



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2017 – 06:51 AM EDT

PDB ID : 4Z8C  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome bound to translation inhibitor oncocin  
Authors : Roy, R.N.; Lomakin, I.B.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : unknown  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

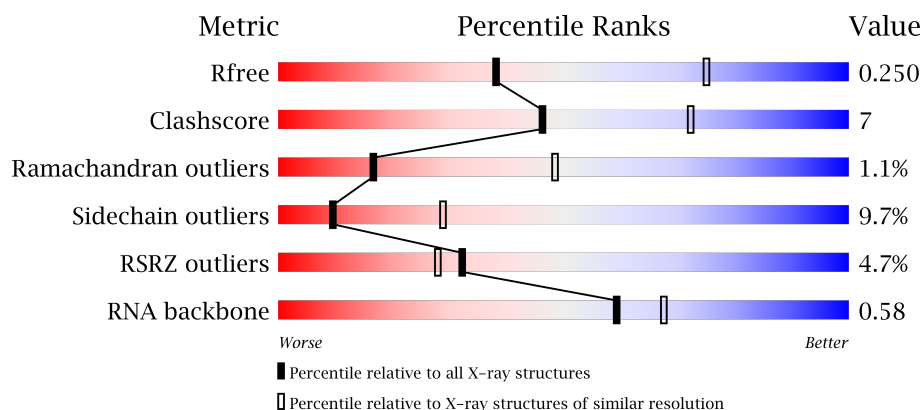
# 1 Overall quality at a glance

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.







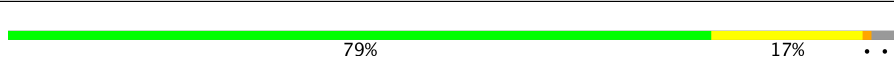
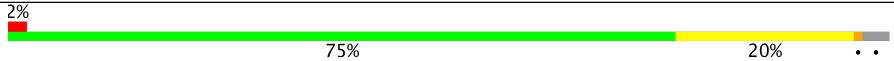
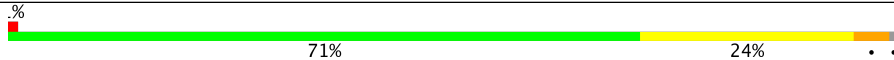
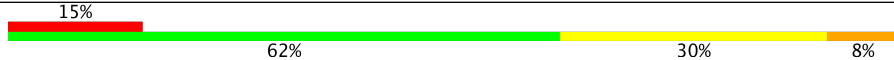
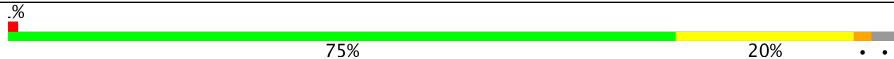
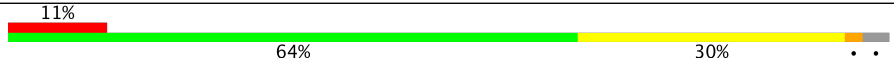
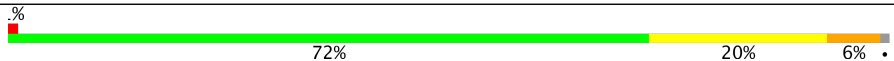
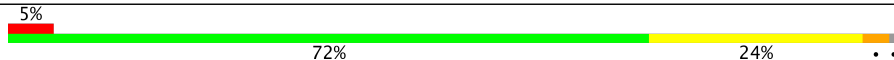


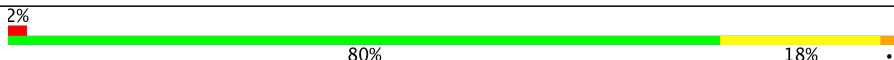
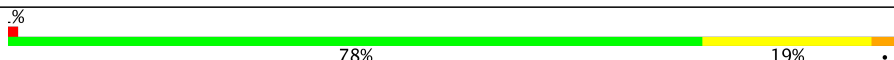
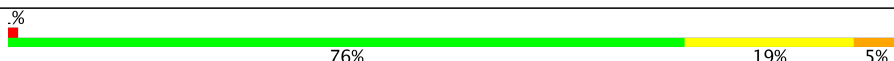
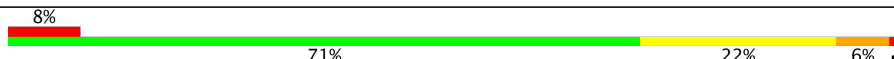
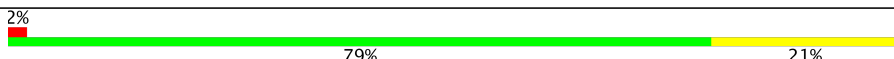

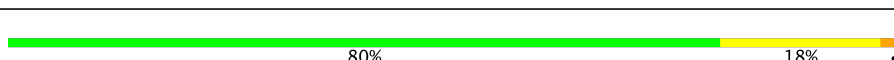
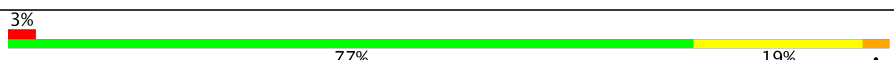
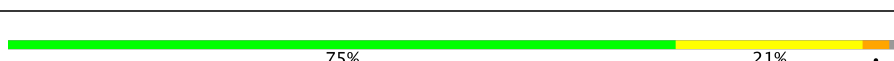
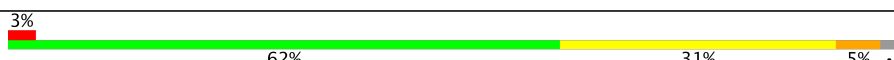
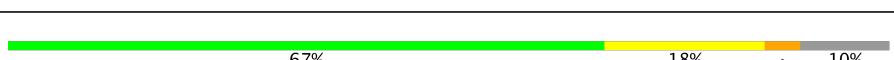
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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>67%</div> <div>23%</div> <div>6%</div> </div>
1	2A	2915	<div> <div>62%</div> <div>29%</div> <div>5%</div> <div>.</div> </div>
2	1B	121	<div> <div>72%</div> <div>25%</div> <div>..</div> </div>
2	2B	121	<div> <div>55%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>

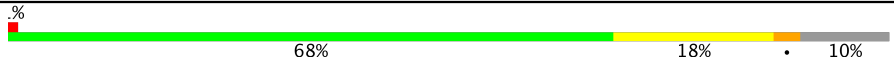



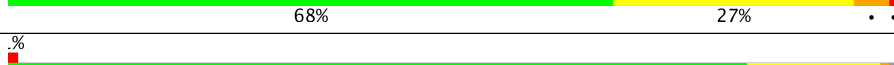
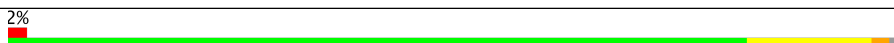
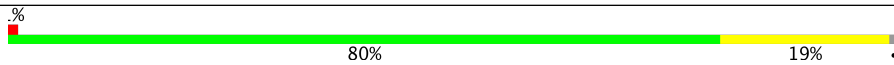



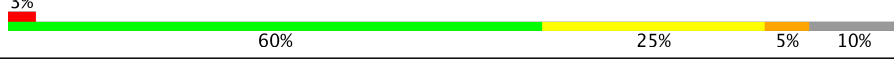

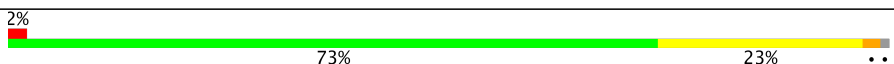



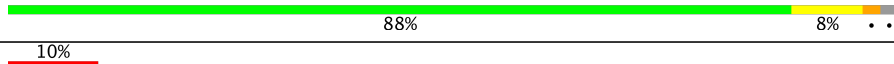

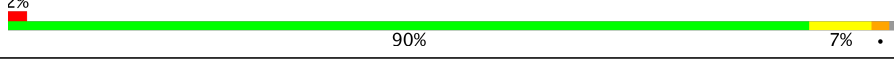



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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	




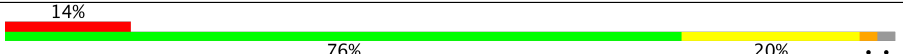
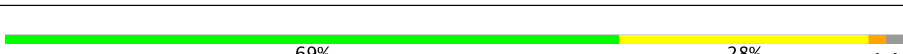
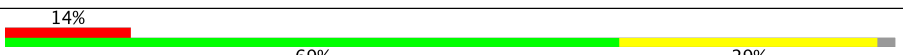
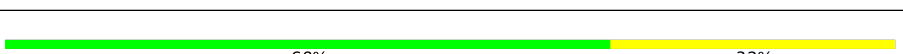
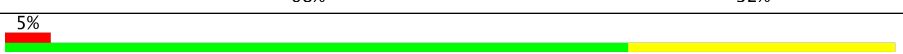

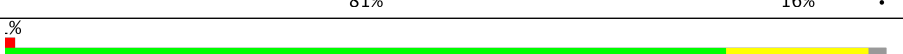
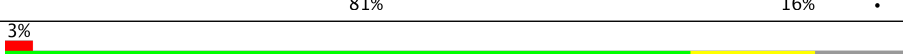
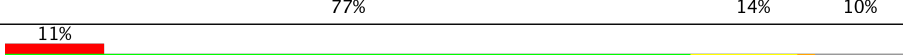
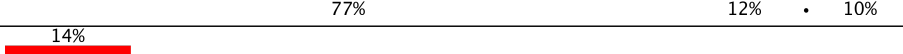
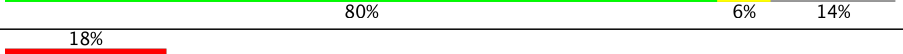





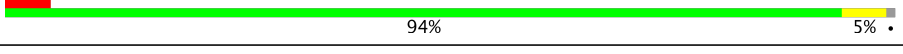
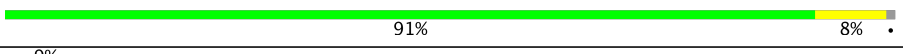
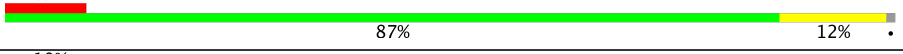
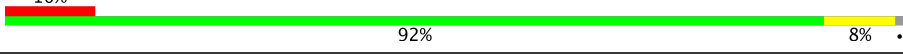
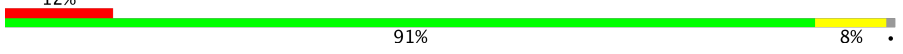

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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	19	
55	2z	19	

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
56	MG	15	101	-	-	-	X
56	MG	1A	3001	-	-	-	X
56	MG	1A	3074	-	-	-	X
56	MG	1A	3092	-	-	-	X
56	MG	1A	3093	-	-	-	X
56	MG	1A	3110	-	-	-	X
56	MG	1A	3129	-	-	-	X
56	MG	1A	3131	-	-	-	X
56	MG	1A	3132	-	-	-	X
56	MG	1A	3162	-	-	-	X
56	MG	1A	3170	-	-	-	X
56	MG	1A	3172	-	-	-	X
56	MG	1A	3177	-	-	-	X
56	MG	1A	3178	-	-	-	X
56	MG	1A	3179	-	-	-	X
56	MG	1A	3182	-	-	-	X
56	MG	1A	3186	-	-	-	X
56	MG	1A	3187	-	-	-	X
56	MG	1A	3203	-	-	-	X
56	MG	1A	3208	-	-	-	X
56	MG	1A	3215	-	-	-	X
56	MG	1A	3225	-	-	-	X
56	MG	1A	3241	-	-	-	X
56	MG	1A	3253	-	-	-	X
56	MG	1A	3267	-	-	-	X
56	MG	1A	3287	-	-	-	X
56	MG	1A	3289	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3312	-	-	-	X
56	MG	1A	3315	-	-	-	X
56	MG	1A	3322	-	-	-	X
56	MG	1A	3329	-	-	-	X
56	MG	1A	3374	-	-	-	X
56	MG	1A	3394	-	-	-	X
56	MG	1A	3411	-	-	-	X
56	MG	1A	3437	-	-	-	X
56	MG	1A	3442	-	-	-	X
56	MG	1A	3444	-	-	-	X
56	MG	1A	3449	-	-	-	X
56	MG	1A	3456	-	-	-	X
56	MG	1A	3459	-	-	-	X
56	MG	1A	3473	-	-	-	X
56	MG	1A	3481	-	-	-	X
56	MG	1A	3518	-	-	-	X
56	MG	1A	3705	-	-	-	X
56	MG	1A	3711	-	-	-	X
56	MG	1A	3797	-	-	-	X
56	MG	1A	3821	-	-	-	X
56	MG	1A	3887	-	-	-	X
56	MG	1A	3888	-	-	-	X
56	MG	1A	3911	-	-	-	X
56	MG	1A	3930	-	-	-	X
56	MG	1A	3931	-	-	-	X
56	MG	1A	3962	-	-	-	X
56	MG	1A	3964	-	-	-	X
56	MG	1A	3968	-	-	-	X
56	MG	1A	3973	-	-	-	X
56	MG	1A	3975	-	-	-	X
56	MG	1A	3980	-	-	-	X
56	MG	1A	3986	-	-	-	X
56	MG	1A	3994	-	-	-	X
56	MG	1A	3995	-	-	-	X
56	MG	1A	4002	-	-	-	X
56	MG	1A	4003	-	-	-	X
56	MG	1A	4007	-	-	-	X
56	MG	1A	4008	-	-	-	X
56	MG	1A	4010	-	-	-	X
56	MG	1A	4011	-	-	-	X
56	MG	1A	4012	-	-	-	X
56	MG	1A	4017	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4018	-	-	-	X
56	MG	1A	4019	-	-	-	X
56	MG	1B	205	-	-	-	X
56	MG	1B	211	-	-	-	X
56	MG	1D	303	-	-	-	X
56	MG	1D	306	-	-	-	X
56	MG	1D	309	-	-	-	X
56	MG	1D	311	-	-	-	X
56	MG	1D	312	-	-	-	X
56	MG	1E	303	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1F	306	-	-	-	X
56	MG	1H	8002	-	-	-	X
56	MG	1P	205	-	-	-	X
56	MG	1P	206	-	-	-	X
56	MG	1R	203	-	-	-	X
56	MG	1U	202	-	-	-	X
56	MG	1U	203	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1U	205	-	-	-	X
56	MG	1W	3005	-	-	-	X
56	MG	1X	102	-	-	-	X
56	MG	1a	1659	-	-	-	X
56	MG	1a	1668	-	-	-	X
56	MG	1a	1739	-	-	-	X
56	MG	1a	1749	-	-	-	X
56	MG	1a	1765	-	-	-	X
56	MG	1a	1814	-	-	-	X
56	MG	1a	1858	-	-	-	X
56	MG	2A	3016	-	-	-	X
56	MG	2A	3017	-	-	-	X
56	MG	2A	3019	-	-	-	X
56	MG	2A	3024	-	-	-	X
56	MG	2A	3027	-	-	-	X
56	MG	2A	3029	-	-	-	X
56	MG	2A	3042	-	-	-	X
56	MG	2A	3063	-	-	-	X
56	MG	2A	3107	-	-	-	X
56	MG	2A	3123	-	-	-	X
56	MG	2A	3139	-	-	-	X
56	MG	2A	3155	-	-	-	X
56	MG	2A	3188	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3191	-	-	-	X
56	MG	2A	3199	-	-	-	X
56	MG	2A	3209	-	-	-	X
56	MG	2A	3214	-	-	-	X
56	MG	2A	3222	-	-	-	X
56	MG	2A	3232	-	-	-	X
56	MG	2A	3233	-	-	-	X
56	MG	2A	3303	-	-	-	X
56	MG	2A	3304	-	-	-	X
56	MG	2A	3318	-	-	-	X
56	MG	2A	3349	-	-	-	X
56	MG	2A	3381	-	-	-	X
56	MG	2A	3416	-	-	-	X
56	MG	2A	3430	-	-	-	X
56	MG	2A	3468	-	-	-	X
56	MG	2A	3470	-	-	-	X
56	MG	2A	3540	-	-	-	X
56	MG	2A	3550	-	-	-	X
56	MG	2A	3554	-	-	-	X
56	MG	2A	3555	-	-	-	X
56	MG	2A	3559	-	-	-	X
56	MG	2A	3561	-	-	-	X
56	MG	2A	3562	-	-	-	X
56	MG	2A	3563	-	-	-	X
56	MG	2D	303	-	-	-	X
56	MG	2F	303	-	-	-	X
56	MG	2P	201	-	-	-	X
56	MG	2U	201	-	-	-	X
56	MG	2a	3011	-	-	-	X
56	MG	2a	3022	-	-	-	X
56	MG	2a	3026	-	-	-	X
56	MG	2a	3105	-	-	-	X
56	MG	2a	3194	-	-	-	X
56	MG	2a	3228	-	-	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288378 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	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

- 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
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1139	709	231	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	0	0	0
			1091	680	225	185	1		
15	2T	131	Total	C	N	O	0	0	0
			1083	675	224	183	1		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			

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

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

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

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

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

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

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

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

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

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

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



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- 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
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	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
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	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
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1095	695	203	193	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
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- 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
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			829	516	155	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
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	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
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	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
			715	447	140	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
			671	424	133	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
			811	519	148	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	84	Total	C	N	O	S	0	0	0
			642	409	119	112	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			187	116	42	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called Initiator Methionine tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Oncocin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	13	Total	C	N	O	0	0	0
			108	72	20	16			
55	2z	13	Total	C	N	O	0	0	0
			108	72	20	16			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	4	Total	Mg	0	0
			4	4		
56	17	1	Total	Mg	0	0
			1	1		
56	1z	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	5	Total	Mg	0	0
			5	5		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	1	Total	Mg	0	0
			1	1		
56	18	3	Total	Mg	0	0
			3	3		
56	1o	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	2h	1	Total 1	Mg 1	0	0
56	1P	6	Total 6	Mg 6	0	0
56	2B	11	Total 11	Mg 11	0	0
56	1q	4	Total 4	Mg 4	0	0
56	2a	263	Total 263	Mg 263	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1E	5	Total 5	Mg 5	0	0
56	2z	1	Total 1	Mg 1	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	6	Total 6	Mg 6	0	0
56	16	2	Total 2	Mg 2	0	0
56	28	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1021	Total 1021	Mg 1021	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	12	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	1D	14	Total 14	Mg 14	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	1	Total 1	Mg 1	0	0
56	1a	276	Total 276	Mg 276	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	4	Total 4	Mg 4	0	0
56	1x	8	Total 8	Mg 8	0	0
56	1R	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	2U	1	Total 1	Mg 1	0	0
56	1G	3	Total 3	Mg 3	0	0
56	2O	3	Total 3	Mg 3	0	0
56	11	1	Total 1	Mg 1	0	0
56	1d	2	Total 2	Mg 2	0	0
56	1H	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2x	4	Total 4	Mg 4	0	0
56	1Z	2	Total 2	Mg 2	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1U	5	Total 5	Mg 5	0	0
56	1O	2	Total 2	Mg 2	0	0
56	1r	2	Total 2	Mg 2	0	0
56	19	3	Total 3	Mg 3	0	0
56	1l	1	Total 1	Mg 1	0	0
56	1F	8	Total 8	Mg 8	0	0
56	10	7	Total 7	Mg 7	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	4	Total 4	Mg 4	0	0
56	2A	566	Total 566	Mg 566	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	24	Total 24	Mg 24	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0

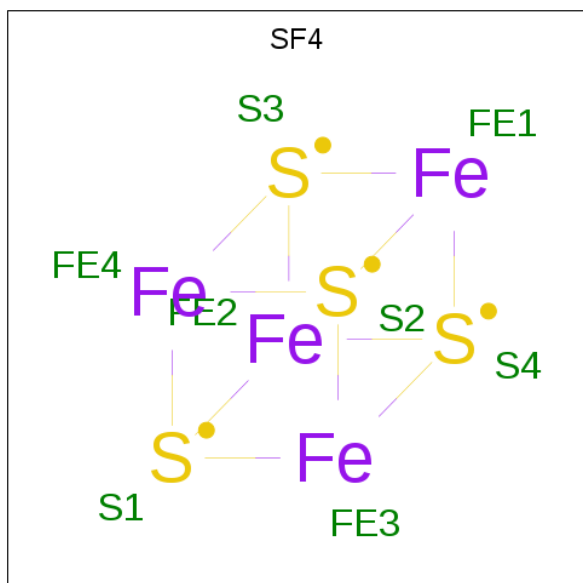
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1n	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	19	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1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

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2088	Total	O	0	0
			2088	2088		
59	1B	38	Total	O	0	0
			38	38		
59	1D	22	Total	O	0	0
			22	22		
59	1E	25	Total	O	0	0
			25	25		
59	1F	16	Total	O	0	0
			16	16		
59	1G	6	Total	O	0	0
			6	6		
59	1H	5	Total	O	0	0
			5	5		
59	1I	1	Total	O	0	0
			1	1		
59	1N	5	Total	O	0	0
			5	5		
59	1O	4	Total	O	0	0
			4	4		
59	1P	21	Total	O	0	0
			21	21		
59	1Q	9	Total	O	0	0
			9	9		
59	1R	9	Total	O	0	0
			9	9		
59	1S	1	Total	O	0	0
			1	1		
59	1T	11	Total	O	0	0
			11	11		
59	1U	13	Total	O	0	0
			13	13		
59	1V	2	Total	O	0	0
			2	2		
59	1W	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1X	5	Total 5	O 5	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	3	Total 3	O 3	0	0
59	10	10	Total 10	O 10	0	0
59	11	4	Total 4	O 4	0	0
59	12	1	Total 1	O 1	0	0
59	13	4	Total 4	O 4	0	0
59	15	5	Total 5	O 5	0	0
59	16	8	Total 8	O 8	0	0
59	17	8	Total 8	O 8	0	0
59	18	13	Total 13	O 13	0	0
59	19	2	Total 2	O 2	0	0
59	1a	319	Total 319	O 319	0	0
59	1b	2	Total 2	O 2	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	4	Total 4	O 4	0	0
59	1e	2	Total 2	O 2	0	0
59	1f	1	Total 1	O 1	0	0
59	1i	1	Total 1	O 1	0	0
59	1j	1	Total 1	O 1	0	0
59	1m	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1o	3	Total 3	O 3	0	0
59	1p	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1v	1	Total 1	O 1	0	0
59	1x	7	Total 7	O 7	0	0
59	1z	2	Total 2	O 2	0	0
59	2A	801	Total 801	O 801	0	0
59	2B	13	Total 13	O 13	0	0
59	2D	20	Total 20	O 20	0	0
59	2E	10	Total 10	O 10	0	0
59	2F	7	Total 7	O 7	0	0
59	2N	1	Total 1	O 1	0	0
59	2O	4	Total 4	O 4	0	0
59	2P	4	Total 4	O 4	0	0
59	2Q	2	Total 2	O 2	0	0
59	2R	3	Total 3	O 3	0	0
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	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2Y	1	Total 1	O 1	0	0
59	2Z	2	Total 2	O 2	0	0
59	20	3	Total 3	O 3	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	27	2	Total 2	O 2	0	0
59	28	4	Total 4	O 4	0	0
59	2a	371	Total 371	O 371	0	0
59	2c	2	Total 2	O 2	0	0
59	2e	3	Total 3	O 3	0	0
59	2h	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2j	1	Total 1	O 1	0	0
59	2k	3	Total 3	O 3	0	0
59	2l	3	Total 3	O 3	0	0
59	2m	1	Total 1	O 1	0	0
59	2n	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	2	Total 2	O 2	0	0
59	2q	2	Total 2	O 2	0	0

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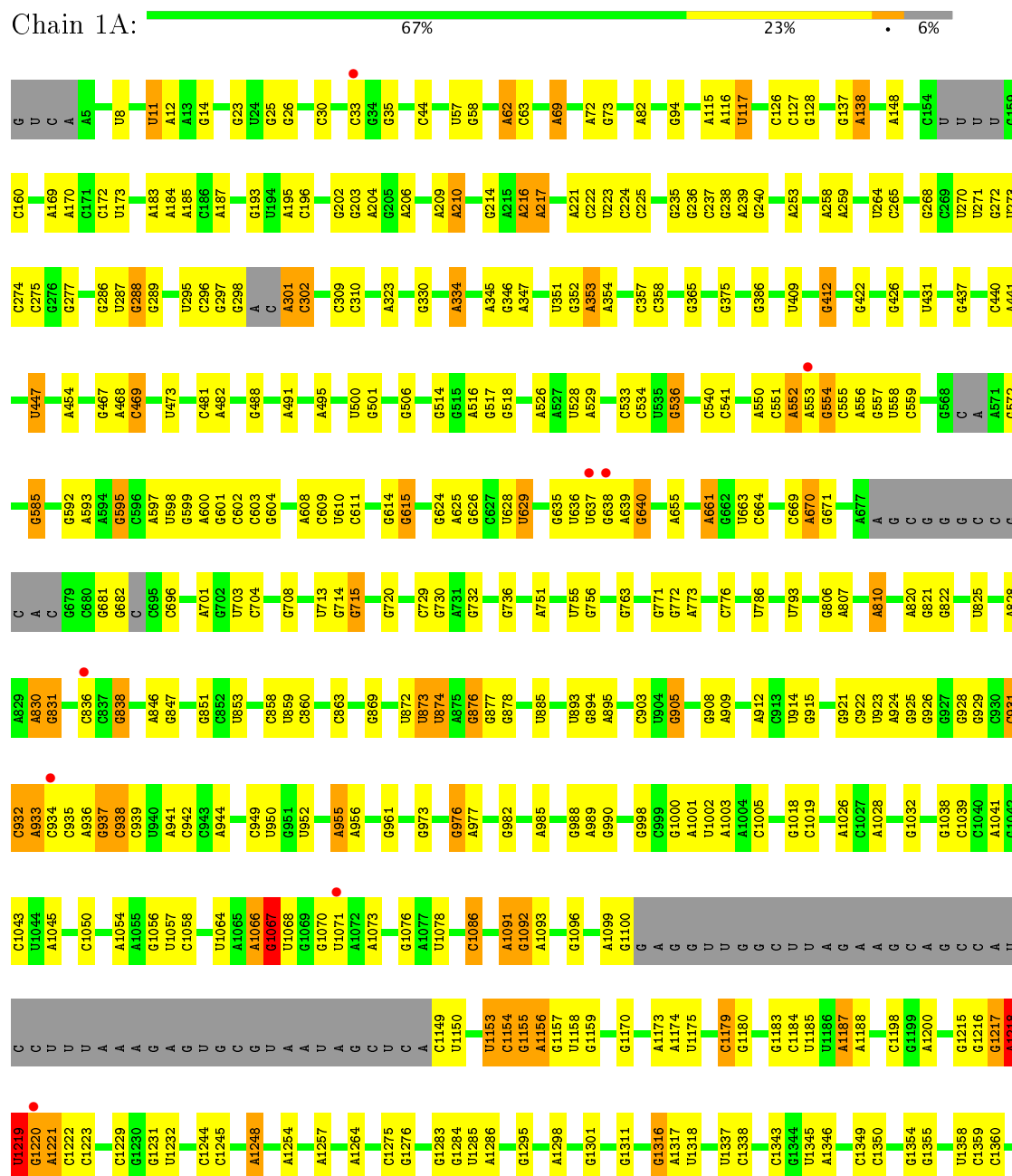
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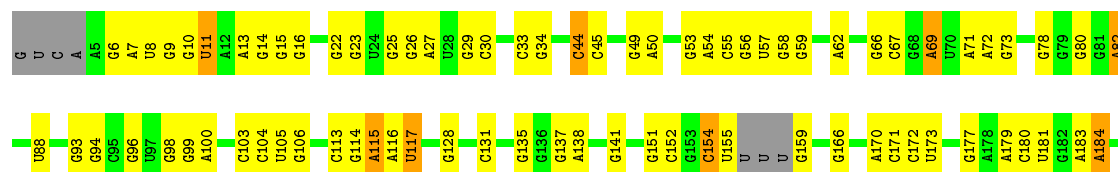
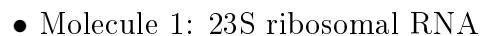
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2r	1	Total 1	O 1	0	0
59	2t	3	Total 3	O 3	0	0
59	2x	3	Total 3	O 3	0	0
59	2z	1	Total 1	O 1	0	0

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

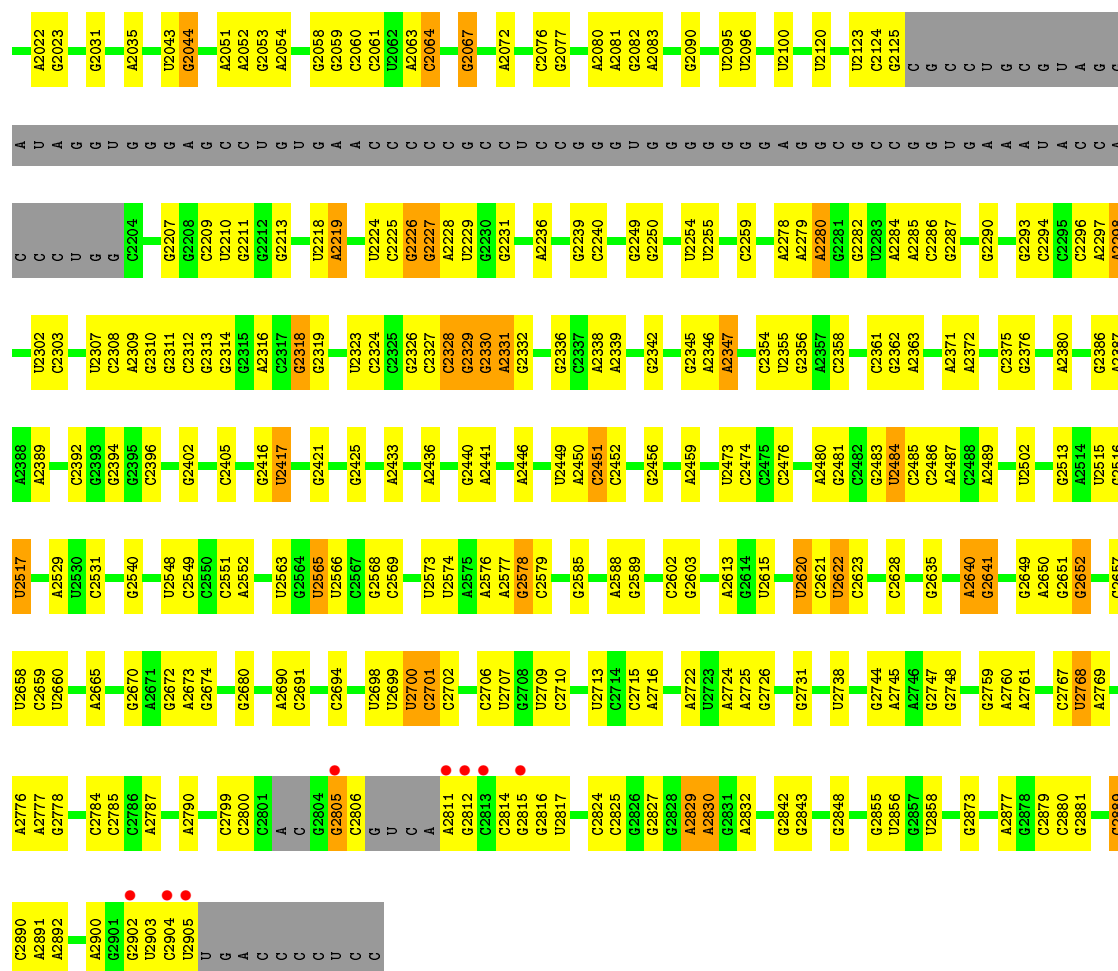
- Molecule 1: 23S ribosomal RNA





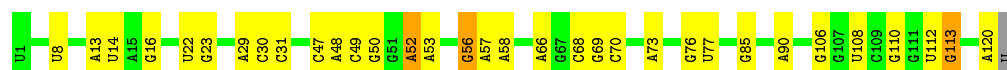


U1835	A1711	A	U1451	A1346	U	U1128	A1066	C980	A885	G756	C555	G436	G298	A187
A1845	G1712	C1582	C1452	G1354	G	A1129	G1067	G961	U872	G763	A556	G437	A299	G193
G1846	G1713	G1585	G1461	G1355	A	A1130	U1068	A962	U873		G557	A438	C300	
G1847	C1462	U1586	C1462	G1356	C1223	A1131	G1069	A963	U874		U558	A448	A301	
G1854	G1716	U1357	U1485	U1357		G1132	U1071	G964	U879	G768	A560	A454	C309	G201
C1873	G1720	C1359	G1466	U1358	U1231	A1133	A1072	U967	U885	G769	C561	A454	C310	G202
A1877	U1735	A1591	G1470	C1360	U1232	G1134	A1073	C968	C886	U770	C	A468	C320	A201
A1878	U1736	U1592	G1474	U1361	U1233	G1135	A1074		U885		A	C470	C320	G203
G1879	U1739	C1593	G1475	A1362	G1235	G1136	G1075	G972	C886		A	C471	C321	A204
G1880	A1744	A1604	G1476	G1369	U1238	U1141	U1077	G976	U885		A	C478	A322	A209
A1889	A1745	G1605	C1477	G1370		U1142	G1078		C886		A	C479	A323	A210
G1890	A1746	A1612	U1476	G1373	C1245	U1143	G1079	G984	U885		A	C478	A324	A217
G1891	A1747	A1615	U1477	U1374	U1150	U1150	U1080	G984	U885		A	C479	A325	
A1898	A1748	A1615	A1490	C1375	G1151	G1151	U1081	A985	U885		A	C478	A326	
G1899	G1753	G1619	G1494	A1376	U1152	U1152	G1082	G988	U885		A	C478	A327	
A1910	C1754	U1624	U1495	G1377	C1154	C1154	G1084	G988	U885		A	C478	A328	
A1911	G1765	A1625	U1496	G1381	G1155	G1155	G1085	G989	U885		A	C478	A329	
G1920	A1766	A1626	U1497	A1382	U1156	U1156	G1086	G991	U885		A	C478	A330	
A1921	U1767	A1626	U1498	G1383	U1157	U1157	G1087	G992	U885		A	C478	A331	
G1927	U1768	C1630	A1501	U1386	U1158	U1158	G1088	G992	U885		A	C478	A332	
A1934	A1769	A1631	A1506	U1387	C1161	C1161	G1089	G1000	U885		A	C478	A333	
C1935	G1775	C1632	C1510	G1388	G1162	G1162	G1090	A1001	U885		A	C478	A334	
G1950	U1787	C1633	G1511	G1389	C1164	C1164	G1091	U1002	U885		A	C478	A335	
G1959	U1788	C1633	G1512	A1286	G1167	G1167	G1092	U1003	U885		A	C478	A336	
C1968	A1803	U1647	U1534	U1397	G1170	G1170	G1093	U1004	U885		A	C478	A337	
U1976	A1810	A1648	A1535	G1407	G1171	G1171	G1094	U1005	U885		A	C478	A338	
U1980	A1811	C1649	U1538	G1408	G1172	G1172	G1095	U1006	U885		A	C478	A339	
U1987	A1812	A1653	U1542	G1409	G1173	G1173	G1096	U1007	U885		A	C478	A340	
C1988	A1813	A1654	U1543	A1410	G1174	G1174	G1097	U1008	U885		A	C478	A341	
A1991	A1814	U1655	U1544	G1413	G1175	G1175	G1098	U1009	U885		A	C478	A342	
A1992	A1815	G1658	U1545	G1414	G1176	G1176	G1099	U1010	U885		A	C478	A343	
U2012	A1816	G1659	U1546	G1415	G1177	G1177	G1101	U1011	U885		A	C478	A344	
G2013	A1817	G1660	U1547	G1416	G1178	G1178	G1102	U1012	U885		A	C478	A345	
U2014	A1818	G1661	U1548	G1417	G1179	G1179	G1103	U1013	U885		A	C478	A346	
C2017	A1819	G1662	U1549	G1418	G1180	G1180	G1104	U1014	U885		A	C478	A347	
G2018	A1820	G1663	U1550	G1419	G1181	G1181	G1105	U1015	U885		A	C478	A348	
	A1821	G1664	U1551	G1420	G1182	G1182	G1106	U1016	U885		A	C478	A349	
	A1822	G1665	U1552	G1421	G1183	G1183	G1107	U1017	U885		A	C478	A350	
	A1823	G1666	U1553	G1422	G1184	G1184	G1108	U1018	U885		A	C478	A351	
	U1826	G1667	U1554	G1423	G1185	G1185	G1109	U1019	U885		A	C478	A352	
	C1827	G1668	U1555	G1424	G1186	G1186	G1110	U1020	U885		A	C478	A353	
	U1828	G1669	U1556	G1425	G1187	G1187	G1111	U1021	U885		A	C478	A354	
	G1829	G1670	U1557	G1426	G1188	G1188	G1112	U1022	U885		A	C478	A355	
	A1830	G1671	U1558	G1427	G1189	G1189	G1113	U1023	U885		A	C478	A356	
	G1831	G1672	U1559	G1428	G1190	G1190	G1114	U1024	U885		A	C478	A357	
	A1832	G1673	U1560	G1429	G1191	G1191	G1115	U1025	U885		A	C478	A358	
	C1833	G1674	U1561	G1430	G1192	G1192	G1116	U1026	U885		A	C478	A359	
	U1834	G1675	U1562	G1431	G1193	G1193	G1117	U1027	U885		A	C478	A360	
	A1835	G1676	U1563	G1432	G1194	G1194	G1118	U1028	U885		A	C478	A361	
	C1836	G1677	U1564	G1433	G1195	G1195	G1119	U1029	U885		A	C478	A362	
	U1837	G1678	U1565	G1434	G1196	G1196	G1120	U1030	U885		A	C478	A363	
	A1838	G1679	U1566	G1435	G1197	G1197	G1121	U1031	U885		A	C478	A364	
	C1839	G1680	U1567	G1436	G1198	G1198	G1122	U1032	U885		A	C478	A365	
	U2015	G1681	U1568	G1437	G1199	G1199	G1123	U1033	U885		A	C478	A366	
	A1839	G1682	U1569	G1438	G1200	G1200	G1124	U1034	U885		A	C478	A367	
	C2016	G1683	U1570	G1439	G1201	G1201	G1125	U1035	U885		A	C478	A368	
	G2017	G1684	U1571	G1440	G1202	G1202	G1126	U1036	U885		A	C478	A369	
	A1840	G1685	U1572	G1441	G1203	G1203	G1127	U1037	U885		A	C478	A370	
	C1841	G1686	U1573	G1442	G1204	G1204	G1128	U1038	U885		A	C478	A371	
	A1842	G1687	U1574	G1443	G1205	G1205	G1129	U1039	U885		A	C478	A372	
	C1843	G1688	U1575	G1444	G1206	G1206	G1130	U1040	U885		A	C478	A373	
	U1844	G1689	U1576	G1445	G1207	G1207	G1131	U1041	U885		A	C478	A374	
	A1845	G1690	U1577	G1446	G1208	G1208	G1132	U1042	U885		A	C478	A375	
	C1846	G1691	U1578	G1447	G1209	G1209	G1133	U1043	U885		A	C478	A376	
	U1847	G1692	U1579	G1448	G1210	G1210	G1134	U1044	U885		A	C478	A377	
	A1848	G1693	U1580	G1449	G1211	G1211	G1135	U1045	U885		A	C478	A378	
	C1849	G1694	U1581	G1450	G1212	G1212	G1136	U1046	U885		A	C478	A379	
	U1850	G1695	U1582	G1451	G1213	G1213	G1137	U1047	U885		A	C478	A380	
	A1851	G1696	U1583	G1452	G1214	G1214	G1138	U1048	U885		A	C478	A381	
	C1852	G1697	U1584	G1453	G1215	G1215	G1139	U1049	U885		A	C478	A382	
	U1853	G1698	U1585	G1454	G1216	G1216	G1140	U1050	U885		A	C478	A383	
	A1854	G1699	U1586	G1455	G1217	G1217	G1141	U1051	U885		A	C478	A384	
	C1855	G1700	U1587	G1456	G1218	G1218	G1142	U1052	U885		A	C478	A385	
	U1856	G1701	U1588	G1457	G1219	G1219	G1143	U1053	U885		A	C478	A386	
	A1857	G1702	U1589	G1458	G1220	G1220	G1144	U1054	U885		A	C478	A387	
	C1858	G1703	U1590	G1459	G1221	G1221	G1145	U1055	U885		A	C478	A388	
	U1859	G1704	U1591	G1460	G1222	G1222	G1146	U1056	U885		A	C478	A389	
	A1860	G1705	U1592	G1461	G1223	G1223	G1147	U1057	U885		A	C478	A390	
	C1861	G1706	U1593	G1462	G1224	G1224	G1148	U1058	U885		A	C478	A391	
	U1862	G1707	U1594	G1463	G1225	G1225	G1149	U1059	U885		A	C478	A392	
	A1863	G1708	U1595	G1464	G1226	G1226	G1150	U1060	U885		A	C478	A393	
	C1864	G1709	U1596	G1465	G1227	G1227	G1151	U1061	U885		A	C478	A394	
	U1865	G1710	U1597	G1466	G1228	G1228	G1152	U1062	U885		A	C478	A395	
	A1866	G1711	U1598	G1467	G1229	G1229	G1153	U1063	U885		A	C478	A396	
	C1867	G1712	U1599	G1468	G1230	G1230	G1154	U1064	U885		A	C478	A397	
	U1868	G1713	U1600	G1469	G1231	G1231	G1155	U1065	U885		A	C478	A398	
	A1869	G1714	U1601	G1470	G1232	G1232	G1156	U1066	U885		A	C478	A399	
	C1869	G1715	U1602	G1471	G1233	G1233	G1157	U1067	U885		A	C478	A400	
	U1870	G1716	U1603	G1472	G1234	G1234	G1158	U1068	U885		A	C478	A401	
	A1871	G1717	U1604	G1473	G1235	G1235	G1159	U1069	U885		A	C478	A402	
	C1871	G1718	U1605	G1474	G1236	G1236	G1160	U1070	U885		A	C478	A403	
	U1872	G1719	U1606	G1475	G1237	G1237	G1161	U1071	U885		A	C478	A404	
	A1873	G1720	U1607	G1476	G1238	G1238	G1162	U1072	U885		A	C478	A405	
	C1873	G1721	U1608	G1477	G1239	G1239	G1163	U1073	U885		A	C478	A406	
	U1874	G1722	U1609	G1478	G1240	G1240	G1164	U1074	U885		A	C478	A407	
	A1875	G1723	U1610	G1479	G1241	G1241	G1165	U1075	U885		A	C478	A408	
	C1875	G1724	U1611	G1480	G1242	G1242	G1166	U1076	U885		A	C478	A409	
	U1876	G1725	U1612	G1481	G1243	G1243	G1167	U1077	U885		A	C478	A410	
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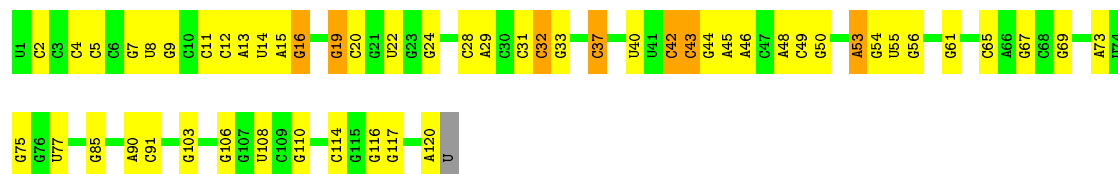
- Molecule 2: 5S ribosomal RNA

Chain 1B: 72% 25% ..



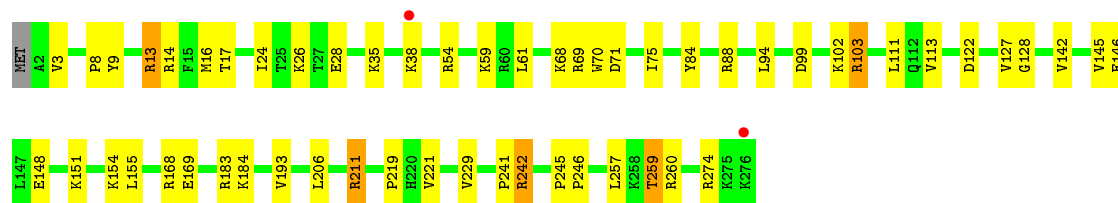
- Molecule 2: 5S ribosomal RNA

Chain 2B: 55% 38% 6% ..

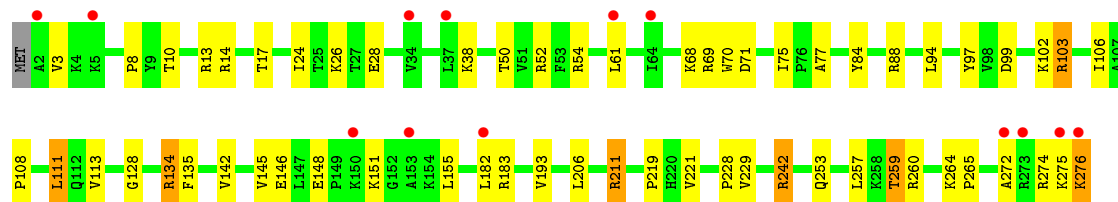
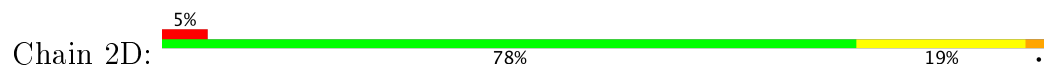


- Molecule 3: 50S ribosomal protein L2

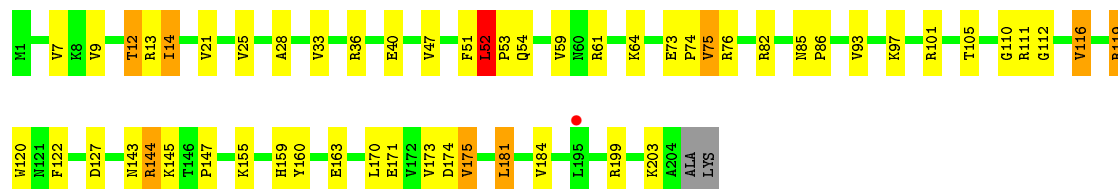
Chain 1D: 79% 18% ..



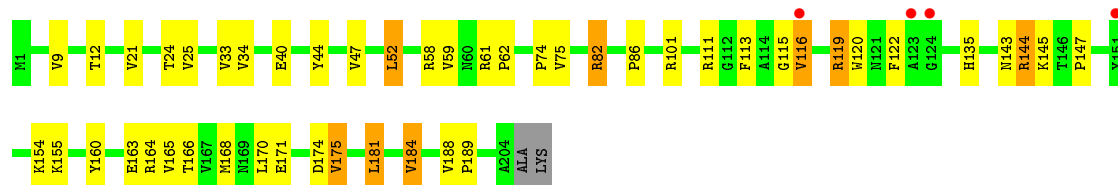
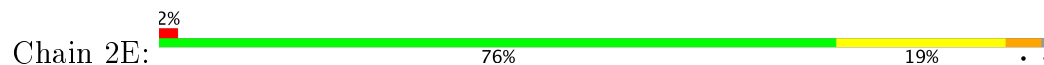
• Molecule 3: 50S ribosomal protein L2



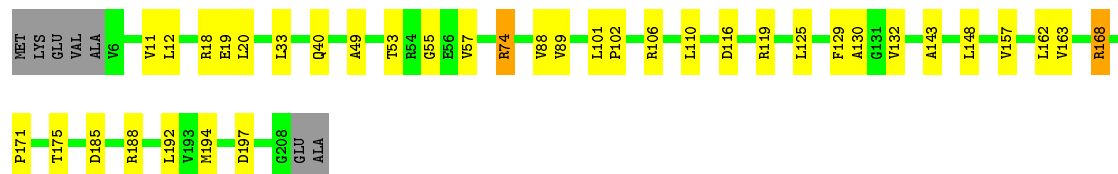
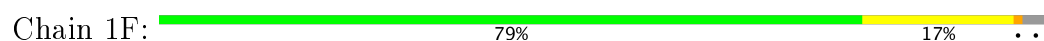
• Molecule 4: 50S ribosomal protein L3



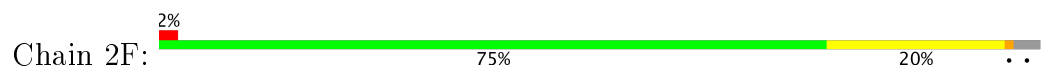
• Molecule 4: 50S ribosomal protein L3

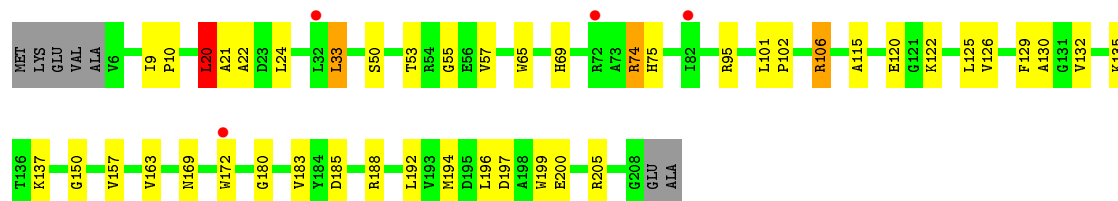


• Molecule 5: 50S ribosomal protein L4

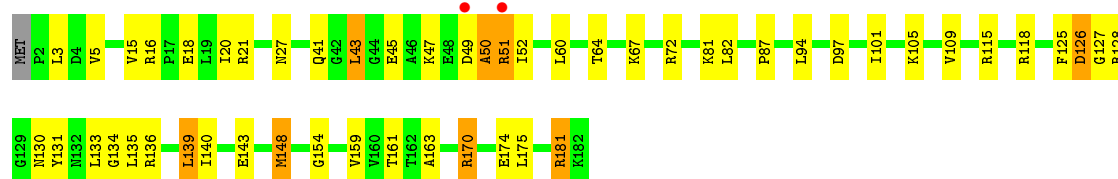


• Molecule 5: 50S ribosomal protein L4

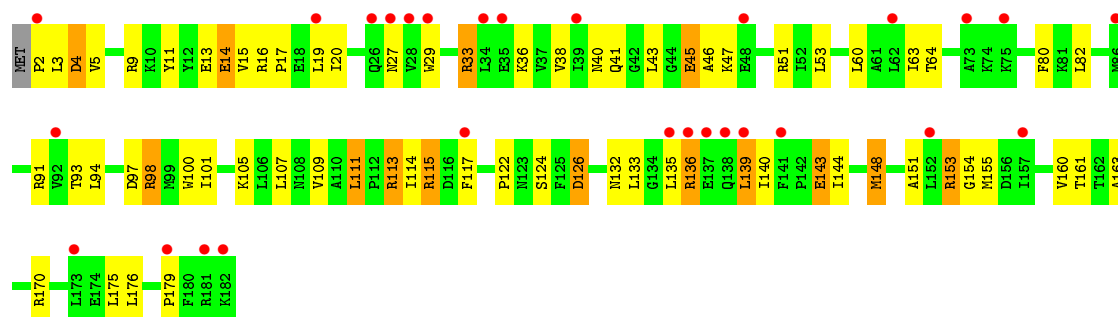




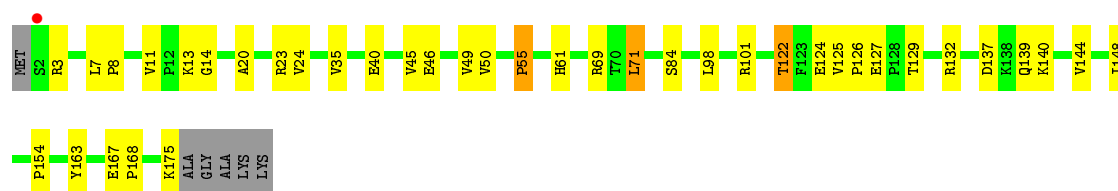
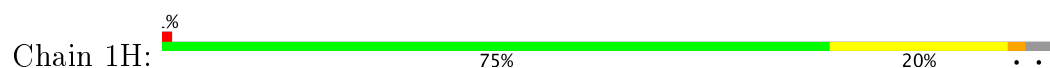
• Molecule 6: 50S ribosomal protein L5



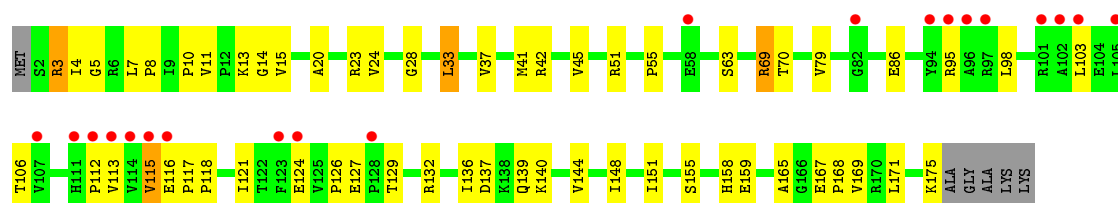
• Molecule 6: 50S ribosomal protein L5



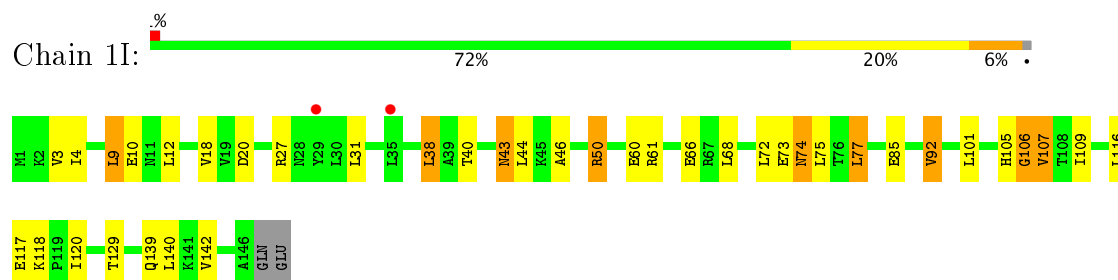
• Molecule 7: 50S ribosomal protein L6



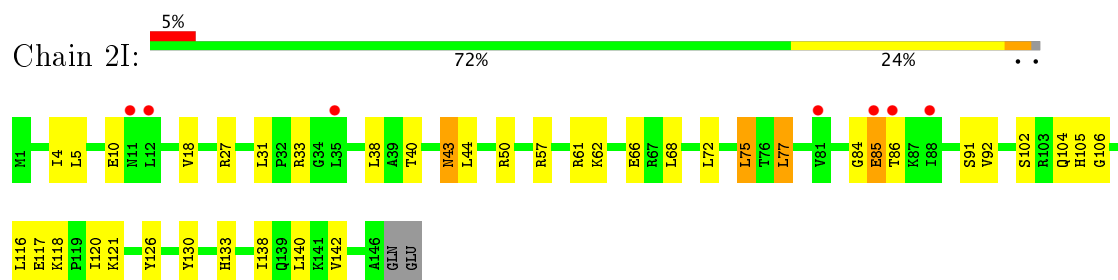
• Molecule 7: 50S ribosomal protein L6



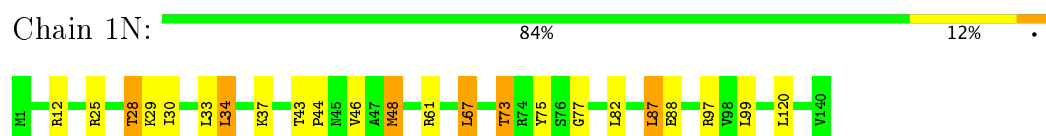
- Molecule 8: 50S ribosomal protein L9



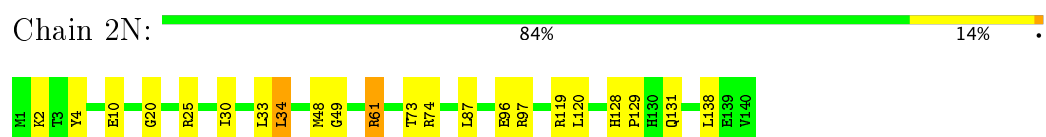
- Molecule 8: 50S ribosomal protein L9



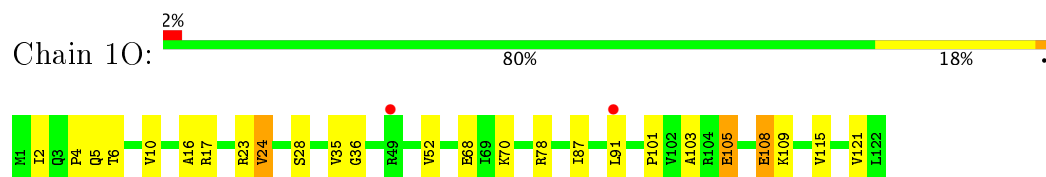
- Molecule 9: 50S ribosomal protein L13



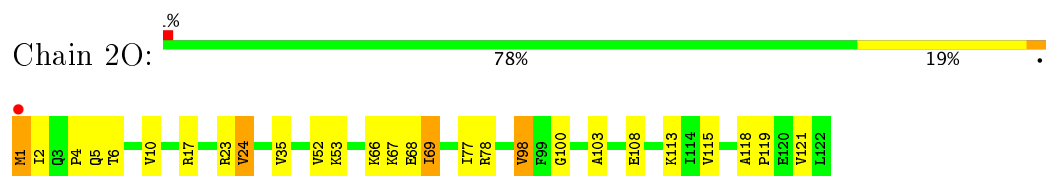
- Molecule 9: 50S ribosomal protein L13



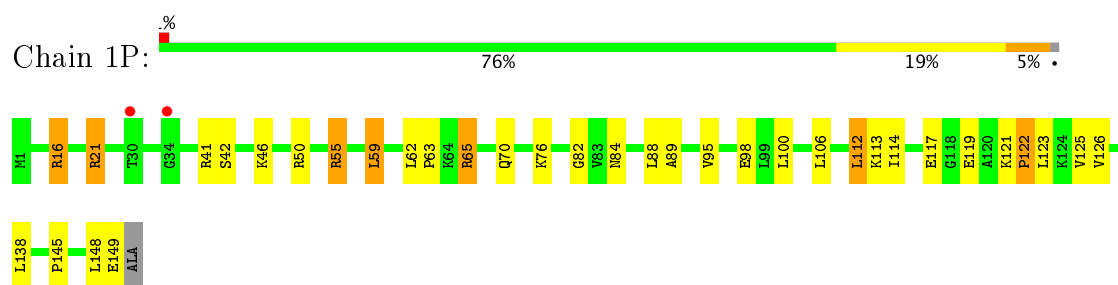
- Molecule 10: 50S ribosomal protein L14



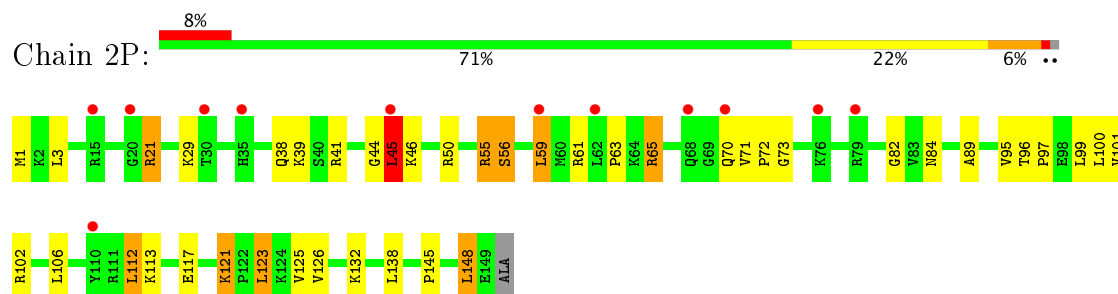
- Molecule 10: 50S ribosomal protein L14



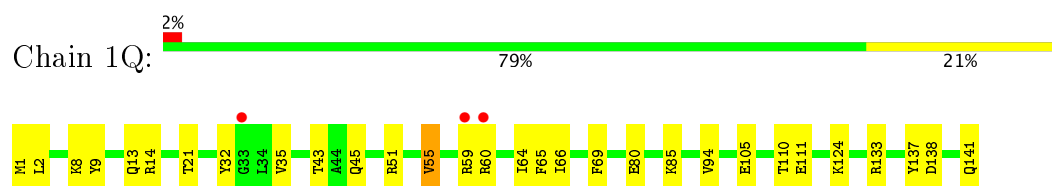
- Molecule 11: 50S ribosomal protein L15



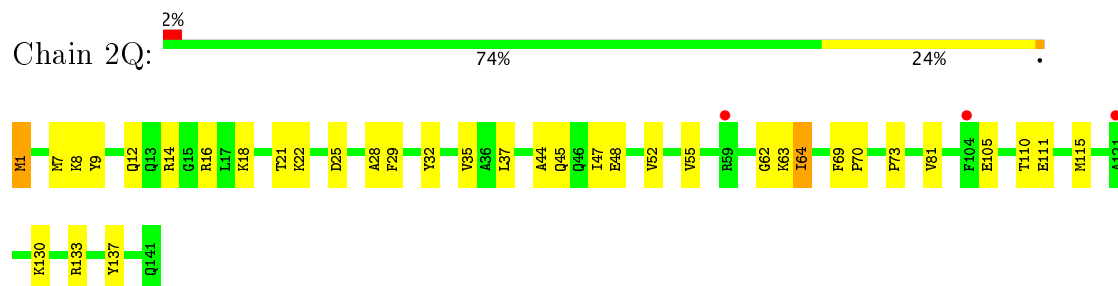
- Molecule 11: 50S ribosomal protein L15



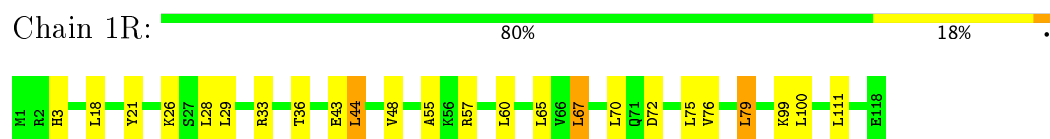
- Molecule 12: 50S ribosomal protein L16



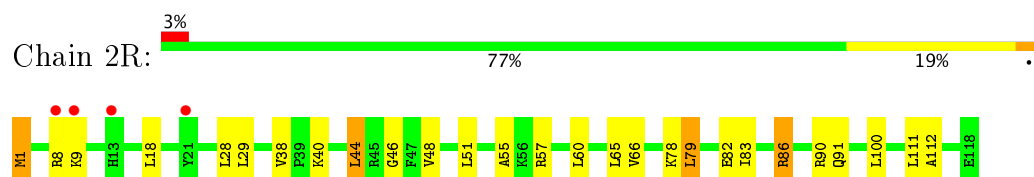
- Molecule 12: 50S ribosomal protein L16



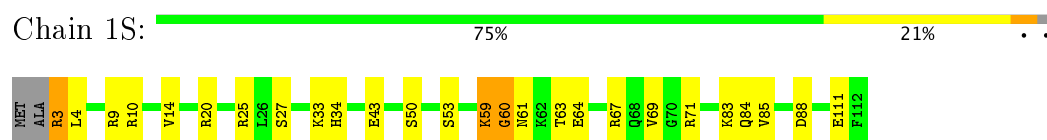
- Molecule 13: 50S ribosomal protein L17



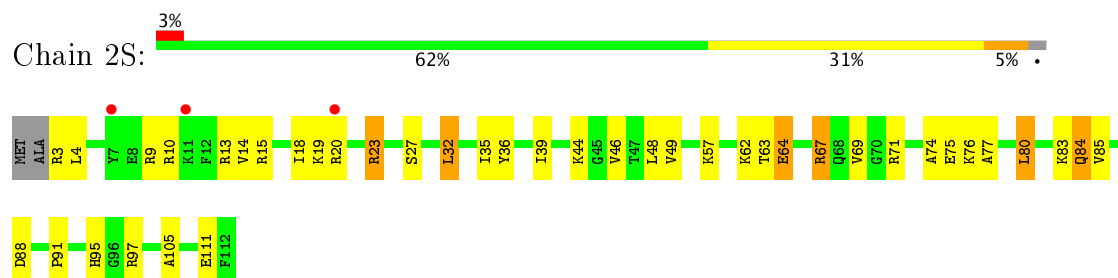
- Molecule 13: 50S ribosomal protein L17



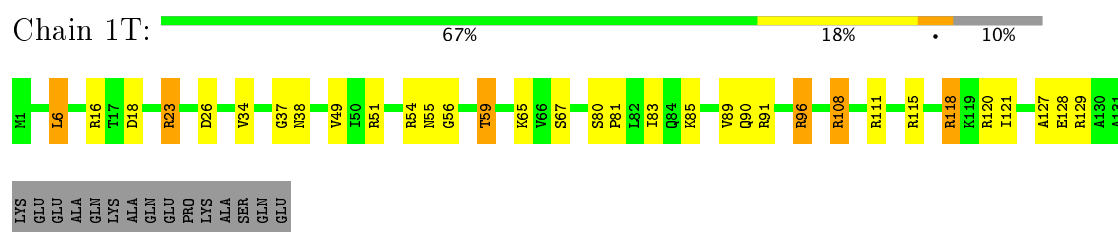
- Molecule 14: 50S ribosomal protein L18



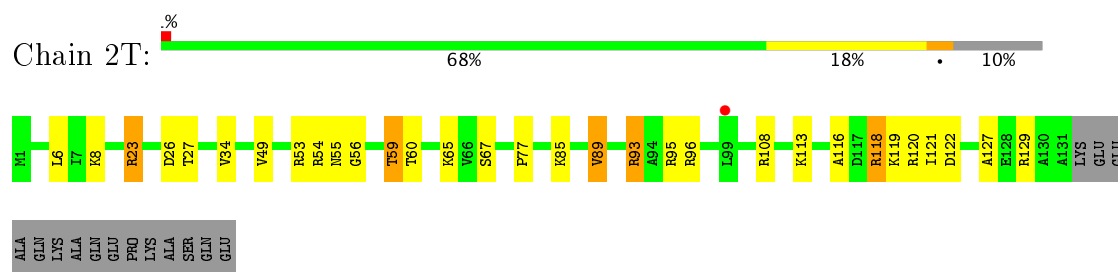
- Molecule 14: 50S ribosomal protein L18



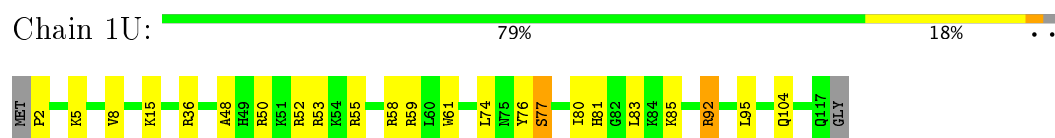
- Molecule 15: 50S ribosomal protein L19



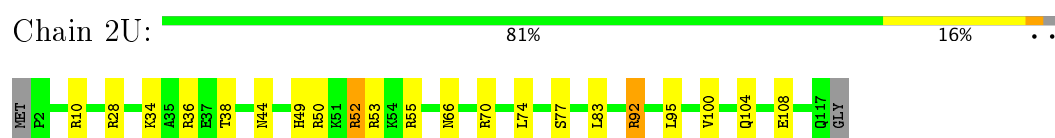
- Molecule 15: 50S ribosomal protein L19



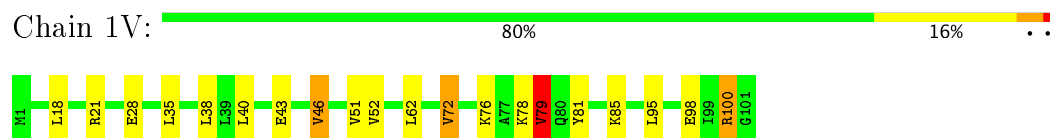
- Molecule 16: 50S ribosomal protein L20



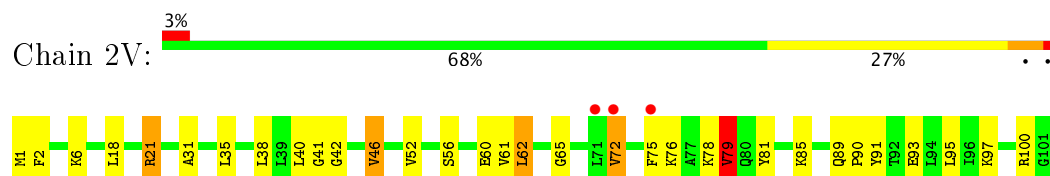
- Molecule 16: 50S ribosomal protein L20



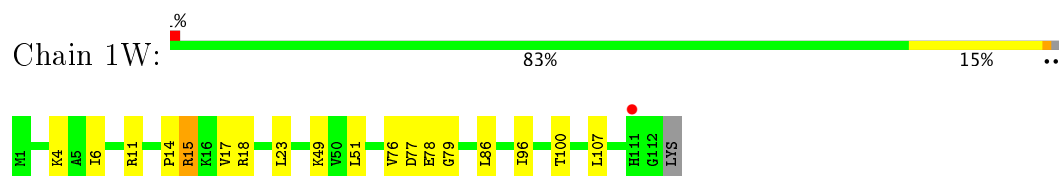
## • Molecule 17: 50S ribosomal protein L21



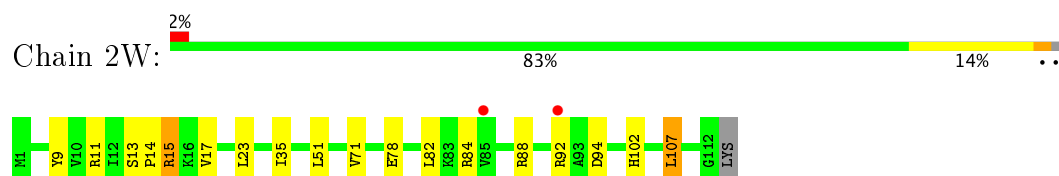
## • Molecule 17: 50S ribosomal protein L21



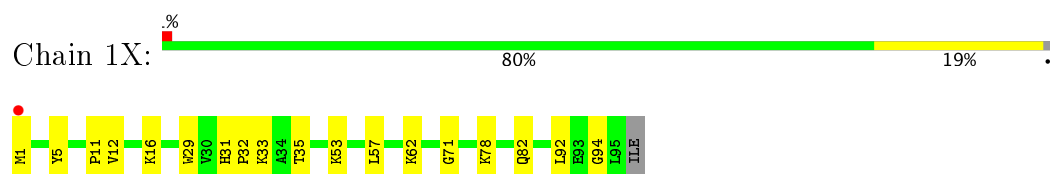
## • Molecule 18: 50S ribosomal protein L22



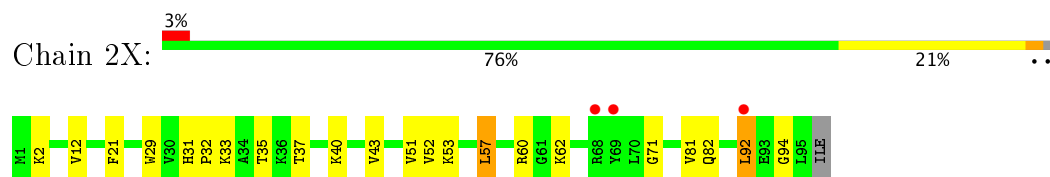
## • Molecule 18: 50S ribosomal protein L22



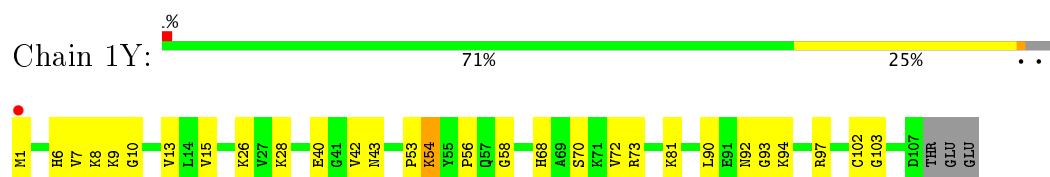
## • Molecule 19: 50S ribosomal protein L23



## • Molecule 19: 50S ribosomal protein L23

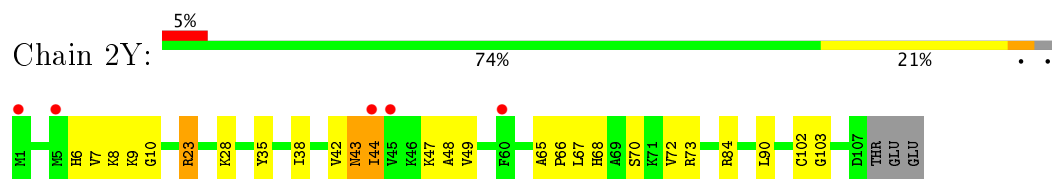


## • Molecule 20: 50S ribosomal protein L24

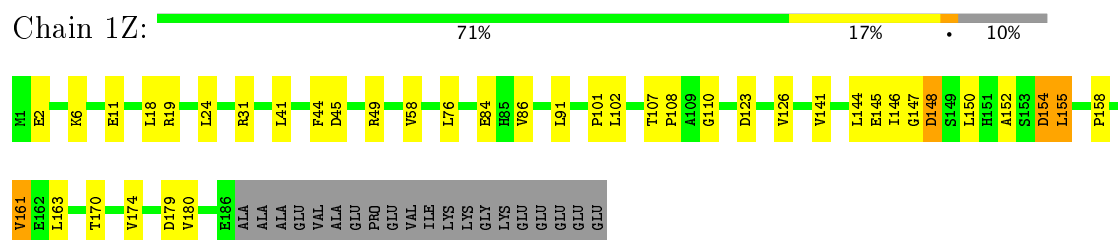




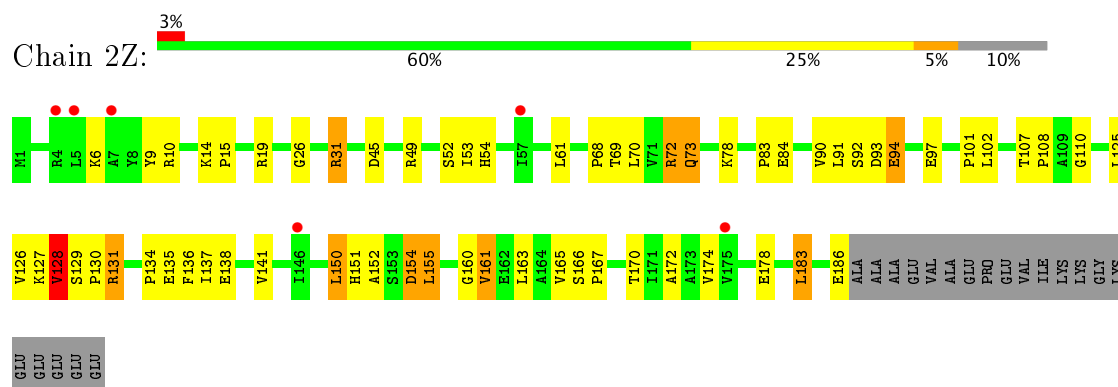
- Molecule 20: 50S ribosomal protein L24



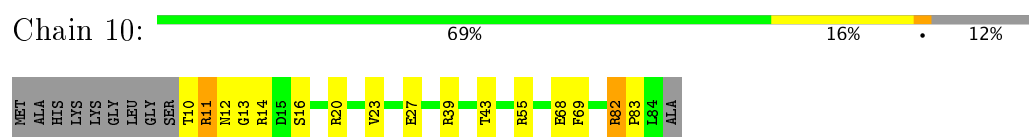
- Molecule 21: 50S ribosomal protein L25



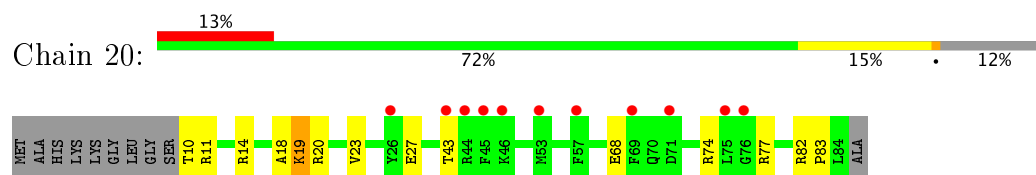
- Molecule 21: 50S ribosomal protein L25



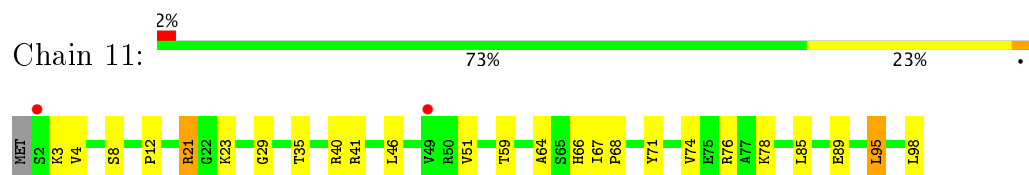
- Molecule 22: 50S ribosomal protein L27



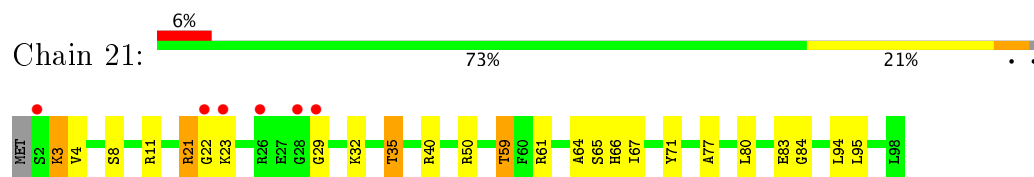
- Molecule 22: 50S ribosomal protein L27



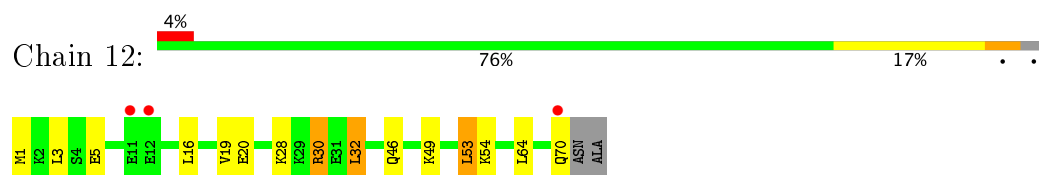
- Molecule 23: 50S ribosomal protein L28



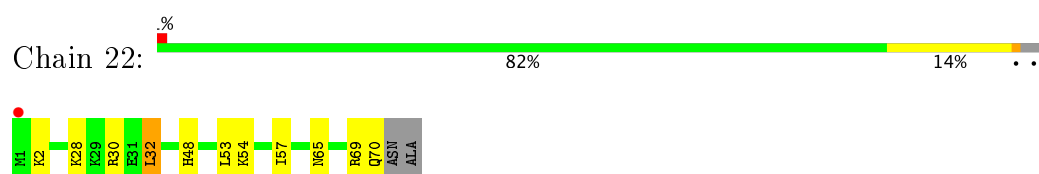
- Molecule 23: 50S ribosomal protein L28



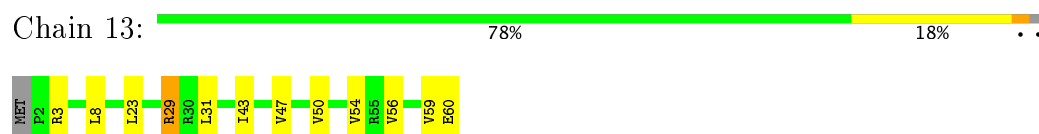
- Molecule 24: 50S ribosomal protein L29



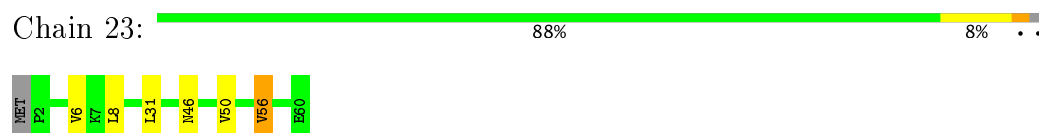
- Molecule 24: 50S ribosomal protein L29



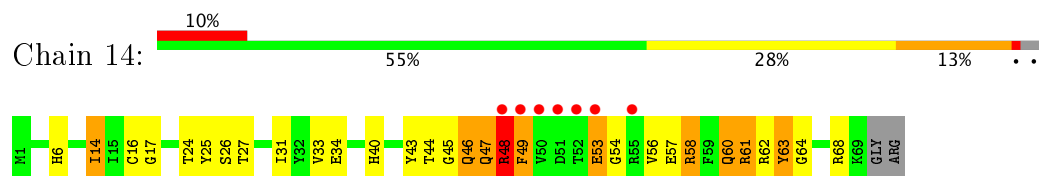
- Molecule 25: 50S ribosomal protein L30



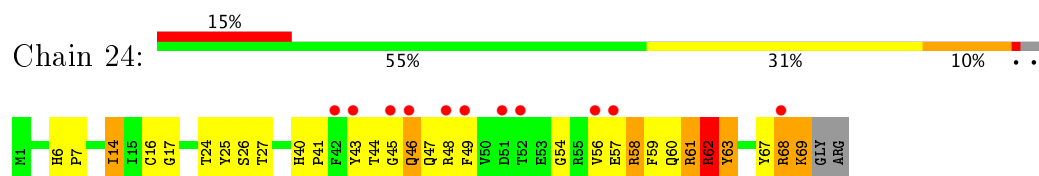
- Molecule 25: 50S ribosomal protein L30



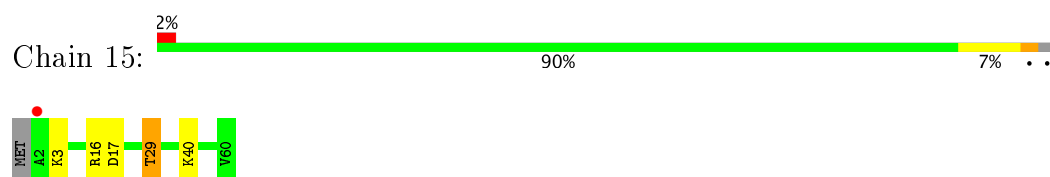
- Molecule 26: 50S ribosomal protein L31



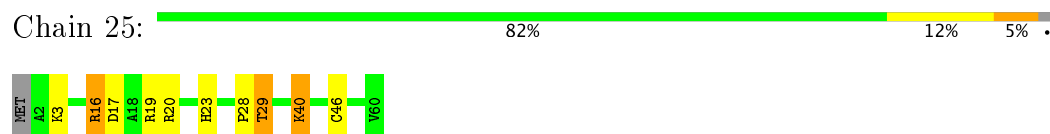
- Molecule 26: 50S ribosomal protein L31



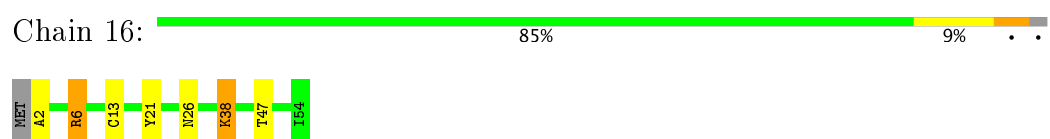
- Molecule 27: 50S ribosomal protein L32



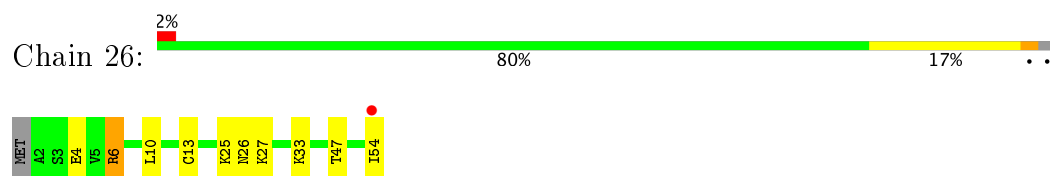
- Molecule 27: 50S ribosomal protein L32



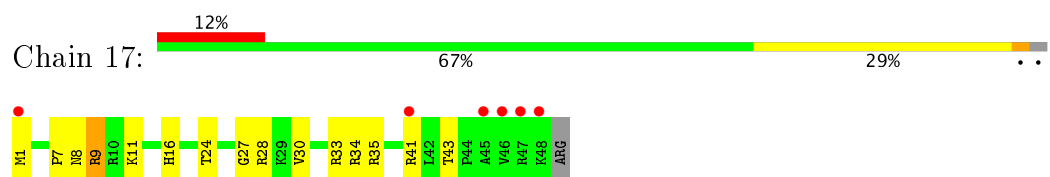
- Molecule 28: 50S ribosomal protein L33



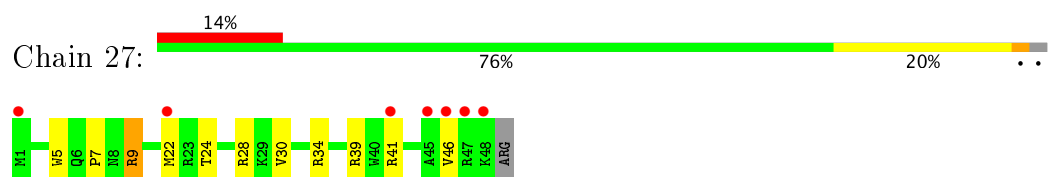
- Molecule 28: 50S ribosomal protein L33



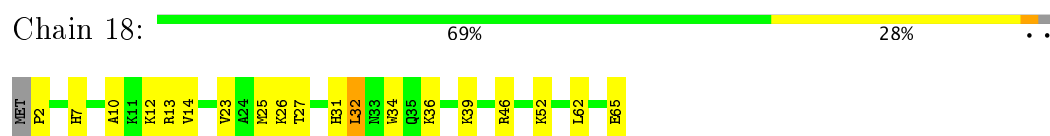
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

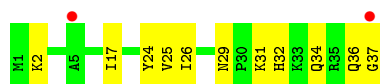




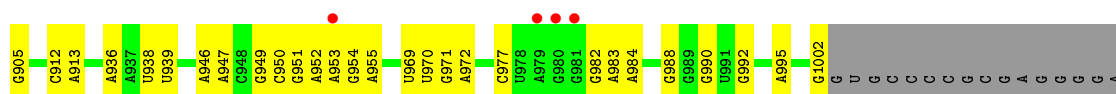
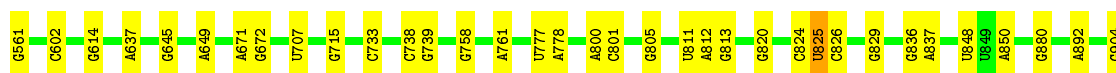
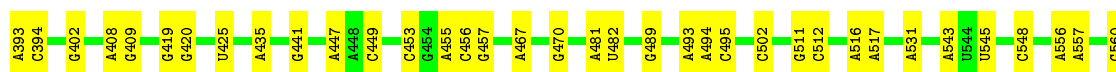
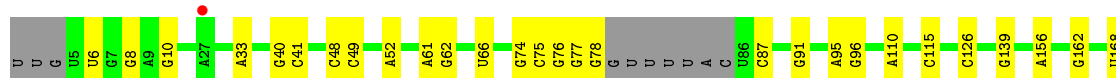
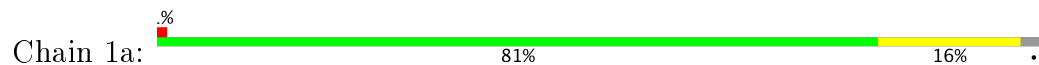
- Molecule 31: 50S ribosomal protein L36



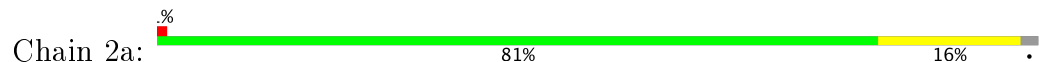
- Molecule 31: 50S ribosomal protein L36

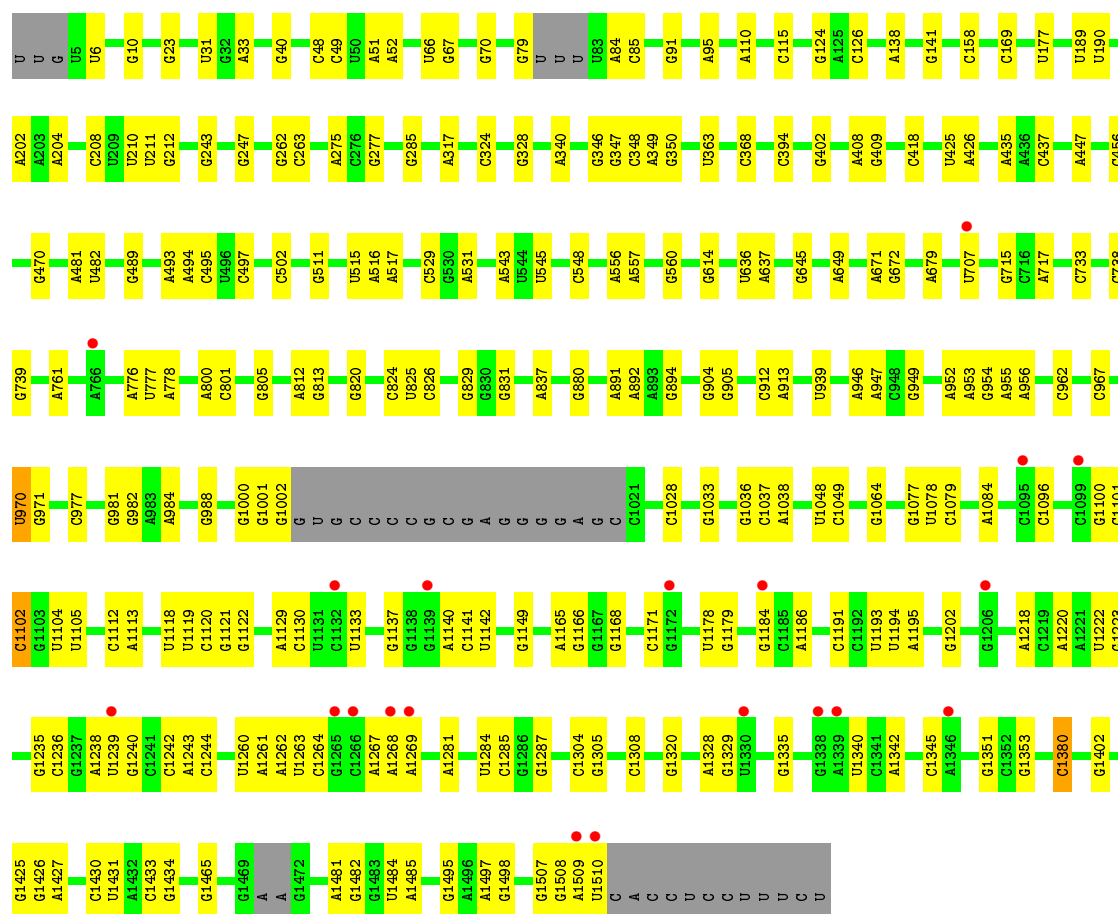


- Molecule 32: 16S ribosomal RNA

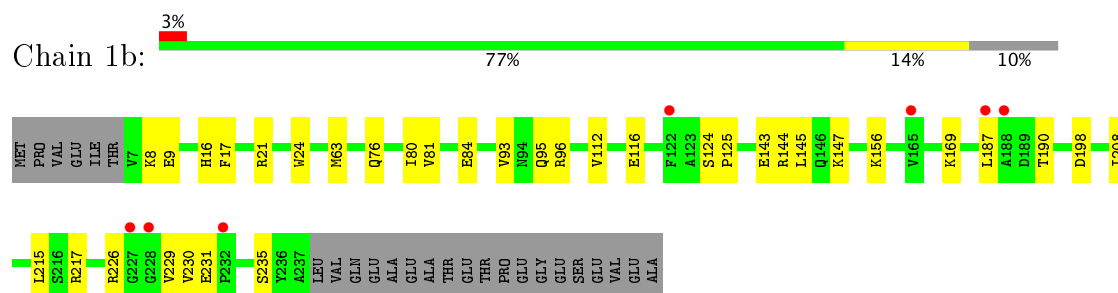


- Molecule 32: 16S ribosomal RNA

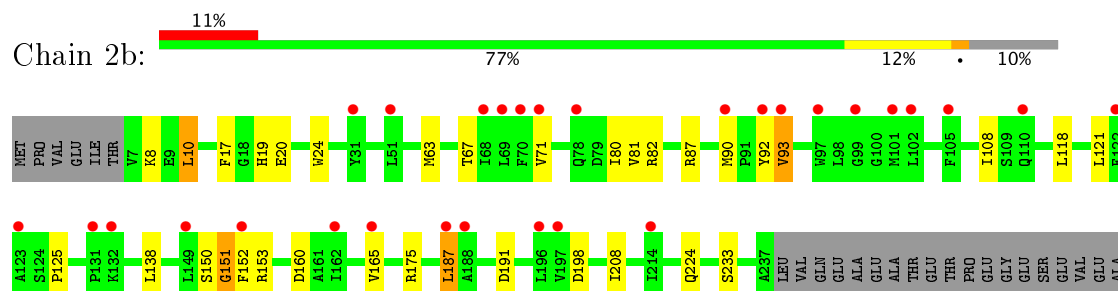




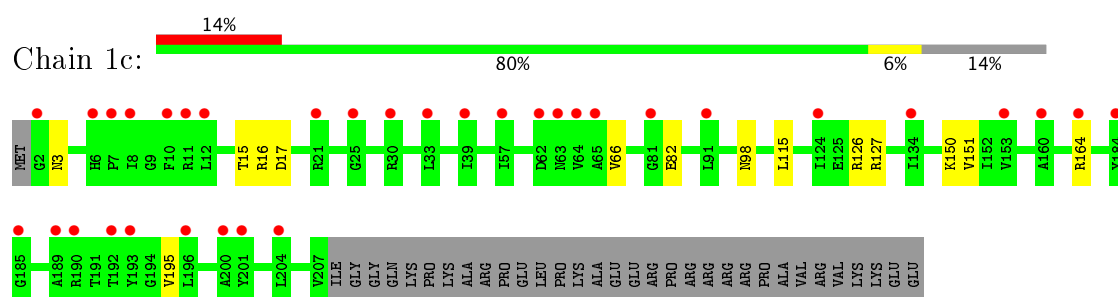
• Molecule 33: 30S ribosomal protein S2



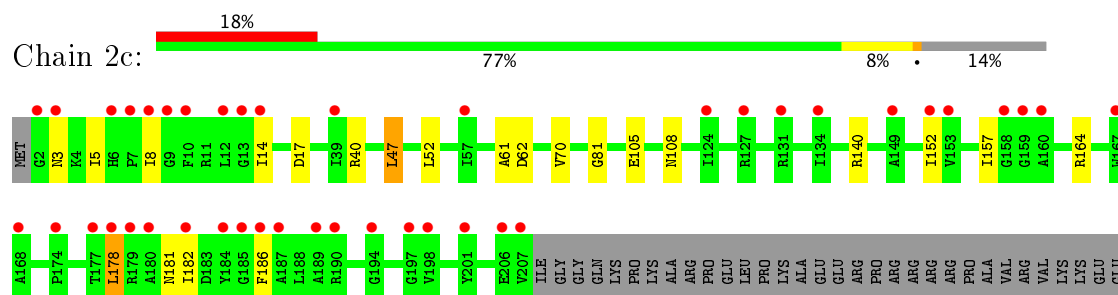
• Molecule 33: 30S ribosomal protein S2



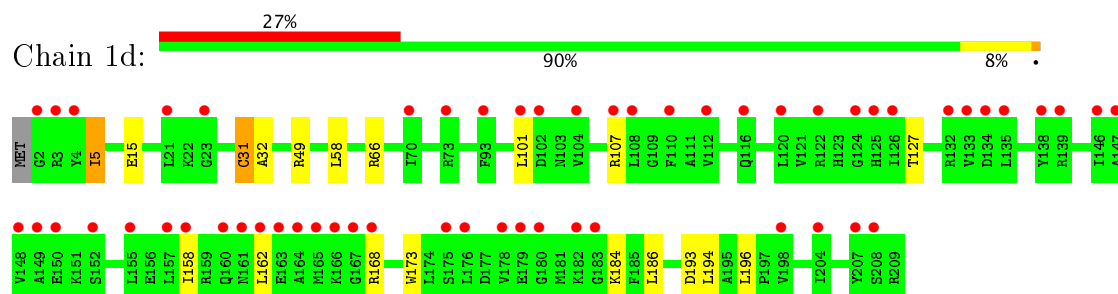
• Molecule 34: 30S ribosomal protein S3



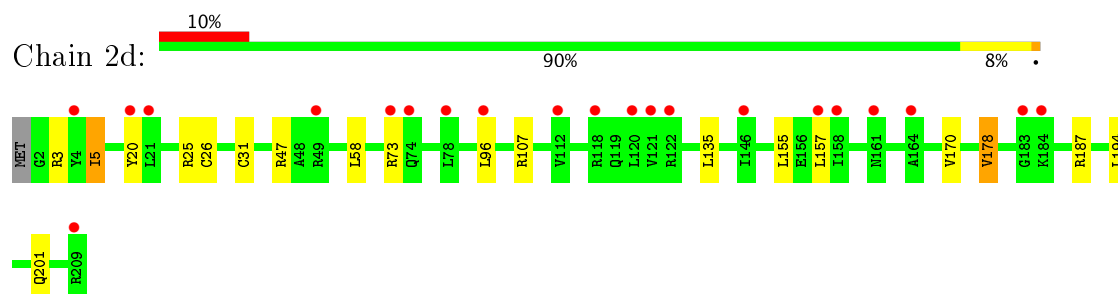
• Molecule 34: 30S ribosomal protein S3



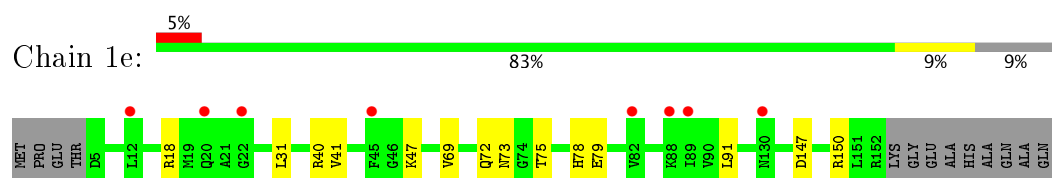
• Molecule 35: 30S ribosomal protein S4



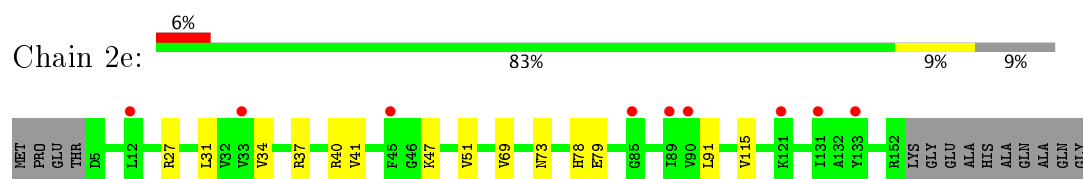
• Molecule 35: 30S ribosomal protein S4



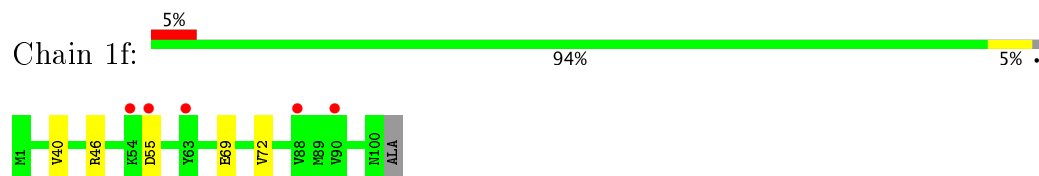
• Molecule 36: 30S ribosomal protein S5



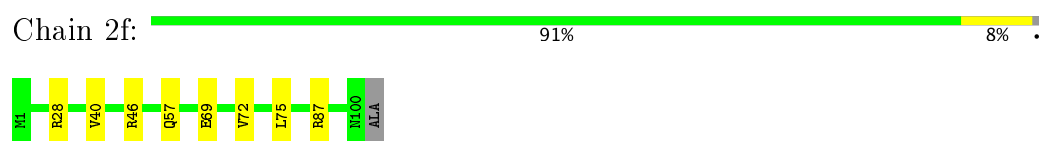
• Molecule 36: 30S ribosomal protein S5



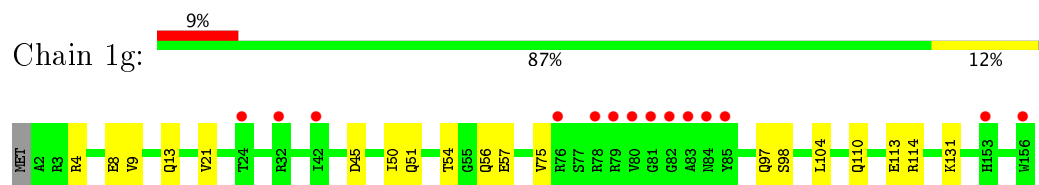
- Molecule 37: 30S ribosomal protein S6



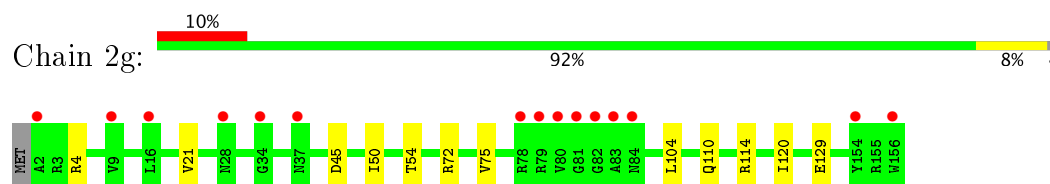
- Molecule 37: 30S ribosomal protein S6



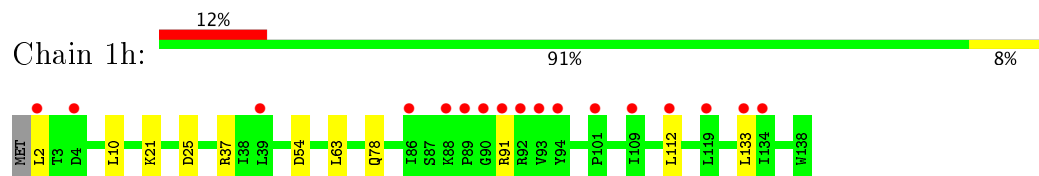
- Molecule 38: 30S ribosomal protein S7



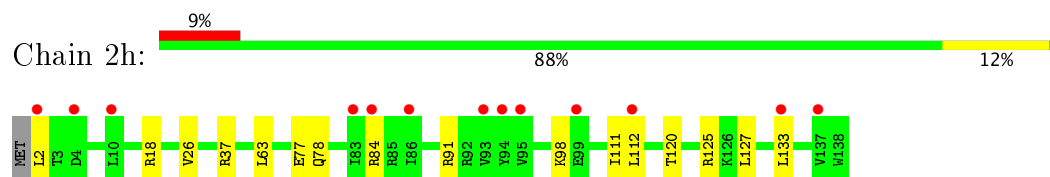
- Molecule 38: 30S ribosomal protein S7



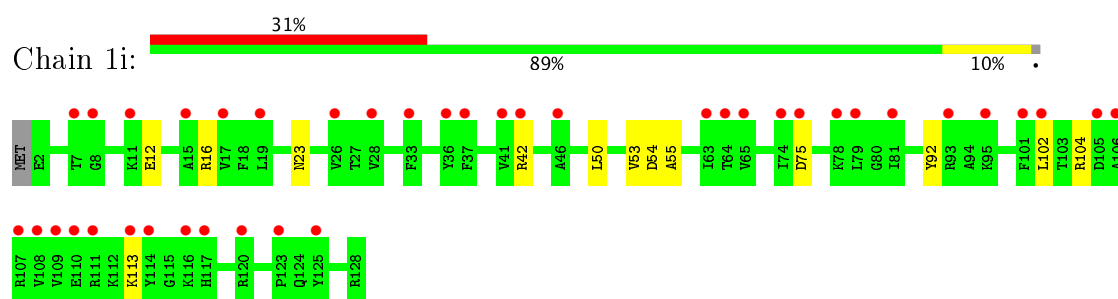
- Molecule 39: 30S ribosomal protein S8



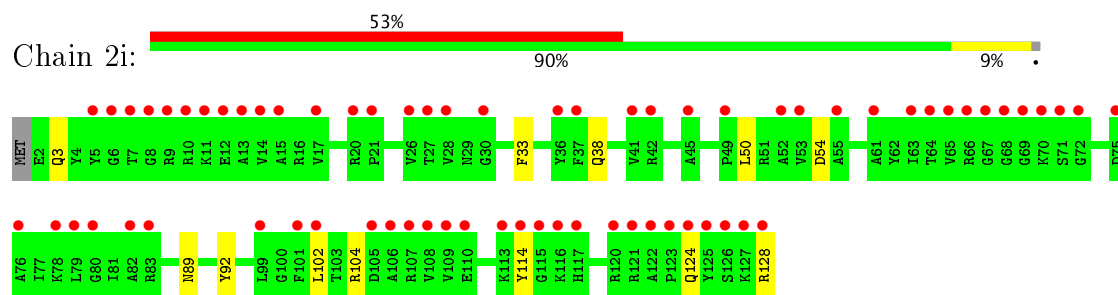
- Molecule 39: 30S ribosomal protein S8



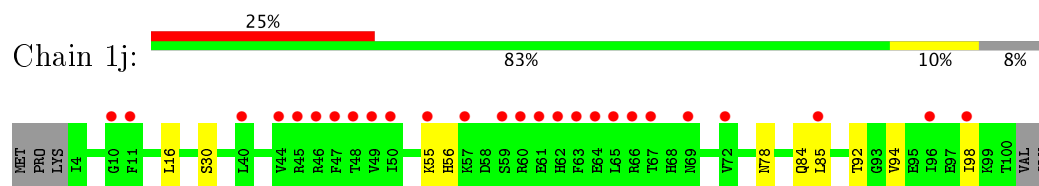
- Molecule 40: 30S ribosomal protein S9



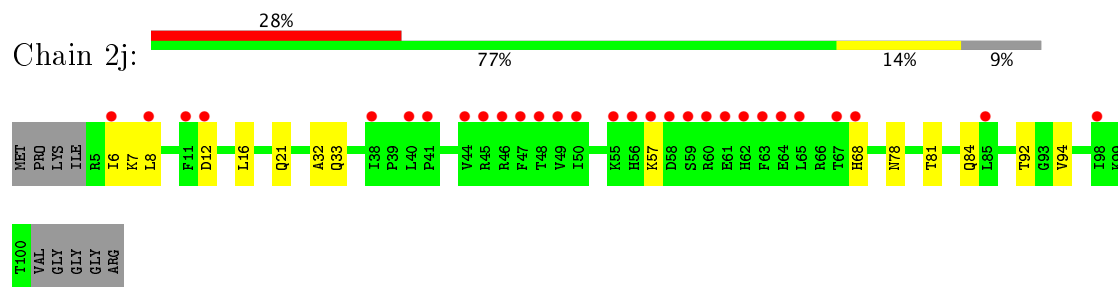
• Molecule 40: 30S ribosomal protein S9



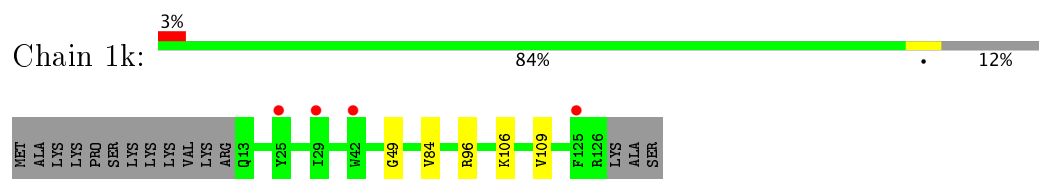
• Molecule 41: 30S ribosomal protein S10



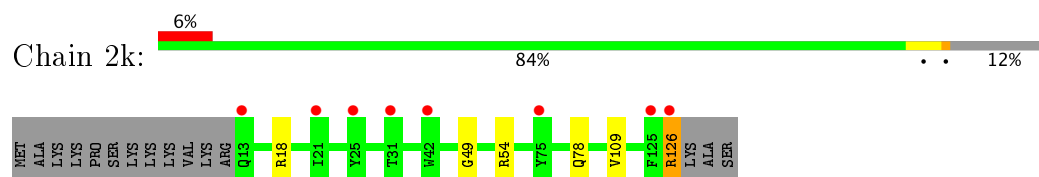
• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11

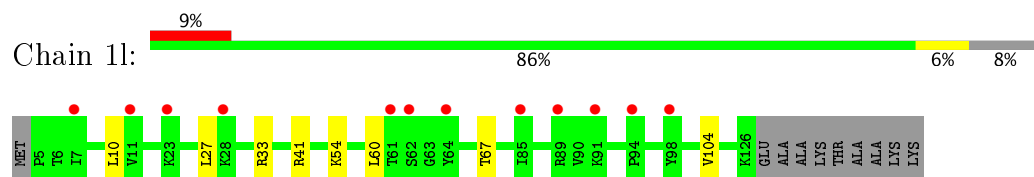


• Molecule 42: 30S ribosomal protein S11

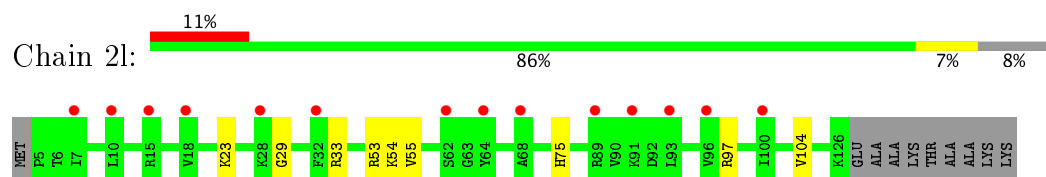




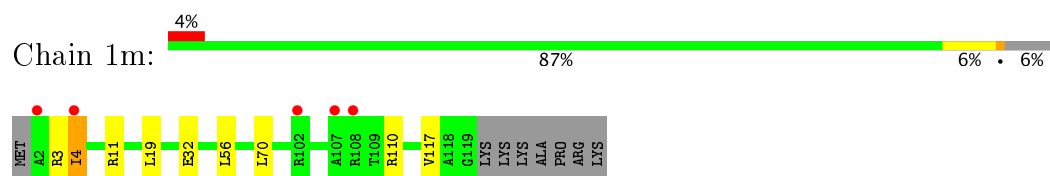
- Molecule 43: 30S ribosomal protein S12



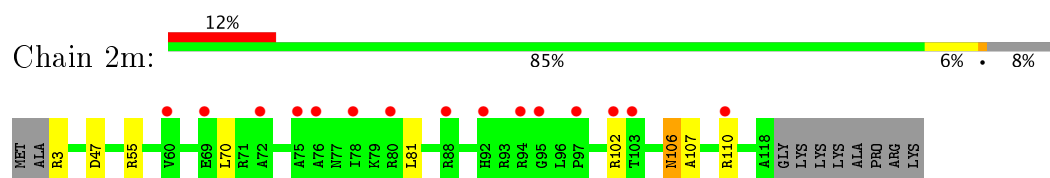
- Molecule 43: 30S ribosomal protein S12



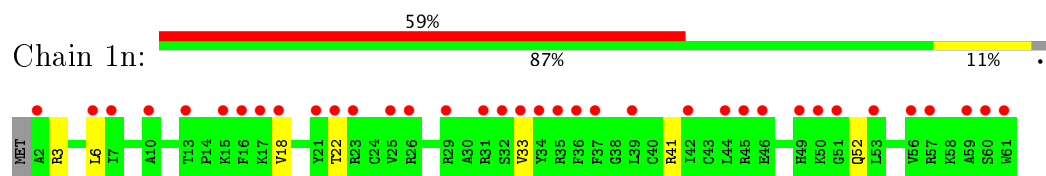
- Molecule 44: 30S ribosomal protein S13



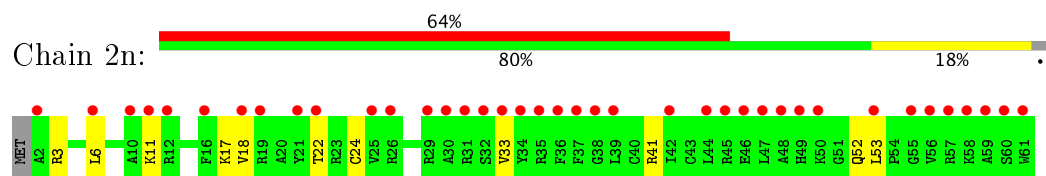
- Molecule 44: 30S ribosomal protein S13



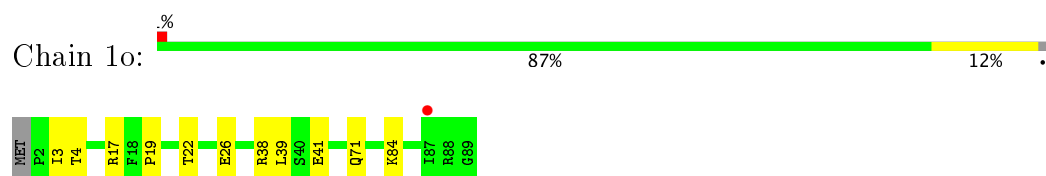
- Molecule 45: 30S ribosomal protein S14 type Z



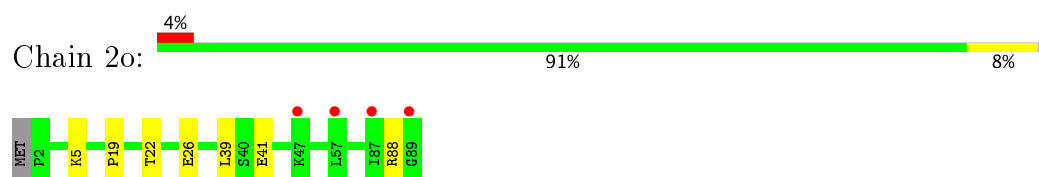
- Molecule 45: 30S ribosomal protein S14 type Z



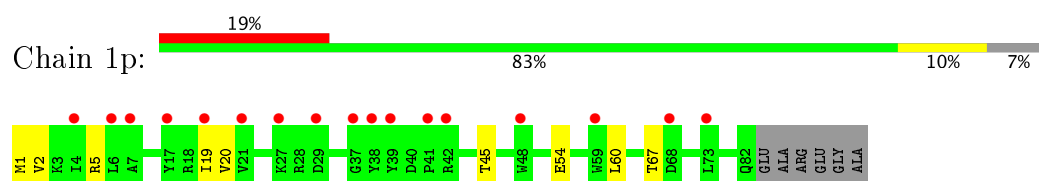
- Molecule 46: 30S ribosomal protein S15



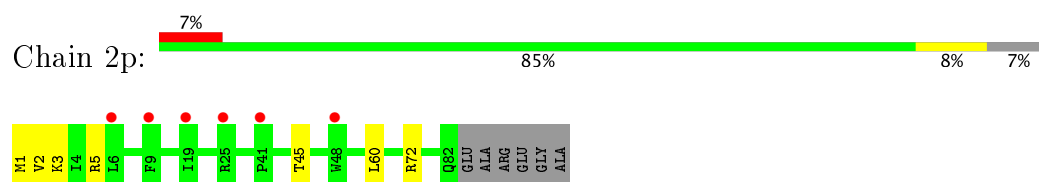
- Molecule 46: 30S ribosomal protein S15



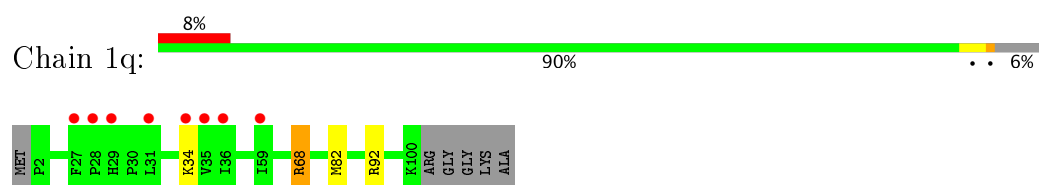
- Molecule 47: 30S ribosomal protein S16



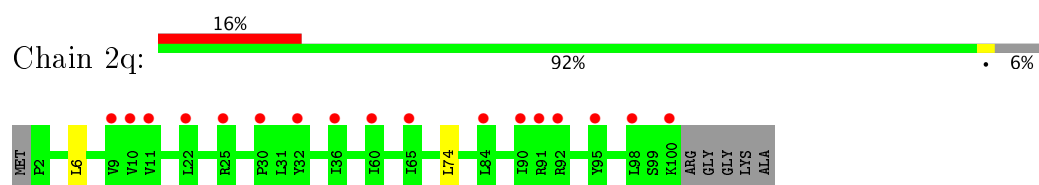
- Molecule 47: 30S ribosomal protein S16



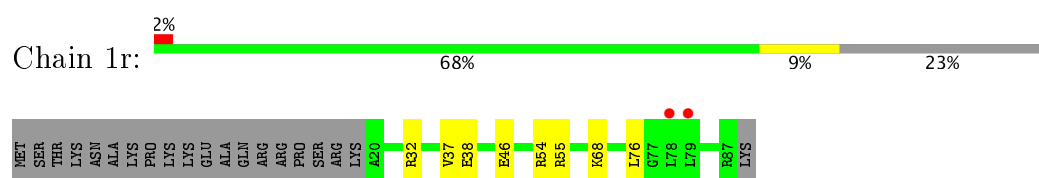
- Molecule 48: 30S ribosomal protein S17



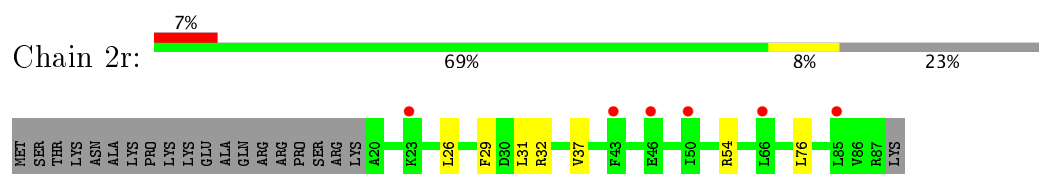
- Molecule 48: 30S ribosomal protein S17




- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18




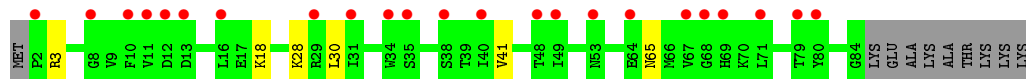
- Molecule 50: 30S ribosomal protein S19

Chain 1s:  80% 11% 10%




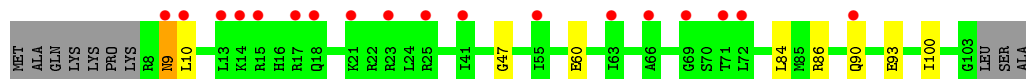
- Molecule 50: 30S ribosomal protein S19

Chain 2s:  25% 83% 6% 11%




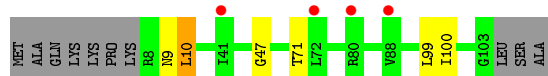
- Molecule 51: 30S ribosomal protein S20

Chain 1t:  17% 82% 8% 9%




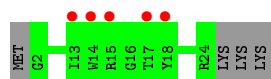
- Molecule 51: 30S ribosomal protein S20

Chain 2t:  4% 85% 5% 9%




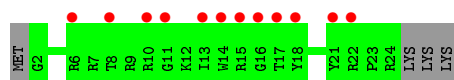
- Molecule 52: 30S ribosomal protein Thx

Chain 1u:  19% 85% 15%



- Molecule 52: 30S ribosomal protein Thx

Chain 2u:  44% 85% 15%



- Molecule 53: mRNA

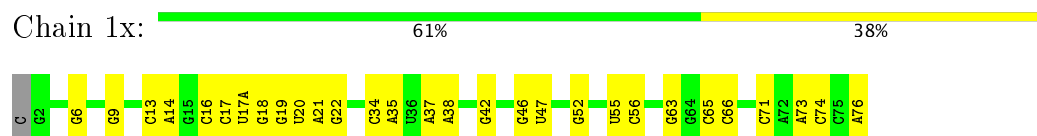
Chain 1v:  4% 13% 8% 79%



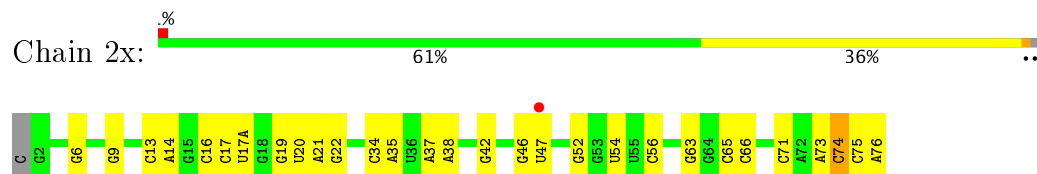
- Molecule 53: mRNA



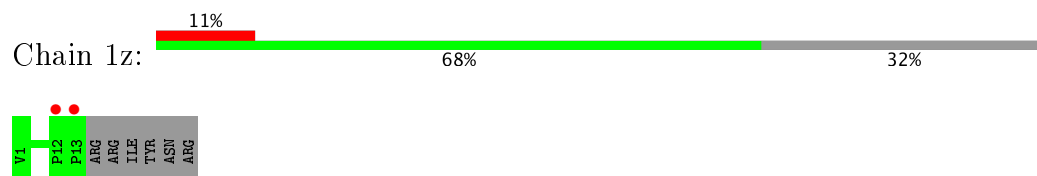
- Molecule 54: Initiator Methionine tRNA



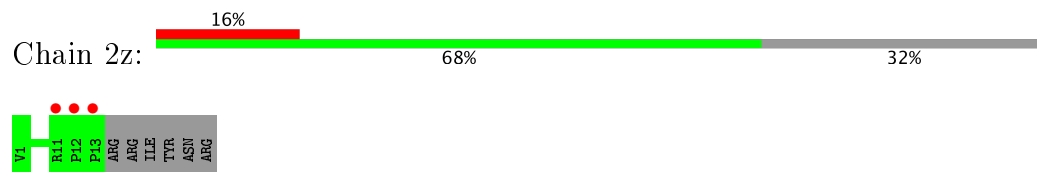
- Molecule 54: Initiator Methionine tRNA



- Molecule 55: Oncocin



- Molecule 55: Oncocin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.14Å 450.73Å 623.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.98 – 2.90 311.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (59.98-2.90) 98.0 (311.74-2.80)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 2.82Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.203 , 0.248 0.207 , 0.250	Depositor DCC
$R_{free}$ test set	63771 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	288378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, SF4, MG, 5MC, 4SU, 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	0.34	0/66249	0.77	19/103407 (0.0%)
1	2A	0.28	0/67298	0.76	12/105044 (0.0%)
2	1B	0.28	0/2877	0.79	0/4488
2	2B	0.30	0/2878	0.79	0/4490
3	1D	0.29	0/2186	0.49	0/2944
3	2D	0.28	0/2192	0.49	0/2951
4	1E	0.36	0/1592	0.51	1/2149 (0.0%)
4	2E	0.26	0/1592	0.49	0/2149
5	1F	0.27	0/1619	0.49	0/2193
5	2F	0.25	0/1615	0.48	0/2188
6	1G	0.23	0/1450	0.46	0/1959
6	2G	0.26	0/1449	0.49	0/1958
7	1H	0.25	0/1356	0.46	0/1834
7	2H	0.24	0/1356	0.45	0/1834
8	1I	0.24	0/1100	0.49	0/1501
8	2I	0.23	0/1076	0.49	0/1471
9	1N	0.27	0/1144	0.46	0/1543
9	2N	0.25	0/1144	0.46	0/1543
10	1O	0.28	0/943	0.48	0/1269
10	2O	0.27	0/943	0.49	0/1269
11	1P	0.27	0/1156	0.50	0/1537
11	2P	0.27	0/1152	0.49	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.27	0/1143	0.47	0/1527
13	1R	0.26	0/982	0.50	0/1312
13	2R	0.25	0/982	0.47	0/1312
14	1S	0.25	0/887	0.48	0/1180
14	2S	0.27	0/880	0.52	0/1172
15	1T	0.27	0/1105	0.45	0/1477
15	2T	0.26	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.45	0/1301
16	2U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	1V	0.28	0/782	0.46	0/1049
17	2V	0.25	0/782	0.44	0/1049
18	1W	0.28	0/897	0.44	0/1205
18	2W	0.26	0/897	0.44	0/1205
19	1X	0.28	0/764	0.46	0/1025
19	2X	0.26	0/764	0.48	1/1025 (0.1%)
20	1Y	0.28	0/819	0.51	0/1095
20	2Y	0.25	0/819	0.47	0/1095
21	1Z	0.25	0/1502	0.45	0/2041
21	2Z	0.24	0/1486	0.44	0/2022
22	10	0.28	0/606	0.50	0/808
22	20	0.26	0/606	0.47	0/808
23	11	0.26	0/762	0.45	0/1014
23	21	0.25	0/762	0.43	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.25	0/590	0.40	0/781
25	13	0.26	0/474	0.43	0/635
25	23	0.24	0/469	0.44	0/630
26	14	0.29	0/571	0.59	0/768
26	24	0.29	0/545	0.58	0/737
27	15	0.29	0/469	0.51	0/635
27	25	0.25	0/469	0.48	0/635
28	16	0.29	0/460	0.43	0/613
28	26	0.26	0/456	0.45	0/608
29	17	0.28	0/426	0.43	0/561
29	27	0.27	0/426	0.44	0/561
30	18	0.29	0/525	0.47	0/691
30	28	0.26	0/525	0.43	0/691
31	19	0.29	0/310	0.44	0/407
31	29	0.25	0/310	0.43	0/407
32	1a	0.25	0/35537	0.77	7/55456 (0.0%)
32	2a	0.25	2/35680 (0.0%)	0.78	33/55681 (0.1%)
33	1b	0.25	0/1820	0.51	0/2468
33	2b	2.71	8/1728 (0.5%)	0.68	3/2352 (0.1%)
34	1c	0.23	0/1504	0.44	0/2047
34	2c	0.25	0/1435	0.51	2/1960 (0.1%)
35	1d	0.24	0/1648	0.48	0/2222
35	2d	0.25	0/1659	0.45	0/2230
36	1e	0.25	0/1145	0.49	0/1543
36	2e	0.26	0/1111	0.50	0/1504
37	1f	0.24	0/819	0.45	0/1111
37	2f	0.24	0/830	0.44	0/1125
38	1g	0.23	0/1198	0.42	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	2g	0.24	0/1185	0.42	0/1602
39	1h	0.23	0/1108	0.45	0/1494
39	2h	0.23	0/1094	0.47	0/1478
40	1i	0.25	0/995	0.49	0/1339
40	2i	0.26	0/949	0.50	0/1284
41	1j	0.24	0/695	0.55	0/950
41	2j	0.25	0/690	0.50	0/943
42	1k	0.24	0/840	0.45	0/1138
42	2k	0.25	0/844	0.51	1/1145 (0.1%)
43	1l	0.24	0/936	0.46	0/1263
43	2l	0.25	0/934	0.51	1/1262 (0.1%)
44	1m	0.23	0/933	0.49	0/1254
44	2m	0.27	0/913	0.47	0/1230
45	1n	0.29	0/491	0.50	0/653
45	2n	0.27	0/467	0.41	0/624
46	1o	0.24	0/726	0.47	0/970
46	2o	0.23	0/739	0.44	0/985
47	1p	0.22	0/686	0.46	0/926
47	2p	0.23	0/693	0.47	0/935
48	1q	0.25	0/824	0.46	0/1105
48	2q	0.24	0/836	0.44	0/1117
49	1r	0.25	0/560	0.48	0/746
49	2r	0.23	0/560	0.44	0/746
50	1s	0.24	0/657	0.52	0/890
50	2s	0.26	0/661	0.53	0/893
51	1t	0.22	0/714	0.52	0/948
51	2t	0.23	0/733	0.44	0/969
52	1u	0.21	0/191	0.45	0/252
52	2u	0.24	0/203	0.42	0/266
53	1v	0.39	0/122	1.03	0/188
53	2v	0.41	0/122	1.09	0/188
54	1x	0.41	0/1725	1.03	10/2689 (0.4%)
54	2x	0.41	0/1725	1.04	11/2689 (0.4%)
55	1z	0.29	0/114	0.54	0/158
55	2z	0.24	0/114	0.48	0/158
All	All	0.35	10/306296 (0.0%)	0.71	101/458216 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
41	2j	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	58.43	2.27	1.39
33	2b	92	TYR	CD2-CE2	54.24	2.20	1.39
33	2b	92	TYR	CE2-CZ	42.19	1.93	1.38
33	2b	92	TYR	CE1-CZ	41.20	1.92	1.38
33	2b	92	TYR	CG-CD1	33.29	1.82	1.39

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.60	157.16	122.30
32	2a	1102	C	N1-C2-O2	14.44	127.57	118.90
32	2a	1137	G	N3-C2-N2	13.03	129.02	119.90
32	2a	1137	G	N1-C2-N2	-12.03	105.38	116.20
32	2a	1137	G	C4-N9-C1'	11.15	141.00	126.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	Peptide
41	2j	32	ALA	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	59154	0	29830	434	0
1	2A	60091	0	30300	592	0
2	1B	2572	0	1306	18	0
2	2B	2573	0	1306	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1D	2136	0	2218	38	0
3	2D	2142	0	2229	39	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	27	0
5	1F	1584	0	1625	21	0
5	2F	1580	0	1619	25	0
6	1G	1425	0	1443	28	0
6	2G	1424	0	1434	48	0
7	1H	1330	0	1407	19	0
7	2H	1330	0	1407	31	0
8	1I	1085	0	1114	17	0
8	2I	1061	0	1080	24	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	11	0
10	1O	933	0	996	16	0
10	2O	933	0	996	17	0
11	1P	1139	0	1223	27	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1178	19	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	8	0
13	2R	968	0	1033	12	0
14	1S	877	0	938	18	0
14	2S	870	0	923	23	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	10	0
16	2U	959	0	1019	15	0
17	1V	771	0	830	9	0
17	2V	771	0	830	18	0
18	1W	886	0	940	10	0
18	2W	886	0	940	8	0
19	1X	750	0	814	13	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	18	0
21	1Z	1470	0	1478	20	0
21	2Z	1454	0	1452	41	0
22	10	598	0	614	11	0
22	20	598	0	614	11	0
23	11	755	0	826	16	0
23	21	755	0	826	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	12	588	0	643	6	0
24	22	588	0	643	4	0
25	13	469	0	518	8	0
25	23	464	0	514	2	0
26	14	558	0	544	20	0
26	24	532	0	503	23	0
27	15	455	0	465	7	0
27	25	455	0	465	9	0
28	16	453	0	473	5	0
28	26	449	0	469	6	0
29	17	418	0	467	10	0
29	27	418	0	467	8	0
30	18	517	0	582	16	0
30	28	517	0	582	14	0
31	19	307	0	335	8	0
31	29	307	0	335	8	0
32	1a	31750	0	16028	0	0
32	2a	31877	0	16086	0	0
33	1b	1786	0	1744	0	0
33	2b	1697	0	1574	0	0
34	1c	1480	0	1400	0	0
34	2c	1412	0	1246	0	0
35	1d	1618	0	1579	0	0
35	2d	1630	0	1633	0	0
36	1e	1129	0	1184	0	0
36	2e	1095	0	1124	0	0
37	1f	806	0	793	0	0
37	2f	817	0	808	0	0
38	1g	1183	0	1165	0	0
38	2g	1167	0	1119	0	0
39	1h	1088	0	1126	0	0
39	2h	1074	0	1100	0	0
40	1i	976	0	973	0	0
40	2i	932	0	891	0	0
41	1j	682	0	598	0	0
41	2j	678	0	612	0	0
42	1k	826	0	829	0	0
42	2k	829	0	825	0	0
43	1l	920	0	958	0	0
43	2l	918	0	947	0	0
44	1m	923	0	962	0	0
44	2m	903	0	923	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1n	482	0	507	0	0
45	2n	459	0	467	0	0
46	1o	715	0	729	0	0
46	2o	728	0	760	0	0
47	1p	671	0	679	0	0
47	2p	677	0	686	0	0
48	1q	811	0	858	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	642	0	629	0	0
50	2s	646	0	644	0	0
51	1t	712	0	759	0	0
51	2t	731	0	807	0	0
52	1u	187	0	186	0	0
52	2u	199	0	208	0	0
53	1v	109	0	55	0	0
53	2v	109	0	55	0	0
54	1x	1625	0	829	0	0
54	2x	1625	0	829	0	0
55	1z	108	0	116	0	0
55	2z	108	0	116	0	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	1	0	0	0	0
56	18	3	0	0	0	0
56	19	3	0	0	0	0
56	1A	1021	0	0	0	0
56	1B	24	0	0	0	0
56	1D	14	0	0	0	0
56	1E	5	0	0	0	0
56	1F	8	0	0	0	0
56	1G	3	0	0	0	0
56	1H	2	0	0	0	0
56	1N	6	0	0	0	0
56	1O	2	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	4	0	0	0	0
56	1T	5	0	0	0	0
56	1U	5	0	0	0	0
56	1V	1	0	0	0	0
56	1W	5	0	0	0	0
56	1X	2	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	276	0	0	0	0
56	1b	2	0	0	0	0
56	1d	2	0	0	0	0
56	1e	3	0	0	0	0
56	1f	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	2	0	0	0	0
56	1q	4	0	0	0	0
56	1r	2	0	0	0	0
56	1t	1	0	0	0	0
56	1x	8	0	0	0	0
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	566	0	0	0	0
56	2B	11	0	0	0	0
56	2D	6	0	0	0	0
56	2E	4	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2U	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	263	0	0	0	0
56	2d	1	0	0	0	0
56	2f	1	0	0	0	0
56	2h	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2q	2	0	0	0	0
56	2t	1	0	0	0	0
56	2x	4	0	0	0	0
56	2z	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	10	0	0	1	0
59	11	4	0	0	0	0
59	12	1	0	0	0	0
59	13	4	0	0	1	0
59	15	5	0	0	0	0
59	16	8	0	0	1	0
59	17	8	0	0	2	0
59	18	13	0	0	0	0
59	19	2	0	0	0	0
59	1A	2088	0	0	61	0
59	1B	38	0	0	4	0
59	1D	22	0	0	0	0
59	1E	25	0	0	4	0
59	1F	16	0	0	0	0
59	1G	6	0	0	0	0
59	1H	5	0	0	1	0
59	1I	1	0	0	0	0
59	1N	5	0	0	0	0
59	1O	4	0	0	0	0
59	1P	21	0	0	1	0
59	1Q	9	0	0	0	0
59	1R	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1S	1	0	0	0	0
59	1T	11	0	0	2	0
59	1U	13	0	0	0	0
59	1V	2	0	0	0	0
59	1W	9	0	0	0	0
59	1X	5	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	3	0	0	0	0
59	1a	319	0	0	0	0
59	1b	2	0	0	0	0
59	1c	1	0	0	0	0
59	1d	4	0	0	0	0
59	1e	2	0	0	0	0
59	1f	1	0	0	0	0
59	1i	1	0	0	0	0
59	1j	1	0	0	0	0
59	1m	1	0	0	0	0
59	1o	3	0	0	0	0
59	1p	1	0	0	0	0
59	1s	1	0	0	0	0
59	1v	1	0	0	0	0
59	1x	7	0	0	0	0
59	1z	2	0	0	0	0
59	20	3	0	0	0	0
59	21	1	0	0	0	0
59	23	2	0	0	0	0
59	25	1	0	0	0	0
59	27	2	0	0	0	0
59	28	4	0	0	0	0
59	2A	801	0	0	45	0
59	2B	13	0	0	0	0
59	2D	20	0	0	1	0
59	2E	10	0	0	1	0
59	2F	7	0	0	0	0
59	2N	1	0	0	0	0
59	2O	4	0	0	0	0
59	2P	4	0	0	0	0
59	2Q	2	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	3	0	0	0	0
59	2Y	1	0	0	0	0
59	2Z	2	0	0	0	0
59	2a	371	0	0	0	0
59	2c	2	0	0	0	0
59	2e	3	0	0	0	0
59	2h	1	0	0	0	0
59	2i	2	0	0	0	0
59	2j	1	0	0	0	0
59	2k	3	0	0	0	0
59	2l	3	0	0	0	0
59	2m	1	0	0	0	0
59	2n	1	0	0	0	0
59	2o	1	0	0	0	0
59	2p	2	0	0	0	0
59	2q	2	0	0	0	0
59	2r	1	0	0	0	0
59	2t	3	0	0	0	0
59	2x	3	0	0	0	0
59	2z	1	0	0	0	0
All	All	288378	0	189976	1793	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 7.

The worst 5 of 1793 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:1098:C:N3	1:2A:1099:A:C8	2.28	1.01
1:2A:1096:G:C5	1:2A:1097:C:C5	2.56	0.94
1:2A:1151:G:C2	1:2A:1152:G:N7	2.38	0.92
1:2A:1096:G:C4	1:2A:1097:C:C5	2.61	0.88
1:2A:1151:G:H2'	1:2A:1152:G:H5'	1.55	0.88

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	38	72
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	32	68
4	2E	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	32	68
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	32	68
5	2F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	32	68
6	1G	179/182 (98%)	161 (90%)	14 (8%)	4 (2%)	8	29
6	2G	179/182 (98%)	159 (89%)	16 (9%)	4 (2%)	8	29
7	1H	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	15	46
7	2H	172/180 (96%)	157 (91%)	13 (8%)	2 (1%)	15	46
8	1I	144/148 (97%)	124 (86%)	15 (10%)	5 (4%)	4	17
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	13	41
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	25	60
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	25	60
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	25	60
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	25	60
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	20	54
14	2S	108/112 (96%)	97 (90%)	6 (6%)	5 (5%)	3	11
15	1T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	18	51
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	18	51
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	17	48
19	2X	93/96 (97%)	91 (98%)	0	2 (2%)	8	29
20	1Y	105/110 (96%)	98 (93%)	5 (5%)	2 (2%)	9	33
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	184/206 (89%)	172 (94%)	12 (6%)	0	100	100
21	2Z	184/206 (89%)	172 (94%)	11 (6%)	1 (0%)	32	68
22	10	73/85 (86%)	69 (94%)	3 (4%)	1 (1%)	13	41
22	20	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	17	48
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	51 (76%)	8 (12%)	8 (12%)	0	1
26	24	67/71 (94%)	53 (79%)	7 (10%)	7 (10%)	0	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8	29
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	195 (85%)	28 (12%)	6 (3%)	6	24
33	2b	229/256 (90%)	190 (83%)	33 (14%)	6 (3%)	6	24
34	1c	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	12	39
34	2c	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	5	21
35	1d	206/209 (99%)	187 (91%)	16 (8%)	3 (2%)	12	39
35	2d	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	12	39
36	1e	146/162 (90%)	128 (88%)	16 (11%)	2 (1%)	13	41
36	2e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	8	30
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	14	43
38	2g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	14	43
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	16 (13%)	2 (2%)	11	37
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	22	57
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	5	19
41	2j	94/105 (90%)	85 (90%)	8 (8%)	1 (1%)	17	48
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	20	54
42	2k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	20	54
43	1l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	20	54
44	2m	114/126 (90%)	100 (88%)	12 (10%)	2 (2%)	10	34
45	1n	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	4	18
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	11	36
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	15	46
46	2o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	7	27
47	1p	80/88 (91%)	66 (82%)	14 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	18	51
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	82/93 (88%)	70 (85%)	12 (15%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	15 (18%)	0	100	100
51	1t	94/106 (89%)	84 (89%)	7 (7%)	3 (3%)	5	19
51	2t	94/106 (89%)	83 (88%)	7 (7%)	4 (4%)	3	12
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
55	1z	11/19 (58%)	11 (100%)	0	0	100	100
55	2z	11/19 (58%)	11 (100%)	0	0	100	100
All	All	11432/12166 (94%)	10579 (92%)	731 (6%)	122 (1%)	17	48

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	126	ASP
7	1H	126	PRO
14	1S	60	GLY
22	10	13	GLY
26	14	45	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	197 (92%)	18 (8%)	13	36
3	2D	216/218 (99%)	198 (92%)	18 (8%)	13	36
4	1E	164/166 (99%)	147 (90%)	17 (10%)	8	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	146 (89%)	18 (11%)	7	22
5	1F	160/166 (96%)	148 (92%)	12 (8%)	16	42
5	2F	159/166 (96%)	146 (92%)	13 (8%)	13	37
6	1G	143/156 (92%)	129 (90%)	14 (10%)	9	28
6	2G	142/156 (91%)	126 (89%)	16 (11%)	7	21
7	1H	144/148 (97%)	135 (94%)	9 (6%)	21	51
7	2H	144/148 (97%)	135 (94%)	9 (6%)	21	51
8	1I	110/124 (89%)	92 (84%)	18 (16%)	2	8
8	2I	104/124 (84%)	97 (93%)	7 (7%)	19	48
9	1N	118/119 (99%)	107 (91%)	11 (9%)	10	31
9	2N	118/119 (99%)	108 (92%)	10 (8%)	12	35
10	1O	100/100 (100%)	95 (95%)	5 (5%)	28	62
10	2O	100/100 (100%)	92 (92%)	8 (8%)	14	38
11	1P	116/116 (100%)	103 (89%)	13 (11%)	7	21
11	2P	115/116 (99%)	100 (87%)	15 (13%)	5	15
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	17	43
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	14	38
13	1R	101/101 (100%)	88 (87%)	13 (13%)	5	15
13	2R	101/101 (100%)	87 (86%)	14 (14%)	4	12
14	1S	87/88 (99%)	80 (92%)	7 (8%)	14	38
14	2S	85/88 (97%)	73 (86%)	12 (14%)	4	12
15	1T	115/127 (91%)	104 (90%)	11 (10%)	10	29
15	2T	113/127 (89%)	103 (91%)	10 (9%)	12	34
16	1U	93/94 (99%)	82 (88%)	11 (12%)	6	18
16	2U	93/94 (99%)	86 (92%)	7 (8%)	16	42
17	1V	80/82 (98%)	66 (82%)	14 (18%)	2	6
17	2V	80/82 (98%)	69 (86%)	11 (14%)	4	12
18	1W	90/92 (98%)	84 (93%)	6 (7%)	19	48
18	2W	90/92 (98%)	83 (92%)	7 (8%)	15	39
19	1X	77/78 (99%)	75 (97%)	2 (3%)	51	83
19	2X	77/78 (99%)	74 (96%)	3 (4%)	37	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	81 (95%)	4 (5%)	30	65
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	17	44
21	1Z	159/179 (89%)	144 (91%)	15 (9%)	10	30
21	2Z	156/179 (87%)	138 (88%)	18 (12%)	6	20
22	10	60/67 (90%)	55 (92%)	5 (8%)	13	36
22	20	60/67 (90%)	58 (97%)	2 (3%)	43	77
23	11	80/83 (96%)	75 (94%)	5 (6%)	21	51
23	21	80/83 (96%)	74 (92%)	6 (8%)	16	42
24	12	65/67 (97%)	57 (88%)	8 (12%)	5	16
24	22	65/67 (97%)	60 (92%)	5 (8%)	15	40
25	13	51/52 (98%)	47 (92%)	4 (8%)	15	39
25	23	50/52 (96%)	47 (94%)	3 (6%)	22	54
26	14	60/63 (95%)	50 (83%)	10 (17%)	2	7
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	10
27	15	50/52 (96%)	48 (96%)	2 (4%)	36	71
27	25	50/52 (96%)	47 (94%)	3 (6%)	22	54
28	16	51/52 (98%)	49 (96%)	2 (4%)	37	72
28	26	50/52 (96%)	48 (96%)	2 (4%)	36	71
29	17	41/42 (98%)	38 (93%)	3 (7%)	16	43
29	27	41/42 (98%)	40 (98%)	1 (2%)	54	84
30	18	54/55 (98%)	48 (89%)	6 (11%)	7	21
30	28	54/55 (98%)	51 (94%)	3 (6%)	25	57
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	48	81
33	1b	177/220 (80%)	148 (84%)	29 (16%)	2	8
33	2b	158/220 (72%)	130 (82%)	28 (18%)	2	6
34	1c	127/188 (68%)	116 (91%)	11 (9%)	12	34
34	2c	108/188 (57%)	92 (85%)	16 (15%)	3	11
35	1d	161/181 (89%)	143 (89%)	18 (11%)	7	21
35	2d	164/181 (91%)	146 (89%)	18 (11%)	7	22
36	1e	113/123 (92%)	101 (89%)	12 (11%)	8	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	106/123 (86%)	95 (90%)	11 (10%)	8	25
37	1f	83/90 (92%)	78 (94%)	5 (6%)	22	54
37	2f	86/90 (96%)	78 (91%)	8 (9%)	10	31
38	1g	111/127 (87%)	94 (85%)	17 (15%)	3	10
38	2g	107/127 (84%)	97 (91%)	10 (9%)	10	31
39	1h	114/119 (96%)	103 (90%)	11 (10%)	10	29
39	2h	111/119 (93%)	95 (86%)	16 (14%)	4	11
40	1i	89/99 (90%)	78 (88%)	11 (12%)	5	16
40	2i	80/99 (81%)	69 (86%)	11 (14%)	4	12
41	1j	60/92 (65%)	53 (88%)	7 (12%)	6	18
41	2j	62/92 (67%)	49 (79%)	13 (21%)	1	4
42	1k	82/99 (83%)	78 (95%)	4 (5%)	29	63
42	2k	82/99 (83%)	77 (94%)	5 (6%)	22	53
43	1l	95/109 (87%)	87 (92%)	8 (8%)	13	36
43	2l	94/109 (86%)	86 (92%)	8 (8%)	12	35
44	1m	90/101 (89%)	81 (90%)	9 (10%)	9	27
44	2m	87/101 (86%)	79 (91%)	8 (9%)	11	32
45	1n	47/50 (94%)	42 (89%)	5 (11%)	8	24
45	2n	43/50 (86%)	33 (77%)	10 (23%)	1	2
46	1o	75/80 (94%)	65 (87%)	10 (13%)	4	13
46	2o	78/80 (98%)	73 (94%)	5 (6%)	20	50
47	1p	67/74 (90%)	58 (87%)	9 (13%)	4	13
47	2p	68/74 (92%)	61 (90%)	7 (10%)	8	25
48	1q	91/97 (94%)	87 (96%)	4 (4%)	33	67
48	2q	94/97 (97%)	92 (98%)	2 (2%)	59	86
49	1r	59/77 (77%)	51 (86%)	8 (14%)	4	12
49	2r	59/77 (77%)	52 (88%)	7 (12%)	6	18
50	1s	65/80 (81%)	55 (85%)	10 (15%)	3	10
50	2s	67/80 (84%)	61 (91%)	6 (9%)	11	33
51	1t	66/82 (80%)	59 (89%)	7 (11%)	8	24
51	2t	71/82 (87%)	68 (96%)	3 (4%)	34	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	16/22 (73%)	16 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
55	1z	13/19 (68%)	13 (100%)	0	100	100
55	2z	13/19 (68%)	13 (100%)	0	100	100
All	All	9161/10104 (91%)	8276 (90%)	885 (10%)	9	29

5 of 885 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	1o	3	ILE
5	2F	197	ASP
41	2j	33	GLN
47	1p	5	ARG
3	2D	61	LEU

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

Mol	Chain	Res	Type
3	2D	253	GLN
15	2T	58	ASN
44	2m	77	ASN
5	2F	69	HIS
8	2I	43	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	357 (13%)	17 (0%)
1	2A	2781/2915 (95%)	405 (14%)	26 (0%)
2	1B	119/121 (98%)	13 (10%)	2 (1%)
2	2B	119/121 (98%)	23 (19%)	2 (1%)
32	1a	1472/1521 (96%)	238 (16%)	0
32	2a	1479/1521 (97%)	240 (16%)	0
53	1v	4/24 (16%)	2 (50%)	0
53	2v	4/24 (16%)	2 (50%)	0
54	1x	75/77 (97%)	26 (34%)	0
54	2x	75/77 (97%)	26 (34%)	0
All	All	8865/9316 (95%)	1332 (15%)	47 (0%)



5 of 1332 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	12	A
1	1A	14	G
1	1A	33	C
1	1A	44	C

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2A	424	G
1	2A	1047	G
1	2A	2700	U
1	2A	669	C
1	2A	1087	G

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
54	5MC	1x	32	54	15,22,23	1.44	1 (6%)	17,32,35	1.16	2 (11%)
54	5MU	1x	54	54	14,22,23	0.76	1 (7%)	16,32,35	2.44	3 (18%)
54	PSU	1x	55	54	16,21,22	1.45	2 (12%)	20,30,33	3.65	6 (30%)
54	4SU	1x	8	54	14,21,22	1.42	2 (14%)	15,30,33	2.45	2 (13%)
54	5MC	2x	32	54	15,22,23	1.38	1 (6%)	17,32,35	1.04	1 (5%)
54	5MU	2x	54	54	14,22,23	0.72	0	16,32,35	2.17	3 (18%)
54	PSU	2x	55	54	16,21,22	1.33	3 (18%)	20,30,33	3.59	5 (25%)
54	4SU	2x	8	54	14,21,22	1.29	2 (14%)	15,30,33	2.37	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	5MC	1x	32	54	-	0/3/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/3/25/26	0/2/2/2
54	5MC	2x	32	54	-	0/3/25/26	0/2/2/2
54	5MU	2x	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2x	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/3/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	55	PSU	C5-C1'	-4.15	1.48	1.52
54	1x	8	4SU	C4-S4	-3.64	1.60	1.67
54	2x	8	4SU	C4-S4	-3.57	1.60	1.67
54	2x	55	PSU	C5-C1'	-3.45	1.49	1.52
54	1x	8	4SU	C2-N3	-3.26	1.31	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	55	PSU	N1-C2-N3	-9.84	121.32	128.40
54	2x	55	PSU	N1-C2-N3	-9.74	121.40	128.40
54	1x	55	PSU	C5-C4-N3	-8.62	118.36	125.43
54	2x	55	PSU	C5-C4-N3	-8.59	118.39	125.43
54	1x	54	5MU	C5-C4-N3	-5.83	118.81	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2352 ligands modelled in this entry, 2350 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2746/2915 (94%)	0.66	10 (0%) 92 92	24, 41, 87, 115	0
1	2A	2790/2915 (95%)	0.23	16 (0%) 89 88	26, 45, 94, 113	0
2	1B	120/121 (99%)	0.47	0 100 100	40, 66, 79, 96	0
2	2B	120/121 (99%)	-0.15	0 100 100	45, 72, 82, 98	0
3	1D	275/276 (99%)	0.55	2 (0%) 87 86	21, 40, 58, 81	0
3	2D	275/276 (99%)	0.53	13 (4%) 32 28	21, 42, 60, 81	0
4	1E	204/206 (99%)	0.35	1 (0%) 90 90	17, 37, 64, 79	0
4	2E	204/206 (99%)	0.39	4 (1%) 65 62	26, 52, 72, 83	0
5	1F	203/210 (96%)	0.38	0 100 100	22, 50, 77, 92	0
5	2F	203/210 (96%)	0.12	4 (1%) 65 62	25, 54, 78, 92	0
6	1G	181/182 (99%)	0.20	2 (1%) 80 79	54, 71, 84, 98	0
6	2G	181/182 (99%)	0.83	28 (15%) 2 1	59, 76, 88, 99	0
7	1H	174/180 (96%)	0.35	1 (0%) 89 88	49, 64, 79, 86	0
7	2H	174/180 (96%)	0.50	20 (11%) 5 4	52, 70, 82, 88	0
8	1I	146/148 (98%)	0.12	2 (1%) 75 74	47, 75, 87, 93	0
8	2I	146/148 (98%)	0.29	7 (4%) 31 27	48, 77, 87, 93	0
9	1N	140/140 (100%)	0.59	0 100 100	30, 46, 70, 78	0
9	2N	140/140 (100%)	0.26	0 100 100	33, 50, 72, 80	0
10	1O	122/122 (100%)	0.52	2 (1%) 72 70	31, 42, 64, 70	0
10	2O	122/122 (100%)	0.22	1 (0%) 86 85	34, 45, 64, 71	0
11	1P	149/150 (99%)	0.51	2 (1%) 77 76	25, 53, 75, 85	0
11	2P	149/150 (99%)	0.72	12 (8%) 13 9	29, 57, 77, 87	0
12	1Q	141/141 (100%)	0.55	3 (2%) 64 60	32, 50, 65, 84	0
12	2Q	141/141 (100%)	0.31	3 (2%) 64 60	36, 53, 68, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.50	0 100 100	27, 40, 56, 67	0
13	2R	118/118 (100%)	0.46	4 (3%) 46 39	29, 43, 57, 69	0
14	1S	110/112 (98%)	0.28	0 100 100	49, 63, 74, 82	0
14	2S	110/112 (98%)	0.08	3 (2%) 55 50	54, 67, 78, 84	0
15	1T	131/146 (89%)	0.37	0 100 100	35, 48, 80, 88	0
15	2T	131/146 (89%)	0.22	1 (0%) 86 85	37, 50, 78, 87	0
16	1U	116/118 (98%)	0.59	0 100 100	29, 39, 57, 78	0
16	2U	116/118 (98%)	0.22	0 100 100	31, 44, 61, 78	0
17	1V	101/101 (100%)	0.42	0 100 100	30, 51, 69, 78	0
17	2V	101/101 (100%)	-0.08	3 (2%) 51 44	33, 57, 72, 79	0
18	1W	112/113 (99%)	0.51	1 (0%) 84 83	28, 37, 59, 90	0
18	2W	112/113 (99%)	0.24	2 (1%) 69 66	30, 40, 60, 90	0
19	1X	95/96 (98%)	0.53	1 (1%) 80 79	31, 47, 68, 80	0
19	2X	95/96 (98%)	0.21	3 (3%) 48 42	35, 50, 71, 81	0
20	1Y	107/110 (97%)	0.16	1 (0%) 84 83	31, 49, 74, 84	0
20	2Y	107/110 (97%)	0.71	5 (4%) 32 28	55, 72, 84, 96	0
21	1Z	186/206 (90%)	-0.07	0 100 100	40, 62, 79, 96	0
21	2Z	186/206 (90%)	0.26	6 (3%) 48 42	67, 81, 94, 101	0
22	10	75/85 (88%)	0.32	0 100 100	23, 38, 53, 67	0
22	20	75/85 (88%)	1.16	11 (14%) 3 2	43, 63, 73, 78	0
23	11	97/98 (98%)	0.57	2 (2%) 64 60	21, 42, 71, 80	0
23	21	97/98 (98%)	0.51	6 (6%) 21 16	33, 54, 77, 86	0
24	12	70/72 (97%)	0.51	3 (4%) 36 31	42, 59, 74, 89	0
24	22	70/72 (97%)	-0.03	1 (1%) 75 74	46, 63, 75, 87	0
25	13	59/60 (98%)	0.43	0 100 100	32, 46, 67, 80	0
25	23	59/60 (98%)	0.38	0 100 100	36, 49, 72, 82	0
26	14	69/71 (97%)	0.31	7 (10%) 8 5	68, 84, 100, 103	0
26	24	69/71 (97%)	0.76	11 (15%) 2 1	73, 86, 100, 104	0
27	15	59/60 (98%)	0.52	1 (1%) 70 68	21, 40, 60, 78	0
27	25	59/60 (98%)	0.18	0 100 100	24, 43, 62, 79	0
28	16	53/54 (98%)	0.22	0 100 100	36, 48, 63, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.04	1 (1%) 67 64	39, 51, 65, 70	0
29	17	48/49 (97%)	1.21	6 (12%) 4 3	26, 31, 67, 76	0
29	27	48/49 (97%)	1.10	7 (14%) 3 2	28, 33, 67, 78	0
30	18	64/65 (98%)	0.70	0 100 100	32, 40, 51, 64	0
30	28	64/65 (98%)	1.15	9 (14%) 3 2	34, 43, 54, 67	0
31	19	37/37 (100%)	0.62	0 100 100	40, 49, 66, 69	0
31	29	37/37 (100%)	0.78	2 (5%) 26 22	44, 53, 67, 71	0
32	1a	1477/1521 (97%)	0.31	16 (1%) 80 79	33, 72, 99, 116	0
32	2a	1483/1521 (97%)	0.34	20 (1%) 77 76	43, 78, 102, 119	0
33	1b	231/256 (90%)	0.11	7 (3%) 51 44	60, 83, 95, 105	0
33	2b	231/256 (90%)	0.77	29 (12%) 4 3	71, 88, 97, 101	0
34	1c	206/239 (86%)	0.82	34 (16%) 2 1	70, 84, 91, 99	0
34	2c	206/239 (86%)	0.80	42 (20%) 1 1	72, 86, 93, 100	0
35	1d	208/209 (99%)	1.26	56 (26%) 1 0	55, 78, 91, 101	0
35	2d	208/209 (99%)	0.65	21 (10%) 8 5	58, 75, 87, 90	0
36	1e	148/162 (91%)	0.59	8 (5%) 26 22	47, 65, 77, 94	0
36	2e	148/162 (91%)	0.58	9 (6%) 22 17	56, 74, 86, 91	0
37	1f	100/101 (99%)	0.35	5 (5%) 30 25	57, 75, 85, 89	0
37	2f	100/101 (99%)	-0.21	0 100 100	60, 76, 86, 90	0
38	1g	155/156 (99%)	0.54	14 (9%) 10 7	66, 80, 93, 101	0
38	2g	155/156 (99%)	0.41	15 (9%) 8 6	69, 81, 94, 99	0
39	1h	137/138 (99%)	0.70	17 (12%) 4 3	56, 68, 80, 85	0
39	2h	137/138 (99%)	0.60	13 (9%) 9 6	58, 75, 83, 89	0
40	1i	127/128 (99%)	1.44	40 (31%) 0 0	66, 87, 94, 99	0
40	2i	127/128 (99%)	2.35	68 (53%) 0 0	65, 88, 96, 100	0
41	1j	97/105 (92%)	1.15	26 (26%) 1 0	65, 86, 96, 104	0
41	2j	96/105 (91%)	1.53	29 (30%) 1 0	75, 92, 99, 103	0
42	1k	114/129 (88%)	0.40	4 (3%) 44 38	45, 69, 82, 94	0
42	2k	114/129 (88%)	0.37	8 (7%) 17 12	52, 76, 88, 91	0
43	1l	122/132 (92%)	0.52	12 (9%) 8 6	47, 65, 76, 88	0
43	2l	122/132 (92%)	0.86	14 (11%) 5 4	52, 67, 77, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	118/126 (93%)	0.44	5 (4%) 37 32	64, 82, 89, 95	0
44	2m	116/126 (92%)	0.52	15 (12%) 4 3	66, 84, 91, 94	0
45	1n	60/61 (98%)	2.35	36 (60%) 0 0	69, 81, 88, 93	0
45	2n	60/61 (98%)	2.74	39 (65%) 0 0	71, 83, 89, 95	0
46	1o	88/89 (98%)	0.26	1 (1%) 80 79	49, 68, 84, 91	0
46	2o	88/89 (98%)	0.28	4 (4%) 34 29	56, 73, 85, 94	0
47	1p	82/88 (93%)	1.16	17 (20%) 1 1	66, 79, 92, 96	0
47	2p	82/88 (93%)	0.74	6 (7%) 16 11	59, 71, 83, 96	0
48	1q	99/105 (94%)	0.58	8 (8%) 13 9	51, 68, 81, 84	0
48	2q	99/105 (94%)	1.08	17 (17%) 2 1	57, 72, 83, 86	0
49	1r	68/88 (77%)	0.38	2 (2%) 52 46	56, 71, 84, 91	0
49	2r	68/88 (77%)	0.68	6 (8%) 11 7	65, 75, 89, 94	0
50	1s	84/93 (90%)	-0.00	0 100 100	71, 83, 92, 98	0
50	2s	83/93 (89%)	1.38	23 (27%) 1 0	80, 92, 101, 108	0
51	1t	96/106 (90%)	0.91	18 (18%) 1 1	61, 74, 88, 90	0
51	2t	96/106 (90%)	0.40	4 (4%) 37 32	54, 73, 85, 90	0
52	1u	23/27 (85%)	1.14	5 (21%) 1 1	71, 80, 85, 87	0
52	2u	23/27 (85%)	2.48	12 (52%) 0 0	72, 82, 87, 89	0
53	1v	5/24 (20%)	1.20	1 (20%) 1 1	57, 67, 94, 101	0
53	2v	5/24 (20%)	2.31	3 (60%) 0 0	61, 70, 95, 102	0
54	1x	72/77 (93%)	0.24	0 100 100	35, 68, 87, 102	0
54	2x	72/77 (93%)	0.21	1 (1%) 75 74	38, 72, 89, 103	0
55	1z	13/19 (68%)	0.93	2 (15%) 2 1	26, 37, 63, 72	0
55	2z	13/19 (68%)	1.74	3 (23%) 1 0	28, 39, 65, 74	0
All	All	20522/21482 (95%)	0.48	965 (4%) 32 28	17, 62, 93, 119	0

The worst 5 of 965 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	9.6
38	1g	79	ARG	7.9
40	2i	7	THR	7.9
52	2u	14	TRP	7.7
41	1j	62	HIS	7.5

## 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
54	PSU	2x	55	20/21	0.86	0.12	-	69,77,85,97	0
54	5MU	2x	54	21/22	0.94	0.16	-	75,81,92,101	0
54	5MC	2x	32	21/22	0.96	0.22	-	61,77,79,91	0
54	4SU	1x	8	20/21	0.95	0.20	-	51,69,76,81	0
54	4SU	2x	8	20/21	0.92	0.15	-	70,77,94,99	0
54	5MC	1x	32	21/22	0.97	0.19	-	48,59,69,81	0
54	5MU	1x	54	21/22	0.94	0.17	-	57,66,80,87	0
54	PSU	1x	55	20/21	0.92	0.17	-	62,73,83,85	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(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3481	1/1	0.93	0.89	57.89	40,40,40,40	0
56	MG	1A	3930	1/1	0.95	0.72	49.16	44,44,44,44	0
56	MG	1A	3374	1/1	0.89	0.79	38.56	64,64,64,64	0
56	MG	1A	3267	1/1	0.98	0.72	38.07	27,27,27,27	0
56	MG	1A	3289	1/1	0.94	0.85	34.56	43,43,43,43	0
56	MG	1A	3074	1/1	0.97	0.71	33.30	51,51,51,51	0
56	MG	1A	3092	1/1	0.89	0.60	31.90	49,49,49,49	0
56	MG	1A	4008	1/1	0.89	1.45	31.40	48,48,48,48	0
56	MG	2A	3554	1/1	0.77	2.20	29.91	51,51,51,51	0
56	MG	1U	205	1/1	0.89	1.04	28.87	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
56	MG	2A	3042	1/1	0.96	0.53	28.41	43,43,43,43	0
56	MG	1A	3962	1/1	0.91	1.01	27.70	52,52,52,52	0
56	MG	1E	303	1/1	0.94	0.99	27.39	58,58,58,58	0
56	MG	2A	3107	1/1	0.92	0.75	25.71	45,45,45,45	0
56	MG	1A	3001	1/1	0.97	0.85	25.68	42,42,42,42	0
56	MG	2a	3022	1/1	0.85	0.70	25.01	73,73,73,73	0
56	MG	1A	3473	1/1	0.94	0.87	24.99	50,50,50,50	0
56	MG	1A	3986	1/1	0.94	0.85	24.95	42,42,42,42	0
56	MG	1A	3178	1/1	0.89	0.71	24.78	41,41,41,41	0
56	MG	1A	3975	1/1	0.96	0.91	24.72	45,45,45,45	0
56	MG	1U	202	1/1	0.90	0.85	24.56	50,50,50,50	0
56	MG	1A	4007	1/1	0.90	0.90	23.77	36,36,36,36	0
56	MG	1F	306	1/1	0.91	0.77	22.72	33,33,33,33	0
56	MG	1A	3187	1/1	0.91	0.64	22.66	46,46,46,46	0
56	MG	1A	3132	1/1	0.68	0.72	22.56	51,51,51,51	0
56	MG	1A	3456	1/1	0.97	0.53	21.83	39,39,39,39	0
56	MG	1D	309	1/1	0.97	0.82	21.81	41,41,41,41	0
56	MG	1A	3093	1/1	0.95	0.52	20.89	47,47,47,47	0
56	MG	1A	4003	1/1	0.94	0.89	20.72	43,43,43,43	0
56	MG	1A	4018	1/1	0.85	0.93	19.89	50,50,50,50	0
56	MG	1A	4017	1/1	0.81	0.93	19.88	60,60,60,60	0
56	MG	2A	3214	1/1	0.90	0.78	18.94	43,43,43,43	0
56	MG	1W	3005	1/1	0.91	0.53	18.81	49,49,49,49	0
56	MG	1A	3110	1/1	0.93	0.70	17.31	55,55,55,55	0
56	MG	1U	204	1/1	0.89	1.10	17.28	42,42,42,42	0
56	MG	1A	4011	1/1	0.95	0.95	17.13	47,47,47,47	0
56	MG	1A	4002	1/1	0.94	0.89	17.09	34,34,34,34	0
56	MG	1A	3322	1/1	0.81	0.62	15.93	50,50,50,50	0
56	MG	2A	3063	1/1	0.95	0.46	15.72	45,45,45,45	0
56	MG	1A	3394	1/1	0.67	0.46	15.30	56,56,56,56	0
56	MG	1A	4010	1/1	0.87	0.57	15.25	41,41,41,41	0
56	MG	1A	3995	1/1	0.82	0.89	14.63	42,42,42,42	0
56	MG	1A	3182	1/1	0.97	0.47	14.25	42,42,42,42	0
56	MG	1a	1765	1/1	0.78	0.51	14.02	57,57,57,57	0
56	MG	1A	3179	1/1	0.94	0.40	13.95	44,44,44,44	0
56	MG	1A	3931	1/1	0.91	0.45	13.72	33,33,33,33	0
56	MG	1A	3241	1/1	0.89	0.39	13.46	42,42,42,42	0
56	MG	2U	201	1/1	0.96	0.69	13.20	48,48,48,48	0
56	MG	1A	3129	1/1	0.89	0.67	12.98	40,40,40,40	0
56	MG	1A	3994	1/1	0.97	0.62	12.00	47,47,47,47	0
56	MG	1P	206	1/1	0.97	0.76	11.97	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
56	MG	1A	3131	1/1	0.86	0.57	11.92	42,42,42,42	0
56	MG	1A	3315	1/1	0.90	0.46	11.67	49,49,49,49	0
56	MG	2A	3027	1/1	0.74	0.89	11.60	51,51,51,51	0
56	MG	2A	3563	1/1	0.94	0.70	11.17	47,47,47,47	0
56	MG	2A	3562	1/1	0.77	0.65	11.15	49,49,49,49	0
56	MG	1F	304	1/1	0.88	0.55	11.12	43,43,43,43	0
56	MG	2A	3139	1/1	0.94	0.31	11.06	45,45,45,45	0
56	MG	1A	3442	1/1	0.73	0.38	10.87	58,58,58,58	0
56	MG	1A	3980	1/1	0.86	0.44	10.80	50,50,50,50	0
56	MG	1A	3186	1/1	0.94	0.43	10.46	32,32,32,32	0
56	MG	2A	3016	1/1	0.93	0.26	10.14	57,57,57,57	0
56	MG	1R	203	1/1	0.91	0.63	9.96	43,43,43,43	0
56	MG	1A	3177	1/1	0.93	0.62	9.90	39,39,39,39	0
56	MG	1A	3444	1/1	0.91	0.59	9.74	36,36,36,36	0
56	MG	1A	3797	1/1	0.96	0.80	9.72	40,40,40,40	0
56	MG	1D	311	1/1	0.87	0.47	9.67	55,55,55,55	0
56	MG	1a	1749	1/1	0.96	0.88	9.66	57,57,57,57	0
56	MG	1A	3215	1/1	0.95	0.23	9.63	51,51,51,51	0
56	MG	1A	4019	1/1	0.94	0.78	9.28	47,47,47,47	0
56	MG	1A	3968	1/1	0.91	0.62	9.12	50,50,50,50	0
56	MG	1A	3203	1/1	0.98	0.28	9.05	32,32,32,32	0
56	MG	1A	3449	1/1	0.93	0.31	8.92	66,66,66,66	0
56	MG	1A	3973	1/1	0.90	0.45	8.74	51,51,51,51	0
56	MG	2A	3222	1/1	0.94	0.61	8.74	36,36,36,36	0
56	MG	2A	3561	1/1	0.96	0.93	8.65	41,41,41,41	0
56	MG	2A	3349	1/1	0.95	0.24	8.65	59,59,59,59	0
56	MG	1D	306	1/1	0.97	0.49	8.52	31,31,31,31	0
56	MG	2a	3228	1/1	0.84	0.40	8.45	69,69,69,69	0
56	MG	2A	3233	1/1	0.91	0.54	8.29	48,48,48,48	0
56	MG	15	101	1/1	0.66	0.49	8.29	58,58,58,58	0
56	MG	1X	102	1/1	0.91	0.47	7.70	53,53,53,53	0
56	MG	1U	203	1/1	0.93	0.51	7.52	47,47,47,47	0
56	MG	1A	3887	1/1	0.92	0.34	7.19	31,31,31,31	0
56	MG	1A	3225	1/1	0.99	0.55	7.11	34,34,34,34	0
56	MG	1a	1668	1/1	0.89	0.30	6.95	59,59,59,59	0
56	MG	1a	1659	1/1	0.92	0.44	6.82	63,63,63,63	0
56	MG	2A	3416	1/1	0.90	0.19	6.73	48,48,48,48	0
56	MG	2A	3430	1/1	0.92	0.30	6.49	45,45,45,45	0
56	MG	1D	303	1/1	0.89	0.43	6.44	47,47,47,47	0
56	MG	1A	3518	1/1	0.90	0.36	6.29	53,53,53,53	0
56	MG	1A	3411	1/1	0.94	0.30	6.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1D	312	1/1	0.98	0.44	6.23	47,47,47,47	0
56	MG	2F	303	1/1	0.89	0.62	6.11	50,50,50,50	0
56	MG	2a	3011	1/1	0.80	0.22	6.07	67,67,67,67	0
56	MG	1A	3287	1/1	0.93	0.35	6.01	27,27,27,27	0
56	MG	2A	3540	1/1	0.77	0.33	5.89	58,58,58,58	0
56	MG	1A	3705	1/1	0.84	0.40	5.82	34,34,34,34	0
56	MG	1a	1858	1/1	0.91	0.26	5.67	52,52,52,52	0
56	MG	1A	3208	1/1	0.97	0.29	5.34	34,34,34,34	0
56	MG	2A	3024	1/1	0.90	0.26	5.33	43,43,43,43	0
56	MG	1A	3162	1/1	0.91	0.41	5.24	38,38,38,38	0
56	MG	1A	3459	1/1	0.83	0.43	5.15	46,46,46,46	0
56	MG	1P	205	1/1	0.96	0.53	5.14	31,31,31,31	0
56	MG	2P	201	1/1	0.96	0.57	5.02	41,41,41,41	0
56	MG	1A	4012	1/1	0.97	0.45	4.88	36,36,36,36	0
56	MG	1H	8002	1/1	0.80	0.42	4.71	79,79,79,79	0
56	MG	1A	3711	1/1	0.94	0.34	4.67	48,48,48,48	0
56	MG	1A	3172	1/1	0.85	0.63	4.66	44,44,44,44	0
56	MG	2A	3029	1/1	0.92	0.24	4.36	48,48,48,48	0
56	MG	1a	1814	1/1	0.95	0.30	4.34	67,67,67,67	0
56	MG	2A	3381	1/1	0.63	0.20	4.06	64,64,64,64	0
56	MG	2A	3550	1/1	0.92	0.50	4.01	42,42,42,42	0
56	MG	2A	3019	1/1	0.98	0.30	4.01	46,46,46,46	0
56	MG	2a	3105	1/1	0.94	0.33	3.99	55,55,55,55	0
56	MG	1A	3253	1/1	0.98	0.26	3.81	31,31,31,31	0
56	MG	1A	3888	1/1	0.86	0.48	3.72	42,42,42,42	0
56	MG	1A	3329	1/1	0.96	0.26	3.68	52,52,52,52	0
56	MG	2A	3304	1/1	0.97	0.28	3.52	41,41,41,41	0
56	MG	2A	3555	1/1	0.81	0.52	3.34	36,36,36,36	0
56	MG	2A	3199	1/1	0.96	0.23	3.32	39,39,39,39	0
56	MG	1A	3821	1/1	0.92	0.29	3.18	23,23,23,23	0
56	MG	1A	3437	1/1	0.92	0.25	3.16	62,62,62,62	0
56	MG	1A	3312	1/1	0.95	0.26	3.10	38,38,38,38	0
56	MG	2A	3470	1/1	0.98	0.27	3.09	44,44,44,44	0
56	MG	2A	3191	1/1	0.90	0.29	3.00	40,40,40,40	0
56	MG	2A	3123	1/1	0.99	0.19	2.92	41,41,41,41	0
56	MG	1B	211	1/1	0.89	0.23	2.87	51,51,51,51	0
56	MG	2a	3194	1/1	0.97	0.21	2.82	72,72,72,72	0
56	MG	2A	3155	1/1	0.96	0.22	2.76	33,33,33,33	0
56	MG	2D	303	1/1	0.92	0.31	2.74	49,49,49,49	0
56	MG	2A	3232	1/1	0.83	0.24	2.72	54,54,54,54	0
56	MG	1a	1739	1/1	0.94	0.29	2.69	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
56	MG	1A	3964	1/1	0.96	0.30	2.65	29,29,29,29	0
56	MG	2A	3559	1/1	0.86	0.31	2.60	54,54,54,54	0
56	MG	2A	3303	1/1	0.98	0.23	2.50	55,55,55,55	0
56	MG	1A	3911	1/1	0.94	0.27	2.47	39,39,39,39	0
56	MG	2a	3026	1/1	0.83	0.26	2.37	64,64,64,64	0
56	MG	2A	3017	1/1	0.89	0.36	2.23	47,47,47,47	0
56	MG	2A	3209	1/1	0.79	0.19	2.22	45,45,45,45	0
56	MG	2A	3468	1/1	0.91	0.20	2.19	56,56,56,56	0
56	MG	1A	3170	1/1	0.83	0.23	2.11	44,44,44,44	0
56	MG	2A	3318	1/1	0.93	0.25	2.11	47,47,47,47	0
56	MG	1B	205	1/1	0.86	0.22	2.07	56,56,56,56	0
56	MG	2A	3188	1/1	0.96	0.23	2.04	35,35,35,35	0
56	MG	1a	1730	1/1	0.97	0.24	1.88	70,70,70,70	0
56	MG	1W	3003	1/1	0.95	0.28	1.86	35,35,35,35	0
56	MG	1A	3860	1/1	0.97	0.23	1.85	29,29,29,29	0
56	MG	2A	3556	1/1	0.84	0.19	1.79	62,62,62,62	0
56	MG	2a	3065	1/1	0.86	0.34	1.77	80,80,80,80	0
56	MG	15	104	1/1	0.87	0.27	1.74	62,62,62,62	0
56	MG	2A	3396	1/1	0.92	0.23	1.74	40,40,40,40	0
56	MG	2A	3558	1/1	0.98	0.32	1.70	34,34,34,34	0
57	ZN	25	501	1/1	0.98	0.21	1.69	54,54,54,54	0
56	MG	1A	3408	1/1	0.81	0.24	1.63	42,42,42,42	0
56	MG	1A	3167	1/1	0.82	0.27	1.56	35,35,35,35	0
56	MG	1A	3292	1/1	0.95	0.27	1.48	17,17,17,17	0
57	ZN	26	102	1/1	0.95	0.20	1.44	56,56,56,56	0
56	MG	1A	3222	1/1	0.95	0.23	1.43	50,50,50,50	0
56	MG	2a	3030	1/1	0.42	0.26	1.41	73,73,73,73	0
56	MG	2A	3427	1/1	0.92	0.24	1.40	56,56,56,56	0
56	MG	2a	3111	1/1	0.98	0.25	1.36	56,56,56,56	0
56	MG	2a	3068	1/1	0.94	0.33	1.33	67,67,67,67	0
56	MG	19	101	1/1	0.98	0.29	1.33	65,65,65,65	0
56	MG	1A	4020	1/1	0.99	0.30	1.31	32,32,32,32	0
56	MG	2a	3027	1/1	0.84	0.28	1.27	70,70,70,70	0
56	MG	1A	3912	1/1	0.94	0.33	1.19	40,40,40,40	0
56	MG	2A	3147	1/1	0.89	0.16	1.18	42,42,42,42	0
56	MG	1x	104	1/1	0.96	0.15	1.14	52,52,52,52	0
56	MG	1A	3809	1/1	0.98	0.21	1.14	45,45,45,45	0
56	MG	1R	202	1/1	0.96	0.29	1.13	52,52,52,52	0
56	MG	1a	1710	1/1	0.88	0.18	1.07	71,71,71,71	0
56	MG	1a	1795	1/1	0.95	0.21	1.04	75,75,75,75	0
56	MG	1q	203	1/1	0.90	0.24	0.99	51,51,51,51	0
56	MG	1A	3258	1/1	0.95	0.24	0.98	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1q	202	1/1	0.91	0.26	0.95	62,62,62,62	0
56	MG	2A	3078	1/1	0.94	0.19	0.91	60,60,60,60	0
56	MG	2a	3257	1/1	0.91	0.16	0.90	90,90,90,90	0
56	MG	1A	3740	1/1	0.94	0.25	0.84	36,36,36,36	0
57	ZN	2Y	501	1/1	0.92	0.19	0.75	85,85,85,85	0
56	MG	2a	3187	1/1	0.88	0.24	0.63	59,59,59,59	0
56	MG	1a	1722	1/1	0.89	0.22	0.57	54,54,54,54	0
56	MG	1A	3813	1/1	0.94	0.21	0.54	56,56,56,56	0
56	MG	2A	3376	1/1	0.93	0.18	0.51	47,47,47,47	0
56	MG	2A	3149	1/1	0.96	0.22	0.48	43,43,43,43	0
56	MG	1A	3250	1/1	0.98	0.20	0.43	34,34,34,34	0
56	MG	2a	3028	1/1	0.99	0.23	0.36	76,76,76,76	0
56	MG	2a	3259	1/1	0.72	0.23	0.34	56,56,56,56	0
56	MG	2A	3486	1/1	0.82	0.18	0.26	57,57,57,57	0
56	MG	1a	1870	1/1	0.95	0.30	0.24	88,88,88,88	0
56	MG	1D	310	1/1	0.85	0.22	0.21	57,57,57,57	0
56	MG	1a	1810	1/1	0.95	0.20	0.19	38,38,38,38	0
56	MG	1A	3683	1/1	0.88	0.22	0.16	58,58,58,58	0
56	MG	2a	3007	1/1	0.98	0.20	0.12	46,46,46,46	0
56	MG	1A	3882	1/1	0.97	0.22	0.11	49,49,49,49	0
56	MG	2A	3326	1/1	0.72	0.21	0.11	42,42,42,42	0
56	MG	2A	3100	1/1	0.95	0.21	0.10	50,50,50,50	0
56	MG	1A	3168	1/1	0.92	0.25	0.07	42,42,42,42	0
56	MG	2A	3292	1/1	0.91	0.19	0.05	42,42,42,42	0
56	MG	2A	3539	1/1	0.95	0.22	0.01	35,35,35,35	0
56	MG	2A	3059	1/1	0.91	0.18	-0.06	48,48,48,48	0
56	MG	1a	1846	1/1	0.92	0.18	-0.06	52,52,52,52	0
56	MG	1A	3010	1/1	0.89	0.22	-0.09	42,42,42,42	0
57	ZN	1Y	201	1/1	0.97	0.19	-0.11	61,61,61,61	0
56	MG	2A	3048	1/1	0.93	0.18	-0.12	56,56,56,56	0
56	MG	2A	3507	1/1	0.94	0.17	-0.15	47,47,47,47	0
56	MG	1A	3321	1/1	0.95	0.24	-0.16	37,37,37,37	0
56	MG	2A	3186	1/1	0.92	0.15	-0.16	36,36,36,36	0
56	MG	1e	3002	1/1	0.95	0.18	-0.18	83,83,83,83	0
56	MG	1a	1673	1/1	0.90	0.16	-0.18	71,71,71,71	0
56	MG	2A	3565	1/1	0.93	0.15	-0.25	52,52,52,52	0
56	MG	1A	3548	1/1	0.97	0.20	-0.26	38,38,38,38	0
56	MG	2a	3255	1/1	0.72	0.18	-0.27	70,70,70,70	0
56	MG	2A	3405	1/1	0.84	0.18	-0.28	63,63,63,63	0
56	MG	1A	3198	1/1	0.95	0.21	-0.30	28,28,28,28	0
57	ZN	16	102	1/1	0.99	0.19	-0.30	29,29,29,29	0
56	MG	1D	308	1/1	0.89	0.20	-0.30	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3373	1/1	0.92	0.17	-0.40	47,47,47,47	0
56	MG	2a	3005	1/1	0.93	0.20	-0.40	62,62,62,62	0
56	MG	1a	1859	1/1	0.95	0.18	-0.40	59,59,59,59	0
56	MG	2a	3184	1/1	0.91	0.14	-0.41	80,80,80,80	0
56	MG	2a	3261	1/1	0.76	0.23	-0.46	74,74,74,74	0
57	ZN	19	103	1/1	0.99	0.22	-0.47	45,45,45,45	0
56	MG	2E	304	1/1	0.94	0.18	-0.48	67,67,67,67	0
56	MG	2A	3262	1/1	0.96	0.18	-0.50	54,54,54,54	0
56	MG	1A	3202	1/1	0.93	0.22	-0.55	43,43,43,43	0
56	MG	2D	302	1/1	0.87	0.19	-0.56	54,54,54,54	0
56	MG	2A	3339	1/1	0.90	0.22	-0.58	31,31,31,31	0
56	MG	1A	3613	1/1	0.84	0.19	-0.62	35,35,35,35	0
56	MG	2A	3171	1/1	0.94	0.15	-0.63	41,41,41,41	0
56	MG	2A	3368	1/1	0.83	0.21	-0.63	29,29,29,29	0
57	ZN	29	501	1/1	0.93	0.16	-0.63	62,62,62,62	0
57	ZN	14	501	1/1	0.97	0.14	-0.68	106,106,106,106	0
56	MG	1A	3645	1/1	0.82	0.21	-0.68	23,23,23,23	0
56	MG	2q	202	1/1	0.79	0.26	-0.70	69,69,69,69	0
56	MG	1A	3022	1/1	0.90	0.23	-0.70	59,59,59,59	0
56	MG	2a	3013	1/1	0.87	0.15	-0.71	72,72,72,72	0
56	MG	2A	3312	1/1	0.97	0.20	-0.72	28,28,28,28	0
56	MG	2A	3293	1/1	0.92	0.16	-0.73	62,62,62,62	0
56	MG	1a	1799	1/1	0.93	0.19	-0.73	61,61,61,61	0
56	MG	1A	3993	1/1	0.97	0.20	-0.75	73,73,73,73	0
56	MG	1A	3567	1/1	0.88	0.20	-0.79	39,39,39,39	0
56	MG	1A	3990	1/1	0.96	0.23	-0.80	36,36,36,36	0
58	SF4	1d	501	8/8	0.98	0.18	-0.81	66,73,85,85	0
56	MG	1A	3843	1/1	0.95	0.18	-0.82	50,50,50,50	0
56	MG	2A	3508	1/1	0.85	0.21	-0.83	56,56,56,56	0
56	MG	2a	3163	1/1	0.90	0.12	-0.84	70,70,70,70	0
56	MG	2A	3106	1/1	0.73	0.14	-0.84	59,59,59,59	0
56	MG	1A	3617	1/1	0.91	0.23	-0.88	27,27,27,27	0
56	MG	2l	202	1/1	0.95	0.24	-0.89	40,40,40,40	0
56	MG	2O	202	1/1	0.99	0.16	-0.90	42,42,42,42	0
56	MG	2a	3232	1/1	0.98	0.13	-0.92	66,66,66,66	0
56	MG	1A	3588	1/1	0.97	0.22	-0.92	33,33,33,33	0
56	MG	1d	502	1/1	0.85	0.13	-0.98	76,76,76,76	0
58	SF4	2d	501	8/8	0.99	0.17	-0.99	56,76,90,91	0
56	MG	1a	1790	1/1	0.94	0.17	-1.01	71,71,71,71	0
56	MG	1A	3538	1/1	0.95	0.21	-1.01	57,57,57,57	0
56	MG	1a	1711	1/1	0.96	0.19	-1.03	49,49,49,49	0
56	MG	2D	301	1/1	0.93	0.16	-1.05	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3575	1/1	0.79	0.21	-1.07	41,41,41,41	0
56	MG	1a	1837	1/1	0.99	0.16	-1.08	37,37,37,37	0
56	MG	2A	3235	1/1	0.78	0.16	-1.10	52,52,52,52	0
56	MG	1B	207	1/1	0.92	0.19	-1.11	33,33,33,33	0
56	MG	2A	3564	1/1	0.81	0.18	-1.11	59,59,59,59	0
56	MG	1a	1629	1/1	0.91	0.13	-1.14	49,49,49,49	0
56	MG	2G	3001	1/1	0.58	0.18	-1.14	58,58,58,58	0
56	MG	2E	301	1/1	0.90	0.18	-1.17	44,44,44,44	0
56	MG	1A	3188	1/1	0.93	0.21	-1.17	43,43,43,43	0
56	MG	2a	3129	1/1	0.95	0.14	-1.18	65,65,65,65	0
56	MG	2A	3533	1/1	0.89	0.22	-1.19	35,35,35,35	0
56	MG	2a	3113	1/1	0.91	0.10	-1.19	65,65,65,65	0
56	MG	2A	3300	1/1	0.84	0.17	-1.20	32,32,32,32	0
57	ZN	15	103	1/1	0.99	0.18	-1.20	43,43,43,43	0
56	MG	1A	3895	1/1	0.82	0.22	-1.23	24,24,24,24	0
57	ZN	2n	501	1/1	0.92	0.12	-1.23	98,98,98,98	0
56	MG	1A	3528	1/1	0.96	0.20	-1.23	54,54,54,54	0
56	MG	1A	3632	1/1	0.82	0.20	-1.26	25,25,25,25	0
56	MG	1A	3607	1/1	0.85	0.20	-1.27	40,40,40,40	0
56	MG	1A	3731	1/1	0.93	0.22	-1.28	23,23,23,23	0
56	MG	1A	4004	1/1	0.95	0.22	-1.30	49,49,49,49	0
56	MG	1a	1665	1/1	0.93	0.14	-1.30	61,61,61,61	0
56	MG	2A	3546	1/1	0.92	0.16	-1.31	44,44,44,44	0
57	ZN	24	501	1/1	0.77	0.10	-1.33	125,125,125,125	0
56	MG	2B	3004	1/1	0.82	0.14	-1.34	75,75,75,75	0
56	MG	1A	3637	1/1	0.94	0.18	-1.36	47,47,47,47	0
56	MG	2A	3398	1/1	0.82	0.16	-1.38	50,50,50,50	0
56	MG	2A	3220	1/1	0.94	0.13	-1.38	45,45,45,45	0
56	MG	2A	3167	1/1	0.94	0.20	-1.38	25,25,25,25	0
56	MG	1A	3578	1/1	0.97	0.17	-1.40	64,64,64,64	0
56	MG	2t	3001	1/1	0.94	0.12	-1.40	50,50,50,50	0
56	MG	2A	3261	1/1	0.94	0.18	-1.41	42,42,42,42	0
56	MG	2a	3108	1/1	0.79	0.09	-1.44	62,62,62,62	0
56	MG	1Q	3004	1/1	0.98	0.18	-1.45	39,39,39,39	0
56	MG	2a	3191	1/1	0.85	0.12	-1.46	54,54,54,54	0
56	MG	1A	3589	1/1	0.96	0.20	-1.46	29,29,29,29	0
56	MG	1A	3767	1/1	0.93	0.20	-1.46	40,40,40,40	0
56	MG	2A	3299	1/1	0.87	0.17	-1.47	46,46,46,46	0
56	MG	2a	3153	1/1	0.81	0.11	-1.51	67,67,67,67	0
56	MG	1A	3196	1/1	0.97	0.20	-1.51	25,25,25,25	0
56	MG	2A	3306	1/1	0.87	0.19	-1.52	48,48,48,48	0
56	MG	1n	502	1/1	0.83	0.24	-1.53	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
56	MG	2a	3048	1/1	0.94	0.17	-1.53	80,80,80,80	0
56	MG	2A	3067	1/1	0.89	0.18	-1.57	52,52,52,52	0
56	MG	2A	3338	1/1	0.93	0.14	-1.65	56,56,56,56	0
57	ZN	1n	501	1/1	0.92	0.11	-1.66	84,84,84,84	0
56	MG	2A	3168	1/1	0.94	0.20	-1.67	47,47,47,47	0
56	MG	2A	3296	1/1	0.96	0.18	-1.69	45,45,45,45	0
56	MG	2A	3301	1/1	0.82	0.15	-1.69	38,38,38,38	0
56	MG	1a	1738	1/1	0.95	0.12	-1.69	64,64,64,64	0
56	MG	2a	3104	1/1	0.86	0.14	-1.70	62,62,62,62	0
56	MG	2A	3184	1/1	0.89	0.19	-1.70	39,39,39,39	0
56	MG	2A	3370	1/1	0.97	0.15	-1.74	44,44,44,44	0
56	MG	1a	1873	1/1	0.72	0.09	-1.76	52,52,52,52	0
56	MG	2a	3034	1/1	0.91	0.17	-1.77	59,59,59,59	0
56	MG	1a	1604	1/1	0.93	0.12	-1.77	69,69,69,69	0
56	MG	1b	3001	1/1	0.85	0.11	-1.79	83,83,83,83	0
56	MG	1A	3233	1/1	0.87	0.19	-1.80	34,34,34,34	0
56	MG	2A	3337	1/1	0.92	0.18	-1.81	46,46,46,46	0
56	MG	2A	3481	1/1	0.97	0.15	-1.82	50,50,50,50	0
56	MG	1A	3935	1/1	0.96	0.19	-1.83	28,28,28,28	0
56	MG	2A	3054	1/1	0.95	0.15	-1.83	49,49,49,49	0
56	MG	2A	3070	1/1	0.94	0.17	-1.88	32,32,32,32	0
56	MG	2Q	3003	1/1	0.95	0.14	-1.89	41,41,41,41	0
56	MG	2a	3076	1/1	0.97	0.16	-1.90	83,83,83,83	0
56	MG	1A	4015	1/1	0.90	0.20	-1.92	15,15,15,15	0
56	MG	1A	3159	1/1	0.97	0.16	-1.93	35,35,35,35	0
56	MG	1a	1664	1/1	0.96	0.12	-1.93	61,61,61,61	0
56	MG	2A	3164	1/1	0.90	0.15	-1.94	64,64,64,64	0
56	MG	2a	3099	1/1	0.92	0.16	-1.96	35,35,35,35	0
56	MG	2A	3208	1/1	0.96	0.13	-1.99	40,40,40,40	0
56	MG	1G	3001	1/1	0.87	0.17	-2.01	48,48,48,48	0
56	MG	1a	1709	1/1	0.92	0.16	-2.03	43,43,43,43	0
56	MG	1a	1815	1/1	0.99	0.10	-2.03	58,58,58,58	0
56	MG	2a	3082	1/1	0.85	0.13	-2.06	61,61,61,61	0
56	MG	2A	3401	1/1	0.69	0.13	-2.07	48,48,48,48	0
56	MG	2F	306	1/1	0.94	0.11	-2.08	40,40,40,40	0
56	MG	2A	3500	1/1	0.98	0.12	-2.14	49,49,49,49	0
56	MG	1t	3001	1/1	0.81	0.13	-2.16	54,54,54,54	0
56	MG	1A	3033	1/1	0.83	0.13	-2.17	57,57,57,57	0
56	MG	1A	3539	1/1	0.86	0.22	-2.17	44,44,44,44	0
56	MG	1r	3001	1/1	0.80	0.15	-2.18	69,69,69,69	0
56	MG	1A	3282	1/1	0.95	0.17	-2.22	52,52,52,52	0
56	MG	1A	3501	1/1	0.95	0.18	-2.23	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
56	MG	10	101	1/1	0.80	0.14	-2.23	61,61,61,61	0
56	MG	2A	3133	1/1	0.94	0.12	-2.23	52,52,52,52	0
56	MG	1A	3054	1/1	0.85	0.18	-2.24	47,47,47,47	0
56	MG	2a	3131	1/1	0.96	0.17	-2.28	44,44,44,44	0
56	MG	1a	1789	1/1	0.97	0.08	-2.30	66,66,66,66	0
56	MG	1A	3819	1/1	0.93	0.10	-2.32	82,82,82,82	0
56	MG	2A	3395	1/1	0.87	0.18	-2.36	33,33,33,33	0
56	MG	1A	3150	1/1	0.86	0.15	-2.37	34,34,34,34	0
56	MG	2A	3547	1/1	0.90	0.15	-2.37	22,22,22,22	0
56	MG	1a	1872	1/1	0.92	0.10	-2.37	53,53,53,53	0
56	MG	1A	3775	1/1	0.99	0.17	-2.41	14,14,14,14	0
56	MG	2l	201	1/1	0.76	0.10	-2.42	63,63,63,63	0
56	MG	2D	305	1/1	0.98	0.14	-2.42	28,28,28,28	0
56	MG	1a	1671	1/1	0.91	0.18	-2.42	38,38,38,38	0
56	MG	1a	1822	1/1	0.80	0.15	-2.42	52,52,52,52	0
56	MG	1a	1874	1/1	0.94	0.07	-2.43	61,61,61,61	0
56	MG	2A	3173	1/1	0.88	0.12	-2.45	52,52,52,52	0
56	MG	2a	3066	1/1	0.90	0.09	-2.46	84,84,84,84	0
56	MG	1A	3734	1/1	0.87	0.21	-2.46	38,38,38,38	0
56	MG	2A	3154	1/1	0.96	0.16	-2.47	32,32,32,32	0
56	MG	2A	3553	1/1	0.91	0.12	-2.47	44,44,44,44	0
56	MG	1a	1728	1/1	0.97	0.13	-2.48	53,53,53,53	0
56	MG	2A	3196	1/1	0.98	0.17	-2.49	35,35,35,35	0
56	MG	1A	3704	1/1	0.79	0.18	-2.59	18,18,18,18	0
56	MG	1A	3612	1/1	0.89	0.16	-2.61	55,55,55,55	0
56	MG	2a	3116	1/1	0.74	0.12	-2.62	62,62,62,62	0
56	MG	2A	3297	1/1	0.92	0.11	-2.62	58,58,58,58	0
56	MG	1a	1687	1/1	0.91	0.16	-2.63	46,46,46,46	0
56	MG	1A	3385	1/1	0.77	0.20	-2.63	59,59,59,59	0
56	MG	2A	3548	1/1	0.91	0.11	-2.63	40,40,40,40	0
56	MG	28	8001	1/1	0.95	0.16	-2.64	54,54,54,54	0
56	MG	1A	4014	1/1	0.99	0.16	-2.64	43,43,43,43	0
56	MG	1a	1847	1/1	0.99	0.10	-2.66	53,53,53,53	0
56	MG	1a	1824	1/1	0.98	0.16	-2.68	52,52,52,52	0
56	MG	1A	3885	1/1	0.96	0.17	-2.69	53,53,53,53	0
56	MG	1A	3221	1/1	0.84	0.16	-2.69	37,37,37,37	0
56	MG	2a	3203	1/1	0.94	0.16	-2.70	69,69,69,69	0
56	MG	2A	3465	1/1	0.78	0.16	-2.70	31,31,31,31	0
56	MG	1A	3756	1/1	0.98	0.15	-2.70	51,51,51,51	0
56	MG	1A	3273	1/1	0.90	0.18	-2.71	36,36,36,36	0
56	MG	2a	3087	1/1	0.88	0.12	-2.71	55,55,55,55	0
56	MG	1B	221	1/1	0.79	0.17	-2.71	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3386	1/1	0.91	0.16	-2.72	30,30,30,30	0
56	MG	1A	3268	1/1	0.86	0.14	-2.72	55,55,55,55	0
56	MG	2A	3392	1/1	0.96	0.13	-2.74	28,28,28,28	0
56	MG	1A	3979	1/1	0.94	0.19	-2.74	49,49,49,49	0
56	MG	2A	3560	1/1	0.90	0.17	-2.75	31,31,31,31	0
56	MG	1A	3195	1/1	0.99	0.17	-2.76	33,33,33,33	0
56	MG	2A	3194	1/1	0.74	0.14	-2.78	44,44,44,44	0
56	MG	2A	3321	1/1	0.85	0.15	-2.78	35,35,35,35	0
56	MG	1A	3192	1/1	0.96	0.19	-2.82	35,35,35,35	0
56	MG	2A	3215	1/1	0.97	0.18	-2.83	39,39,39,39	0
56	MG	2x	3004	1/1	0.95	0.13	-2.85	42,42,42,42	0
56	MG	2A	3536	1/1	0.93	0.12	-2.89	38,38,38,38	0
56	MG	1A	3566	1/1	0.96	0.17	-2.90	23,23,23,23	0
56	MG	1A	3658	1/1	0.88	0.19	-2.91	18,18,18,18	0
56	MG	1A	3954	1/1	0.95	0.11	-2.91	51,51,51,51	0
56	MG	2a	3212	1/1	0.95	0.10	-2.92	54,54,54,54	0
56	MG	1A	3907	1/1	0.97	0.15	-2.93	15,15,15,15	0
56	MG	2A	3329	1/1	0.91	0.14	-2.93	37,37,37,37	0
56	MG	2A	3090	1/1	0.97	0.15	-2.94	45,45,45,45	0
56	MG	1a	1718	1/1	0.97	0.15	-2.95	48,48,48,48	0
56	MG	1A	3753	1/1	0.96	0.19	-2.95	68,68,68,68	0
56	MG	1A	3651	1/1	0.98	0.15	-2.95	21,21,21,21	0
56	MG	1A	3618	1/1	0.91	0.19	-2.98	18,18,18,18	0
56	MG	2F	305	1/1	0.84	0.12	-2.99	41,41,41,41	0
56	MG	1A	3551	1/1	0.95	0.20	-2.99	33,33,33,33	0
56	MG	1A	3608	1/1	0.94	0.19	-3.01	25,25,25,25	0
56	MG	2A	3112	1/1	0.85	0.13	-3.02	39,39,39,39	0
56	MG	2a	3208	1/1	0.95	0.13	-3.03	58,58,58,58	0
56	MG	1a	1677	1/1	0.74	0.12	-3.03	66,66,66,66	0
56	MG	2a	3244	1/1	0.94	0.17	-3.03	67,67,67,67	0
56	MG	1A	3750	1/1	0.91	0.15	-3.05	21,21,21,21	0
56	MG	1A	3615	1/1	0.88	0.18	-3.06	39,39,39,39	0
56	MG	2a	3077	1/1	0.78	0.11	-3.07	59,59,59,59	0
56	MG	1a	1755	1/1	0.92	0.09	-3.10	79,79,79,79	0
56	MG	1a	1635	1/1	0.94	0.16	-3.11	50,50,50,50	0
56	MG	2A	3212	1/1	0.94	0.15	-3.11	23,23,23,23	0
56	MG	2A	3428	1/1	0.93	0.14	-3.14	49,49,49,49	0
56	MG	2A	3552	1/1	0.95	0.11	-3.15	22,22,22,22	0
56	MG	2A	3320	1/1	0.93	0.14	-3.17	33,33,33,33	0
56	MG	1A	3989	1/1	0.95	0.13	-3.18	25,25,25,25	0
56	MG	2A	3335	1/1	0.97	0.17	-3.23	40,40,40,40	0
56	MG	2A	3317	1/1	0.92	0.15	-3.25	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
56	MG	1A	3790	1/1	0.97	0.18	-3.27	48,48,48,48	0
56	MG	2A	3206	1/1	0.93	0.12	-3.29	41,41,41,41	0
56	MG	2A	3189	1/1	0.93	0.13	-3.32	34,34,34,34	0
56	MG	2A	3534	1/1	0.98	0.09	-3.33	64,64,64,64	0
56	MG	1A	3722	1/1	0.89	0.19	-3.34	22,22,22,22	0
56	MG	2a	3183	1/1	0.98	0.14	-3.34	37,37,37,37	0
56	MG	2A	3058	1/1	0.94	0.16	-3.37	37,37,37,37	0
56	MG	1A	3606	1/1	0.79	0.19	-3.37	32,32,32,32	0
56	MG	1a	1684	1/1	0.94	0.10	-3.38	48,48,48,48	0
56	MG	2A	3359	1/1	0.94	0.12	-3.38	50,50,50,50	0
56	MG	2a	3193	1/1	0.97	0.12	-3.43	47,47,47,47	0
56	MG	1a	1724	1/1	0.84	0.09	-3.45	76,76,76,76	0
56	MG	1F	305	1/1	0.90	0.15	-3.49	44,44,44,44	0
56	MG	2A	3446	1/1	0.93	0.10	-3.50	42,42,42,42	0
56	MG	1A	3621	1/1	0.90	0.14	-3.53	18,18,18,18	0
56	MG	1X	101	1/1	0.96	0.18	-3.55	45,45,45,45	0
56	MG	1A	3893	1/1	0.95	0.18	-3.55	30,30,30,30	0
56	MG	1A	3727	1/1	0.95	0.19	-3.57	26,26,26,26	0
56	MG	1A	3280	1/1	0.90	0.14	-3.60	34,34,34,34	0
56	MG	1a	1715	1/1	0.95	0.07	-3.60	39,39,39,39	0
56	MG	1A	3780	1/1	0.63	0.14	-3.61	43,43,43,43	0
56	MG	2A	3052	1/1	0.99	0.14	-3.64	43,43,43,43	0
56	MG	1A	3565	1/1	0.94	0.18	-3.64	45,45,45,45	0
56	MG	2B	3006	1/1	0.93	0.09	-3.68	58,58,58,58	0
56	MG	1a	1666	1/1	0.90	0.11	-3.69	71,71,71,71	0
56	MG	1A	3733	1/1	0.93	0.13	-3.70	35,35,35,35	0
56	MG	2A	3369	1/1	0.83	0.15	-3.71	31,31,31,31	0
56	MG	1A	3193	1/1	0.94	0.16	-3.72	23,23,23,23	0
56	MG	1a	1716	1/1	0.99	0.08	-3.73	53,53,53,53	0
56	MG	1Q	3002	1/1	0.97	0.11	-3.74	44,44,44,44	0
56	MG	2a	3260	1/1	0.93	0.08	-3.74	72,72,72,72	0
56	MG	2A	3542	1/1	0.88	0.15	-3.75	42,42,42,42	0
56	MG	2A	3499	1/1	0.89	0.14	-3.77	47,47,47,47	0
56	MG	1A	3963	1/1	0.97	0.16	-3.78	14,14,14,14	0
56	MG	1a	1813	1/1	0.93	0.16	-3.81	59,59,59,59	0
56	MG	1A	3792	1/1	0.91	0.16	-3.82	79,79,79,79	0
56	MG	1A	3665	1/1	0.81	0.20	-3.89	22,22,22,22	0
56	MG	2a	3118	1/1	0.90	0.17	-3.91	38,38,38,38	0
56	MG	1A	3547	1/1	0.83	0.16	-3.93	54,54,54,54	0
56	MG	2f	3001	1/1	0.96	0.09	-3.97	59,59,59,59	0
56	MG	1A	3317	1/1	0.95	0.18	-3.97	34,34,34,34	0
56	MG	1A	3910	1/1	0.94	0.14	-3.99	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
56	MG	2A	3377	1/1	0.95	0.11	-4.01	43,43,43,43	0
56	MG	1A	3181	1/1	0.97	0.16	-4.02	24,24,24,24	0
56	MG	1A	3672	1/1	0.98	0.12	-4.05	13,13,13,13	0
56	MG	1A	3791	1/1	0.97	0.17	-4.09	20,20,20,20	0
56	MG	1A	3897	1/1	0.97	0.18	-4.09	29,29,29,29	0
56	MG	1A	3401	1/1	0.96	0.14	-4.14	46,46,46,46	0
56	MG	2a	3230	1/1	0.92	0.14	-4.16	50,50,50,50	0
56	MG	1A	3537	1/1	0.95	0.15	-4.16	32,32,32,32	0
56	MG	1A	3774	1/1	0.97	0.12	-4.22	20,20,20,20	0
56	MG	2A	3205	1/1	0.96	0.12	-4.22	51,51,51,51	0
56	MG	1A	3730	1/1	0.91	0.15	-4.23	30,30,30,30	0
56	MG	1a	1720	1/1	0.94	0.10	-4.23	50,50,50,50	0
56	MG	2A	3385	1/1	0.95	0.14	-4.26	35,35,35,35	0
56	MG	2a	3213	1/1	0.96	0.10	-4.26	67,67,67,67	0
56	MG	2A	3310	1/1	0.88	0.14	-4.27	31,31,31,31	0
56	MG	2A	3295	1/1	0.83	0.14	-4.27	48,48,48,48	0
56	MG	1A	4009	1/1	0.97	0.17	-4.28	56,56,56,56	0
56	MG	1A	3770	1/1	0.97	0.17	-4.30	36,36,36,36	0
56	MG	1A	3205	1/1	0.94	0.17	-4.31	41,41,41,41	0
56	MG	1A	3768	1/1	0.97	0.15	-4.32	10,10,10,10	0
56	MG	2A	3420	1/1	0.98	0.12	-4.33	53,53,53,53	0
56	MG	2A	3268	1/1	0.88	0.16	-4.35	55,55,55,55	0
56	MG	1a	1731	1/1	0.95	0.11	-4.41	57,57,57,57	0
56	MG	1E	305	1/1	0.93	0.14	-4.42	31,31,31,31	0
56	MG	1A	3309	1/1	0.97	0.10	-4.43	20,20,20,20	0
56	MG	2A	3531	1/1	0.95	0.09	-4.46	52,52,52,52	0
56	MG	1A	3999	1/1	0.89	0.14	-4.46	21,21,21,21	0
56	MG	1A	3327	1/1	0.80	0.13	-4.51	73,73,73,73	0
56	MG	2A	3502	1/1	0.89	0.13	-4.54	35,35,35,35	0
56	MG	2A	3429	1/1	0.90	0.12	-4.54	58,58,58,58	0
56	MG	1A	3822	1/1	0.78	0.15	-4.55	46,46,46,46	0
56	MG	1A	3761	1/1	0.93	0.10	-4.59	66,66,66,66	0
56	MG	1A	3597	1/1	0.93	0.12	-4.60	48,48,48,48	0
56	MG	2A	3126	1/1	0.80	0.11	-4.60	50,50,50,50	0
56	MG	2a	3142	1/1	0.96	0.14	-4.61	51,51,51,51	0
56	MG	1A	3604	1/1	0.97	0.14	-4.72	27,27,27,27	0
56	MG	2A	3324	1/1	0.95	0.12	-4.74	34,34,34,34	0
56	MG	1a	1697	1/1	0.94	0.10	-4.79	52,52,52,52	0
56	MG	2A	3115	1/1	0.93	0.13	-4.79	35,35,35,35	0
56	MG	1A	3933	1/1	0.93	0.13	-4.80	42,42,42,42	0
56	MG	1F	302	1/1	0.96	0.15	-4.85	51,51,51,51	0
56	MG	1D	307	1/1	0.95	0.13	-4.88	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1663	1/1	0.98	0.08	-4.88	76,76,76,76	0
56	MG	1a	1641	1/1	0.97	0.08	-4.90	55,55,55,55	0
56	MG	1a	1675	1/1	0.92	0.15	-4.92	56,56,56,56	0
56	MG	1A	3227	1/1	0.94	0.15	-4.93	41,41,41,41	0
56	MG	2A	3270	1/1	0.90	0.11	-4.94	45,45,45,45	0
56	MG	2a	3134	1/1	0.86	0.11	-4.94	59,59,59,59	0
56	MG	1A	3169	1/1	0.98	0.17	-4.94	21,21,21,21	0
56	MG	1A	3283	1/1	0.90	0.13	-4.96	44,44,44,44	0
56	MG	1A	3624	1/1	0.94	0.17	-4.99	18,18,18,18	0
56	MG	2A	3110	1/1	0.80	0.17	-4.99	45,45,45,45	0
56	MG	1A	3550	1/1	0.98	0.16	-5.03	33,33,33,33	0
56	MG	2A	3150	1/1	0.98	0.15	-5.05	30,30,30,30	0
56	MG	1A	3248	1/1	0.94	0.12	-5.07	26,26,26,26	0
56	MG	1A	3194	1/1	0.98	0.17	-5.07	32,32,32,32	0
56	MG	2a	3093	1/1	0.89	0.10	-5.11	50,50,50,50	0
56	MG	1A	3723	1/1	0.92	0.18	-5.16	8,8,8,8	0
56	MG	2A	3068	1/1	0.92	0.12	-5.26	39,39,39,39	0
56	MG	2A	3302	1/1	0.90	0.16	-5.26	41,41,41,41	0
56	MG	1A	3739	1/1	0.96	0.16	-5.27	30,30,30,30	0
56	MG	2a	3132	1/1	0.96	0.10	-5.28	65,65,65,65	0
56	MG	1a	1856	1/1	0.96	0.16	-5.29	43,43,43,43	0
56	MG	1A	3826	1/1	0.93	0.16	-5.36	37,37,37,37	0
56	MG	2A	3130	1/1	0.90	0.12	-5.39	39,39,39,39	0
56	MG	1A	3908	1/1	0.99	0.16	-5.42	40,40,40,40	0
56	MG	1a	1876	1/1	0.83	0.12	-5.43	80,80,80,80	0
56	MG	1A	3969	1/1	0.96	0.11	-5.43	18,18,18,18	0
56	MG	2A	3221	1/1	0.92	0.09	-5.43	47,47,47,47	0
56	MG	2A	3278	1/1	0.93	0.12	-5.44	31,31,31,31	0
56	MG	1A	3859	1/1	0.96	0.12	-5.50	24,24,24,24	0
56	MG	1A	3629	1/1	0.98	0.14	-5.51	27,27,27,27	0
56	MG	1A	3996	1/1	0.91	0.09	-5.54	40,40,40,40	0
56	MG	2A	3471	1/1	0.95	0.14	-5.57	34,34,34,34	0
56	MG	1A	3157	1/1	0.98	0.15	-5.67	28,28,28,28	0
56	MG	1a	1669	1/1	0.93	0.12	-5.70	46,46,46,46	0
56	MG	1A	3158	1/1	0.97	0.13	-5.73	24,24,24,24	0
56	MG	2a	3139	1/1	0.87	0.12	-5.74	70,70,70,70	0
56	MG	2a	3179	1/1	0.95	0.12	-5.75	49,49,49,49	0
56	MG	1A	3288	1/1	0.96	0.15	-5.76	40,40,40,40	0
56	MG	1A	3460	1/1	0.90	0.15	-5.78	36,36,36,36	0
56	MG	1A	3659	1/1	0.96	0.09	-5.80	23,23,23,23	0
56	MG	2A	3291	1/1	0.94	0.15	-5.81	36,36,36,36	0
56	MG	1A	3670	1/1	0.93	0.13	-5.89	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
56	MG	1A	3596	1/1	0.94	0.11	-5.91	49,49,49,49	0
56	MG	1A	3839	1/1	0.95	0.14	-5.92	40,40,40,40	0
56	MG	2A	3518	1/1	0.96	0.11	-5.96	42,42,42,42	0
56	MG	2A	3519	1/1	0.97	0.06	-5.97	45,45,45,45	0
56	MG	1A	3622	1/1	0.97	0.13	-6.00	22,22,22,22	0
56	MG	1A	3535	1/1	0.95	0.11	-6.01	41,41,41,41	0
56	MG	2A	3263	1/1	0.95	0.09	-6.08	56,56,56,56	0
56	MG	2a	3049	1/1	0.90	0.10	-6.09	64,64,64,64	0
56	MG	1A	3559	1/1	0.97	0.14	-6.21	51,51,51,51	0
56	MG	2A	3442	1/1	0.92	0.11	-6.25	50,50,50,50	0
56	MG	1A	3616	1/1	0.93	0.14	-6.25	22,22,22,22	0
56	MG	2A	3283	1/1	0.94	0.11	-6.28	48,48,48,48	0
56	MG	1A	3611	1/1	0.91	0.11	-6.28	58,58,58,58	0
56	MG	2A	3051	1/1	0.95	0.10	-6.29	40,40,40,40	0
56	MG	1A	3626	1/1	0.95	0.16	-6.33	25,25,25,25	0
56	MG	1A	3906	1/1	0.93	0.16	-6.44	49,49,49,49	0
56	MG	2A	3273	1/1	0.88	0.06	-6.44	41,41,41,41	0
56	MG	1A	3546	1/1	0.97	0.19	-6.45	36,36,36,36	0
56	MG	2A	3344	1/1	0.97	0.14	-6.54	39,39,39,39	0
56	MG	1A	3811	1/1	0.93	0.09	-6.55	39,39,39,39	0
56	MG	1A	3694	1/1	0.99	0.13	-6.58	16,16,16,16	0
56	MG	1a	1607	1/1	0.85	0.10	-6.72	78,78,78,78	0
56	MG	2A	3351	1/1	0.99	0.11	-6.75	37,37,37,37	0
56	MG	1a	1691	1/1	0.88	0.12	-6.83	27,27,27,27	0
56	MG	1A	3610	1/1	0.79	0.10	-6.83	37,37,37,37	0
56	MG	2A	3062	1/1	0.95	0.10	-6.86	39,39,39,39	0
56	MG	1A	3922	1/1	0.97	0.13	-6.86	19,19,19,19	0
56	MG	1A	3581	1/1	0.96	0.10	-6.88	37,37,37,37	0
56	MG	1A	3263	1/1	0.89	0.14	-6.90	37,37,37,37	0
56	MG	1A	3293	1/1	0.95	0.13	-6.98	27,27,27,27	0
56	MG	1a	1752	1/1	0.97	0.06	-6.98	72,72,72,72	0
56	MG	1B	210	1/1	0.95	0.14	-7.03	49,49,49,49	0
56	MG	1a	1808	1/1	0.95	0.11	-7.08	52,52,52,52	0
56	MG	2A	3345	1/1	0.97	0.12	-7.12	35,35,35,35	0
56	MG	2A	3421	1/1	0.98	0.09	-7.13	59,59,59,59	0
56	MG	1A	3681	1/1	0.98	0.13	-7.16	14,14,14,14	0
56	MG	1a	1871	1/1	0.91	0.11	-7.17	46,46,46,46	0
56	MG	2A	3460	1/1	0.70	0.10	-7.17	54,54,54,54	0
56	MG	1a	1632	1/1	0.97	0.13	-7.17	41,41,41,41	0
56	MG	2A	3099	1/1	0.97	0.10	-7.19	30,30,30,30	0
56	MG	1A	3679	1/1	0.95	0.13	-7.26	25,25,25,25	0
56	MG	1A	3874	1/1	0.88	0.16	-7.29	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
56	MG	1A	3825	1/1	0.96	0.12	-7.32	30,30,30,30	0
56	MG	1A	3793	1/1	0.93	0.10	-7.43	40,40,40,40	0
56	MG	2a	3090	1/1	0.93	0.10	-7.45	42,42,42,42	0
56	MG	2A	3487	1/1	0.90	0.08	-7.51	32,32,32,32	0
56	MG	1A	3161	1/1	0.96	0.09	-7.60	33,33,33,33	0
56	MG	1A	3336	1/1	0.93	0.14	-7.83	49,49,49,49	0
56	MG	1A	3639	1/1	0.93	0.12	-7.98	25,25,25,25	0
56	MG	1a	1603	1/1	0.95	0.09	-8.01	57,57,57,57	0
56	MG	1A	3151	1/1	0.94	0.08	-8.23	47,47,47,47	0
56	MG	2a	3251	1/1	0.90	0.08	-8.24	57,57,57,57	0
56	MG	1A	3676	1/1	0.88	0.16	-8.25	50,50,50,50	0
56	MG	1B	218	1/1	0.95	0.12	-8.30	39,39,39,39	0
56	MG	1A	3660	1/1	0.97	0.10	-8.35	11,11,11,11	0
56	MG	20	8001	1/1	0.92	0.08	-8.52	65,65,65,65	0
56	MG	1A	3749	1/1	0.92	0.12	-8.52	27,27,27,27	0
56	MG	1A	3217	1/1	0.94	0.12	-8.55	42,42,42,42	0
56	MG	1A	3576	1/1	0.98	0.12	-8.58	19,19,19,19	0
56	MG	1A	3553	1/1	0.99	0.14	-8.65	44,44,44,44	0
56	MG	1A	3190	1/1	0.95	0.15	-8.79	44,44,44,44	0
56	MG	1A	3803	1/1	0.96	0.08	-9.12	29,29,29,29	0
56	MG	1B	220	1/1	0.92	0.14	-9.38	70,70,70,70	0
56	MG	1A	3900	1/1	0.93	0.11	-9.46	66,66,66,66	0
56	MG	2A	3485	1/1	0.90	0.13	-9.70	38,38,38,38	0
56	MG	1A	3262	1/1	0.85	0.06	-9.86	66,66,66,66	0
56	MG	1A	3648	1/1	0.83	0.13	-9.99	20,20,20,20	0
56	MG	1A	3569	1/1	0.93	0.07	-10.32	45,45,45,45	0
56	MG	2a	3103	1/1	0.93	0.12	-10.37	69,69,69,69	0
56	MG	1A	3631	1/1	0.94	0.12	-10.54	19,19,19,19	0
56	MG	1A	3978	1/1	0.95	0.12	-10.93	29,29,29,29	0
56	MG	1a	1700	1/1	0.94	0.10	-10.94	36,36,36,36	0
56	MG	1A	3275	1/1	0.94	0.09	-10.97	25,25,25,25	0
56	MG	1A	3872	1/1	0.92	0.12	-11.13	28,28,28,28	0
56	MG	1A	3757	1/1	0.85	0.11	-11.42	39,39,39,39	0
56	MG	1A	3690	1/1	0.98	0.15	-11.74	48,48,48,48	0
56	MG	1A	3752	1/1	0.95	0.10	-11.96	50,50,50,50	0
56	MG	1A	3643	1/1	0.95	0.13	-12.02	19,19,19,19	0
56	MG	1A	3056	1/1	0.93	0.12	-12.05	62,62,62,62	0
56	MG	1A	3716	1/1	0.96	0.12	-12.19	43,43,43,43	0
56	MG	1A	3789	1/1	0.96	0.08	-12.81	26,26,26,26	0
56	MG	1A	3294	1/1	0.92	0.10	-13.29	23,23,23,23	0
56	MG	1A	3561	1/1	0.97	0.10	-13.90	44,44,44,44	0
56	MG	2A	3406	1/1	0.96	0.07	-15.50	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1661	1/1	0.94	0.09	-16.18	15,15,15,15	0
56	MG	1A	3271	1/1	0.97	0.08	-16.19	17,17,17,17	0
56	MG	1A	3602	1/1	0.93	0.10	-16.32	45,45,45,45	0
56	MG	2A	3163	1/1	0.98	0.08	-21.60	33,33,33,33	0
56	MG	1A	3541	1/1	0.91	0.07	-26.45	48,48,48,48	0
56	MG	2A	3011	1/1	0.75	0.35	-	61,61,61,61	0
56	MG	1A	3156	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	1a	1775	1/1	0.81	0.35	-	80,80,80,80	0
56	MG	1A	3745	1/1	0.85	0.68	-	71,71,71,71	0
56	MG	1a	1865	1/1	0.91	0.17	-	69,69,69,69	0
56	MG	1A	3045	1/1	0.89	0.10	-	70,70,70,70	0
56	MG	2A	3475	1/1	0.94	0.18	-	35,35,35,35	0
56	MG	2A	3342	1/1	0.79	0.26	-	63,63,63,63	0
56	MG	1A	3136	1/1	0.92	0.16	-	60,60,60,60	0
56	MG	2A	3148	1/1	0.83	0.26	-	63,63,63,63	0
56	MG	1A	3871	1/1	0.91	0.26	-	60,60,60,60	0
56	MG	1A	3710	1/1	0.97	0.24	-	39,39,39,39	0
56	MG	1A	3113	1/1	0.92	0.14	-	63,63,63,63	0
56	MG	2A	3236	1/1	0.83	0.06	-	91,91,91,91	0
56	MG	1A	3592	1/1	0.96	0.26	-	47,47,47,47	0
56	MG	1a	1746	1/1	0.95	0.23	-	55,55,55,55	0
56	MG	2F	301	1/1	0.93	0.11	-	57,57,57,57	0
56	MG	2A	3135	1/1	0.91	0.13	-	61,61,61,61	0
56	MG	2A	3219	1/1	0.90	0.30	-	44,44,44,44	0
56	MG	1A	3965	1/1	0.87	0.43	-	53,53,53,53	0
56	MG	1A	3357	1/1	0.70	0.21	-	68,68,68,68	0
56	MG	2A	3549	1/1	0.97	0.27	-	43,43,43,43	0
56	MG	1a	1809	1/1	0.94	0.18	-	62,62,62,62	0
56	MG	1A	3542	1/1	0.87	0.15	-	26,26,26,26	0
56	MG	1A	3837	1/1	0.93	0.08	-	62,62,62,62	0
56	MG	2a	3015	1/1	0.80	0.15	-	67,67,67,67	0
56	MG	1a	1605	1/1	0.96	0.13	-	55,55,55,55	0
56	MG	1A	3960	1/1	0.94	0.67	-	53,53,53,53	0
56	MG	1A	3974	1/1	0.91	0.12	-	30,30,30,30	0
56	MG	1A	3720	1/1	0.97	0.10	-	45,45,45,45	0
56	MG	2a	3130	1/1	0.98	0.08	-	43,43,43,43	0
56	MG	1A	3423	1/1	0.90	0.22	-	57,57,57,57	0
56	MG	2a	3165	1/1	0.93	0.15	-	52,52,52,52	0
56	MG	1A	3122	1/1	0.93	0.23	-	58,58,58,58	0
56	MG	2a	3055	1/1	0.90	0.05	-	98,98,98,98	0
56	MG	2A	3180	1/1	0.92	0.09	-	37,37,37,37	0
56	MG	2A	3095	1/1	0.95	0.19	-	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
56	MG	1A	3759	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	1A	3834	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	2A	3443	1/1	0.48	0.23	-	56,56,56,56	0
56	MG	2a	3125	1/1	0.81	0.11	-	60,60,60,60	0
56	MG	1A	3005	1/1	0.80	0.24	-	58,58,58,58	0
56	MG	2A	3527	1/1	0.91	0.26	-	51,51,51,51	0
56	MG	1A	3098	1/1	0.87	0.18	-	52,52,52,52	0
56	MG	1a	1863	1/1	0.95	0.11	-	51,51,51,51	0
56	MG	1A	3375	1/1	0.91	0.62	-	51,51,51,51	0
56	MG	1A	3032	1/1	0.61	0.16	-	63,63,63,63	0
56	MG	1A	3290	1/1	0.80	0.51	-	37,37,37,37	0
56	MG	2A	3473	1/1	0.81	0.14	-	64,64,64,64	0
56	MG	2A	3239	1/1	0.84	0.11	-	60,60,60,60	0
56	MG	1a	1828	1/1	0.83	0.11	-	61,61,61,61	0
56	MG	1A	3035	1/1	0.67	0.67	-	53,53,53,53	0
56	MG	1A	3012	1/1	0.94	0.21	-	47,47,47,47	0
56	MG	2a	3035	1/1	0.85	0.10	-	69,69,69,69	0
56	MG	2A	3031	1/1	0.82	0.15	-	51,51,51,51	0
56	MG	2a	3078	1/1	0.96	0.14	-	47,47,47,47	0
56	MG	2A	3325	1/1	0.93	0.18	-	52,52,52,52	0
56	MG	2a	3033	1/1	0.98	0.41	-	53,53,53,53	0
56	MG	2A	3388	1/1	0.79	0.21	-	45,45,45,45	0
56	MG	1A	3719	1/1	0.97	0.13	-	38,38,38,38	0
56	MG	2A	3279	1/1	0.93	0.12	-	62,62,62,62	0
56	MG	2a	3147	1/1	0.95	0.08	-	73,73,73,73	0
56	MG	1A	3695	1/1	0.95	0.23	-	41,41,41,41	0
56	MG	1x	108	1/1	0.88	0.14	-	70,70,70,70	0
56	MG	2a	3140	1/1	0.93	0.08	-	63,63,63,63	0
56	MG	2a	3189	1/1	0.90	0.21	-	51,51,51,51	0
56	MG	1a	1682	1/1	0.92	0.12	-	46,46,46,46	0
56	MG	1a	1771	1/1	0.82	0.16	-	63,63,63,63	0
56	MG	1A	3350	1/1	0.89	0.14	-	54,54,54,54	0
56	MG	2A	3049	1/1	0.82	0.14	-	52,52,52,52	0
56	MG	1a	1791	1/1	0.90	0.07	-	99,99,99,99	0
56	MG	1D	305	1/1	0.92	0.28	-	39,39,39,39	0
56	MG	1A	3089	1/1	0.91	0.45	-	55,55,55,55	0
56	MG	2A	3414	1/1	0.94	0.07	-	49,49,49,49	0
56	MG	1A	3024	1/1	0.84	0.20	-	63,63,63,63	0
56	MG	2A	3002	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	1B	209	1/1	0.84	0.32	-	62,62,62,62	0
56	MG	1a	1616	1/1	0.94	0.27	-	74,74,74,74	0
56	MG	2A	3444	1/1	0.99	0.21	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	214	1/1	0.92	0.08	-	68,68,68,68	0
56	MG	1B	208	1/1	0.87	0.25	-	56,56,56,56	0
56	MG	1a	1844	1/1	0.97	0.10	-	43,43,43,43	0
56	MG	1A	3609	1/1	0.92	0.17	-	22,22,22,22	0
56	MG	1A	3832	1/1	0.91	0.11	-	57,57,57,57	0
56	MG	19	102	1/1	0.94	0.13	-	51,51,51,51	0
56	MG	2A	3435	1/1	0.94	0.07	-	53,53,53,53	0
56	MG	2A	3526	1/1	0.97	0.09	-	49,49,49,49	0
56	MG	1A	3020	1/1	0.89	0.13	-	54,54,54,54	0
56	MG	1A	3865	1/1	0.85	0.25	-	68,68,68,68	0
56	MG	2A	3020	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	2a	3196	1/1	0.92	0.17	-	90,90,90,90	0
56	MG	1A	3414	1/1	0.93	0.11	-	65,65,65,65	0
56	MG	1A	3988	1/1	0.91	0.74	-	45,45,45,45	0
56	MG	1A	3476	1/1	0.95	0.23	-	53,53,53,53	0
56	MG	2a	3058	1/1	0.80	0.17	-	87,87,87,87	0
56	MG	1A	3453	1/1	0.96	0.17	-	18,18,18,18	0
56	MG	1A	3077	1/1	0.86	0.24	-	69,69,69,69	0
56	MG	2A	3394	1/1	0.97	0.22	-	54,54,54,54	0
56	MG	2A	3026	1/1	0.92	0.17	-	51,51,51,51	0
56	MG	1A	3507	1/1	0.89	0.89	-	64,64,64,64	0
56	MG	1A	3139	1/1	0.93	0.41	-	41,41,41,41	0
56	MG	2A	3340	1/1	0.94	0.16	-	56,56,56,56	0
56	MG	1A	3101	1/1	0.86	0.29	-	55,55,55,55	0
56	MG	1a	1727	1/1	0.88	0.13	-	54,54,54,54	0
56	MG	1a	1774	1/1	0.94	0.09	-	76,76,76,76	0
56	MG	2a	3158	1/1	0.84	0.11	-	74,74,74,74	0
56	MG	1A	3855	1/1	0.83	0.19	-	84,84,84,84	0
56	MG	1A	3061	1/1	0.94	0.17	-	44,44,44,44	0
56	MG	1A	3244	1/1	0.96	0.12	-	67,67,67,67	0
56	MG	1A	3878	1/1	0.87	0.19	-	43,43,43,43	0
56	MG	1A	3876	1/1	0.89	0.22	-	79,79,79,79	0
56	MG	1A	3482	1/1	0.82	0.18	-	48,48,48,48	0
56	MG	2a	3052	1/1	0.81	0.08	-	95,95,95,95	0
56	MG	2A	3264	1/1	0.87	0.10	-	64,64,64,64	0
56	MG	1A	3049	1/1	0.93	0.28	-	48,48,48,48	0
56	MG	1A	3047	1/1	0.92	0.17	-	67,67,67,67	0
56	MG	2a	3240	1/1	0.87	0.23	-	81,81,81,81	0
56	MG	2a	3135	1/1	0.89	0.11	-	60,60,60,60	0
56	MG	2a	3071	1/1	0.93	0.30	-	59,59,59,59	0
56	MG	1A	3118	1/1	0.84	0.15	-	68,68,68,68	0
56	MG	1G	3002	1/1	0.84	0.15	-	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
56	MG	2h	3001	1/1	0.90	0.15	-	62,62,62,62	0
56	MG	2A	3372	1/1	0.97	0.18	-	45,45,45,45	0
56	MG	1A	3896	1/1	0.91	0.18	-	19,19,19,19	0
56	MG	1A	3633	1/1	0.89	0.22	-	71,71,71,71	0
56	MG	2a	3253	1/1	0.95	0.31	-	56,56,56,56	0
56	MG	2a	3210	1/1	0.81	0.11	-	62,62,62,62	0
56	MG	1A	3216	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	2a	3143	1/1	0.95	0.20	-	88,88,88,88	0
56	MG	1A	3094	1/1	0.93	0.33	-	51,51,51,51	0
56	MG	1A	3088	1/1	0.98	0.44	-	60,60,60,60	0
56	MG	1A	3276	1/1	0.91	0.28	-	38,38,38,38	0
56	MG	2a	3010	1/1	0.91	0.12	-	74,74,74,74	0
56	MG	1A	3255	1/1	0.90	0.12	-	58,58,58,58	0
56	MG	1A	3781	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	2A	3566	1/1	0.97	0.11	-	62,62,62,62	0
56	MG	1a	1816	1/1	0.97	0.12	-	40,40,40,40	0
56	MG	1a	1723	1/1	0.77	0.16	-	85,85,85,85	0
56	MG	1A	3123	1/1	0.88	0.19	-	44,44,44,44	0
56	MG	2A	3089	1/1	0.94	0.18	-	40,40,40,40	0
56	MG	1A	3701	1/1	0.96	0.09	-	68,68,68,68	0
56	MG	2k	8001	1/1	0.97	0.05	-	83,83,83,83	0
56	MG	1a	1734	1/1	0.95	0.10	-	45,45,45,45	0
56	MG	2A	3014	1/1	0.93	0.06	-	66,66,66,66	0
56	MG	1A	3947	1/1	0.93	0.36	-	43,43,43,43	0
56	MG	1a	1681	1/1	0.94	0.06	-	55,55,55,55	0
56	MG	1A	3055	1/1	0.95	0.65	-	59,59,59,59	0
56	MG	1A	3738	1/1	0.91	0.17	-	37,37,37,37	0
56	MG	2z	101	1/1	0.96	0.68	-	54,54,54,54	0
56	MG	1H	8001	1/1	0.85	0.09	-	58,58,58,58	0
56	MG	2A	3367	1/1	0.93	0.17	-	50,50,50,50	0
56	MG	2A	3424	1/1	0.96	0.14	-	80,80,80,80	0
56	MG	1a	1802	1/1	0.82	0.13	-	76,76,76,76	0
56	MG	1A	3247	1/1	0.97	0.61	-	43,43,43,43	0
56	MG	2A	3494	1/1	0.95	0.10	-	56,56,56,56	0
56	MG	1A	3155	1/1	0.97	0.19	-	37,37,37,37	0
56	MG	1A	3345	1/1	0.92	0.09	-	60,60,60,60	0
56	MG	2a	3155	1/1	0.90	0.10	-	79,79,79,79	0
56	MG	2A	3521	1/1	0.94	0.16	-	44,44,44,44	0
56	MG	2a	3164	1/1	0.91	0.10	-	82,82,82,82	0
56	MG	2A	3450	1/1	0.91	0.08	-	62,62,62,62	0
56	MG	1A	3175	1/1	0.95	0.39	-	35,35,35,35	0
56	MG	1A	3620	1/1	0.98	0.11	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3765	1/1	0.91	0.10	-	44,44,44,44	0
56	MG	2A	3314	1/1	0.93	0.19	-	56,56,56,56	0
56	MG	2A	3012	1/1	0.94	0.24	-	53,53,53,53	0
56	MG	1A	3270	1/1	0.82	0.18	-	34,34,34,34	0
56	MG	2A	3528	1/1	0.94	0.25	-	49,49,49,49	0
56	MG	2a	3144	1/1	0.96	0.09	-	56,56,56,56	0
56	MG	1a	1679	1/1	0.89	0.20	-	57,57,57,57	0
56	MG	1A	3487	1/1	0.96	0.31	-	63,63,63,63	0
56	MG	1A	3976	1/1	0.93	0.28	-	69,69,69,69	0
56	MG	1A	3957	1/1	0.94	0.13	-	42,42,42,42	0
56	MG	1A	3590	1/1	0.96	0.06	-	47,47,47,47	0
56	MG	1A	3462	1/1	0.84	0.07	-	57,57,57,57	0
56	MG	2a	3019	1/1	0.93	0.11	-	73,73,73,73	0
56	MG	1A	3848	1/1	0.95	0.24	-	61,61,61,61	0
56	MG	1a	1741	1/1	0.84	0.14	-	63,63,63,63	0
56	MG	1Q	3001	1/1	0.90	0.29	-	38,38,38,38	0
56	MG	1A	3226	1/1	0.83	0.10	-	41,41,41,41	0
56	MG	1A	3396	1/1	0.81	0.24	-	67,67,67,67	0
56	MG	2a	3258	1/1	0.89	0.21	-	69,69,69,69	0
56	MG	2a	3032	1/1	0.90	0.22	-	50,50,50,50	0
56	MG	1A	3398	1/1	0.90	0.56	-	43,43,43,43	0
56	MG	1A	3016	1/1	0.96	0.23	-	61,61,61,61	0
56	MG	1A	3923	1/1	0.73	0.24	-	53,53,53,53	0
56	MG	1A	3545	1/1	0.90	0.17	-	17,17,17,17	0
56	MG	2A	3319	1/1	0.89	0.17	-	58,58,58,58	0
56	MG	1A	3773	1/1	0.94	0.27	-	80,80,80,80	0
56	MG	1a	1623	1/1	0.74	0.19	-	72,72,72,72	0
56	MG	2A	3379	1/1	0.97	0.09	-	42,42,42,42	0
56	MG	1a	1707	1/1	0.85	0.11	-	67,67,67,67	0
56	MG	1A	3771	1/1	0.92	0.49	-	71,71,71,71	0
56	MG	1a	1751	1/1	0.75	0.18	-	61,61,61,61	0
56	MG	1A	3387	1/1	0.88	1.26	-	56,56,56,56	0
56	MG	1a	1758	1/1	0.91	0.07	-	82,82,82,82	0
56	MG	2A	3039	1/1	0.80	0.20	-	49,49,49,49	0
56	MG	1A	3135	1/1	0.87	0.34	-	64,64,64,64	0
56	MG	2a	3243	1/1	0.95	0.10	-	67,67,67,67	0
56	MG	1B	203	1/1	0.90	0.21	-	61,61,61,61	0
56	MG	1a	1729	1/1	0.99	0.22	-	35,35,35,35	0
56	MG	2A	3466	1/1	0.99	0.15	-	69,69,69,69	0
56	MG	1A	3028	1/1	0.78	0.43	-	46,46,46,46	0
56	MG	2A	3226	1/1	0.94	0.21	-	57,57,57,57	0
56	MG	1A	3619	1/1	0.79	0.14	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1606	1/1	0.89	0.12	-	76,76,76,76	0
56	MG	1a	1811	1/1	0.94	0.14	-	55,55,55,55	0
56	MG	2A	3267	1/1	0.92	0.15	-	39,39,39,39	0
56	MG	2A	3478	1/1	0.96	0.16	-	44,44,44,44	0
56	MG	2a	3220	1/1	0.93	0.10	-	63,63,63,63	0
56	MG	1A	3812	1/1	0.96	0.07	-	51,51,51,51	0
56	MG	1A	3446	1/1	0.82	0.32	-	62,62,62,62	0
56	MG	2A	3162	1/1	0.85	0.25	-	50,50,50,50	0
56	MG	1A	3458	1/1	0.89	0.23	-	46,46,46,46	0
56	MG	2A	3336	1/1	0.89	0.12	-	36,36,36,36	0
56	MG	2A	3079	1/1	0.95	0.33	-	52,52,52,52	0
56	MG	1A	3393	1/1	0.94	0.50	-	52,52,52,52	0
56	MG	1A	3531	1/1	0.93	0.22	-	33,33,33,33	0
56	MG	2a	3122	1/1	0.97	0.18	-	72,72,72,72	0
56	MG	1A	3953	1/1	0.80	0.30	-	71,71,71,71	0
56	MG	1A	3977	1/1	0.72	0.57	-	53,53,53,53	0
56	MG	1A	3472	1/1	0.85	0.67	-	83,83,83,83	0
56	MG	2Q	3005	1/1	0.94	0.52	-	52,52,52,52	0
56	MG	1A	3391	1/1	0.92	0.17	-	35,35,35,35	0
56	MG	1A	3506	1/1	0.95	0.14	-	58,58,58,58	0
56	MG	1O	3002	1/1	0.95	0.21	-	46,46,46,46	0
56	MG	1A	3220	1/1	0.89	0.15	-	60,60,60,60	0
56	MG	2A	3094	1/1	0.89	0.25	-	46,46,46,46	0
56	MG	1l	201	1/1	0.90	0.14	-	58,58,58,58	0
56	MG	1A	3373	1/1	0.97	0.06	-	48,48,48,48	0
56	MG	2A	3159	1/1	0.93	0.18	-	37,37,37,37	0
56	MG	1a	1851	1/1	0.97	0.11	-	74,74,74,74	0
56	MG	1a	1797	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1a	1609	1/1	0.81	0.20	-	63,63,63,63	0
56	MG	1a	1647	1/1	0.94	0.19	-	56,56,56,56	0
56	MG	2A	3145	1/1	0.64	0.22	-	77,77,77,77	0
56	MG	1a	1820	1/1	0.90	0.14	-	54,54,54,54	0
56	MG	1a	1776	1/1	0.77	0.18	-	69,69,69,69	0
56	MG	1A	3699	1/1	0.88	0.12	-	47,47,47,47	0
56	MG	2A	3334	1/1	0.75	0.18	-	58,58,58,58	0
56	MG	2a	3177	1/1	0.96	0.06	-	44,44,44,44	0
56	MG	1A	3041	1/1	0.92	0.22	-	55,55,55,55	0
56	MG	2A	3037	1/1	0.94	0.07	-	46,46,46,46	0
56	MG	1a	1806	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	1A	3836	1/1	0.93	0.19	-	35,35,35,35	0
56	MG	1A	3316	1/1	0.95	0.26	-	48,48,48,48	0
56	MG	1A	3879	1/1	0.97	0.21	-	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
56	MG	1A	4001	1/1	0.88	0.81	-	43,43,43,43	0
56	MG	1a	1832	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	2A	3417	1/1	0.96	0.13	-	70,70,70,70	0
56	MG	1A	3277	1/1	0.93	0.87	-	48,48,48,48	0
56	MG	1A	3432	1/1	0.92	0.15	-	58,58,58,58	0
56	MG	2A	3438	1/1	0.97	0.18	-	62,62,62,62	0
56	MG	1A	3380	1/1	0.85	0.39	-	63,63,63,63	0
56	MG	1A	3689	1/1	0.94	0.12	-	55,55,55,55	0
56	MG	2A	3142	1/1	0.84	0.19	-	50,50,50,50	0
56	MG	1A	3485	1/1	0.93	0.13	-	55,55,55,55	0
56	MG	1A	3905	1/1	0.94	0.12	-	51,51,51,51	0
56	MG	2A	3457	1/1	0.98	0.12	-	45,45,45,45	0
56	MG	1A	3291	1/1	0.91	0.52	-	48,48,48,48	0
56	MG	2A	3201	1/1	0.90	0.12	-	47,47,47,47	0
56	MG	2A	3085	1/1	0.92	0.27	-	53,53,53,53	0
56	MG	2a	3127	1/1	0.95	0.18	-	61,61,61,61	0
56	MG	2a	3085	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	1A	3209	1/1	0.94	0.60	-	40,40,40,40	0
56	MG	2A	3129	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	1a	1852	1/1	0.92	0.13	-	70,70,70,70	0
56	MG	1A	3246	1/1	0.87	0.20	-	58,58,58,58	0
56	MG	2A	3004	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	2A	3210	1/1	0.30	0.17	-	63,63,63,63	0
56	MG	1A	3591	1/1	0.91	0.12	-	77,77,77,77	0
56	MG	1A	3742	1/1	0.95	0.20	-	35,35,35,35	0
56	MG	1A	3758	1/1	0.89	0.12	-	65,65,65,65	0
56	MG	1a	1794	1/1	0.90	0.16	-	67,67,67,67	0
56	MG	1A	3025	1/1	0.97	0.15	-	57,57,57,57	0
56	MG	1A	3071	1/1	0.97	0.18	-	44,44,44,44	0
56	MG	1A	3925	1/1	0.95	0.16	-	42,42,42,42	0
56	MG	1A	3909	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	1A	3845	1/1	0.89	0.12	-	42,42,42,42	0
56	MG	1A	3383	1/1	0.95	0.20	-	56,56,56,56	0
56	MG	2a	3133	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	1A	3053	1/1	0.92	0.22	-	53,53,53,53	0
56	MG	1A	3741	1/1	0.90	0.20	-	19,19,19,19	0
56	MG	1a	1753	1/1	0.94	0.08	-	70,70,70,70	0
56	MG	1A	3861	1/1	0.95	0.18	-	48,48,48,48	0
56	MG	1a	1689	1/1	0.83	0.11	-	65,65,65,65	0
56	MG	2A	3350	1/1	0.96	0.14	-	34,34,34,34	0
56	MG	1A	3478	1/1	0.91	0.39	-	65,65,65,65	0
56	MG	1a	1760	1/1	0.84	0.12	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3286	1/1	0.98	0.38	-	36,36,36,36	0
56	MG	1A	3264	1/1	0.93	0.39	-	38,38,38,38	0
56	MG	2A	3274	1/1	0.92	0.12	-	64,64,64,64	0
56	MG	2a	3185	1/1	0.56	0.16	-	67,67,67,67	0
56	MG	2A	3557	1/1	0.88	0.09	-	64,64,64,64	0
56	MG	1A	3429	1/1	0.48	0.32	-	70,70,70,70	0
56	MG	2A	3093	1/1	0.90	0.10	-	55,55,55,55	0
56	MG	1a	1818	1/1	0.95	0.16	-	63,63,63,63	0
56	MG	1A	3206	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	1A	3579	1/1	0.93	0.14	-	45,45,45,45	0
56	MG	1A	3185	1/1	0.86	0.10	-	41,41,41,41	0
56	MG	1A	3483	1/1	0.89	0.49	-	54,54,54,54	0
56	MG	1a	1849	1/1	0.86	0.10	-	53,53,53,53	0
56	MG	1A	3653	1/1	0.92	0.15	-	25,25,25,25	0
56	MG	2a	3238	1/1	0.87	0.15	-	55,55,55,55	0
56	MG	1a	1645	1/1	0.96	0.11	-	67,67,67,67	0
56	MG	1A	3829	1/1	0.95	0.26	-	55,55,55,55	0
56	MG	1a	1785	1/1	0.94	0.26	-	63,63,63,63	0
56	MG	2B	3007	1/1	0.83	0.24	-	56,56,56,56	0
56	MG	1A	3493	1/1	0.93	0.15	-	65,65,65,65	0
56	MG	2A	3124	1/1	0.92	0.25	-	54,54,54,54	0
56	MG	1a	1639	1/1	0.94	0.15	-	62,62,62,62	0
56	MG	1A	3296	1/1	0.70	0.18	-	55,55,55,55	0
56	MG	1A	3087	1/1	0.92	0.57	-	57,57,57,57	0
56	MG	1a	1798	1/1	0.93	0.10	-	71,71,71,71	0
56	MG	1A	3838	1/1	0.76	0.21	-	66,66,66,66	0
56	MG	2A	3216	1/1	0.86	0.44	-	45,45,45,45	0
56	MG	1A	3021	1/1	0.93	1.05	-	48,48,48,48	0
56	MG	1A	3367	1/1	0.85	0.11	-	66,66,66,66	0
56	MG	1A	3967	1/1	0.93	0.11	-	19,19,19,19	0
56	MG	1A	3928	1/1	0.91	0.09	-	62,62,62,62	0
56	MG	1A	3103	1/1	0.89	0.21	-	50,50,50,50	0
56	MG	1A	3564	1/1	0.82	0.19	-	35,35,35,35	0
56	MG	2A	3363	1/1	0.94	0.17	-	61,61,61,61	0
56	MG	1A	3555	1/1	0.89	0.13	-	46,46,46,46	0
56	MG	1A	3755	1/1	0.82	0.10	-	66,66,66,66	0
56	MG	1A	3496	1/1	0.96	0.13	-	88,88,88,88	0
56	MG	2A	3140	1/1	0.93	0.10	-	58,58,58,58	0
56	MG	1A	3684	1/1	0.93	0.11	-	50,50,50,50	0
56	MG	2A	3127	1/1	0.88	0.16	-	57,57,57,57	0
56	MG	1A	3530	1/1	0.94	0.26	-	51,51,51,51	0
56	MG	1A	3532	1/1	0.97	0.10	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3574	1/1	0.97	0.21	-	48,48,48,48	0
56	MG	1A	3249	1/1	0.90	0.25	-	42,42,42,42	0
56	MG	1A	3338	1/1	0.70	0.34	-	54,54,54,54	0
56	MG	1A	3764	1/1	0.97	0.16	-	41,41,41,41	0
56	MG	1A	3802	1/1	0.96	0.11	-	77,77,77,77	0
56	MG	2A	3493	1/1	0.82	0.23	-	58,58,58,58	0
56	MG	1A	3744	1/1	0.92	0.11	-	53,53,53,53	0
56	MG	1A	3696	1/1	0.95	0.12	-	65,65,65,65	0
56	MG	1A	3265	1/1	0.96	0.14	-	51,51,51,51	0
56	MG	1A	3433	1/1	0.73	0.14	-	71,71,71,71	0
56	MG	2A	3244	1/1	0.94	0.10	-	63,63,63,63	0
56	MG	1A	3894	1/1	0.90	0.10	-	41,41,41,41	0
56	MG	2a	3018	1/1	0.81	0.19	-	49,49,49,49	0
56	MG	2A	3153	1/1	0.94	0.17	-	33,33,33,33	0
56	MG	1A	3076	1/1	0.89	0.48	-	58,58,58,58	0
56	MG	1A	3779	1/1	0.85	0.27	-	54,54,54,54	0
56	MG	2a	3242	1/1	0.93	0.12	-	61,61,61,61	0
56	MG	2a	3205	1/1	0.86	0.22	-	74,74,74,74	0
56	MG	2A	3246	1/1	0.86	0.17	-	36,36,36,36	0
56	MG	1A	3332	1/1	0.86	0.11	-	55,55,55,55	0
56	MG	1A	3036	1/1	0.90	0.42	-	55,55,55,55	0
56	MG	2A	3413	1/1	0.97	0.23	-	62,62,62,62	0
56	MG	2a	3069	1/1	0.89	0.34	-	95,95,95,95	0
56	MG	2A	3409	1/1	0.96	0.16	-	50,50,50,50	0
56	MG	1A	3392	1/1	0.62	0.77	-	52,52,52,52	0
56	MG	2a	3115	1/1	0.92	0.14	-	54,54,54,54	0
56	MG	1A	3067	1/1	0.84	0.19	-	46,46,46,46	0
56	MG	1A	3434	1/1	0.82	0.20	-	70,70,70,70	0
56	MG	1A	3095	1/1	0.81	0.32	-	50,50,50,50	0
56	MG	1A	3662	1/1	0.95	0.28	-	44,44,44,44	0
56	MG	1A	3390	1/1	0.86	0.72	-	40,40,40,40	0
56	MG	1a	1646	1/1	0.90	0.15	-	57,57,57,57	0
56	MG	1A	3199	1/1	0.96	0.20	-	37,37,37,37	0
56	MG	1A	3365	1/1	0.87	0.24	-	46,46,46,46	0
56	MG	1A	3027	1/1	0.79	0.34	-	54,54,54,54	0
56	MG	2a	3150	1/1	0.97	0.18	-	51,51,51,51	0
56	MG	1A	3614	1/1	0.86	0.23	-	37,37,37,37	0
56	MG	1a	1721	1/1	0.84	0.13	-	59,59,59,59	0
56	MG	10	103	1/1	0.92	0.10	-	75,75,75,75	0
56	MG	1W	3002	1/1	0.80	0.20	-	55,55,55,55	0
56	MG	2A	3461	1/1	0.91	0.14	-	47,47,47,47	0
56	MG	1A	3200	1/1	0.88	0.12	-	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
56	MG	1A	3426	1/1	0.93	0.28	-	46,46,46,46	0
56	MG	2A	3121	1/1	0.96	0.18	-	32,32,32,32	0
56	MG	10	107	1/1	0.94	0.16	-	55,55,55,55	0
56	MG	2A	3015	1/1	0.91	0.22	-	52,52,52,52	0
56	MG	1A	3646	1/1	0.98	0.14	-	10,10,10,10	0
56	MG	2A	3358	1/1	0.82	0.27	-	59,59,59,59	0
56	MG	1a	1784	1/1	0.92	0.14	-	56,56,56,56	0
56	MG	1A	3445	1/1	0.69	0.29	-	63,63,63,63	0
56	MG	1A	3842	1/1	0.89	0.22	-	56,56,56,56	0
56	MG	1A	3295	1/1	0.92	0.18	-	50,50,50,50	0
56	MG	1B	206	1/1	0.98	0.26	-	46,46,46,46	0
56	MG	2A	3227	1/1	0.87	0.17	-	47,47,47,47	0
56	MG	2A	3515	1/1	0.70	0.09	-	63,63,63,63	0
56	MG	2a	3110	1/1	0.92	0.13	-	68,68,68,68	0
56	MG	2A	3080	1/1	0.90	0.16	-	48,48,48,48	0
56	MG	1A	3798	1/1	0.91	0.07	-	61,61,61,61	0
56	MG	2A	3479	1/1	0.94	0.38	-	50,50,50,50	0
56	MG	1A	3521	1/1	0.53	0.33	-	75,75,75,75	0
56	MG	1A	3174	1/1	0.98	0.66	-	37,37,37,37	0
56	MG	1A	3048	1/1	0.96	0.24	-	45,45,45,45	0
56	MG	1A	3344	1/1	0.89	0.10	-	72,72,72,72	0
56	MG	1A	3807	1/1	0.91	0.12	-	57,57,57,57	0
56	MG	2a	3256	1/1	0.77	0.13	-	94,94,94,94	0
56	MG	2a	3079	1/1	0.85	0.06	-	69,69,69,69	0
56	MG	1a	1750	1/1	0.84	0.38	-	64,64,64,64	0
56	MG	1A	3961	1/1	0.72	0.21	-	60,60,60,60	0
56	MG	1a	1869	1/1	0.89	0.16	-	64,64,64,64	0
56	MG	1A	3404	1/1	0.87	0.34	-	48,48,48,48	0
56	MG	2A	3366	1/1	0.98	0.20	-	69,69,69,69	0
56	MG	1A	3691	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	2a	3186	1/1	0.91	0.14	-	48,48,48,48	0
56	MG	2A	3354	1/1	0.92	0.11	-	63,63,63,63	0
56	MG	1A	3418	1/1	0.94	0.10	-	66,66,66,66	0
56	MG	1a	1829	1/1	0.96	0.24	-	47,47,47,47	0
56	MG	2A	3211	1/1	0.85	0.29	-	63,63,63,63	0
56	MG	1a	1867	1/1	0.91	0.11	-	80,80,80,80	0
56	MG	1A	3788	1/1	0.94	0.15	-	23,23,23,23	0
56	MG	2Z	3001	1/1	0.98	0.11	-	68,68,68,68	0
56	MG	2A	3256	1/1	0.86	0.15	-	34,34,34,34	0
56	MG	2A	3175	1/1	0.93	0.24	-	52,52,52,52	0
56	MG	1A	3623	1/1	0.97	0.25	-	25,25,25,25	0
56	MG	1A	3543	1/1	0.93	0.18	-	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
56	MG	1A	4016	1/1	0.93	0.47	-	37,37,37,37	0
56	MG	1F	303	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	1a	1617	1/1	0.82	0.30	-	78,78,78,78	0
56	MG	1a	1701	1/1	0.89	0.17	-	54,54,54,54	0
56	MG	2A	3285	1/1	0.96	0.19	-	39,39,39,39	0
56	MG	2A	3480	1/1	0.97	0.14	-	46,46,46,46	0
56	MG	2I	204	1/1	0.89	0.12	-	64,64,64,64	0
56	MG	1A	3514	1/1	0.90	0.18	-	53,53,53,53	0
56	MG	2A	3071	1/1	0.80	0.17	-	68,68,68,68	0
56	MG	1A	3866	1/1	0.96	0.15	-	37,37,37,37	0
56	MG	2A	3357	1/1	0.90	0.20	-	65,65,65,65	0
56	MG	1a	1836	1/1	0.92	0.16	-	41,41,41,41	0
56	MG	2a	3062	1/1	0.95	0.11	-	59,59,59,59	0
56	MG	1a	1841	1/1	0.91	0.18	-	64,64,64,64	0
56	MG	2A	3489	1/1	0.90	0.07	-	63,63,63,63	0
56	MG	1A	3144	1/1	0.89	0.36	-	54,54,54,54	0
56	MG	1A	3810	1/1	0.90	0.06	-	48,48,48,48	0
56	MG	2A	3535	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	1a	1712	1/1	0.97	0.16	-	25,25,25,25	0
56	MG	1A	3259	1/1	0.98	0.16	-	38,38,38,38	0
56	MG	1a	1840	1/1	0.95	0.20	-	41,41,41,41	0
56	MG	1a	1713	1/1	0.98	0.13	-	63,63,63,63	0
56	MG	2A	3469	1/1	0.93	0.11	-	51,51,51,51	0
56	MG	1A	3278	1/1	0.82	0.13	-	56,56,56,56	0
56	MG	1A	3732	1/1	0.93	0.22	-	45,45,45,45	0
56	MG	1A	3402	1/1	0.88	0.15	-	58,58,58,58	0
56	MG	2A	3213	1/1	0.68	0.15	-	59,59,59,59	0
56	MG	2A	3152	1/1	0.97	0.10	-	58,58,58,58	0
56	MG	1a	1800	1/1	0.83	0.18	-	57,57,57,57	0
56	MG	1a	1733	1/1	0.92	0.12	-	65,65,65,65	0
56	MG	2a	3235	1/1	0.61	0.15	-	68,68,68,68	0
56	MG	2A	3459	1/1	0.97	0.11	-	49,49,49,49	0
56	MG	1A	3070	1/1	0.65	0.17	-	72,72,72,72	0
56	MG	2a	3128	1/1	0.93	0.11	-	38,38,38,38	0
56	MG	2B	3005	1/1	0.92	0.16	-	53,53,53,53	0
56	MG	1a	1672	1/1	0.82	0.15	-	58,58,58,58	0
56	MG	2A	3426	1/1	0.94	0.12	-	62,62,62,62	0
56	MG	2B	3010	1/1	0.93	0.32	-	50,50,50,50	0
56	MG	2a	3247	1/1	0.92	0.11	-	71,71,71,71	0
56	MG	1a	1633	1/1	0.90	0.14	-	38,38,38,38	0
56	MG	2A	3390	1/1	0.93	0.18	-	56,56,56,56	0
56	MG	1A	3636	1/1	0.96	0.16	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1868	1/1	0.91	0.12	-	66,66,66,66	0
56	MG	1A	3323	1/1	0.90	0.36	-	58,58,58,58	0
56	MG	1A	3166	1/1	0.69	0.15	-	55,55,55,55	0
56	MG	1F	308	1/1	0.80	0.62	-	55,55,55,55	0
56	MG	1A	3841	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	1A	3938	1/1	0.96	0.18	-	44,44,44,44	0
56	MG	2F	304	1/1	0.73	0.24	-	53,53,53,53	0
56	MG	1A	3347	1/1	0.95	0.16	-	60,60,60,60	0
56	MG	1A	3835	1/1	0.98	0.10	-	66,66,66,66	0
56	MG	1A	3795	1/1	0.94	0.15	-	64,64,64,64	0
56	MG	1a	1630	1/1	0.87	0.28	-	56,56,56,56	0
56	MG	1A	3729	1/1	0.87	0.17	-	48,48,48,48	0
56	MG	1A	3498	1/1	0.71	0.37	-	67,67,67,67	0
56	MG	18	101	1/1	0.87	0.11	-	63,63,63,63	0
56	MG	1A	3668	1/1	0.85	0.12	-	60,60,60,60	0
56	MG	2a	3136	1/1	0.98	0.09	-	51,51,51,51	0
56	MG	1A	3058	1/1	0.97	0.12	-	50,50,50,50	0
56	MG	1A	3862	1/1	0.85	0.21	-	62,62,62,62	0
56	MG	1a	1803	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	2a	3029	1/1	0.87	0.28	-	69,69,69,69	0
56	MG	1a	1614	1/1	0.77	0.33	-	68,68,68,68	0
56	MG	2A	3257	1/1	0.75	0.19	-	62,62,62,62	0
56	MG	2A	3097	1/1	0.86	0.13	-	51,51,51,51	0
56	MG	2A	3445	1/1	0.64	0.16	-	71,71,71,71	0
56	MG	1A	3504	1/1	0.96	0.11	-	60,60,60,60	0
56	MG	2A	3030	1/1	0.88	0.09	-	50,50,50,50	0
56	MG	1A	3164	1/1	0.59	0.15	-	64,64,64,64	0
56	MG	2A	3289	1/1	0.91	0.20	-	58,58,58,58	0
56	MG	2a	3206	1/1	0.85	0.09	-	63,63,63,63	0
56	MG	2a	3017	1/1	0.96	0.23	-	70,70,70,70	0
56	MG	2A	3204	1/1	0.93	0.11	-	44,44,44,44	0
56	MG	1a	1862	1/1	0.83	0.13	-	65,65,65,65	0
56	MG	1D	313	1/1	0.90	0.58	-	56,56,56,56	0
56	MG	1A	3475	1/1	0.94	0.55	-	53,53,53,53	0
56	MG	1A	3698	1/1	0.88	0.07	-	48,48,48,48	0
56	MG	1A	3853	1/1	0.95	0.14	-	46,46,46,46	0
56	MG	1A	3138	1/1	0.94	0.59	-	55,55,55,55	0
56	MG	1A	3284	1/1	0.88	0.10	-	41,41,41,41	0
56	MG	2A	3309	1/1	0.83	0.18	-	31,31,31,31	0
56	MG	1A	3509	1/1	0.83	0.23	-	71,71,71,71	0
56	MG	2A	3437	1/1	0.92	0.12	-	57,57,57,57	0
56	MG	1A	3817	1/1	0.95	0.23	-	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
56	MG	1A	3664	1/1	0.94	0.14	-	15,15,15,15	0
56	MG	2q	201	1/1	0.90	0.17	-	58,58,58,58	0
56	MG	2A	3050	1/1	0.96	0.16	-	38,38,38,38	0
56	MG	2A	3234	1/1	0.87	0.39	-	48,48,48,48	0
56	MG	2A	3404	1/1	0.94	0.10	-	43,43,43,43	0
56	MG	1B	222	1/1	0.90	0.09	-	70,70,70,70	0
56	MG	2A	3286	1/1	0.95	0.13	-	32,32,32,32	0
56	MG	1A	3465	1/1	0.90	0.19	-	44,44,44,44	0
56	MG	2a	3250	1/1	0.90	0.15	-	61,61,61,61	0
56	MG	2A	3383	1/1	0.93	0.22	-	66,66,66,66	0
56	MG	1A	3864	1/1	0.96	0.07	-	55,55,55,55	0
56	MG	1A	3508	1/1	0.71	0.44	-	57,57,57,57	0
56	MG	1E	302	1/1	0.93	0.10	-	48,48,48,48	0
56	MG	1a	1678	1/1	0.92	0.07	-	43,43,43,43	0
56	MG	2A	3200	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	1A	3356	1/1	0.97	0.16	-	42,42,42,42	0
56	MG	2A	3423	1/1	0.95	0.06	-	66,66,66,66	0
56	MG	1a	1875	1/1	0.86	0.26	-	82,82,82,82	0
56	MG	2O	203	1/1	0.94	0.13	-	40,40,40,40	0
56	MG	2A	3119	1/1	0.88	0.13	-	61,61,61,61	0
56	MG	1A	3502	1/1	0.93	0.35	-	63,63,63,63	0
56	MG	2A	3096	1/1	0.79	0.16	-	40,40,40,40	0
56	MG	1A	3776	1/1	0.94	0.13	-	20,20,20,20	0
56	MG	26	101	1/1	0.90	0.10	-	57,57,57,57	0
56	MG	1A	4006	1/1	0.95	0.16	-	45,45,45,45	0
56	MG	2a	3149	1/1	0.93	0.12	-	65,65,65,65	0
56	MG	2A	3240	1/1	0.81	0.15	-	63,63,63,63	0
56	MG	2A	3125	1/1	0.98	0.20	-	56,56,56,56	0
56	MG	2a	3061	1/1	0.96	0.10	-	73,73,73,73	0
56	MG	2A	3008	1/1	0.73	0.12	-	64,64,64,64	0
56	MG	2A	3364	1/1	0.80	0.15	-	60,60,60,60	0
56	MG	2A	3076	1/1	0.69	0.20	-	60,60,60,60	0
56	MG	2A	3488	1/1	0.94	0.20	-	63,63,63,63	0
56	MG	2a	3039	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	1A	3573	1/1	0.94	0.24	-	47,47,47,47	0
56	MG	1a	1756	1/1	0.90	0.11	-	75,75,75,75	0
56	MG	2B	3011	1/1	0.88	0.18	-	83,83,83,83	0
56	MG	2a	3109	1/1	0.95	0.12	-	47,47,47,47	0
56	MG	2A	3245	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	1A	3490	1/1	0.89	0.12	-	66,66,66,66	0
56	MG	1A	3652	1/1	0.98	0.10	-	36,36,36,36	0
56	MG	2a	3045	1/1	0.91	0.22	-	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
56	MG	2A	3229	1/1	0.76	0.21	-	55,55,55,55	0
56	MG	2a	3084	1/1	0.97	0.22	-	56,56,56,56	0
56	MG	13	101	1/1	0.95	0.13	-	49,49,49,49	0
56	MG	2A	3280	1/1	0.94	0.11	-	63,63,63,63	0
56	MG	1A	3685	1/1	0.87	0.26	-	73,73,73,73	0
56	MG	2a	3234	1/1	0.91	0.13	-	66,66,66,66	0
56	MG	1A	3650	1/1	0.95	0.18	-	19,19,19,19	0
56	MG	1a	1719	1/1	0.99	0.14	-	53,53,53,53	0
56	MG	2a	3214	1/1	0.68	0.20	-	97,97,97,97	0
56	MG	1A	3858	1/1	0.99	0.23	-	46,46,46,46	0
56	MG	1A	3427	1/1	0.83	0.15	-	53,53,53,53	0
56	MG	1A	3450	1/1	0.81	0.19	-	45,45,45,45	0
56	MG	2a	3046	1/1	0.85	0.09	-	65,65,65,65	0
56	MG	1A	3050	1/1	0.78	0.28	-	48,48,48,48	0
56	MG	1A	3527	1/1	0.63	0.19	-	41,41,41,41	0
56	MG	1A	3510	1/1	0.96	0.24	-	55,55,55,55	0
56	MG	1a	1656	1/1	0.96	0.06	-	57,57,57,57	0
56	MG	1A	3355	1/1	0.89	0.13	-	53,53,53,53	0
56	MG	1A	3471	1/1	0.84	0.09	-	74,74,74,74	0
56	MG	15	102	1/1	0.94	0.68	-	40,40,40,40	0
56	MG	2A	3266	1/1	0.81	0.13	-	71,71,71,71	0
56	MG	1A	3352	1/1	0.83	0.12	-	58,58,58,58	0
56	MG	1A	3751	1/1	0.84	0.13	-	39,39,39,39	0
56	MG	2A	3512	1/1	0.94	0.11	-	44,44,44,44	0
56	MG	1A	3148	1/1	0.94	0.15	-	62,62,62,62	0
56	MG	1A	3197	1/1	0.81	0.13	-	50,50,50,50	0
56	MG	2a	3094	1/1	0.91	0.17	-	49,49,49,49	0
56	MG	1A	3700	1/1	0.93	0.07	-	63,63,63,63	0
56	MG	2A	3484	1/1	0.86	0.14	-	82,82,82,82	0
56	MG	1P	202	1/1	0.91	0.20	-	55,55,55,55	0
56	MG	1A	3627	1/1	0.93	0.14	-	20,20,20,20	0
56	MG	2A	3380	1/1	0.85	0.27	-	74,74,74,74	0
56	MG	1A	3085	1/1	0.98	0.60	-	47,47,47,47	0
56	MG	1A	3484	1/1	0.97	0.17	-	48,48,48,48	0
56	MG	2A	3007	1/1	0.95	0.60	-	46,46,46,46	0
56	MG	2a	3053	1/1	0.94	0.14	-	85,85,85,85	0
56	MG	2a	3146	1/1	0.83	0.15	-	57,57,57,57	0
56	MG	2a	3126	1/1	0.96	0.21	-	41,41,41,41	0
56	MG	1A	3536	1/1	0.92	0.20	-	68,68,68,68	0
56	MG	1B	223	1/1	0.83	0.12	-	59,59,59,59	0
56	MG	1a	1667	1/1	0.88	0.15	-	65,65,65,65	0
56	MG	1A	3937	1/1	0.91	0.16	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3505	1/1	0.91	0.10	-	65,65,65,65	0
56	MG	1a	1834	1/1	0.95	0.20	-	63,63,63,63	0
56	MG	1q	204	1/1	0.94	0.27	-	52,52,52,52	0
56	MG	2A	3503	1/1	0.92	0.08	-	59,59,59,59	0
56	MG	2A	3003	1/1	0.88	0.11	-	53,53,53,53	0
56	MG	1a	1644	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	2A	3514	1/1	0.89	0.13	-	60,60,60,60	0
56	MG	1A	3034	1/1	0.60	0.23	-	73,73,73,73	0
56	MG	1A	3470	1/1	0.83	0.13	-	52,52,52,52	0
56	MG	1a	1745	1/1	0.81	0.19	-	79,79,79,79	0
56	MG	1a	1650	1/1	0.96	0.26	-	57,57,57,57	0
56	MG	2A	3218	1/1	0.82	0.56	-	62,62,62,62	0
56	MG	1A	3421	1/1	0.81	0.14	-	47,47,47,47	0
56	MG	1A	3229	1/1	0.98	0.12	-	50,50,50,50	0
56	MG	1A	3230	1/1	0.83	0.56	-	46,46,46,46	0
56	MG	1a	1655	1/1	0.95	0.11	-	56,56,56,56	0
56	MG	2A	3472	1/1	0.92	0.09	-	39,39,39,39	0
56	MG	1A	3457	1/1	0.82	0.15	-	72,72,72,72	0
56	MG	1A	3068	1/1	0.91	0.70	-	44,44,44,44	0
56	MG	1A	3556	1/1	0.92	0.12	-	59,59,59,59	0
56	MG	2A	3131	1/1	0.80	0.17	-	52,52,52,52	0
56	MG	1a	1736	1/1	0.94	0.22	-	41,41,41,41	0
56	MG	1A	3360	1/1	0.86	0.23	-	47,47,47,47	0
56	MG	2x	3001	1/1	0.89	0.14	-	66,66,66,66	0
56	MG	2A	3044	1/1	0.93	0.75	-	48,48,48,48	0
56	MG	2A	3407	1/1	0.87	0.18	-	40,40,40,40	0
56	MG	1A	3339	1/1	0.90	0.18	-	56,56,56,56	0
56	MG	2A	3276	1/1	0.98	0.15	-	42,42,42,42	0
56	MG	1A	3308	1/1	0.94	0.34	-	50,50,50,50	0
56	MG	1a	1768	1/1	0.96	0.18	-	72,72,72,72	0
56	MG	2a	3041	1/1	0.92	0.28	-	73,73,73,73	0
56	MG	1a	1839	1/1	0.97	0.12	-	56,56,56,56	0
56	MG	2A	3252	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	2A	3491	1/1	0.95	0.04	-	47,47,47,47	0
56	MG	1A	3212	1/1	0.96	0.07	-	39,39,39,39	0
56	MG	2a	3003	1/1	0.93	0.19	-	57,57,57,57	0
56	MG	1A	3783	1/1	0.90	0.18	-	37,37,37,37	0
56	MG	1a	1638	1/1	0.91	0.11	-	63,63,63,63	0
56	MG	2A	3408	1/1	0.92	0.16	-	62,62,62,62	0
56	MG	1A	3039	1/1	0.84	0.30	-	49,49,49,49	0
56	MG	2a	3217	1/1	0.87	0.12	-	83,83,83,83	0
56	MG	1A	3818	1/1	0.87	0.16	-	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
56	MG	1A	3702	1/1	0.98	0.14	-	44,44,44,44	0
56	MG	1A	3480	1/1	0.95	0.09	-	56,56,56,56	0
56	MG	1a	1651	1/1	0.84	0.28	-	54,54,54,54	0
56	MG	2A	3282	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	2a	3254	1/1	0.56	0.23	-	71,71,71,71	0
56	MG	2A	3073	1/1	0.90	0.18	-	55,55,55,55	0
56	MG	1a	1622	1/1	0.98	0.17	-	90,90,90,90	0
56	MG	2x	3003	1/1	0.83	0.12	-	73,73,73,73	0
56	MG	1E	304	1/1	0.91	0.17	-	57,57,57,57	0
56	MG	2A	3197	1/1	0.92	0.24	-	57,57,57,57	0
56	MG	1A	3210	1/1	0.94	0.21	-	43,43,43,43	0
56	MG	1A	3673	1/1	0.95	0.26	-	65,65,65,65	0
56	MG	1A	3331	1/1	0.88	0.20	-	57,57,57,57	0
56	MG	1A	3125	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	1A	3715	1/1	0.87	0.15	-	63,63,63,63	0
56	MG	1A	3325	1/1	0.91	0.10	-	74,74,74,74	0
56	MG	1A	3425	1/1	0.90	0.14	-	63,63,63,63	0
56	MG	1A	3171	1/1	0.98	0.25	-	38,38,38,38	0
56	MG	2a	3162	1/1	0.80	0.20	-	75,75,75,75	0
56	MG	1E	301	1/1	0.92	0.14	-	15,15,15,15	0
56	MG	2A	3375	1/1	0.93	0.17	-	48,48,48,48	0
56	MG	1A	3945	1/1	0.96	0.21	-	60,60,60,60	0
56	MG	1A	3666	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	1A	3915	1/1	0.90	0.22	-	58,58,58,58	0
56	MG	1Z	8002	1/1	0.91	0.12	-	67,67,67,67	0
56	MG	1a	1821	1/1	0.85	0.07	-	49,49,49,49	0
56	MG	1A	3314	1/1	0.89	0.30	-	55,55,55,55	0
56	MG	1A	3191	1/1	0.95	0.16	-	37,37,37,37	0
56	MG	1a	1864	1/1	0.90	0.15	-	73,73,73,73	0
56	MG	1A	3515	1/1	0.89	0.37	-	48,48,48,48	0
56	MG	2a	3223	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	1A	3359	1/1	0.86	0.32	-	53,53,53,53	0
56	MG	2A	3108	1/1	0.96	0.12	-	46,46,46,46	0
56	MG	1A	3464	1/1	0.75	1.11	-	76,76,76,76	0
56	MG	2A	3203	1/1	0.89	0.09	-	43,43,43,43	0
56	MG	1A	3982	1/1	0.92	0.32	-	49,49,49,49	0
56	MG	1a	1683	1/1	0.98	0.12	-	68,68,68,68	0
56	MG	1A	3066	1/1	0.82	0.61	-	53,53,53,53	0
56	MG	1A	3815	1/1	0.70	0.13	-	67,67,67,67	0
56	MG	1A	3997	1/1	0.85	0.22	-	50,50,50,50	0
56	MG	2A	3482	1/1	0.96	0.26	-	60,60,60,60	0
56	MG	2a	3262	1/1	0.94	0.09	-	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
56	MG	1A	3563	1/1	0.88	0.14	-	46,46,46,46	0
56	MG	1B	217	1/1	0.97	0.18	-	50,50,50,50	0
56	MG	2A	3464	1/1	0.95	0.10	-	50,50,50,50	0
56	MG	1W	3001	1/1	0.95	0.32	-	34,34,34,34	0
56	MG	2a	3152	1/1	0.81	0.15	-	84,84,84,84	0
56	MG	2A	3315	1/1	0.83	0.22	-	55,55,55,55	0
56	MG	2a	3120	1/1	0.94	0.12	-	63,63,63,63	0
56	MG	1A	3409	1/1	0.82	0.12	-	51,51,51,51	0
56	MG	1A	3522	1/1	0.85	0.12	-	69,69,69,69	0
56	MG	1A	3747	1/1	0.91	0.17	-	29,29,29,29	0
56	MG	2A	3066	1/1	0.89	0.18	-	55,55,55,55	0
56	MG	2A	3225	1/1	0.86	0.14	-	63,63,63,63	0
56	MG	2A	3504	1/1	0.93	0.08	-	56,56,56,56	0
56	MG	2A	3313	1/1	0.94	0.09	-	53,53,53,53	0
56	MG	1A	3763	1/1	0.89	0.09	-	43,43,43,43	0
56	MG	1A	3903	1/1	0.94	0.17	-	19,19,19,19	0
56	MG	1A	3800	1/1	0.97	0.10	-	50,50,50,50	0
56	MG	2a	3222	1/1	0.96	0.16	-	46,46,46,46	0
56	MG	1A	3305	1/1	0.90	0.20	-	43,43,43,43	0
56	MG	1A	3096	1/1	0.91	0.36	-	50,50,50,50	0
56	MG	1D	314	1/1	0.96	0.35	-	63,63,63,63	0
56	MG	1A	3641	1/1	0.93	0.11	-	39,39,39,39	0
56	MG	2A	3074	1/1	0.80	0.26	-	57,57,57,57	0
56	MG	1A	3932	1/1	0.91	0.35	-	20,20,20,20	0
56	MG	1a	1843	1/1	0.90	0.08	-	74,74,74,74	0
56	MG	2A	3378	1/1	0.95	0.17	-	66,66,66,66	0
56	MG	2a	3036	1/1	0.82	0.27	-	72,72,72,72	0
56	MG	2A	3105	1/1	0.93	0.27	-	54,54,54,54	0
56	MG	1A	3726	1/1	0.88	0.24	-	64,64,64,64	0
56	MG	2A	3255	1/1	0.88	0.15	-	52,52,52,52	0
56	MG	2a	3123	1/1	0.79	0.15	-	81,81,81,81	0
56	MG	2A	3516	1/1	0.91	0.15	-	59,59,59,59	0
56	MG	2A	3458	1/1	0.98	0.08	-	54,54,54,54	0
56	MG	1A	3431	1/1	0.89	0.29	-	64,64,64,64	0
56	MG	1A	3785	1/1	0.84	0.14	-	72,72,72,72	0
56	MG	2a	3073	1/1	0.65	0.14	-	61,61,61,61	0
56	MG	10	102	1/1	0.94	0.14	-	60,60,60,60	0
56	MG	2A	3374	1/1	0.96	0.25	-	37,37,37,37	0
56	MG	2a	3168	1/1	0.91	0.08	-	71,71,71,71	0
56	MG	1A	3709	1/1	0.78	0.20	-	45,45,45,45	0
56	MG	1A	3311	1/1	0.89	0.17	-	65,65,65,65	0
56	MG	2a	3002	1/1	0.94	0.24	-	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
56	MG	2A	3043	1/1	0.99	0.19	-	49,49,49,49	0
56	MG	1A	3371	1/1	0.90	0.15	-	56,56,56,56	0
56	MG	2a	3025	1/1	0.90	0.10	-	60,60,60,60	0
56	MG	1a	1757	1/1	0.77	0.14	-	63,63,63,63	0
56	MG	2a	3202	1/1	0.92	0.18	-	72,72,72,72	0
56	MG	2A	3195	1/1	0.71	0.15	-	48,48,48,48	0
56	MG	2A	3330	1/1	0.97	0.23	-	47,47,47,47	0
56	MG	2a	3070	1/1	0.71	0.14	-	69,69,69,69	0
56	MG	1A	3407	1/1	0.93	0.10	-	41,41,41,41	0
56	MG	1A	3091	1/1	0.96	0.11	-	51,51,51,51	0
56	MG	1A	3142	1/1	0.87	0.61	-	57,57,57,57	0
56	MG	1A	3760	1/1	0.97	0.17	-	36,36,36,36	0
56	MG	1a	1624	1/1	0.89	0.60	-	62,62,62,62	0
56	MG	1R	201	1/1	0.95	0.27	-	63,63,63,63	0
56	MG	1A	3201	1/1	0.96	0.15	-	49,49,49,49	0
56	MG	2A	3436	1/1	0.91	0.16	-	58,58,58,58	0
56	MG	2A	3092	1/1	0.80	0.12	-	54,54,54,54	0
56	MG	1A	3165	1/1	0.73	0.25	-	53,53,53,53	0
56	MG	1A	3492	1/1	0.96	0.57	-	52,52,52,52	0
56	MG	1a	1825	1/1	0.97	0.07	-	43,43,43,43	0
56	MG	1A	3707	1/1	0.96	0.20	-	70,70,70,70	0
56	MG	1a	1769	1/1	0.89	0.09	-	87,87,87,87	0
56	MG	1A	3235	1/1	0.87	0.16	-	46,46,46,46	0
56	MG	1A	3306	1/1	0.86	0.26	-	41,41,41,41	0
56	MG	2a	3207	1/1	0.85	0.15	-	73,73,73,73	0
56	MG	1T	204	1/1	0.89	0.19	-	67,67,67,67	0
56	MG	1A	3272	1/1	0.98	0.22	-	29,29,29,29	0
56	MG	2A	3389	1/1	0.81	0.24	-	77,77,77,77	0
56	MG	25	502	1/1	0.95	0.29	-	47,47,47,47	0
56	MG	1A	3218	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	1A	3104	1/1	0.90	0.09	-	55,55,55,55	0
56	MG	2a	3248	1/1	0.91	0.15	-	65,65,65,65	0
56	MG	2a	3229	1/1	0.89	0.18	-	51,51,51,51	0
56	MG	1A	3468	1/1	0.86	0.24	-	57,57,57,57	0
56	MG	1A	3919	1/1	0.95	0.30	-	49,49,49,49	0
56	MG	2A	3141	1/1	0.79	0.15	-	74,74,74,74	0
56	MG	2A	3075	1/1	0.93	0.14	-	59,59,59,59	0
56	MG	1a	1804	1/1	0.94	0.11	-	52,52,52,52	0
56	MG	1A	3674	1/1	0.96	0.15	-	52,52,52,52	0
56	MG	1a	1627	1/1	0.72	0.14	-	67,67,67,67	0
56	MG	1A	3828	1/1	0.98	0.08	-	67,67,67,67	0
56	MG	2A	3172	1/1	0.94	0.27	-	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
56	MG	1A	3160	1/1	0.93	0.12	-	40,40,40,40	0
56	MG	1A	3970	1/1	0.97	1.04	-	30,30,30,30	0
56	MG	1A	3724	1/1	0.94	0.20	-	58,58,58,58	0
56	MG	1A	3605	1/1	0.86	0.20	-	33,33,33,33	0
56	MG	1A	3337	1/1	0.91	0.32	-	57,57,57,57	0
56	MG	1A	3869	1/1	0.92	0.09	-	42,42,42,42	0
56	MG	1A	3419	1/1	0.93	0.20	-	56,56,56,56	0
56	MG	2A	3399	1/1	0.96	0.12	-	31,31,31,31	0
56	MG	2A	3284	1/1	0.91	0.10	-	62,62,62,62	0
56	MG	2a	3180	1/1	0.81	0.19	-	61,61,61,61	0
56	MG	1A	3951	1/1	0.93	0.31	-	70,70,70,70	0
56	MG	1A	3784	1/1	0.93	0.21	-	33,33,33,33	0
56	MG	1A	3013	1/1	0.80	0.26	-	70,70,70,70	0
56	MG	2E	303	1/1	0.96	0.19	-	26,26,26,26	0
56	MG	2A	3331	1/1	0.97	0.16	-	48,48,48,48	0
56	MG	2A	3509	1/1	0.78	0.19	-	62,62,62,62	0
56	MG	1A	3890	1/1	0.87	0.21	-	37,37,37,37	0
56	MG	1A	3863	1/1	0.90	0.21	-	78,78,78,78	0
56	MG	2A	3046	1/1	0.94	0.26	-	64,64,64,64	0
56	MG	1A	3877	1/1	0.93	0.13	-	42,42,42,42	0
56	MG	1A	3857	1/1	0.80	0.21	-	32,32,32,32	0
56	MG	2A	3009	1/1	0.85	0.41	-	60,60,60,60	0
56	MG	2A	3028	1/1	0.89	0.14	-	52,52,52,52	0
56	MG	1a	1652	1/1	0.98	0.20	-	48,48,48,48	0
56	MG	2a	3145	1/1	0.91	0.10	-	61,61,61,61	0
56	MG	16	101	1/1	0.95	0.17	-	45,45,45,45	0
56	MG	1A	3941	1/1	0.89	0.12	-	65,65,65,65	0
56	MG	2A	3122	1/1	0.71	0.17	-	66,66,66,66	0
56	MG	1A	3769	1/1	0.83	0.20	-	90,90,90,90	0
56	MG	1A	3934	1/1	0.97	0.12	-	33,33,33,33	0
56	MG	1A	3920	1/1	0.94	0.15	-	64,64,64,64	0
56	MG	1A	3899	1/1	0.96	0.24	-	47,47,47,47	0
56	MG	2A	3497	1/1	0.85	0.18	-	54,54,54,54	0
56	MG	1A	3956	1/1	0.93	0.18	-	53,53,53,53	0
56	MG	2A	3525	1/1	0.91	0.15	-	63,63,63,63	0
56	MG	1A	3983	1/1	0.91	0.18	-	55,55,55,55	0
56	MG	2a	3138	1/1	0.79	0.13	-	81,81,81,81	0
56	MG	1a	1779	1/1	0.95	0.11	-	82,82,82,82	0
56	MG	2a	3173	1/1	0.78	0.56	-	74,74,74,74	0
56	MG	1A	3823	1/1	0.94	0.29	-	43,43,43,43	0
56	MG	1A	3998	1/1	0.89	0.27	-	75,75,75,75	0
56	MG	1x	103	1/1	0.96	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1q	201	1/1	0.90	0.18	-	51,51,51,51	0
56	MG	2a	3042	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	2a	3233	1/1	0.97	0.10	-	61,61,61,61	0
56	MG	2A	3247	1/1	0.91	0.54	-	59,59,59,59	0
56	MG	1a	1801	1/1	0.92	0.19	-	59,59,59,59	0
56	MG	1a	1688	1/1	0.92	0.11	-	56,56,56,56	0
56	MG	2A	3332	1/1	0.78	0.13	-	38,38,38,38	0
56	MG	1A	3376	1/1	0.96	0.19	-	53,53,53,53	0
56	MG	2a	3161	1/1	0.68	0.12	-	102,102,102,102	0
56	MG	1A	3153	1/1	0.96	0.11	-	24,24,24,24	0
56	MG	2a	3012	1/1	0.91	0.13	-	66,66,66,66	0
56	MG	1A	3257	1/1	0.92	0.17	-	44,44,44,44	0
56	MG	1A	3266	1/1	0.93	0.10	-	44,44,44,44	0
56	MG	1A	3918	1/1	0.85	0.40	-	71,71,71,71	0
56	MG	2a	3031	1/1	0.53	0.17	-	65,65,65,65	0
56	MG	1A	3361	1/1	0.84	0.19	-	66,66,66,66	0
56	MG	1A	3717	1/1	0.97	0.17	-	59,59,59,59	0
56	MG	1A	3313	1/1	0.96	0.37	-	53,53,53,53	0
56	MG	1A	3413	1/1	0.94	0.13	-	41,41,41,41	0
56	MG	2A	3134	1/1	0.93	0.07	-	51,51,51,51	0
56	MG	1A	3219	1/1	0.86	0.27	-	59,59,59,59	0
56	MG	2A	3537	1/1	0.97	0.16	-	37,37,37,37	0
56	MG	2a	3209	1/1	0.95	0.14	-	70,70,70,70	0
56	MG	1A	3677	1/1	0.98	0.15	-	51,51,51,51	0
56	MG	1x	105	1/1	0.93	0.21	-	57,57,57,57	0
56	MG	1A	3240	1/1	0.94	0.16	-	49,49,49,49	0
56	MG	1A	3599	1/1	0.94	0.23	-	37,37,37,37	0
56	MG	2a	3014	1/1	0.52	0.12	-	65,65,65,65	0
56	MG	1A	3728	1/1	0.97	0.20	-	52,52,52,52	0
56	MG	1A	3735	1/1	0.93	0.16	-	36,36,36,36	0
56	MG	1a	1780	1/1	0.94	0.29	-	68,68,68,68	0
56	MG	1A	3080	1/1	0.95	0.31	-	50,50,50,50	0
56	MG	2A	3418	1/1	0.90	0.13	-	57,57,57,57	0
56	MG	1A	3236	1/1	0.89	0.45	-	46,46,46,46	0
56	MG	1A	3319	1/1	0.96	0.10	-	57,57,57,57	0
56	MG	2A	3352	1/1	0.70	0.17	-	68,68,68,68	0
56	MG	1a	1845	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	1A	3520	1/1	0.62	0.14	-	75,75,75,75	0
56	MG	1A	3152	1/1	0.93	0.14	-	50,50,50,50	0
56	MG	1N	3006	1/1	0.82	0.64	-	71,71,71,71	0
56	MG	2A	3207	1/1	0.91	0.12	-	44,44,44,44	0
56	MG	10	105	1/1	0.75	0.17	-	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
56	MG	2A	3538	1/1	0.95	0.19	-	22,22,22,22	0
56	MG	12	3001	1/1	0.70	0.42	-	61,61,61,61	0
56	MG	2A	3265	1/1	0.93	0.19	-	37,37,37,37	0
56	MG	1A	3552	1/1	0.69	0.22	-	50,50,50,50	0
56	MG	1A	3452	1/1	0.93	0.13	-	56,56,56,56	0
56	MG	1A	3721	1/1	0.90	0.18	-	55,55,55,55	0
56	MG	1A	3598	1/1	0.89	0.16	-	51,51,51,51	0
56	MG	1A	3102	1/1	0.88	0.13	-	60,60,60,60	0
56	MG	2a	3075	1/1	0.66	0.15	-	72,72,72,72	0
56	MG	1A	3713	1/1	0.95	0.14	-	40,40,40,40	0
56	MG	1a	1796	1/1	0.90	0.38	-	86,86,86,86	0
56	MG	1A	3638	1/1	0.95	0.29	-	41,41,41,41	0
56	MG	2A	3513	1/1	0.82	0.14	-	61,61,61,61	0
56	MG	2A	3520	1/1	0.97	0.08	-	42,42,42,42	0
56	MG	2A	3517	1/1	0.97	0.15	-	56,56,56,56	0
56	MG	1A	3173	1/1	0.95	0.19	-	62,62,62,62	0
56	MG	2Y	502	1/1	0.94	0.21	-	52,52,52,52	0
56	MG	16	103	1/1	0.96	0.10	-	68,68,68,68	0
56	MG	1A	3400	1/1	0.88	0.15	-	45,45,45,45	0
56	MG	1a	1732	1/1	0.67	0.24	-	74,74,74,74	0
56	MG	1a	1680	1/1	0.97	0.14	-	53,53,53,53	0
56	MG	1a	1835	1/1	0.98	0.07	-	73,73,73,73	0
56	MG	2a	3192	1/1	0.90	0.10	-	60,60,60,60	0
56	MG	2a	3114	1/1	0.93	0.23	-	53,53,53,53	0
56	MG	1A	3105	1/1	0.83	0.22	-	61,61,61,61	0
56	MG	1P	203	1/1	0.96	0.11	-	65,65,65,65	0
56	MG	1T	203	1/1	0.70	0.18	-	61,61,61,61	0
56	MG	1A	3466	1/1	0.92	0.09	-	40,40,40,40	0
56	MG	1A	3870	1/1	0.96	0.12	-	53,53,53,53	0
56	MG	1A	3850	1/1	0.94	0.15	-	41,41,41,41	0
56	MG	1A	3844	1/1	0.94	0.13	-	71,71,71,71	0
56	MG	1A	3007	1/1	0.87	0.28	-	56,56,56,56	0
56	MG	1A	3568	1/1	0.93	0.21	-	42,42,42,42	0
56	MG	1A	3586	1/1	0.94	0.14	-	57,57,57,57	0
56	MG	1A	3580	1/1	0.97	0.22	-	46,46,46,46	0
56	MG	1a	1610	1/1	0.89	0.13	-	53,53,53,53	0
56	MG	1A	3856	1/1	0.95	0.08	-	69,69,69,69	0
56	MG	2A	3136	1/1	0.96	0.09	-	54,54,54,54	0
56	MG	2A	3322	1/1	0.92	0.14	-	67,67,67,67	0
56	MG	1A	3649	1/1	0.92	0.14	-	71,71,71,71	0
56	MG	1a	1782	1/1	0.93	0.18	-	43,43,43,43	0
56	MG	2A	3241	1/1	0.84	0.17	-	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
56	MG	1A	3519	1/1	0.86	0.31	-	62,62,62,62	0
56	MG	2a	3117	1/1	0.90	0.10	-	58,58,58,58	0
56	MG	2x	3002	1/1	0.84	0.13	-	65,65,65,65	0
56	MG	1a	1817	1/1	0.96	0.30	-	52,52,52,52	0
56	MG	2A	3384	1/1	0.95	0.06	-	45,45,45,45	0
56	MG	2a	3218	1/1	0.97	0.14	-	62,62,62,62	0
56	MG	1A	3256	1/1	0.98	0.17	-	43,43,43,43	0
56	MG	2a	3188	1/1	0.94	0.11	-	60,60,60,60	0
56	MG	1Q	3003	1/1	0.77	0.77	-	51,51,51,51	0
56	MG	2a	3021	1/1	0.94	0.48	-	60,60,60,60	0
56	MG	2A	3346	1/1	0.89	0.18	-	62,62,62,62	0
56	MG	1A	3342	1/1	0.95	0.36	-	52,52,52,52	0
56	MG	1A	3682	1/1	0.87	0.14	-	51,51,51,51	0
56	MG	1A	3326	1/1	0.96	0.09	-	53,53,53,53	0
56	MG	1A	3540	1/1	0.98	0.32	-	45,45,45,45	0
56	MG	1a	1693	1/1	0.96	0.14	-	52,52,52,52	0
56	MG	1r	3002	1/1	0.83	0.22	-	55,55,55,55	0
56	MG	1a	1714	1/1	0.98	0.09	-	68,68,68,68	0
56	MG	2A	3151	1/1	0.96	0.27	-	47,47,47,47	0
56	MG	1A	3251	1/1	0.90	0.20	-	30,30,30,30	0
56	MG	2A	3387	1/1	0.96	0.21	-	63,63,63,63	0
56	MG	1A	3926	1/1	0.99	0.31	-	38,38,38,38	0
56	MG	1A	3078	1/1	0.94	0.07	-	62,62,62,62	0
56	MG	1a	1773	1/1	0.81	0.21	-	77,77,77,77	0
56	MG	1A	3243	1/1	0.85	0.86	-	46,46,46,46	0
56	MG	1A	3992	1/1	0.87	0.16	-	55,55,55,55	0
56	MG	1A	3655	1/1	0.91	0.29	-	48,48,48,48	0
56	MG	1A	3073	1/1	0.96	0.24	-	51,51,51,51	0
56	MG	1A	3778	1/1	0.80	0.20	-	23,23,23,23	0
56	MG	1A	3354	1/1	0.93	0.09	-	43,43,43,43	0
56	MG	1A	3119	1/1	0.80	0.37	-	65,65,65,65	0
56	MG	2A	3137	1/1	0.96	0.12	-	51,51,51,51	0
56	MG	1A	3991	1/1	0.90	0.15	-	52,52,52,52	0
56	MG	2A	3316	1/1	0.98	0.21	-	57,57,57,57	0
56	MG	2A	3541	1/1	0.96	0.33	-	42,42,42,42	0
56	MG	1a	1717	1/1	0.81	0.10	-	63,63,63,63	0
56	MG	1a	1670	1/1	0.94	0.18	-	43,43,43,43	0
56	MG	2A	3157	1/1	0.90	0.17	-	43,43,43,43	0
56	MG	1A	3601	1/1	0.97	0.22	-	44,44,44,44	0
56	MG	1A	3517	1/1	0.96	0.65	-	43,43,43,43	0
56	MG	1a	1631	1/1	0.97	0.12	-	36,36,36,36	0
56	MG	2a	3169	1/1	0.96	0.69	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3455	1/1	0.31	0.27	-	69,69,69,69	0
56	MG	1A	3489	1/1	0.84	0.11	-	51,51,51,51	0
56	MG	1a	1737	1/1	0.92	0.07	-	57,57,57,57	0
56	MG	2a	3252	1/1	0.96	0.12	-	70,70,70,70	0
56	MG	1A	3766	1/1	0.91	0.19	-	49,49,49,49	0
56	MG	2A	3371	1/1	0.84	0.13	-	56,56,56,56	0
56	MG	18	102	1/1	0.84	0.29	-	57,57,57,57	0
56	MG	1Z	8001	1/1	0.90	0.22	-	69,69,69,69	0
56	MG	2A	3453	1/1	0.90	0.15	-	61,61,61,61	0
56	MG	1A	3420	1/1	0.83	0.11	-	56,56,56,56	0
56	MG	1A	3009	1/1	0.92	0.28	-	56,56,56,56	0
56	MG	2a	3040	1/1	0.94	0.15	-	39,39,39,39	0
56	MG	10	104	1/1	0.84	0.22	-	43,43,43,43	0
56	MG	1A	3901	1/1	0.91	0.12	-	44,44,44,44	0
56	MG	1a	1692	1/1	0.95	0.09	-	57,57,57,57	0
56	MG	2A	3410	1/1	0.89	0.21	-	56,56,56,56	0
56	MG	1A	3851	1/1	0.95	0.17	-	62,62,62,62	0
56	MG	1a	1763	1/1	0.92	0.36	-	69,69,69,69	0
56	MG	1A	3403	1/1	0.85	0.08	-	59,59,59,59	0
56	MG	1A	3558	1/1	0.96	0.10	-	61,61,61,61	0
56	MG	1A	3772	1/1	0.91	0.12	-	60,60,60,60	0
56	MG	1a	1812	1/1	0.94	0.22	-	49,49,49,49	0
56	MG	2A	3179	1/1	0.88	0.13	-	46,46,46,46	0
56	MG	2A	3447	1/1	0.91	0.12	-	62,62,62,62	0
56	MG	2A	3391	1/1	0.97	0.18	-	48,48,48,48	0
56	MG	1A	3958	1/1	0.87	0.16	-	64,64,64,64	0
56	MG	2a	3083	1/1	0.92	0.26	-	51,51,51,51	0
56	MG	2a	3063	1/1	0.89	0.11	-	77,77,77,77	0
56	MG	1a	1634	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	1A	3107	1/1	0.93	0.27	-	58,58,58,58	0
56	MG	1A	3948	1/1	0.97	0.15	-	28,28,28,28	0
56	MG	2A	3348	1/1	0.96	0.17	-	52,52,52,52	0
56	MG	1A	3461	1/1	0.88	0.25	-	71,71,71,71	0
56	MG	1A	3463	1/1	0.97	0.08	-	80,80,80,80	0
56	MG	2A	3328	1/1	0.84	0.19	-	57,57,57,57	0
56	MG	2A	3025	1/1	0.91	0.45	-	67,67,67,67	0
56	MG	1A	3224	1/1	0.93	0.18	-	35,35,35,35	0
56	MG	2A	3452	1/1	0.85	0.16	-	69,69,69,69	0
56	MG	2A	3111	1/1	0.94	0.28	-	68,68,68,68	0
56	MG	1T	201	1/1	0.95	0.19	-	41,41,41,41	0
56	MG	2a	3124	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	2A	3492	1/1	0.92	0.08	-	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
56	MG	19	104	1/1	0.98	0.13	-	31,31,31,31	0
56	MG	2A	3298	1/1	0.87	0.13	-	49,49,49,49	0
56	MG	2a	3198	1/1	0.90	0.06	-	63,63,63,63	0
56	MG	1D	302	1/1	0.91	0.70	-	65,65,65,65	0
56	MG	1A	3952	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	1a	1805	1/1	0.94	0.19	-	67,67,67,67	0
56	MG	1a	1640	1/1	0.86	0.20	-	51,51,51,51	0
56	MG	1A	3384	1/1	0.90	0.13	-	69,69,69,69	0
56	MG	1A	3069	1/1	0.96	0.28	-	39,39,39,39	0
56	MG	1a	1649	1/1	0.84	0.37	-	63,63,63,63	0
56	MG	1A	3827	1/1	0.94	0.13	-	31,31,31,31	0
56	MG	1A	3630	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	1A	3635	1/1	0.98	0.11	-	46,46,46,46	0
56	MG	2a	3107	1/1	0.97	0.07	-	57,57,57,57	0
56	MG	2A	3072	1/1	0.91	0.17	-	48,48,48,48	0
56	MG	1A	3847	1/1	0.89	0.17	-	46,46,46,46	0
56	MG	2A	3132	1/1	0.93	0.26	-	53,53,53,53	0
56	MG	1A	3940	1/1	0.92	0.17	-	63,63,63,63	0
56	MG	1A	3816	1/1	0.95	0.18	-	68,68,68,68	0
56	MG	2A	3522	1/1	0.87	0.11	-	70,70,70,70	0
56	MG	2A	3128	1/1	0.90	0.17	-	60,60,60,60	0
56	MG	1a	1744	1/1	0.89	0.17	-	61,61,61,61	0
56	MG	2a	3081	1/1	0.94	0.16	-	52,52,52,52	0
56	MG	2a	3241	1/1	0.77	0.42	-	95,95,95,95	0
56	MG	1A	4005	1/1	0.93	0.12	-	58,58,58,58	0
56	MG	1A	3204	1/1	0.96	0.26	-	37,37,37,37	0
56	MG	1A	3324	1/1	0.90	0.24	-	57,57,57,57	0
56	MG	1a	1842	1/1	0.94	0.21	-	73,73,73,73	0
56	MG	1A	3086	1/1	0.96	0.53	-	44,44,44,44	0
56	MG	1a	1625	1/1	0.97	0.07	-	52,52,52,52	0
56	MG	2A	3308	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	2A	3551	1/1	0.72	0.23	-	57,57,57,57	0
56	MG	1A	3052	1/1	0.86	0.13	-	59,59,59,59	0
56	MG	2a	3102	1/1	0.93	0.24	-	47,47,47,47	0
56	MG	1a	1735	1/1	0.96	0.13	-	66,66,66,66	0
56	MG	2A	3529	1/1	0.95	0.10	-	68,68,68,68	0
56	MG	2A	3146	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	1A	3985	1/1	0.88	0.17	-	66,66,66,66	0
56	MG	1A	3443	1/1	0.93	0.47	-	48,48,48,48	0
56	MG	1A	3663	1/1	0.96	0.12	-	55,55,55,55	0
56	MG	1A	3351	1/1	0.93	0.18	-	62,62,62,62	0
56	MG	1A	3927	1/1	0.90	0.18	-	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
56	MG	2A	3402	1/1	0.89	0.40	-	62,62,62,62	0
56	MG	1A	3099	1/1	0.89	0.12	-	39,39,39,39	0
56	MG	1a	1833	1/1	0.97	0.13	-	59,59,59,59	0
56	MG	2a	3092	1/1	0.71	0.18	-	87,87,87,87	0
56	MG	2A	3193	1/1	0.95	0.11	-	32,32,32,32	0
56	MG	2a	3121	1/1	0.89	0.19	-	63,63,63,63	0
56	MG	1A	3364	1/1	0.94	0.15	-	44,44,44,44	0
56	MG	1B	201	1/1	0.87	0.10	-	50,50,50,50	0
56	MG	2a	3237	1/1	0.96	0.07	-	52,52,52,52	0
56	MG	1a	1708	1/1	0.91	0.12	-	61,61,61,61	0
56	MG	1A	3043	1/1	0.74	0.37	-	52,52,52,52	0
56	MG	11	4000	1/1	0.91	0.09	-	43,43,43,43	0
56	MG	1A	3786	1/1	0.92	0.15	-	57,57,57,57	0
56	MG	2a	3176	1/1	0.88	0.17	-	56,56,56,56	0
56	MG	1A	3004	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	2A	3432	1/1	0.97	0.16	-	61,61,61,61	0
56	MG	2A	3523	1/1	0.86	0.39	-	56,56,56,56	0
56	MG	1A	3824	1/1	0.95	0.18	-	33,33,33,33	0
56	MG	1A	3852	1/1	0.94	0.17	-	16,16,16,16	0
56	MG	2A	3182	1/1	0.91	0.28	-	52,52,52,52	0
56	MG	1A	3884	1/1	0.75	0.14	-	53,53,53,53	0
56	MG	2A	3327	1/1	0.96	0.19	-	36,36,36,36	0
56	MG	1a	1850	1/1	0.95	0.10	-	59,59,59,59	0
56	MG	1A	3310	1/1	0.98	0.30	-	44,44,44,44	0
56	MG	2A	3198	1/1	0.87	0.18	-	41,41,41,41	0
56	MG	1A	3603	1/1	0.90	0.10	-	60,60,60,60	0
56	MG	2A	3393	1/1	0.94	0.13	-	63,63,63,63	0
56	MG	1A	3111	1/1	0.75	0.22	-	68,68,68,68	0
56	MG	1a	1783	1/1	0.81	0.16	-	57,57,57,57	0
56	MG	1a	1766	1/1	0.91	0.28	-	60,60,60,60	0
56	MG	2A	3088	1/1	0.88	0.17	-	51,51,51,51	0
56	MG	1A	3405	1/1	0.83	0.14	-	54,54,54,54	0
56	MG	1R	204	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	1A	3304	1/1	0.97	0.17	-	34,34,34,34	0
56	MG	2a	3016	1/1	0.87	0.16	-	65,65,65,65	0
56	MG	1a	1690	1/1	0.83	0.16	-	63,63,63,63	0
56	MG	1A	3040	1/1	0.91	0.39	-	45,45,45,45	0
56	MG	1A	3708	1/1	0.95	0.18	-	63,63,63,63	0
56	MG	2A	3156	1/1	0.83	0.17	-	49,49,49,49	0
56	MG	1A	3984	1/1	0.87	0.12	-	47,47,47,47	0
56	MG	1a	1855	1/1	0.93	0.10	-	55,55,55,55	0
56	MG	1A	3334	1/1	0.92	0.17	-	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
56	MG	1a	1620	1/1	0.91	0.09	-	58,58,58,58	0
56	MG	1A	3006	1/1	0.90	0.24	-	57,57,57,57	0
56	MG	1A	3748	1/1	0.94	0.13	-	37,37,37,37	0
56	MG	1A	3386	1/1	0.93	0.28	-	63,63,63,63	0
56	MG	2A	3056	1/1	0.88	0.13	-	38,38,38,38	0
56	MG	2A	3356	1/1	0.88	0.13	-	60,60,60,60	0
56	MG	1A	3972	1/1	0.97	0.66	-	42,42,42,42	0
56	MG	1A	3570	1/1	0.78	0.18	-	66,66,66,66	0
56	MG	1a	1706	1/1	0.82	0.22	-	64,64,64,64	0
56	MG	1A	3395	1/1	0.97	0.50	-	37,37,37,37	0
56	MG	2A	3250	1/1	0.74	0.16	-	64,64,64,64	0
56	MG	2A	3006	1/1	0.82	0.10	-	64,64,64,64	0
56	MG	1a	1861	1/1	0.93	0.17	-	58,58,58,58	0
56	MG	1A	3146	1/1	0.86	0.18	-	65,65,65,65	0
56	MG	2A	3415	1/1	0.93	0.16	-	60,60,60,60	0
56	MG	2A	3454	1/1	0.96	0.12	-	56,56,56,56	0
56	MG	1a	1637	1/1	0.91	0.31	-	53,53,53,53	0
56	MG	1A	3656	1/1	0.98	0.20	-	33,33,33,33	0
56	MG	1b	3002	1/1	0.82	0.12	-	76,76,76,76	0
56	MG	17	101	1/1	0.87	0.28	-	57,57,57,57	0
56	MG	1A	3495	1/1	0.93	0.11	-	66,66,66,66	0
56	MG	1A	3854	1/1	0.89	0.26	-	53,53,53,53	0
56	MG	2A	3081	1/1	0.94	0.08	-	44,44,44,44	0
56	MG	1A	3686	1/1	0.94	0.13	-	46,46,46,46	0
56	MG	1A	3808	1/1	0.94	0.21	-	51,51,51,51	0
56	MG	1x	107	1/1	0.86	0.38	-	61,61,61,61	0
56	MG	1A	3714	1/1	0.98	0.21	-	46,46,46,46	0
56	MG	2l	203	1/1	0.83	0.22	-	60,60,60,60	0
56	MG	1A	3447	1/1	0.93	0.15	-	63,63,63,63	0
56	MG	1A	3137	1/1	0.91	0.34	-	51,51,51,51	0
56	MG	2a	3088	1/1	0.96	0.22	-	54,54,54,54	0
56	MG	2A	3040	1/1	0.89	0.15	-	53,53,53,53	0
56	MG	2A	3495	1/1	0.89	0.12	-	71,71,71,71	0
56	MG	1A	3242	1/1	0.85	0.12	-	33,33,33,33	0
56	MG	1A	3261	1/1	0.79	0.34	-	62,62,62,62	0
56	MG	1A	3042	1/1	0.93	0.83	-	44,44,44,44	0
56	MG	1A	3801	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	2a	3221	1/1	0.83	0.12	-	66,66,66,66	0
56	MG	1A	3939	1/1	0.82	0.40	-	69,69,69,69	0
56	MG	1A	3706	1/1	0.94	0.13	-	22,22,22,22	0
56	MG	1A	3697	1/1	0.88	0.14	-	58,58,58,58	0
56	MG	2a	3227	1/1	0.94	0.19	-	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
56	MG	1A	3737	1/1	0.92	0.19	-	24,24,24,24	0
56	MG	1A	3516	1/1	0.83	0.27	-	53,53,53,53	0
56	MG	1A	3297	1/1	0.87	0.31	-	70,70,70,70	0
56	MG	2A	3449	1/1	0.86	0.12	-	60,60,60,60	0
56	MG	2a	3236	1/1	0.93	0.14	-	62,62,62,62	0
56	MG	2A	3023	1/1	0.89	0.18	-	61,61,61,61	0
56	MG	1A	3916	1/1	0.98	0.17	-	52,52,52,52	0
56	MG	2a	3190	1/1	0.94	0.20	-	52,52,52,52	0
56	MG	1a	1657	1/1	0.89	0.10	-	71,71,71,71	0
56	MG	1A	3143	1/1	0.95	0.26	-	52,52,52,52	0
56	MG	1A	3417	1/1	0.63	0.48	-	58,58,58,58	0
56	MG	1A	3366	1/1	0.96	0.09	-	46,46,46,46	0
56	MG	1a	1611	1/1	0.88	0.10	-	78,78,78,78	0
56	MG	1A	4000	1/1	0.90	0.14	-	61,61,61,61	0
56	MG	2A	3425	1/1	0.94	0.19	-	47,47,47,47	0
56	MG	2a	3038	1/1	0.82	0.17	-	57,57,57,57	0
56	MG	1B	224	1/1	0.96	0.12	-	44,44,44,44	0
56	MG	1a	1767	1/1	0.95	0.14	-	64,64,64,64	0
56	MG	1a	1704	1/1	0.82	0.18	-	54,54,54,54	0
56	MG	1A	3512	1/1	0.91	0.28	-	60,60,60,60	0
56	MG	2A	3498	1/1	0.93	0.13	-	49,49,49,49	0
56	MG	1a	1838	1/1	0.92	0.33	-	66,66,66,66	0
56	MG	1A	3880	1/1	0.97	0.14	-	55,55,55,55	0
56	MG	1A	3112	1/1	0.95	0.27	-	40,40,40,40	0
56	MG	1a	1636	1/1	0.97	0.20	-	44,44,44,44	0
56	MG	1e	3003	1/1	0.92	0.21	-	68,68,68,68	0
56	MG	1A	3127	1/1	0.93	0.50	-	53,53,53,53	0
56	MG	1A	3917	1/1	0.94	0.15	-	31,31,31,31	0
56	MG	2A	3038	1/1	0.83	0.11	-	58,58,58,58	0
56	MG	1a	1725	1/1	0.87	0.17	-	59,59,59,59	0
56	MG	1A	3260	1/1	0.95	0.22	-	58,58,58,58	0
56	MG	1x	101	1/1	0.97	0.30	-	51,51,51,51	0
56	MG	1A	3422	1/1	0.97	0.09	-	51,51,51,51	0
56	MG	1A	3526	1/1	0.85	0.21	-	32,32,32,32	0
56	MG	2A	3143	1/1	0.88	0.11	-	48,48,48,48	0
56	MG	2A	3183	1/1	0.92	0.14	-	56,56,56,56	0
56	MG	1A	3867	1/1	0.88	0.21	-	30,30,30,30	0
56	MG	1A	3415	1/1	0.88	0.11	-	50,50,50,50	0
56	MG	1a	1754	1/1	0.88	0.10	-	81,81,81,81	0
56	MG	1A	3084	1/1	0.93	0.12	-	50,50,50,50	0
56	MG	1A	3438	1/1	0.97	0.29	-	58,58,58,58	0
56	MG	2a	3201	1/1	0.83	0.39	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1827	1/1	0.91	0.10	-	71,71,71,71	0
56	MG	1A	3886	1/1	0.93	0.35	-	33,33,33,33	0
56	MG	1a	1748	1/1	0.87	0.20	-	52,52,52,52	0
56	MG	1A	3725	1/1	0.87	0.18	-	42,42,42,42	0
56	MG	1O	3001	1/1	0.88	0.26	-	45,45,45,45	0
56	MG	2a	3054	1/1	0.92	0.07	-	89,89,89,89	0
56	MG	1a	1793	1/1	0.92	0.09	-	77,77,77,77	0
56	MG	1A	3881	1/1	0.85	0.10	-	55,55,55,55	0
56	MG	2A	3231	1/1	0.93	0.20	-	45,45,45,45	0
56	MG	1A	3130	1/1	0.85	0.36	-	58,58,58,58	0
56	MG	2A	3451	1/1	0.97	0.17	-	61,61,61,61	0
56	MG	2A	3277	1/1	0.94	0.24	-	41,41,41,41	0
56	MG	1B	202	1/1	0.93	0.19	-	52,52,52,52	0
56	MG	2a	3200	1/1	0.96	0.11	-	49,49,49,49	0
56	MG	1A	3180	1/1	0.94	0.47	-	33,33,33,33	0
56	MG	2a	3020	1/1	0.85	0.16	-	49,49,49,49	0
56	MG	2A	3259	1/1	0.96	0.15	-	72,72,72,72	0
56	MG	2A	3064	1/1	0.94	0.23	-	56,56,56,56	0
56	MG	1a	1764	1/1	0.91	0.44	-	68,68,68,68	0
56	MG	1A	3163	1/1	0.83	0.14	-	32,32,32,32	0
56	MG	1a	1612	1/1	0.92	0.09	-	65,65,65,65	0
56	MG	1a	1788	1/1	0.91	0.64	-	76,76,76,76	0
56	MG	1A	3593	1/1	0.96	0.22	-	35,35,35,35	0
56	MG	2A	3441	1/1	0.93	0.08	-	58,58,58,58	0
56	MG	1A	4013	1/1	0.89	0.23	-	49,49,49,49	0
56	MG	2A	3018	1/1	0.87	0.19	-	50,50,50,50	0
56	MG	1A	3736	1/1	0.96	0.17	-	38,38,38,38	0
56	MG	1A	3072	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	2a	3249	1/1	0.95	0.12	-	61,61,61,61	0
56	MG	1A	3299	1/1	0.92	0.13	-	61,61,61,61	0
56	MG	1a	1628	1/1	0.79	0.15	-	61,61,61,61	0
56	MG	1A	3097	1/1	0.89	0.29	-	55,55,55,55	0
56	MG	1A	3499	1/1	0.81	0.16	-	62,62,62,62	0
56	MG	1B	215	1/1	0.95	0.16	-	31,31,31,31	0
56	MG	1f	3001	1/1	0.65	0.13	-	68,68,68,68	0
56	MG	2A	3102	1/1	0.85	0.15	-	52,52,52,52	0
56	MG	2a	3225	1/1	0.94	0.14	-	59,59,59,59	0
56	MG	2a	3009	1/1	0.97	0.23	-	65,65,65,65	0
56	MG	2a	3050	1/1	0.90	0.41	-	93,93,93,93	0
56	MG	2A	3287	1/1	0.75	0.14	-	56,56,56,56	0
56	MG	2a	3167	1/1	0.89	0.58	-	80,80,80,80	0
56	MG	2A	3353	1/1	0.70	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
56	MG	1A	3023	1/1	0.58	0.19	-	50,50,50,50	0
56	MG	2A	3434	1/1	0.96	0.23	-	63,63,63,63	0
56	MG	1A	3430	1/1	0.90	0.12	-	62,62,62,62	0
56	MG	1A	3410	1/1	0.89	0.14	-	49,49,49,49	0
56	MG	1A	3079	1/1	0.79	0.14	-	58,58,58,58	0
56	MG	2a	3072	1/1	0.69	0.12	-	77,77,77,77	0
56	MG	1A	3549	1/1	0.85	0.19	-	48,48,48,48	0
56	MG	2A	3238	1/1	0.84	0.14	-	60,60,60,60	0
56	MG	1B	212	1/1	0.96	0.20	-	54,54,54,54	0
56	MG	2A	3001	1/1	0.76	0.21	-	45,45,45,45	0
56	MG	2A	3158	1/1	0.88	0.17	-	47,47,47,47	0
56	MG	2A	3035	1/1	0.87	0.12	-	58,58,58,58	0
56	MG	2a	3089	1/1	0.93	0.09	-	66,66,66,66	0
56	MG	1A	3030	1/1	0.95	0.24	-	49,49,49,49	0
56	MG	2A	3333	1/1	0.85	0.16	-	51,51,51,51	0
56	MG	1x	106	1/1	0.87	0.21	-	63,63,63,63	0
56	MG	1a	1743	1/1	0.97	0.11	-	56,56,56,56	0
56	MG	1B	216	1/1	0.99	0.22	-	54,54,54,54	0
56	MG	2A	3113	1/1	0.67	0.17	-	64,64,64,64	0
56	MG	2a	3098	1/1	0.88	0.30	-	50,50,50,50	0
56	MG	2a	3211	1/1	0.95	0.12	-	61,61,61,61	0
56	MG	2a	3224	1/1	0.94	0.17	-	54,54,54,54	0
56	MG	1a	1759	1/1	0.91	0.18	-	70,70,70,70	0
56	MG	1A	3534	1/1	0.86	0.23	-	35,35,35,35	0
56	MG	1A	3943	1/1	0.94	0.17	-	68,68,68,68	0
56	MG	2A	3248	1/1	0.95	0.22	-	56,56,56,56	0
56	MG	1a	1602	1/1	0.86	0.35	-	64,64,64,64	0
56	MG	1A	3820	1/1	0.90	0.11	-	57,57,57,57	0
56	MG	2B	3008	1/1	0.96	0.19	-	47,47,47,47	0
56	MG	1a	1726	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	1A	3642	1/1	0.92	0.19	-	58,58,58,58	0
56	MG	2d	502	1/1	0.96	0.23	-	40,40,40,40	0
56	MG	1A	3494	1/1	0.88	0.34	-	51,51,51,51	0
56	MG	1A	3298	1/1	0.95	0.28	-	50,50,50,50	0
56	MG	2a	3215	1/1	0.92	0.24	-	56,56,56,56	0
56	MG	1A	3274	1/1	0.85	0.21	-	41,41,41,41	0
56	MG	1a	1787	1/1	0.94	0.16	-	58,58,58,58	0
56	MG	1A	3075	1/1	0.92	0.18	-	71,71,71,71	0
56	MG	1A	3062	1/1	0.91	0.13	-	48,48,48,48	0
56	MG	1A	3833	1/1	0.76	0.15	-	78,78,78,78	0
56	MG	1a	1613	1/1	0.97	0.06	-	60,60,60,60	0
56	MG	1A	3026	1/1	0.85	0.14	-	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
56	MG	2A	3061	1/1	0.42	0.27	-	68,68,68,68	0
56	MG	10	106	1/1	0.90	0.37	-	61,61,61,61	0
56	MG	2Q	3001	1/1	0.93	0.33	-	48,48,48,48	0
56	MG	1A	3044	1/1	0.79	1.11	-	45,45,45,45	0
56	MG	1A	3562	1/1	0.93	0.12	-	55,55,55,55	0
56	MG	2A	3166	1/1	0.96	0.26	-	49,49,49,49	0
56	MG	1A	3348	1/1	0.97	0.13	-	47,47,47,47	0
56	MG	1A	3372	1/1	0.81	0.53	-	57,57,57,57	0
56	MG	2A	3403	1/1	0.92	0.18	-	62,62,62,62	0
56	MG	2A	3033	1/1	0.92	0.32	-	61,61,61,61	0
56	MG	1A	3279	1/1	0.93	0.19	-	28,28,28,28	0
56	MG	1A	3211	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	1A	3399	1/1	0.70	0.31	-	58,58,58,58	0
56	MG	1A	3149	1/1	0.85	0.16	-	55,55,55,55	0
56	MG	1A	3743	1/1	0.96	0.38	-	57,57,57,57	0
56	MG	2a	3171	1/1	0.94	0.11	-	68,68,68,68	0
56	MG	1a	1826	1/1	0.97	0.15	-	36,36,36,36	0
56	MG	2A	3253	1/1	0.96	0.24	-	43,43,43,43	0
56	MG	2A	3467	1/1	0.97	0.11	-	46,46,46,46	0
56	MG	2A	3021	1/1	0.88	0.28	-	58,58,58,58	0
56	MG	2A	3077	1/1	0.94	0.20	-	64,64,64,64	0
56	MG	1a	1747	1/1	0.97	0.09	-	56,56,56,56	0
56	MG	2A	3165	1/1	0.93	0.22	-	49,49,49,49	0
56	MG	1o	3002	1/1	0.95	0.11	-	44,44,44,44	0
56	MG	1A	3239	1/1	0.91	0.56	-	36,36,36,36	0
56	MG	2A	3419	1/1	0.93	0.07	-	56,56,56,56	0
56	MG	1A	3585	1/1	0.97	0.13	-	51,51,51,51	0
56	MG	1A	3346	1/1	0.92	0.10	-	63,63,63,63	0
56	MG	2B	3009	1/1	0.92	0.23	-	63,63,63,63	0
56	MG	1a	1848	1/1	0.94	0.23	-	57,57,57,57	0
56	MG	1A	3448	1/1	0.87	0.17	-	49,49,49,49	0
56	MG	2A	3439	1/1	0.95	0.08	-	68,68,68,68	0
56	MG	2A	3169	1/1	0.84	0.25	-	33,33,33,33	0
56	MG	2A	3055	1/1	0.89	0.30	-	40,40,40,40	0
56	MG	1A	3525	1/1	0.89	0.15	-	60,60,60,60	0
56	MG	2A	3290	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	2A	3036	1/1	0.70	0.10	-	74,74,74,74	0
56	MG	1A	3479	1/1	0.82	0.41	-	38,38,38,38	0
56	MG	2a	3001	1/1	0.80	0.19	-	60,60,60,60	0
56	MG	1A	3349	1/1	0.70	0.17	-	73,73,73,73	0
56	MG	2A	3382	1/1	0.97	0.11	-	42,42,42,42	0
56	MG	2A	3490	1/1	0.90	0.30	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3184	1/1	0.96	0.20	-	52,52,52,52	0
56	MG	1A	3949	1/1	0.95	0.15	-	48,48,48,48	0
56	MG	1A	3377	1/1	0.77	0.24	-	61,61,61,61	0
56	MG	1A	3051	1/1	0.96	0.61	-	50,50,50,50	0
56	MG	1A	3389	1/1	0.96	0.61	-	45,45,45,45	0
56	MG	2a	3080	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	2a	3056	1/1	0.76	0.12	-	85,85,85,85	0
56	MG	1A	3379	1/1	0.85	0.28	-	61,61,61,61	0
56	MG	2a	3239	1/1	0.97	0.05	-	76,76,76,76	0
56	MG	2A	3362	1/1	0.97	0.17	-	57,57,57,57	0
56	MG	2A	3524	1/1	0.91	0.11	-	41,41,41,41	0
56	MG	2A	3254	1/1	0.79	0.28	-	40,40,40,40	0
56	MG	1A	3687	1/1	0.99	0.13	-	48,48,48,48	0
56	MG	1A	3213	1/1	0.89	0.13	-	33,33,33,33	0
56	MG	1A	3654	1/1	0.86	0.18	-	67,67,67,67	0
56	MG	1A	3688	1/1	0.98	0.16	-	41,41,41,41	0
56	MG	1A	3412	1/1	0.93	0.56	-	45,45,45,45	0
56	MG	1a	1770	1/1	0.94	0.07	-	67,67,67,67	0
56	MG	1A	3513	1/1	0.75	0.34	-	57,57,57,57	0
56	MG	2A	3223	1/1	0.96	0.42	-	50,50,50,50	0
56	MG	2a	3067	1/1	0.91	0.10	-	88,88,88,88	0
56	MG	2A	3360	1/1	0.92	0.14	-	58,58,58,58	0
56	MG	1A	3320	1/1	0.87	0.06	-	93,93,93,93	0
56	MG	2A	3177	1/1	0.90	0.22	-	48,48,48,48	0
56	MG	2A	3116	1/1	0.93	0.12	-	47,47,47,47	0
56	MG	2a	3178	1/1	0.94	0.15	-	59,59,59,59	0
56	MG	1A	3269	1/1	0.98	0.11	-	36,36,36,36	0
56	MG	1A	3814	1/1	0.96	0.24	-	56,56,56,56	0
56	MG	2A	3456	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	2B	3003	1/1	0.78	0.21	-	73,73,73,73	0
56	MG	2A	3034	1/1	0.82	0.25	-	54,54,54,54	0
56	MG	2a	3182	1/1	0.97	0.15	-	51,51,51,51	0
56	MG	2A	3190	1/1	0.92	0.20	-	54,54,54,54	0
56	MG	1A	3189	1/1	0.92	0.18	-	39,39,39,39	0
56	MG	1A	3577	1/1	0.97	0.23	-	60,60,60,60	0
56	MG	2A	3082	1/1	0.88	0.19	-	41,41,41,41	0
56	MG	1A	3363	1/1	0.78	0.18	-	68,68,68,68	0
56	MG	1A	3929	1/1	0.89	0.20	-	58,58,58,58	0
56	MG	2A	3098	1/1	0.90	0.12	-	51,51,51,51	0
56	MG	1N	3005	1/1	0.94	0.10	-	51,51,51,51	0
56	MG	1a	1807	1/1	0.83	0.17	-	60,60,60,60	0
56	MG	2A	3202	1/1	0.96	0.16	-	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
56	MG	1A	3234	1/1	0.92	0.10	-	43,43,43,43	0
56	MG	2a	3096	1/1	0.68	0.22	-	80,80,80,80	0
56	MG	2a	3119	1/1	0.96	0.28	-	56,56,56,56	0
56	MG	1T	202	1/1	0.84	0.13	-	55,55,55,55	0
56	MG	1T	205	1/1	0.89	0.27	-	65,65,65,65	0
56	MG	1a	1703	1/1	0.80	0.14	-	62,62,62,62	0
56	MG	1A	3428	1/1	0.88	0.11	-	65,65,65,65	0
56	MG	1a	1685	1/1	0.94	0.16	-	53,53,53,53	0
56	MG	1A	3667	1/1	0.96	0.13	-	49,49,49,49	0
56	MG	2A	3187	1/1	0.82	1.30	-	49,49,49,49	0
56	MG	2A	3104	1/1	0.82	0.56	-	54,54,54,54	0
56	MG	2A	3275	1/1	0.95	0.12	-	60,60,60,60	0
56	MG	1D	304	1/1	0.71	0.52	-	58,58,58,58	0
56	MG	1a	1695	1/1	0.92	0.23	-	50,50,50,50	0
56	MG	2A	3013	1/1	0.84	0.17	-	68,68,68,68	0
56	MG	1a	1615	1/1	0.90	0.18	-	55,55,55,55	0
56	MG	1A	3120	1/1	0.81	0.50	-	41,41,41,41	0
56	MG	2A	3411	1/1	0.93	0.14	-	64,64,64,64	0
56	MG	2A	3109	1/1	0.95	0.15	-	64,64,64,64	0
56	MG	1A	3330	1/1	0.84	0.13	-	41,41,41,41	0
56	MG	2A	3144	1/1	0.91	0.31	-	51,51,51,51	0
56	MG	1A	3544	1/1	0.89	0.13	-	36,36,36,36	0
56	MG	1A	3223	1/1	0.97	0.24	-	33,33,33,33	0
56	MG	1A	3680	1/1	0.98	0.10	-	42,42,42,42	0
56	MG	1a	1642	1/1	0.84	0.12	-	69,69,69,69	0
56	MG	1a	1658	1/1	0.91	0.35	-	67,67,67,67	0
56	MG	1A	3115	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	2A	3010	1/1	0.89	0.10	-	56,56,56,56	0
56	MG	1A	3114	1/1	0.93	0.14	-	52,52,52,52	0
56	MG	2a	3006	1/1	0.84	0.10	-	62,62,62,62	0
56	MG	1A	3944	1/1	0.90	0.08	-	68,68,68,68	0
56	MG	2A	3288	1/1	0.89	0.14	-	57,57,57,57	0
56	MG	1A	3406	1/1	0.88	0.10	-	50,50,50,50	0
56	MG	1a	1860	1/1	0.94	0.21	-	55,55,55,55	0
56	MG	2A	3343	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	2A	3181	1/1	0.96	0.10	-	39,39,39,39	0
56	MG	1d	503	1/1	0.99	0.11	-	52,52,52,52	0
56	MG	1A	3474	1/1	0.91	0.37	-	39,39,39,39	0
56	MG	1A	3693	1/1	0.98	0.17	-	21,21,21,21	0
56	MG	1A	3595	1/1	0.95	0.31	-	56,56,56,56	0
56	MG	2A	3463	1/1	0.95	0.04	-	57,57,57,57	0
56	MG	1a	1830	1/1	0.96	0.25	-	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
56	MG	1a	1866	1/1	0.95	0.17	-	61,61,61,61	0
56	MG	1A	3488	1/1	0.89	0.13	-	65,65,65,65	0
56	MG	1A	3846	1/1	0.85	0.08	-	78,78,78,78	0
56	MG	2A	3281	1/1	0.94	0.22	-	59,59,59,59	0
56	MG	1A	3038	1/1	0.92	0.10	-	52,52,52,52	0
56	MG	1A	3703	1/1	0.86	0.15	-	49,49,49,49	0
56	MG	2A	3086	1/1	0.83	0.30	-	49,49,49,49	0
56	MG	1A	3368	1/1	0.90	0.24	-	25,25,25,25	0
56	MG	2a	3097	1/1	0.90	0.21	-	71,71,71,71	0
56	MG	2A	3474	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	1a	1823	1/1	0.94	0.18	-	69,69,69,69	0
56	MG	1A	3806	1/1	0.91	0.28	-	61,61,61,61	0
56	MG	1A	3644	1/1	0.96	0.20	-	19,19,19,19	0
56	MG	2a	3023	1/1	0.82	0.17	-	65,65,65,65	0
56	MG	2A	3400	1/1	0.90	0.49	-	48,48,48,48	0
56	MG	1A	3583	1/1	0.83	0.10	-	55,55,55,55	0
56	MG	2A	3501	1/1	0.68	0.16	-	85,85,85,85	0
56	MG	2A	3272	1/1	0.90	0.23	-	46,46,46,46	0
56	MG	1z	101	1/1	0.77	0.40	-	76,76,76,76	0
56	MG	2A	3341	1/1	0.86	0.17	-	52,52,52,52	0
56	MG	1a	1621	1/1	0.86	0.23	-	68,68,68,68	0
56	MG	2N	8001	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	2a	3197	1/1	0.95	0.12	-	58,58,58,58	0
56	MG	2a	3195	1/1	0.97	0.06	-	43,43,43,43	0
56	MG	1A	3109	1/1	0.94	0.31	-	55,55,55,55	0
56	MG	1A	3307	1/1	0.95	0.30	-	59,59,59,59	0
56	MG	2A	3271	1/1	0.83	0.15	-	27,27,27,27	0
56	MG	1A	3830	1/1	0.93	0.26	-	63,63,63,63	0
56	MG	1A	3134	1/1	0.93	0.51	-	45,45,45,45	0
56	MG	1A	3397	1/1	0.91	0.71	-	49,49,49,49	0
56	MG	1A	3237	1/1	0.94	0.13	-	46,46,46,46	0
56	MG	1a	1698	1/1	0.92	0.14	-	55,55,55,55	0
56	MG	2A	3230	1/1	0.93	0.09	-	47,47,47,47	0
56	MG	2a	3246	1/1	0.94	0.07	-	62,62,62,62	0
56	MG	1A	3090	1/1	0.94	0.43	-	53,53,53,53	0
56	MG	1A	3214	1/1	0.96	0.25	-	60,60,60,60	0
56	MG	1A	3777	1/1	0.91	0.13	-	49,49,49,49	0
56	MG	1D	301	1/1	0.89	0.18	-	56,56,56,56	0
56	MG	1A	3381	1/1	0.89	0.17	-	47,47,47,47	0
56	MG	2a	3156	1/1	0.76	0.10	-	72,72,72,72	0
56	MG	2a	3141	1/1	0.87	0.18	-	73,73,73,73	0
56	MG	1A	3640	1/1	0.86	0.20	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3942	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	2A	3532	1/1	0.96	0.09	-	51,51,51,51	0
56	MG	2A	3114	1/1	0.84	0.13	-	57,57,57,57	0
56	MG	2A	3005	1/1	0.87	0.13	-	54,54,54,54	0
56	MG	2A	3060	1/1	0.95	0.14	-	43,43,43,43	0
56	MG	2A	3530	1/1	0.84	0.12	-	46,46,46,46	0
56	MG	2a	3175	1/1	0.91	0.08	-	62,62,62,62	0
56	MG	1A	3511	1/1	0.81	0.13	-	76,76,76,76	0
56	MG	1A	3587	1/1	0.97	0.11	-	40,40,40,40	0
56	MG	1a	1778	1/1	0.93	0.26	-	57,57,57,57	0
56	MG	2A	3170	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	1A	3018	1/1	0.77	0.12	-	59,59,59,59	0
56	MG	1a	1854	1/1	0.83	0.09	-	82,82,82,82	0
56	MG	1a	1686	1/1	0.90	0.17	-	49,49,49,49	0
56	MG	1A	3469	1/1	0.96	0.13	-	49,49,49,49	0
56	MG	1A	3378	1/1	0.86	0.49	-	69,69,69,69	0
56	MG	1A	3647	1/1	0.83	0.21	-	74,74,74,74	0
56	MG	2a	3064	1/1	0.94	0.08	-	77,77,77,77	0
56	MG	1A	3231	1/1	0.94	1.03	-	49,49,49,49	0
56	MG	2a	3091	1/1	0.81	0.25	-	61,61,61,61	0
56	MG	2A	3433	1/1	0.90	0.14	-	65,65,65,65	0
56	MG	1a	1694	1/1	0.79	0.16	-	78,78,78,78	0
56	MG	1A	3003	1/1	0.91	0.18	-	46,46,46,46	0
56	MG	1A	3424	1/1	0.95	0.15	-	61,61,61,61	0
56	MG	1A	3082	1/1	0.67	0.17	-	56,56,56,56	0
56	MG	2a	3044	1/1	0.84	0.21	-	71,71,71,71	0
56	MG	1a	1761	1/1	0.92	0.21	-	86,86,86,86	0
56	MG	1A	3600	1/1	0.86	0.20	-	54,54,54,54	0
56	MG	2A	3087	1/1	0.82	0.21	-	59,59,59,59	0
56	MG	1a	1601	1/1	0.93	0.10	-	53,53,53,53	0
56	MG	2A	3477	1/1	0.91	0.19	-	57,57,57,57	0
56	MG	1A	3121	1/1	0.88	0.85	-	38,38,38,38	0
56	MG	1a	1853	1/1	0.96	0.14	-	57,57,57,57	0
56	MG	1A	3455	1/1	0.90	0.16	-	63,63,63,63	0
56	MG	1A	3328	1/1	0.82	0.11	-	65,65,65,65	0
56	MG	2A	3323	1/1	0.89	0.10	-	48,48,48,48	0
56	MG	1A	3891	1/1	0.94	0.08	-	62,62,62,62	0
56	MG	1A	3254	1/1	0.92	0.33	-	34,34,34,34	0
56	MG	1A	3981	1/1	0.91	0.24	-	50,50,50,50	0
56	MG	1A	3029	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	2A	3032	1/1	0.93	0.14	-	53,53,53,53	0
56	MG	2A	3057	1/1	0.95	0.23	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1742	1/1	0.90	0.18	-	51,51,51,51	0
56	MG	13	102	1/1	0.87	0.14	-	56,56,56,56	0
56	MG	1A	3063	1/1	0.98	0.05	-	53,53,53,53	0
56	MG	2A	3422	1/1	0.98	0.30	-	57,57,57,57	0
56	MG	2A	3176	1/1	0.91	0.14	-	43,43,43,43	0
56	MG	1A	3491	1/1	0.94	0.42	-	61,61,61,61	0
56	MG	1a	1786	1/1	0.92	0.52	-	92,92,92,92	0
56	MG	1A	3503	1/1	0.87	0.11	-	62,62,62,62	0
56	MG	1a	1740	1/1	0.98	0.07	-	47,47,47,47	0
56	MG	2a	3263	1/1	0.96	0.23	-	71,71,71,71	0
56	MG	1a	1626	1/1	0.76	0.12	-	80,80,80,80	0
56	MG	1A	3116	1/1	0.95	0.29	-	41,41,41,41	0
56	MG	1A	3117	1/1	0.90	0.19	-	48,48,48,48	0
56	MG	1A	3133	1/1	0.88	0.33	-	59,59,59,59	0
56	MG	1A	3799	1/1	0.98	0.33	-	42,42,42,42	0
56	MG	2a	3157	1/1	0.81	0.14	-	74,74,74,74	0
56	MG	1A	3524	1/1	0.92	0.16	-	54,54,54,54	0
56	MG	15	105	1/1	0.81	0.10	-	49,49,49,49	0
56	MG	1A	3081	1/1	0.93	0.30	-	58,58,58,58	0
56	MG	1A	3746	1/1	0.97	0.18	-	7,7,7,7	0
56	MG	1a	1648	1/1	0.95	0.11	-	47,47,47,47	0
56	MG	1A	3883	1/1	0.84	0.59	-	58,58,58,58	0
56	MG	1A	3059	1/1	0.90	0.13	-	46,46,46,46	0
56	MG	1A	3358	1/1	0.90	0.70	-	44,44,44,44	0
56	MG	1A	3014	1/1	0.88	0.33	-	53,53,53,53	0
56	MG	2a	3204	1/1	0.92	0.14	-	64,64,64,64	0
56	MG	1a	1762	1/1	0.93	0.07	-	89,89,89,89	0
56	MG	2A	3448	1/1	0.87	0.14	-	56,56,56,56	0
56	MG	1A	3529	1/1	0.98	0.24	-	48,48,48,48	0
56	MG	1A	3571	1/1	0.99	0.22	-	25,25,25,25	0
56	MG	1A	3628	1/1	0.94	0.18	-	28,28,28,28	0
56	MG	2A	3069	1/1	0.93	0.11	-	37,37,37,37	0
56	MG	2a	3172	1/1	0.96	0.14	-	60,60,60,60	0
56	MG	2a	3199	1/1	0.99	0.16	-	62,62,62,62	0
56	MG	1P	201	1/1	0.69	0.40	-	47,47,47,47	0
56	MG	2A	3347	1/1	0.92	0.10	-	60,60,60,60	0
56	MG	1A	3950	1/1	0.96	0.16	-	41,41,41,41	0
56	MG	2A	3258	1/1	0.74	0.13	-	30,30,30,30	0
56	MG	2a	3037	1/1	0.87	0.15	-	53,53,53,53	0
56	MG	1N	3004	1/1	0.92	0.23	-	36,36,36,36	0
56	MG	2A	3084	1/1	0.93	0.20	-	54,54,54,54	0
56	MG	2A	3496	1/1	0.91	0.08	-	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
56	MG	1A	3300	1/1	0.91	0.14	-	54,54,54,54	0
56	MG	1A	3669	1/1	0.95	0.11	-	46,46,46,46	0
56	MG	2a	3137	1/1	0.92	0.09	-	67,67,67,67	0
56	MG	1A	3064	1/1	0.93	0.41	-	40,40,40,40	0
56	MG	2A	3242	1/1	0.97	0.15	-	52,52,52,52	0
56	MG	1A	3971	1/1	0.91	0.10	-	62,62,62,62	0
56	MG	1A	3782	1/1	0.96	0.17	-	34,34,34,34	0
56	MG	1A	3302	1/1	0.89	0.48	-	41,41,41,41	0
56	MG	1A	3017	1/1	0.93	0.15	-	40,40,40,40	0
56	MG	1A	3477	1/1	0.94	0.29	-	66,66,66,66	0
56	MG	2D	304	1/1	0.88	0.30	-	42,42,42,42	0
56	MG	1B	204	1/1	0.79	0.28	-	54,54,54,54	0
56	MG	1A	3889	1/1	0.86	0.37	-	60,60,60,60	0
56	MG	1a	1608	1/1	0.85	0.28	-	59,59,59,59	0
56	MG	1A	3183	1/1	0.85	0.73	-	44,44,44,44	0
56	MG	2a	3154	1/1	0.95	0.45	-	87,87,87,87	0
56	MG	1A	3382	1/1	0.98	0.08	-	40,40,40,40	0
56	MG	1A	3353	1/1	0.93	0.24	-	58,58,58,58	0
56	MG	2A	3545	1/1	0.98	0.19	-	39,39,39,39	0
56	MG	1A	3904	1/1	0.96	0.12	-	27,27,27,27	0
56	MG	1A	3946	1/1	0.97	0.23	-	41,41,41,41	0
56	MG	2A	3397	1/1	0.91	0.17	-	66,66,66,66	0
56	MG	1A	3718	1/1	0.91	0.13	-	41,41,41,41	0
56	MG	2a	3024	1/1	0.87	0.17	-	76,76,76,76	0
56	MG	1A	3333	1/1	0.91	0.26	-	70,70,70,70	0
56	MG	1A	3369	1/1	0.97	0.51	-	40,40,40,40	0
56	MG	2A	3260	1/1	0.94	0.14	-	72,72,72,72	0
56	MG	1A	3388	1/1	0.87	0.10	-	53,53,53,53	0
56	MG	2A	3365	1/1	0.62	0.13	-	63,63,63,63	0
56	MG	1a	1831	1/1	0.96	0.12	-	54,54,54,54	0
56	MG	2a	3100	1/1	0.77	0.15	-	66,66,66,66	0
56	MG	1A	3671	1/1	0.94	0.32	-	56,56,56,56	0
56	MG	1A	3057	1/1	0.66	0.70	-	50,50,50,50	0
56	MG	1A	3678	1/1	0.95	0.16	-	61,61,61,61	0
56	MG	1V	201	1/1	0.89	0.30	-	45,45,45,45	0
56	MG	1A	3523	1/1	0.82	0.17	-	59,59,59,59	0
56	MG	2A	3120	1/1	0.99	0.25	-	45,45,45,45	0
56	MG	2a	3043	1/1	0.65	0.20	-	65,65,65,65	0
56	MG	1A	3560	1/1	0.70	0.13	-	45,45,45,45	0
56	MG	1A	3584	1/1	0.95	0.17	-	33,33,33,33	0
56	MG	2A	3311	1/1	0.93	0.21	-	42,42,42,42	0
56	MG	1A	4021	1/1	0.95	0.12	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1e	3001	1/1	0.92	0.13	-	69,69,69,69	0
56	MG	2a	3219	1/1	0.94	0.14	-	52,52,52,52	0
56	MG	2A	3294	1/1	0.89	0.17	-	37,37,37,37	0
56	MG	1A	3245	1/1	0.94	0.14	-	49,49,49,49	0
56	MG	1A	3440	1/1	0.80	0.10	-	66,66,66,66	0
56	MG	1A	3451	1/1	0.80	0.88	-	66,66,66,66	0
56	MG	2a	3004	1/1	0.92	0.16	-	46,46,46,46	0
56	MG	1A	3675	1/1	0.82	0.11	-	79,79,79,79	0
56	MG	2A	3174	1/1	0.85	0.12	-	45,45,45,45	0
56	MG	1a	1705	1/1	0.74	0.09	-	73,73,73,73	0
56	MG	2A	3065	1/1	0.91	0.12	-	35,35,35,35	0
56	MG	1A	3902	1/1	0.94	0.10	-	45,45,45,45	0
56	MG	1A	3500	1/1	0.92	0.23	-	55,55,55,55	0
56	MG	2A	3045	1/1	0.92	0.46	-	48,48,48,48	0
56	MG	1B	219	1/1	0.87	0.07	-	60,60,60,60	0
56	MG	1a	1781	1/1	0.91	0.28	-	46,46,46,46	0
56	MG	2a	3060	1/1	0.93	0.20	-	86,86,86,86	0
56	MG	1A	3657	1/1	0.88	0.17	-	49,49,49,49	0
56	MG	2a	3095	1/1	0.95	0.23	-	45,45,45,45	0
56	MG	1A	3362	1/1	0.89	0.18	-	56,56,56,56	0
56	MG	2A	3185	1/1	0.90	0.19	-	52,52,52,52	0
56	MG	2A	3192	1/1	0.99	0.14	-	29,29,29,29	0
56	MG	1A	3019	1/1	0.94	0.13	-	49,49,49,49	0
56	MG	1A	3435	1/1	0.97	0.12	-	56,56,56,56	0
56	MG	2A	3103	1/1	0.79	0.37	-	53,53,53,53	0
56	MG	1A	3924	1/1	0.73	0.14	-	66,66,66,66	0
56	MG	1A	3065	1/1	0.89	0.34	-	49,49,49,49	0
56	MG	2A	3307	1/1	0.94	0.20	-	35,35,35,35	0
56	MG	1A	3692	1/1	0.94	0.14	-	33,33,33,33	0
56	MG	1A	3762	1/1	0.99	0.16	-	45,45,45,45	0
56	MG	1A	3875	1/1	0.85	0.30	-	83,83,83,83	0
56	MG	1A	3126	1/1	0.64	0.16	-	53,53,53,53	0
56	MG	1A	3625	1/1	0.91	0.15	-	22,22,22,22	0
56	MG	1A	3303	1/1	0.89	0.30	-	63,63,63,63	0
56	MG	2a	3047	1/1	0.83	0.21	-	63,63,63,63	0
56	MG	2a	3008	1/1	0.73	0.19	-	67,67,67,67	0
56	MG	1A	3557	1/1	0.93	0.19	-	31,31,31,31	0
56	MG	1A	3285	1/1	0.95	0.20	-	54,54,54,54	0
56	MG	2A	3053	1/1	0.91	0.14	-	55,55,55,55	0
56	MG	2A	3117	1/1	0.75	0.14	-	53,53,53,53	0
56	MG	1A	3661	1/1	0.93	0.19	-	36,36,36,36	0
56	MG	1W	3004	1/1	0.95	0.46	-	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
56	MG	1A	3572	1/1	0.97	0.17	-	50,50,50,50	0
56	MG	2A	3505	1/1	0.89	0.15	-	57,57,57,57	0
56	MG	2D	306	1/1	0.94	0.08	-	68,68,68,68	0
56	MG	2A	3161	1/1	0.97	0.24	-	32,32,32,32	0
56	MG	1A	3318	1/1	0.90	0.29	-	52,52,52,52	0
56	MG	2a	3181	1/1	0.89	0.18	-	47,47,47,47	0
56	MG	1A	3754	1/1	0.97	0.18	-	18,18,18,18	0
56	MG	2A	3228	1/1	0.81	0.19	-	57,57,57,57	0
56	MG	1A	3141	1/1	0.90	0.19	-	66,66,66,66	0
56	MG	1A	3281	1/1	0.84	0.42	-	53,53,53,53	0
56	MG	1A	3340	1/1	0.94	0.24	-	47,47,47,47	0
56	MG	2A	3462	1/1	0.98	0.22	-	60,60,60,60	0
56	MG	2a	3086	1/1	0.82	0.21	-	64,64,64,64	0
56	MG	1A	3486	1/1	0.82	0.14	-	67,67,67,67	0
56	MG	1A	3232	1/1	0.98	0.61	-	43,43,43,43	0
56	MG	2A	3269	1/1	0.86	0.14	-	41,41,41,41	0
56	MG	1A	3913	1/1	0.86	0.16	-	64,64,64,64	0
56	MG	1A	3840	1/1	0.87	0.17	-	63,63,63,63	0
56	MG	2a	3170	1/1	0.81	0.14	-	77,77,77,77	0
56	MG	1a	1699	1/1	0.94	0.07	-	71,71,71,71	0
56	MG	1a	1676	1/1	0.65	0.11	-	74,74,74,74	0
56	MG	1A	3533	1/1	0.91	0.22	-	51,51,51,51	0
56	MG	2a	3216	1/1	0.86	0.25	-	56,56,56,56	0
56	MG	2A	3361	1/1	0.88	0.20	-	54,54,54,54	0
56	MG	2a	3166	1/1	0.90	0.13	-	66,66,66,66	0
56	MG	1A	3936	1/1	0.78	0.19	-	64,64,64,64	0
56	MG	1A	3106	1/1	0.80	0.17	-	64,64,64,64	0
56	MG	1a	1772	1/1	0.94	0.23	-	78,78,78,78	0
56	MG	1A	3343	1/1	0.92	0.18	-	77,77,77,77	0
56	MG	1A	3416	1/1	0.91	0.12	-	60,60,60,60	0
56	MG	1A	3228	1/1	0.89	0.15	-	59,59,59,59	0
56	MG	2a	3226	1/1	0.97	0.07	-	58,58,58,58	0
56	MG	1A	3002	1/1	0.77	0.25	-	53,53,53,53	0
56	MG	2A	3224	1/1	0.89	0.13	-	42,42,42,42	0
56	MG	2A	3041	1/1	0.84	0.41	-	53,53,53,53	0
56	MG	1A	3921	1/1	0.91	0.26	-	55,55,55,55	0
56	MG	1A	3787	1/1	0.93	0.14	-	74,74,74,74	0
56	MG	2A	3243	1/1	0.94	0.17	-	63,63,63,63	0
56	MG	2A	3091	1/1	0.76	0.23	-	49,49,49,49	0
56	MG	2A	3355	1/1	0.94	0.20	-	73,73,73,73	0
56	MG	1A	3335	1/1	0.96	0.15	-	55,55,55,55	0
56	MG	2A	3440	1/1	0.94	0.29	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3178	1/1	0.90	0.09	-	34,34,34,34	0
56	MG	1A	3436	1/1	0.94	0.17	-	61,61,61,61	0
56	MG	1a	1654	1/1	0.89	0.13	-	78,78,78,78	0
56	MG	1A	3796	1/1	0.99	0.12	-	16,16,16,16	0
56	MG	1A	3008	1/1	0.92	0.46	-	58,58,58,58	0
56	MG	1A	3898	1/1	0.94	0.15	-	25,25,25,25	0
56	MG	2A	3249	1/1	0.89	0.14	-	59,59,59,59	0
56	MG	2A	3543	1/1	0.94	0.21	-	56,56,56,56	0
56	MG	1A	3207	1/1	0.90	0.10	-	30,30,30,30	0
56	MG	1A	3497	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	1A	3959	1/1	0.77	0.08	-	79,79,79,79	0
56	MG	1A	3011	1/1	0.95	0.10	-	67,67,67,67	0
56	MG	1N	3003	1/1	0.88	0.20	-	42,42,42,42	0
56	MG	2a	3101	1/1	0.95	0.16	-	53,53,53,53	0
56	MG	1A	3015	1/1	0.97	0.10	-	52,52,52,52	0
56	MG	2A	3101	1/1	0.92	0.23	-	57,57,57,57	0
56	MG	1k	3001	1/1	0.64	0.17	-	70,70,70,70	0
56	MG	1A	3252	1/1	0.95	0.15	-	28,28,28,28	0
56	MG	1A	3892	1/1	0.97	0.15	-	43,43,43,43	0
56	MG	1A	3454	1/1	0.93	0.48	-	66,66,66,66	0
56	MG	2A	3506	1/1	0.94	0.33	-	56,56,56,56	0
56	MG	1A	3794	1/1	0.94	0.14	-	68,68,68,68	0
56	MG	1A	3031	1/1	0.80	0.36	-	61,61,61,61	0
56	MG	1A	3140	1/1	0.92	0.41	-	62,62,62,62	0
56	MG	2a	3159	1/1	0.72	0.20	-	85,85,85,85	0
56	MG	2A	3237	1/1	0.95	0.15	-	41,41,41,41	0
56	MG	2a	3160	1/1	0.92	0.25	-	74,74,74,74	0
56	MG	2O	201	1/1	0.88	0.10	-	48,48,48,48	0
56	MG	2A	3412	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	1a	1618	1/1	0.86	0.12	-	64,64,64,64	0
56	MG	1a	1674	1/1	0.94	0.13	-	54,54,54,54	0
56	MG	2A	3510	1/1	0.81	0.15	-	34,34,34,34	0
56	MG	1A	3046	1/1	0.92	0.32	-	65,65,65,65	0
56	MG	1A	3554	1/1	0.95	0.14	-	80,80,80,80	0
56	MG	2A	3160	1/1	0.91	0.21	-	52,52,52,52	0
56	MG	2a	3074	1/1	0.99	0.18	-	74,74,74,74	0
56	MG	1a	1702	1/1	0.79	0.34	-	82,82,82,82	0
56	MG	2a	3151	1/1	0.93	0.16	-	92,92,92,92	0
56	MG	2A	3138	1/1	0.90	0.14	-	54,54,54,54	0
56	MG	1N	3001	1/1	0.91	0.27	-	42,42,42,42	0
56	MG	1A	3124	1/1	0.83	0.58	-	56,56,56,56	0
56	MG	1x	102	1/1	0.90	0.30	-	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
56	MG	1G	3003	1/1	0.91	0.16	-	45,45,45,45	0
56	MG	1A	3712	1/1	0.94	0.14	-	43,43,43,43	0
56	MG	2A	3305	1/1	0.90	0.12	-	42,42,42,42	0
56	MG	2A	3431	1/1	0.98	0.19	-	68,68,68,68	0
56	MG	2a	3112	1/1	0.95	0.13	-	45,45,45,45	0
56	MG	1P	204	1/1	0.94	0.12	-	47,47,47,47	0
56	MG	2A	3483	1/1	0.77	0.18	-	54,54,54,54	0
56	MG	1a	1777	1/1	0.91	0.24	-	28,28,28,28	0
56	MG	1A	3831	1/1	0.94	0.15	-	70,70,70,70	0
56	MG	1B	213	1/1	0.81	0.18	-	110,110,110,110	0
56	MG	2F	302	1/1	0.93	0.21	-	47,47,47,47	0
56	MG	2A	3544	1/1	0.93	0.18	-	45,45,45,45	0
56	MG	1a	1653	1/1	0.91	0.13	-	60,60,60,60	0
56	MG	2a	3051	1/1	0.89	0.10	-	76,76,76,76	0
56	MG	1A	3370	1/1	0.94	0.13	-	66,66,66,66	0
56	MG	1N	3002	1/1	0.72	0.51	-	48,48,48,48	0
56	MG	1A	3873	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	1a	1819	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	1A	3914	1/1	0.95	0.15	-	38,38,38,38	0
56	MG	1U	201	1/1	0.89	0.19	-	51,51,51,51	0
56	MG	1F	307	1/1	0.68	0.26	-	59,59,59,59	0
56	MG	1A	3439	1/1	0.74	0.12	-	51,51,51,51	0
56	MG	1o	3001	1/1	0.76	0.15	-	74,74,74,74	0
56	MG	2B	3002	1/1	0.86	0.14	-	61,61,61,61	0
56	MG	2A	3118	1/1	0.84	0.21	-	75,75,75,75	0
56	MG	1A	3805	1/1	0.95	0.28	-	41,41,41,41	0
56	MG	2B	3001	1/1	0.60	0.20	-	65,65,65,65	0
56	MG	2a	3106	1/1	0.97	0.22	-	63,63,63,63	0
56	MG	2a	3245	1/1	0.95	0.22	-	62,62,62,62	0
56	MG	1A	3301	1/1	0.86	0.16	-	53,53,53,53	0
56	MG	1A	3083	1/1	0.81	0.33	-	56,56,56,56	0
56	MG	1A	3987	1/1	0.95	0.27	-	38,38,38,38	0
56	MG	2Q	3004	1/1	0.95	0.26	-	42,42,42,42	0
56	MG	1A	3966	1/1	0.82	0.98	-	47,47,47,47	0
56	MG	1A	3594	1/1	0.96	0.11	-	62,62,62,62	0
56	MG	1A	3849	1/1	0.92	0.17	-	73,73,73,73	0
56	MG	1A	3128	1/1	0.85	0.15	-	56,56,56,56	0
56	MG	1a	1696	1/1	0.95	0.16	-	70,70,70,70	0
56	MG	2A	3476	1/1	0.95	0.19	-	33,33,33,33	0
56	MG	1A	3154	1/1	0.91	0.13	-	28,28,28,28	0
56	MG	1A	3060	1/1	0.81	0.55	-	67,67,67,67	0
56	MG	2A	3251	1/1	0.95	0.09	-	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
56	MG	1a	1857	1/1	0.92	0.25	-	73,73,73,73	0
56	MG	1A	3634	1/1	0.94	0.18	-	56,56,56,56	0
56	MG	1A	3341	1/1	0.93	0.10	-	64,64,64,64	0
56	MG	1a	1643	1/1	0.83	0.14	-	76,76,76,76	0
56	MG	1A	3804	1/1	0.93	0.12	-	31,31,31,31	0
56	MG	1A	3100	1/1	0.85	0.12	-	48,48,48,48	0
56	MG	2a	3059	1/1	0.98	0.11	-	83,83,83,83	0
56	MG	18	103	1/1	0.93	0.30	-	52,52,52,52	0
56	MG	2A	3022	1/1	0.89	0.15	-	51,51,51,51	0
56	MG	2a	3148	1/1	0.96	0.07	-	72,72,72,72	0
56	MG	1A	3955	1/1	0.85	0.15	-	63,63,63,63	0
56	MG	2A	3217	1/1	0.85	0.12	-	56,56,56,56	0
56	MG	1a	1619	1/1	0.97	0.23	-	54,54,54,54	0
56	MG	1A	3868	1/1	0.93	0.18	-	44,44,44,44	0
56	MG	1a	1792	1/1	0.83	0.10	-	54,54,54,54	0
56	MG	1A	3238	1/1	0.86	0.98	-	45,45,45,45	0
56	MG	2a	3057	1/1	0.95	0.12	-	96,96,96,96	0
56	MG	1A	3147	1/1	0.92	0.23	-	54,54,54,54	0
56	MG	2A	3083	1/1	0.84	0.14	-	49,49,49,49	0
56	MG	1A	3467	1/1	0.81	0.23	-	71,71,71,71	0
56	MG	1A	3037	1/1	0.89	0.13	-	58,58,58,58	0
56	MG	1a	1660	1/1	0.89	0.14	-	50,50,50,50	0
56	MG	2a	3231	1/1	0.87	0.17	-	75,75,75,75	0
56	MG	1A	3441	1/1	0.92	0.25	-	72,72,72,72	0
56	MG	1A	3582	1/1	0.96	0.16	-	45,45,45,45	0
56	MG	1F	301	1/1	0.89	0.12	-	52,52,52,52	0
56	MG	2A	3047	1/1	0.79	0.21	-	65,65,65,65	0
56	MG	1A	3108	1/1	0.95	0.30	-	56,56,56,56	0
56	MG	1A	3145	1/1	0.49	0.18	-	77,77,77,77	0
56	MG	1A	3176	1/1	0.96	0.86	-	40,40,40,40	0
56	MG	2Q	3002	1/1	0.97	0.13	-	39,39,39,39	0
56	MG	2A	3511	1/1	0.78	0.14	-	52,52,52,52	0
56	MG	2E	302	1/1	0.93	0.15	-	59,59,59,59	0
56	MG	2a	3174	1/1	0.93	0.19	-	69,69,69,69	0
56	MG	1a	1662	1/1	0.87	0.15	-	61,61,61,61	0

## 6.5 Other polymers

There are no such residues in this entry.