	0.99	0.10	-	47,47,47,47	0
55	MG	1a	3086	1/1	0.97	0.33	-	68,68,68,68	0
55	MG	1a	3053	1/1	0.88	0.23	-	82,82,82,82	0
55	MG	2a	1625	1/1	0.73	0.31	-	70,70,70,70	0
55	MG	1F	316	1/1	0.94	0.10	-	69,69,69,69	0
55	MG	2A	3575	1/1	0.91	0.20	-	48,48,48,48	0
55	MG	2A	3281	1/1	0.93	0.10	-	61,61,61,61	0
55	MG	2a	1627	1/1	0.99	0.26	-	84,84,84,84	0
55	MG	1A	3685	1/1	0.97	0.12	-	52,52,52,52	0
55	MG	2A	3173	1/1	0.95	0.56	-	42,42,42,42	0
55	MG	2A	3564	1/1	0.86	0.89	-	57,57,57,57	0
55	MG	2A	3272	1/1	0.94	0.10	-	41,41,41,41	0
55	MG	2A	3394	1/1	0.86	0.19	-	65,65,65,65	0
55	MG	2A	3027	1/1	0.82	0.25	-	70,70,70,70	0
55	MG	2a	1756	1/1	0.86	0.13	-	69,69,69,69	0
55	MG	1A	3735	1/1	0.94	0.35	-	27,27,27,27	0
55	MG	2A	3134	1/1	0.84	0.79	-	70,70,70,70	0
55	MG	2A	3659	1/1	0.91	0.16	-	73,73,73,73	0
55	MG	2A	3392	1/1	0.93	0.19	-	31,31,31,31	0
55	MG	2A	3376	1/1	0.97	0.11	-	31,31,31,31	0
55	MG	2A	3793	1/1	0.92	0.28	-	67,67,67,67	0
55	MG	1A	3536	1/1	0.96	0.08	-	44,44,44,44	0
55	MG	1A	3575	1/1	0.93	0.32	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1a	3046	1/1	0.94	0.26	-	54,54,54,54	0
55	MG	2A	3555	1/1	0.80	0.54	-	52,52,52,52	0
55	MG	2A	3674	1/1	0.95	0.17	-	66,66,66,66	0
55	MG	2A	3247	1/1	0.97	0.16	-	35,35,35,35	0
55	MG	2a	1619	1/1	0.93	0.33	-	72,72,72,72	0
55	MG	2A	3581	1/1	0.97	0.08	-	72,72,72,72	0
55	MG	2A	3336	1/1	0.97	0.21	-	56,56,56,56	0
55	MG	1A	3788	1/1	0.89	0.07	-	48,48,48,48	0
55	MG	1A	3746	1/1	0.95	0.14	-	31,31,31,31	0
55	MG	2A	3686	1/1	0.89	0.08	-	95,95,95,95	0
55	MG	1a	3114	1/1	0.70	0.11	-	74,74,74,74	0
55	MG	1R	205	1/1	0.91	0.26	-	34,34,34,34	0
55	MG	2A	3795	1/1	0.95	0.12	-	72,72,72,72	0
55	MG	1a	3184	1/1	0.75	0.10	-	73,73,73,73	0
55	MG	1A	3705	1/1	0.96	0.26	-	48,48,48,48	0
55	MG	1A	3158	1/1	0.95	0.15	-	37,37,37,37	0
55	MG	1a	3116	1/1	0.91	0.44	-	76,76,76,76	0
55	MG	2a	1640	1/1	0.91	0.70	-	61,61,61,61	0
55	MG	2A	3125	1/1	0.93	1.06	-	58,58,58,58	0
55	MG	1A	3900	1/1	0.77	0.23	-	58,58,58,58	0
55	MG	2a	1632	1/1	0.89	0.22	-	75,75,75,75	0
55	MG	2A	3508	1/1	0.94	0.55	-	57,57,57,57	0
55	MG	2a	1759	1/1	0.88	0.15	-	72,72,72,72	0
55	MG	1A	3586	1/1	0.92	0.07	-	59,59,59,59	0
55	MG	2A	3114	1/1	0.81	0.29	-	62,62,62,62	0
55	MG	2A	3769	1/1	0.91	0.18	-	75,75,75,75	0
55	MG	2A	3573	1/1	0.92	0.13	-	71,71,71,71	0
55	MG	10	107	1/1	0.94	0.18	-	57,57,57,57	0
55	MG	2A	3435	1/1	0.89	0.29	-	76,76,76,76	0
55	MG	2A	3298	1/1	0.95	0.12	-	56,56,56,56	0
55	MG	2A	3621	1/1	0.90	0.50	-	54,54,54,54	0
55	MG	1a	3164	1/1	0.97	0.14	-	61,61,61,61	0
55	MG	1A	3224	1/1	0.99	0.07	-	73,73,73,73	0
55	MG	1A	3753	1/1	0.82	0.17	-	67,67,67,67	0
55	MG	2a	1770	1/1	0.64	0.18	-	75,75,75,75	0
55	MG	1A	3253	1/1	0.80	0.24	-	53,53,53,53	0
55	MG	1A	3072	1/1	0.85	0.17	-	43,43,43,43	0
55	MG	2A	3243	1/1	0.96	0.07	-	72,72,72,72	0
56	A	1B	3025	1/23	0.89	0.59	-	57,57,57,57	0
55	MG	1a	3095	1/1	0.90	0.14	-	62,62,62,62	0
55	MG	1A	3691	1/1	0.92	0.12	-	26,26,26,26	0
55	MG	2a	1777	1/1	0.87	0.11	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3264	1/1	0.96	0.11	-	65,65,65,65	0
55	MG	1A	3318	1/1	0.95	0.24	-	61,61,61,61	0
55	MG	2A	3072	1/1	0.81	0.32	-	57,57,57,57	0
55	MG	1A	3917	1/1	0.70	0.30	-	36,36,36,36	0
55	MG	1A	3898	1/1	0.93	0.36	-	63,63,63,63	0
55	MG	1A	3856	1/1	0.85	0.33	-	46,46,46,46	0
55	MG	2A	3234	1/1	0.96	0.19	-	45,45,45,45	0
55	MG	2A	3779	1/1	0.79	0.08	-	72,72,72,72	0
55	MG	1f	8001	1/1	0.91	0.21	-	60,60,60,60	0
55	MG	2A	3248	1/1	0.78	0.05	-	81,81,81,81	0
55	MG	2A	3093	1/1	0.94	0.39	-	46,46,46,46	0
55	MG	2A	3302	1/1	0.87	0.15	-	44,44,44,44	0
55	MG	1A	3274	1/1	0.98	0.18	-	27,27,27,27	0
55	MG	1A	3445	1/1	0.91	0.17	-	65,65,65,65	0
55	MG	1a	3097	1/1	0.94	0.10	-	61,61,61,61	0
55	MG	1a	3140	1/1	0.87	0.20	-	84,84,84,84	0
55	MG	2a	1790	1/1	0.93	0.44	-	80,80,80,80	0
55	MG	2a	1704	1/1	0.94	0.14	-	68,68,68,68	0
55	MG	2A	3071	1/1	0.88	0.55	-	62,62,62,62	0
55	MG	2a	1769	1/1	0.96	0.27	-	76,76,76,76	0
55	MG	2A	3268	1/1	0.87	0.15	-	69,69,69,69	0
55	MG	2A	3224	1/1	0.82	0.17	-	69,69,69,69	0
55	MG	2A	3790	1/1	0.89	0.05	-	71,71,71,71	0
55	MG	2a	1700	1/1	0.98	0.13	-	76,76,76,76	0
55	MG	2A	3610	1/1	0.84	0.11	-	81,81,81,81	0
55	MG	1B	3011	1/1	0.98	0.15	-	48,48,48,48	0
55	MG	2A	3148	1/1	0.86	0.33	-	57,57,57,57	0
55	MG	1A	3774	1/1	0.97	0.25	-	45,45,45,45	0
55	MG	2A	3781	1/1	0.97	0.07	-	51,51,51,51	0
55	MG	2A	3369	1/1	0.92	0.12	-	58,58,58,58	0
55	MG	2o	3001	1/1	0.88	0.18	-	60,60,60,60	0
55	MG	2A	3542	1/1	0.85	0.15	-	88,88,88,88	0
55	MG	2A	3500	1/1	0.93	0.31	-	41,41,41,41	0
55	MG	1B	3018	1/1	0.95	0.10	-	37,37,37,37	0
55	MG	1a	3161	1/1	0.41	0.78	-	77,77,77,77	0
55	MG	1A	3719	1/1	0.93	0.09	-	45,45,45,45	0
55	MG	1a	3143	1/1	0.83	0.10	-	87,87,87,87	0
55	MG	1G	3002	1/1	0.92	0.07	-	62,62,62,62	0
55	MG	2A	3356	1/1	0.94	0.19	-	43,43,43,43	0
55	MG	2A	3632	1/1	0.81	0.25	-	97,97,97,97	0
55	MG	2A	3152	1/1	0.85	0.45	-	59,59,59,59	0
55	MG	1A	3612	1/1	0.90	0.07	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	2A	3656	1/1	0.94	0.11	-	42,42,42,42	0
55	MG	1A	3777	1/1	0.95	0.05	-	41,41,41,41	0
55	MG	1A	3226	1/1	0.92	0.48	-	31,31,31,31	0
55	MG	2a	1747	1/1	0.65	0.23	-	94,94,94,94	0
55	MG	1a	3051	1/1	0.98	0.41	-	57,57,57,57	0
55	MG	1a	3101	1/1	0.96	0.13	-	39,39,39,39	0
55	MG	1A	3841	1/1	0.95	0.08	-	64,64,64,64	0
55	MG	2B	3010	1/1	0.91	0.07	-	72,72,72,72	0
55	MG	2A	3818	1/1	0.93	0.23	-	57,57,57,57	0
55	MG	2A	3090	1/1	0.39	0.41	-	76,76,76,76	0
55	MG	1a	3170	1/1	0.82	0.28	-	82,82,82,82	0
55	MG	2A	3588	1/1	0.92	0.22	-	67,67,67,67	0
55	MG	2A	3388	1/1	0.98	0.14	-	60,60,60,60	0
55	MG	1A	3657	1/1	0.96	0.06	-	50,50,50,50	0
55	MG	2A	3370	1/1	0.96	0.11	-	76,76,76,76	0
55	MG	1A	3606	1/1	0.98	0.17	-	56,56,56,56	0
55	MG	2a	1709	1/1	0.96	0.15	-	82,82,82,82	0
55	MG	1A	3595	1/1	0.91	0.10	-	67,67,67,67	0
55	MG	2A	3004	1/1	0.73	0.28	-	56,56,56,56	0
55	MG	1B	3010	1/1	0.96	0.04	-	59,59,59,59	0
55	MG	1A	3665	1/1	0.97	0.25	-	51,51,51,51	0
55	MG	1A	3537	1/1	0.96	0.29	-	38,38,38,38	0
55	MG	1d	504	1/1	0.83	0.27	-	75,75,75,75	0
55	MG	1A	3893	1/1	0.86	0.06	-	103,103,103,103	0
55	MG	2A	3751	1/1	0.89	0.17	-	67,67,67,67	0
55	MG	2W	3001	1/1	0.89	0.21	-	60,60,60,60	0
55	MG	2A	3327	1/1	0.94	0.33	-	67,67,67,67	0
55	MG	2A	3345	1/1	0.89	0.21	-	81,81,81,81	0
55	MG	2A	3488	1/1	0.97	0.12	-	58,58,58,58	0
55	MG	1A	3385	1/1	0.92	0.12	-	57,57,57,57	0
55	MG	2A	3598	1/1	0.90	0.12	-	62,62,62,62	0
55	MG	2A	3140	1/1	0.82	0.33	-	61,61,61,61	0
55	MG	1A	3557	1/1	0.95	0.10	-	24,24,24,24	0
55	MG	2a	1761	1/1	0.90	0.21	-	67,67,67,67	0
55	MG	1A	3061	1/1	0.96	0.27	-	47,47,47,47	0
55	MG	1A	3826	1/1	0.96	0.12	-	59,59,59,59	0
55	MG	1A	3033	1/1	0.91	0.59	-	45,45,45,45	0
55	MG	2A	3256	1/1	0.82	0.11	-	84,84,84,84	0
55	MG	1A	3371	1/1	0.91	0.19	-	63,63,63,63	0
55	MG	2A	3747	1/1	0.83	0.07	-	75,75,75,75	0
55	MG	2A	3774	1/1	0.92	0.21	-	79,79,79,79	0
55	MG	1A	3843	1/1	0.97	0.20	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	1A	3588	1/1	0.94	0.14	-	62,62,62,62	0
55	MG	1A	3915	1/1	0.97	0.21	-	60,60,60,60	0
55	MG	2a	1607	1/1	0.88	0.25	-	52,52,52,52	0
55	MG	1A	3424	1/1	0.95	0.04	-	62,62,62,62	0
55	MG	2G	3002	1/1	0.70	0.26	-	90,90,90,90	0
55	MG	1A	3749	1/1	0.99	0.05	-	36,36,36,36	0
55	MG	1a	3186	1/1	0.80	0.08	-	69,69,69,69	0
55	MG	1A	3828	1/1	0.96	0.17	-	61,61,61,61	0
55	MG	2A	3718	1/1	0.93	0.08	-	83,83,83,83	0
55	MG	2A	3305	1/1	0.84	0.07	-	84,84,84,84	0
55	MG	1A	3360	1/1	0.98	0.12	-	21,21,21,21	0
55	MG	1a	3109	1/1	0.93	0.24	-	53,53,53,53	0
55	MG	1A	3524	1/1	0.88	0.17	-	52,52,52,52	0
55	MG	1A	3831	1/1	0.86	0.42	-	51,51,51,51	0
55	MG	1A	3755	1/1	0.96	0.07	-	69,69,69,69	0
55	MG	1A	3051	1/1	0.92	0.57	-	30,30,30,30	0
55	MG	1A	3888	1/1	0.98	0.11	-	47,47,47,47	0
55	MG	1A	3088	1/1	0.88	0.64	-	30,30,30,30	0
56	A	2A	3821	1/23	0.93	0.17	-	79,79,79,79	0
55	MG	1l	201	1/1	0.92	0.23	-	74,74,74,74	0
55	MG	2a	1712	1/1	0.93	0.33	-	69,69,69,69	0
55	MG	1T	201	1/1	0.96	0.19	-	54,54,54,54	0
55	MG	1A	3474	1/1	0.91	0.20	-	69,69,69,69	0
55	MG	1A	3503	1/1	0.66	0.40	-	77,77,77,77	0
55	MG	2A	3357	1/1	0.87	0.14	-	50,50,50,50	0
55	MG	2a	1644	1/1	0.77	0.18	-	67,67,67,67	0
55	MG	1A	3248	1/1	0.81	0.40	-	51,51,51,51	0
55	MG	2A	3660	1/1	0.87	0.20	-	71,71,71,71	0
55	MG	2A	3782	1/1	0.86	0.15	-	82,82,82,82	0
55	MG	2A	3197	1/1	0.91	0.21	-	48,48,48,48	0
55	MG	1A	3398	1/1	0.85	0.24	-	37,37,37,37	0
55	MG	2A	3623	1/1	0.95	0.31	-	66,66,66,66	0
55	MG	2A	3626	1/1	0.94	0.17	-	60,60,60,60	0
55	MG	1a	3222	1/1	0.84	0.43	-	62,62,62,62	0
55	MG	1A	3520	1/1	0.94	0.18	-	56,56,56,56	0
55	MG	1A	3390	1/1	0.96	0.14	-	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.