



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 26, 2019 – 03:44 AM EDT

PDB ID : 5J4C  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with cisplatin (soaked) and bound to mRNA and A-, P- and E-site tRNAs at 2.8Å resolution  
Authors : Melnikov, S.V.; Soll, D.; Steitz, T.A.; Polikanov, Y.S.  
Deposited on : 2016-03-31  
Resolution : 2.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

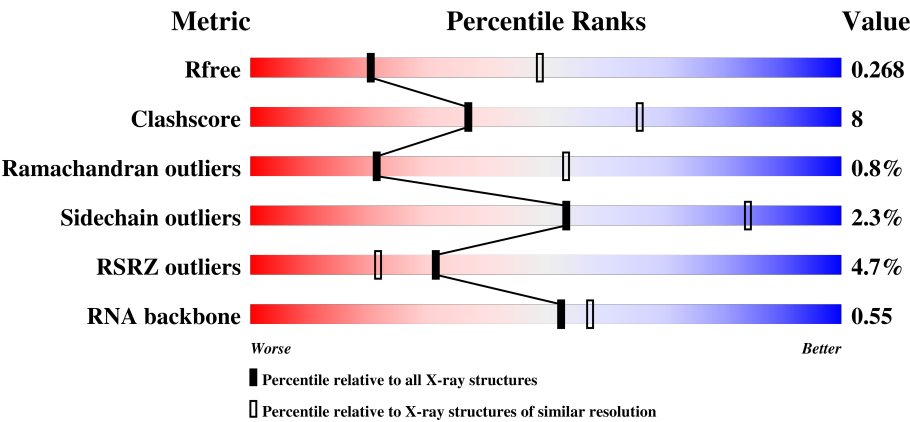
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



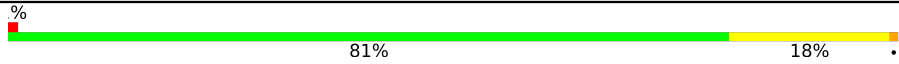
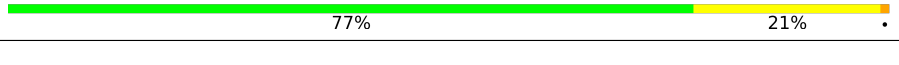
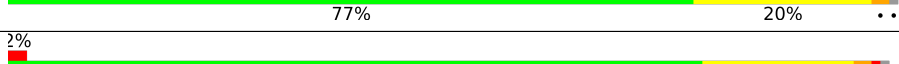
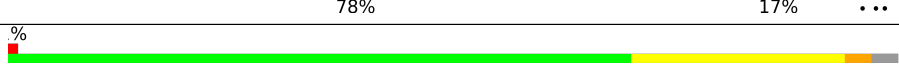
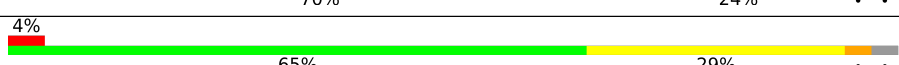


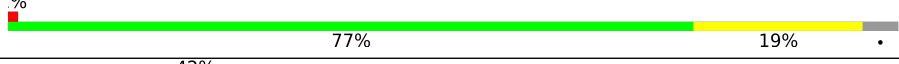
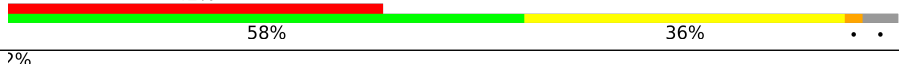


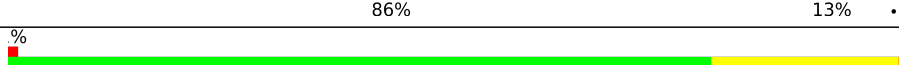
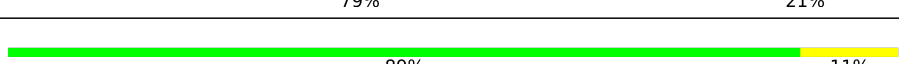
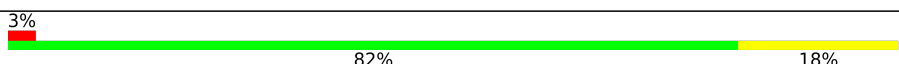
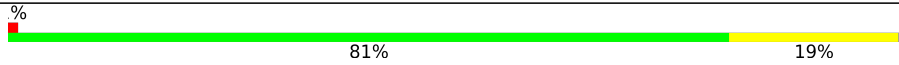

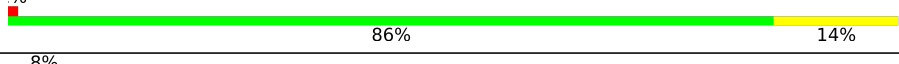




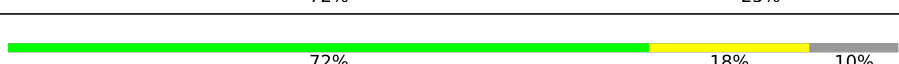



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)
RNA backbone	2636	1064 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div><div>2%</div><div><div></div><div>64%</div><div>28%</div><div>6%</div><div>.</div></div></div>
1	2A	2915	<div><div>%</div><div><div></div><div>53%</div><div>36%</div><div>7%</div><div>.</div></div></div>
2	1B	121	<div><div></div><div><div></div><div>66%</div><div>31%</div><div>...</div></div></div>
2	2B	121	<div><div>%</div><div><div></div><div>49%</div><div>40%</div><div>11%</div><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	
















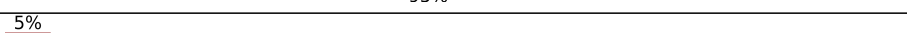
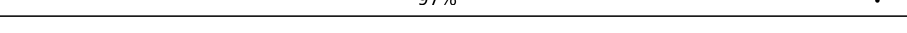


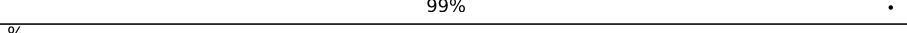
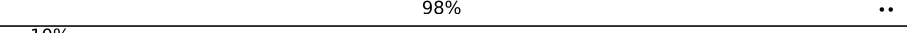
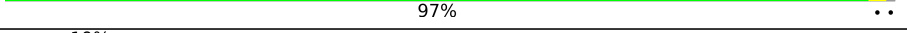
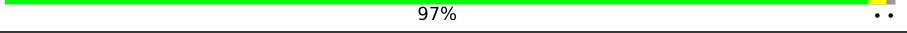
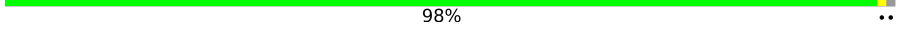
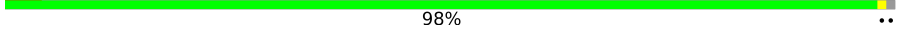
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Mol	Chain	Length	Quality of chain
15	2T	146	<div> <div>3%</div> <div>74%</div> <div>16%</div> <div>10%</div> </div>
16	1U	118	<div> <div>%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
16	2U	118	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
17	1V	101	<div> <div>82%</div> <div>16%</div> <div>..</div> </div>
17	2V	101	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
18	1W	113	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
18	2W	113	<div> <div>%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
19	1X	96	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>
19	2X	96	<div> <div>5%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
20	1Y	110	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
20	2Y	110	<div> <div>3%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
21	1Z	206	<div> <div>3%</div> <div>60%</div> <div>14%</div> <div>25%</div> </div>
21	2Z	206	<div> <div>12%</div> <div>52%</div> <div>24%</div> <div>.</div> <div>22%</div> </div>
22	10	85	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
22	20	85	<div> <div>%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
23	11	98	<div> <div>3%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
23	21	98	<div> <div>4%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
24	12	72	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
24	22	72	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
25	13	60	<div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
25	23	60	<div> <div>8%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
26	14	71	<div> <div>18%</div> <div>62%</div> <div>28%</div> <div>7%</div> <div>.</div> </div>
26	24	71	<div> <div>21%</div> <div>63%</div> <div>27%</div> <div>7%</div> <div>.</div> </div>
27	15	60	<div> <div>2%</div> <div>83%</div> <div>12%</div> <div>..</div> </div>
27	25	60	<div> <div>78%</div> <div>17%</div> <div>..</div> </div>

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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	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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	10	102	-	-	-	X
56	MG	15	102	-	-	-	X
56	MG	16	102	-	-	-	X
56	MG	1A	3091	-	-	-	X
56	MG	1A	3112	-	-	-	X
56	MG	1A	3151	-	-	-	X
56	MG	1A	3222	-	-	-	X
56	MG	1A	3251	-	-	-	X
56	MG	1A	3312	-	-	-	X
56	MG	1A	3351	-	-	-	X
56	MG	1A	3366	-	-	-	X
56	MG	1A	3367	-	-	-	X
56	MG	1A	3369	-	-	-	X
56	MG	1A	3370	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3383	-	-	-	X
56	MG	1A	3392	-	-	-	X
56	MG	1A	3417	-	-	-	X
56	MG	1A	3560	-	-	-	X
56	MG	1A	3575	-	-	-	X
56	MG	1A	3688	-	-	-	X
56	MG	1A	4066	-	-	-	X
56	MG	1A	4114	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4146	-	-	-	X
56	MG	1A	4186	-	-	-	X
56	MG	1B	227	-	-	-	X
56	MG	1a	1602	-	-	-	X
56	MG	1a	1615	-	-	-	X
56	MG	1a	1723	-	-	-	X
56	MG	1w	103	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	23	3001	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3195	-	-	-	X
56	MG	2A	3214	-	-	-	X
56	MG	2A	3248	-	-	-	X
56	MG	2A	3251	-	-	-	X
56	MG	2A	3270	-	-	-	X
56	MG	2A	3301	-	-	-	X
56	MG	2A	3343	-	-	-	X
56	MG	2A	3377	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3387	-	-	-	X
56	MG	2A	3394	-	-	-	X
56	MG	2A	3411	-	-	-	X
56	MG	2A	3456	-	-	-	X
56	MG	2A	3479	-	-	-	X
56	MG	2A	3495	-	-	-	X
56	MG	2A	3792	-	-	-	X
56	MG	2A	3823	-	-	-	X
56	MG	2B	3011	-	-	-	X
56	MG	2a	3026	-	-	-	X
56	MG	2a	3029	-	-	-	X
56	MG	2a	3031	-	-	-	X
56	MG	2a	3034	-	-	-	X
56	MG	2a	3057	-	-	-	X
56	MG	2a	3060	-	-	-	X
56	MG	2a	3064	-	-	-	X
56	MG	2a	3086	-	-	-	X
56	MG	2a	3222	-	-	-	X
56	MG	2l	3001	-	-	-	X
56	MG	2v	102	-	-	-	X
56	MG	2v	103	-	-	-	X
56	MG	2w	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	CPT	1a	1930	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 301288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total 1592	C 713	N 285	O 518	P 74	S 2	0	0	0
54	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
54	2w	72	Total 1544	C 690	N 278	O 502	P 72	S 2	0	0	0
54	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	8	Total	Mg	0	0
			8	8		
56	17	4	Total	Mg	0	0
			4	4		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	7	Total	Mg	0	0
			7	7		
56	20	3	Total	Mg	0	0
			3	3		
56	18	3	Total	Mg	0	0
			3	3		
56	2W	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1P	3	Total 3	Mg 3	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2w	7	Total 7	Mg 7	0	0
56	2a	236	Total 236	Mg 236	0	0
56	1E	13	Total 13	Mg 13	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	2	Total 2	Mg 2	0	0
56	28	3	Total 3	Mg 3	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1A	1254	Total 1254	Mg 1254	0	0
56	1t	1	Total 1	Mg 1	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	1X	6	Total 6	Mg 6	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	12	2	Total 2	Mg 2	0	0
56	1y	5	Total 5	Mg 5	0	0
56	1S	3	Total 3	Mg 3	0	0
56	25	4	Total 4	Mg 4	0	0
56	2T	1	Total 1	Mg 1	0	0
56	1D	12	Total 12	Mg 12	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	1V	2	Total 2	Mg 2	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1w	11	Total 11	Mg 11	0	0
56	1a	330	Total 330	Mg 330	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	15	4	Total 4	Mg 4	0	0
56	1x	18	Total 18	Mg 18	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1s	1	Total 1	Mg 1	0	0

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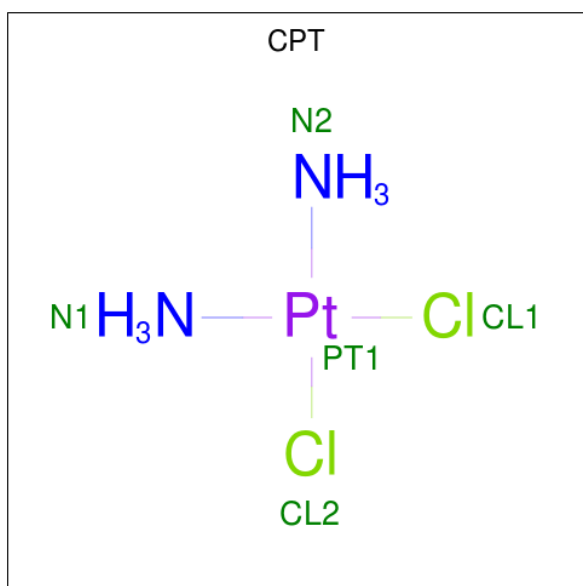
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1m	1	Total 1	Mg 1	0	0
56	2U	6	Total 6	Mg 6	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2n	1	Total 1	Mg 1	0	0
56	1H	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	6	Total 6	Mg 6	0	0
56	2R	2	Total 2	Mg 2	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	3	Total 3	Mg 3	0	0
56	2q	4	Total 4	Mg 4	0	0
56	1U	6	Total 6	Mg 6	0	0
56	2r	1	Total 1	Mg 1	0	0
56	1O	5	Total 5	Mg 5	0	0
56	27	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1l	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2V	1	Total 1 Mg 1	0	0
56	1F	10	Total 10 Mg 10	0	0
56	10	7	Total 7 Mg 7	0	0
56	2t	1	Total 1 Mg 1	0	0
56	1Q	5	Total 5 Mg 5	0	0
56	2A	919	Total 919 Mg 919	0	0
56	23	3	Total 3 Mg 3	0	0
56	2Z	1	Total 1 Mg 1	0	0
56	1B	36	Total 36 Mg 36	0	0
56	2y	7	Total 7 Mg 7	0	0
56	1c	2	Total 2 Mg 2	0	0
56	2v	6	Total 6 Mg 6	0	0

- Molecule 57 is Cisplatin (three-letter code: CPT) (formula:  $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total	K	0	0
			1	1		
58	2A	1	Total	K	0	0
			1	1		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

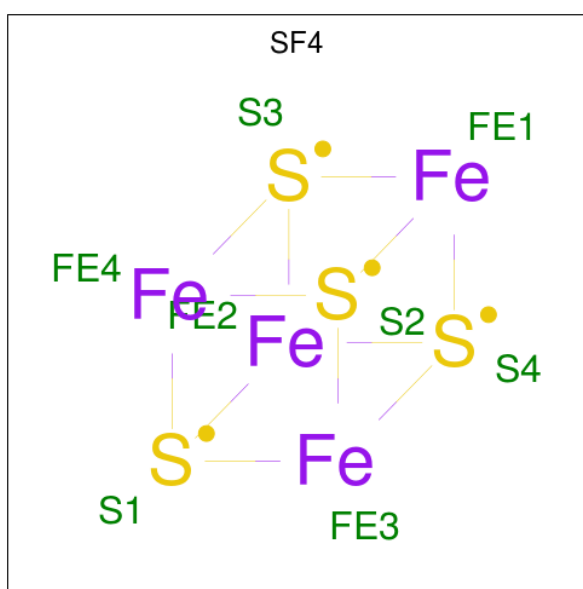
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	24	1	Total 1	Zn 1	0	0
59	2n	1	Total 1	Zn 1	0	0
59	2Y	1	Total 1	Zn 1	0	0
59	16	1	Total 1	Zn 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total 8	Fe 4	S 4	0	0
60	2d	1	Total 8	Fe 4	S 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2273	Total 2273	O 2273	0	0
61	1B	70	Total 70	O 70	0	0
61	1D	28	Total 28	O 28	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	27	Total 27	O 27	0	0
61	1F	15	Total 15	O 15	0	0
61	1G	7	Total 7	O 7	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	3	Total 3	O 3	0	0
61	1O	6	Total 6	O 6	0	0
61	1P	23	Total 23	O 23	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	15	Total 15	O 15	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	10	Total 10	O 10	0	0
61	1U	16	Total 16	O 16	0	0
61	1V	11	Total 11	O 11	0	0
61	1W	13	Total 13	O 13	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	5	Total 5	O 5	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	12	Total 12	O 12	0	0
61	11	14	Total 14	O 14	0	0
61	12	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	5	Total 5	O 5	0	0
61	14	1	Total 1	O 1	0	0
61	15	7	Total 7	O 7	0	0
61	16	2	Total 2	O 2	0	0
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61	18	10	Total 10	O 10	0	0
61	1a	520	Total 520	O 520	0	0
61	1b	1	Total 1	O 1	0	0
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61	1e	1	Total 1	O 1	0	0
61	1g	2	Total 2	O 2	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	10	Total 10	O 10	0	0
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61	1o	2	Total 2	O 2	0	0
61	1p	2	Total 2	O 2	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1x	15	Total 15	O 15	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1393	Total 1393	O 1393	0	0
61	2B	28	Total 28	O 28	0	0
61	2D	29	Total 29	O 29	0	0
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61	2F	17	Total 17	O 17	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	16	Total 16	O 16	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	7	Total 7	O 7	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	2	Total 2	O 2	0	0
61	2W	4	Total 4	O 4	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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61	23	1	Total 1	O 1	0	0
61	25	3	Total 3	O 3	0	0
61	27	3	Total 3	O 3	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
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61	2e	2	Total 2	O 2	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	4	Total 4	O 4	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	3	Total 3	O 3	0	0
61	2x	9	Total 9	O 9	0	0

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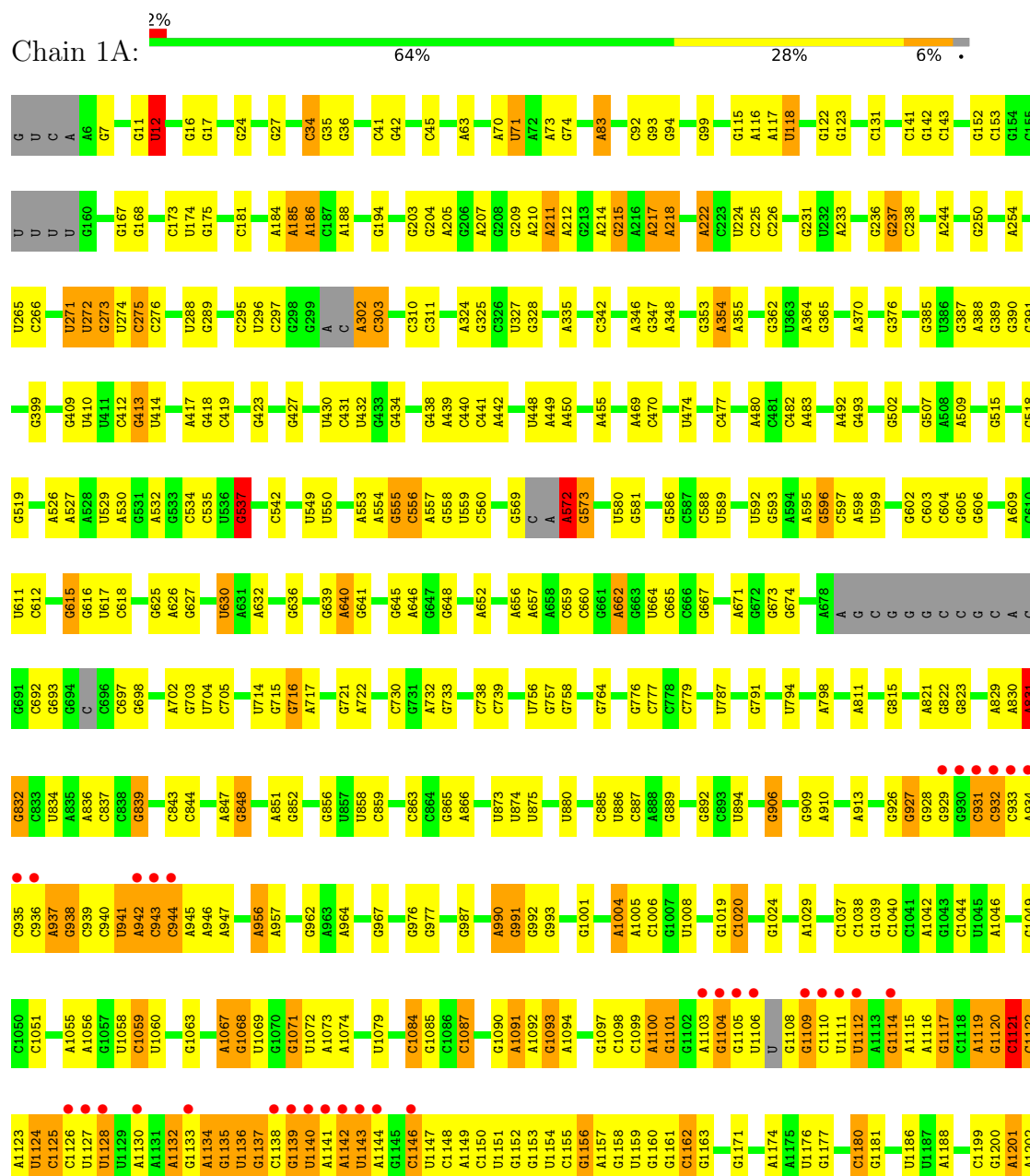
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	20	Total	O	0	0
			20	20		

### 3 Residue-property plots

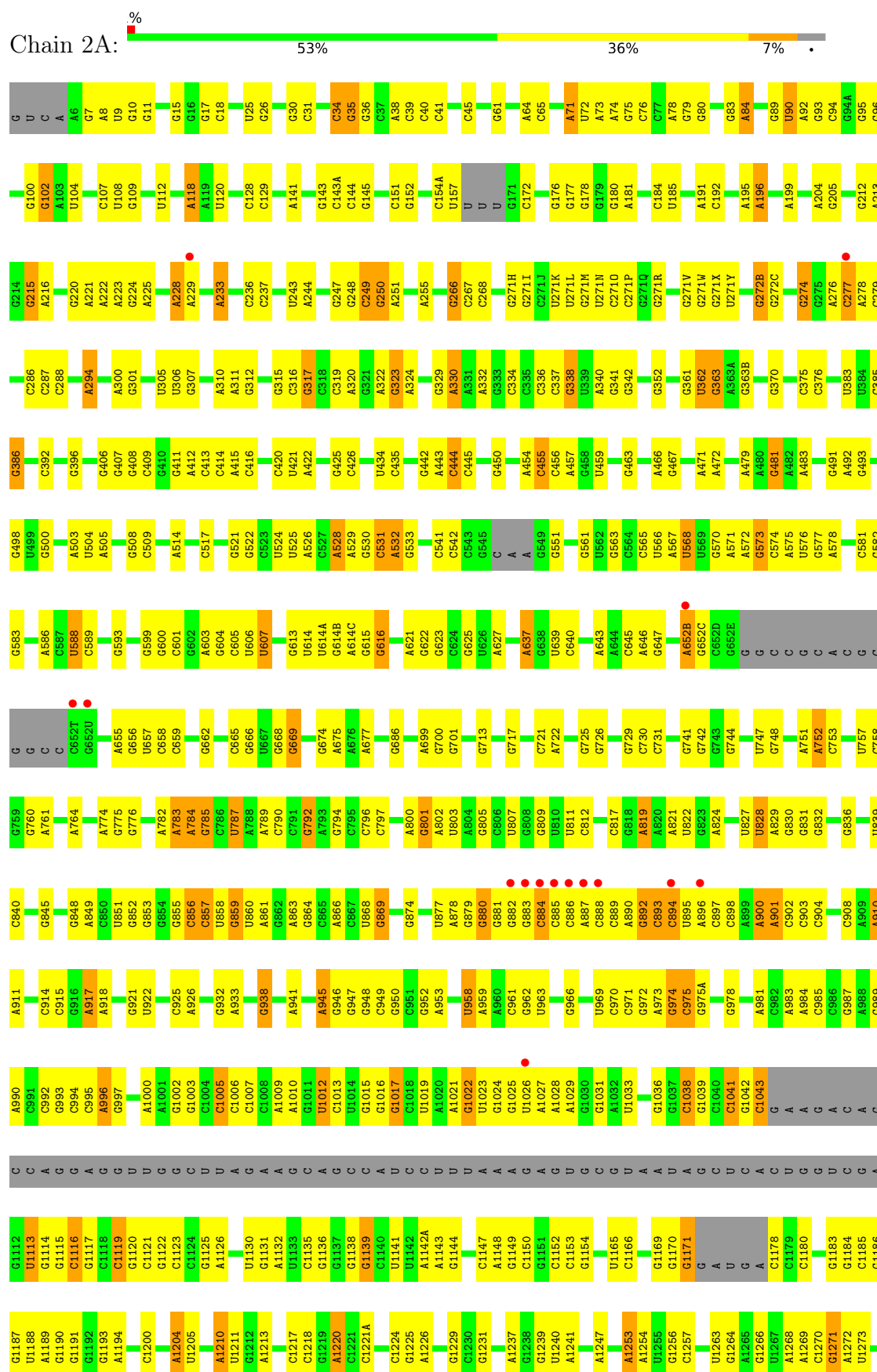
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

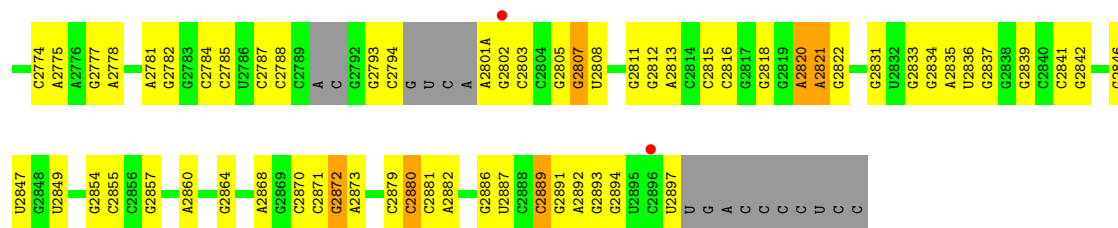




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G2848	A2746	U2616	C2487	A2348	G2263	G2177	G2091	A1975	G1832	G1714	G	U1452	A1332	U1211
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G2857	U2857	G2618	C2489	C2362	U2274	G2181	C2095	U1980	G1845	A1716	A	U1338	U1339	U1213
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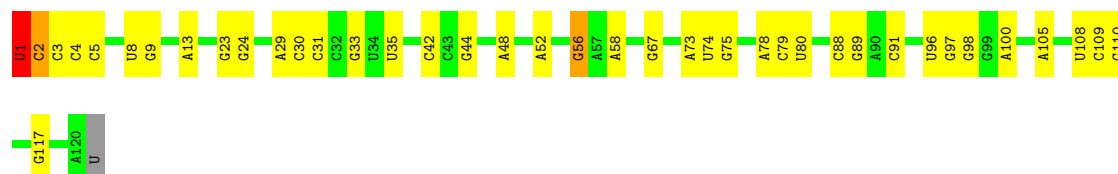


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U2728	C2624	A2425	A2425	G2330	U2242	G2145	G2067	U1968	G1849	G1529				G1437	
G2732	G2625	G2428	G2428	G2331	U2243	C2146	U2068	A1969	G1857	G1530				G1441	
A2733	C2628	A2430	A2430	G2332	A2247	U2150	G2070	U1970	G1858	C1531				U1352	
U2739	G2630	G2436	G2436	G2333	U2249	G2151	A2071	A1972	G1861	C1532				A1353	
A2740	A2632	U2437	U2437	G2334	G2250	G2152	U2074	G1973	U1865	U				A1354	
A2741	C2633	A2438	A2438	U2344	U2265	G2153	U2075	C1974	G1866	A				G1355	
C2742	G2638	C2440	C2440	G2345	U2268	G2154		U1981	G1867	G1533				G1356	
U2750	C2646	C2441	C2441	G2346	U2275	G2155	G2094	G1982	A1877	G1537				A1359	
G2751	U2647	C2442	C2442	G2347	G2276	G2156	C2095	U1993	G1878	C1538				A1360	
C2755	C2648	G2443	G2443	C2350	G2277	A2158	U2096	G1994	G1879	G1539				G1364	
U2756	U2649	G2444	G2444	G2351	G2278	G2159	C2097	C1996	C1880	U1540				A1365	
A2757	G2650	G2445	G2445	G2352	A2278	C2160	U2098	G1997	C1881	G1541				A1366	
U2758	A2654	A2448	A2448	G2353	C2283	G2161	U2099	C1998	A1889	A1542				A1367	
C2759	G2655	A2453	A2453	G2354	C2284	G2162	G2100	C1999	A1890	G1546				G1368	
G2761	C2658	C2461	C2461	G2355	C2285	G2163	G2104	G2010	G1899	C1547				G1369	
A2764	A2662	U2554	U2554	G2356	C2286	U2167	C2105	U2011	A1900	G1557				G1370	
A2765	G2663	U2555	U2555	G2357	C2287	A2169	G2106	G2012	A1664	C1558				G1371	
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C2769	C2665	U2557	U2557	G2359	A2288	A2171	C2111	A2020	A1668	C1465				A1373	
G2770	C2677	C2558	C2558	G2370	G2289	U2172	G2112	G2021	A1669	C1466				A1469	
		C2559	C2559	G2371	G2290	A2173	U2113	U2022	A1670	C1467				C1468	
				G2375	U2291	C2174	A2114	G2023	C1674	U1578				A1384	
				A2376	C2292	C2175	G2115	G2024	A1671	A1579				G1385	
					C2294	C2176	A2176	C2025	A1688	C1582				C1386	
						C2177	A2177		A1689					U1394	
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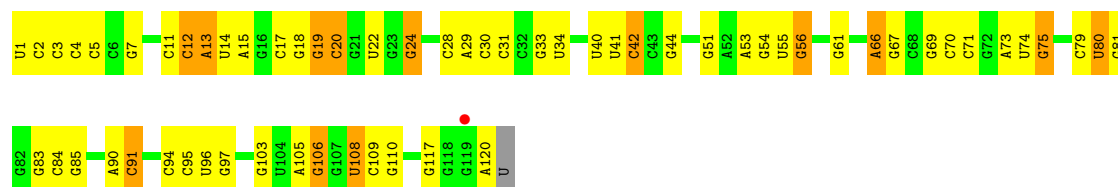
• Molecule 2: 5S ribosomal RNA

Chain 1B: 66% 31% ...



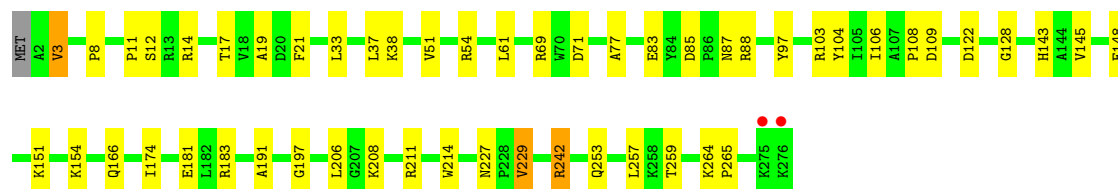
• Molecule 2: 5S ribosomal RNA

Chain 2B: % 49% 40% 11% .



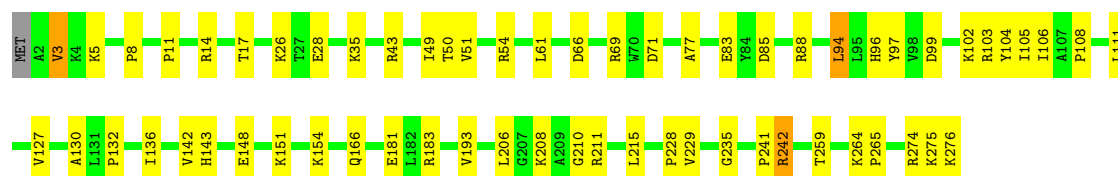
• Molecule 3: 50S ribosomal protein L2

Chain 1D: % 81% 18% .



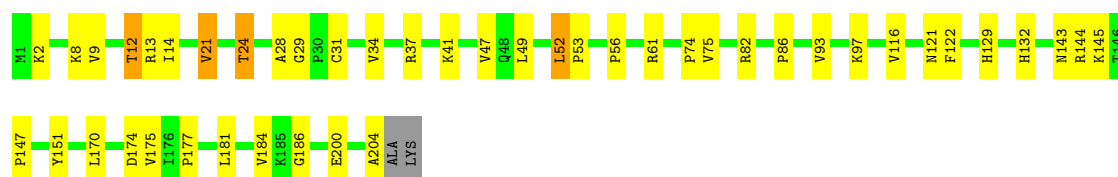
• Molecule 3: 50S ribosomal protein L2

Chain 2D: 77% 21% .

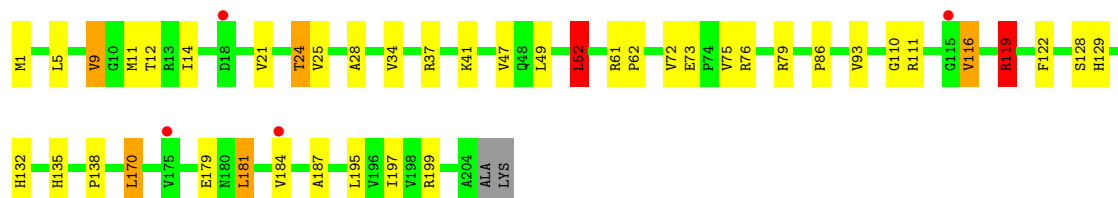
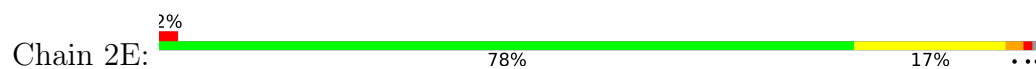


• Molecule 4: 50S ribosomal protein L3

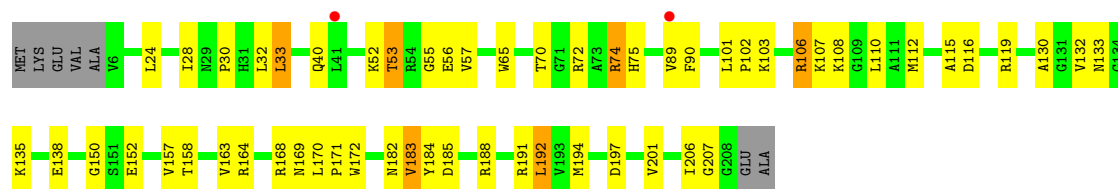
Chain 1E: 77% 20% ..



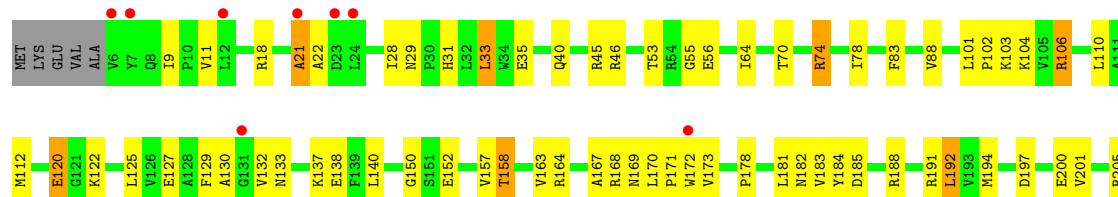
• Molecule 4: 50S ribosomal protein L3



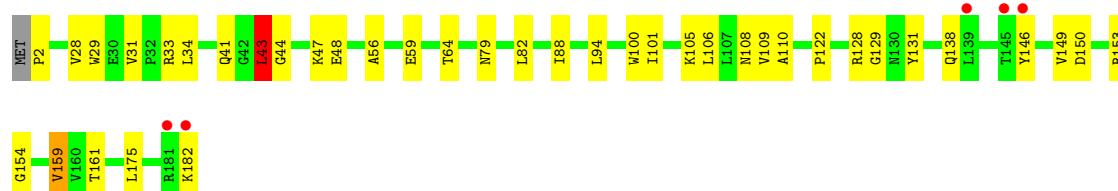
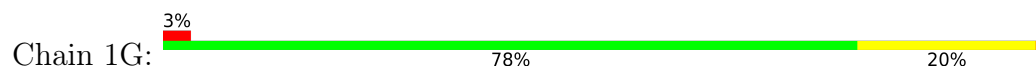
• Molecule 5: 50S ribosomal protein L4



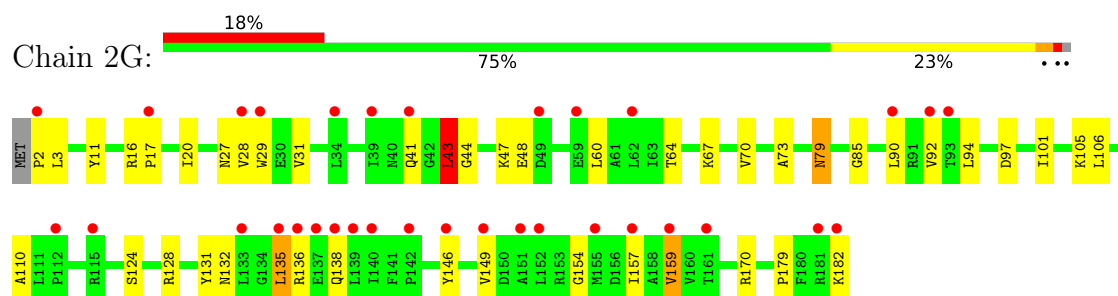
• Molecule 5: 50S ribosomal protein L4



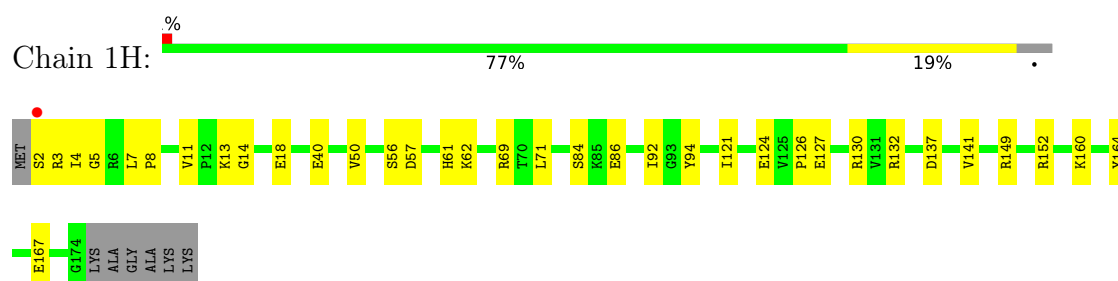
• Molecule 6: 50S ribosomal protein L5



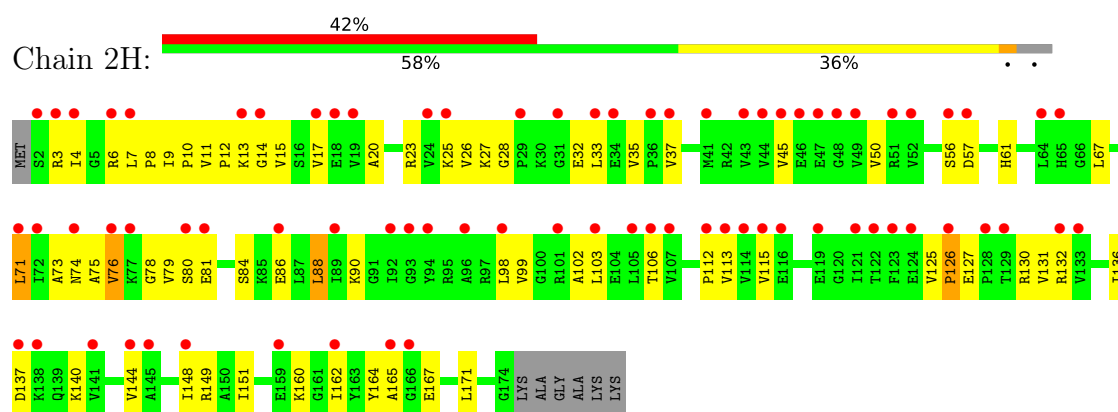
- Molecule 6: 50S ribosomal protein L5



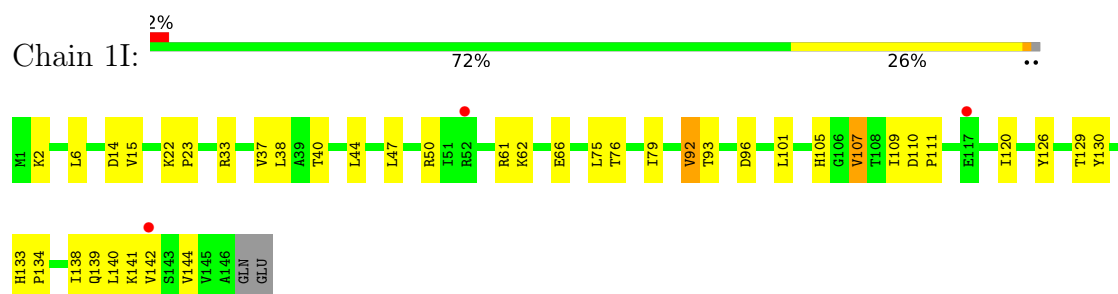
- Molecule 7: 50S ribosomal protein L6



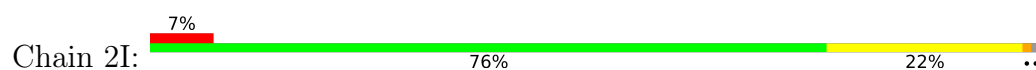
- Molecule 7: 50S ribosomal protein L6

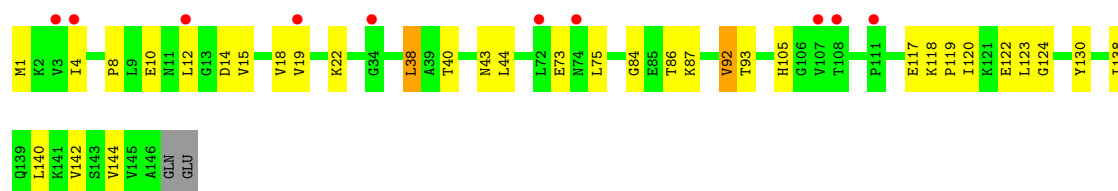


- Molecule 8: 50S ribosomal protein L9



- Molecule 8: 50S ribosomal protein L9





- Molecule 9: 50S ribosomal protein L13

Chain 1N: 86% 13% .



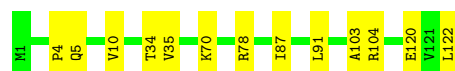
- Molecule 9: 50S ribosomal protein L13

Chain 2N: 79% 21% .



- Molecule 10: 50S ribosomal protein L14

Chain 1O: 89% 11%



- Molecule 10: 50S ribosomal protein L14

Chain 2O: 82% 18% 3%



- Molecule 11: 50S ribosomal protein L15

Chain 1P: 81% 19% .



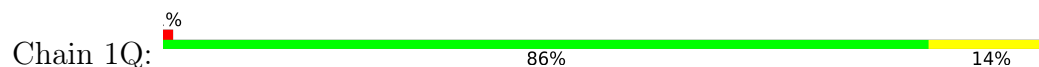
- Molecule 11: 50S ribosomal protein L15

Chain 2P: 71% 27% 15% .

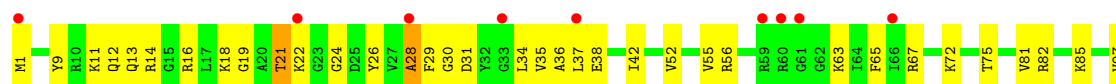




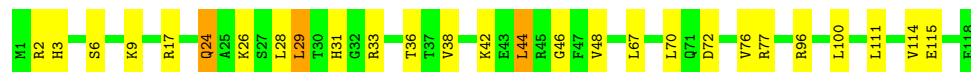
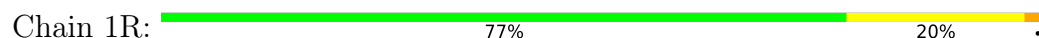
- Molecule 12: 50S ribosomal protein L16



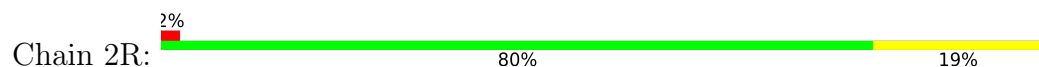
- Molecule 12: 50S ribosomal protein L16



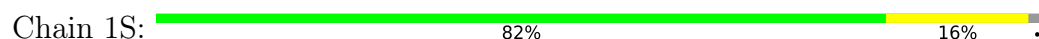
- Molecule 13: 50S ribosomal protein L17



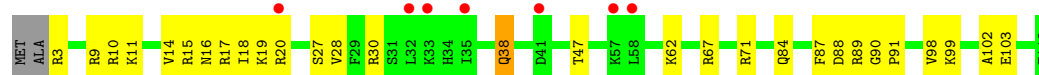
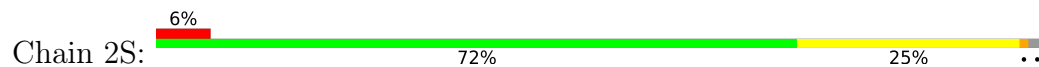
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

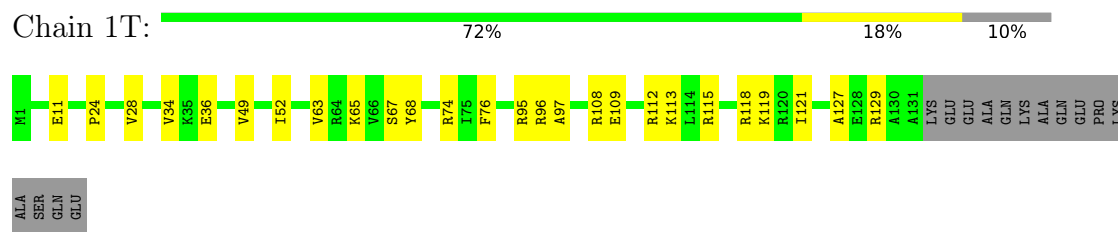


- Molecule 14: 50S ribosomal protein L18

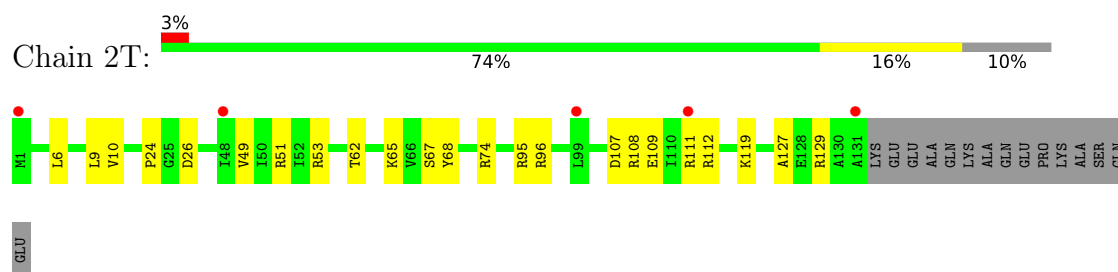


- Molecule 15: 50S ribosomal protein L19

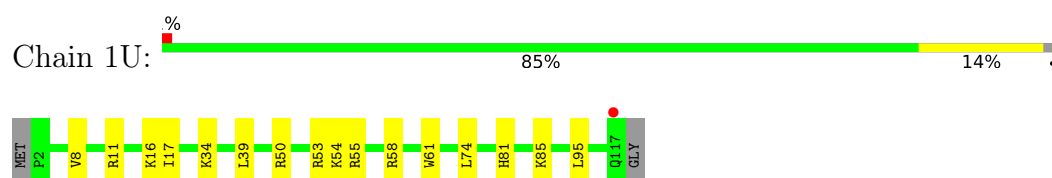




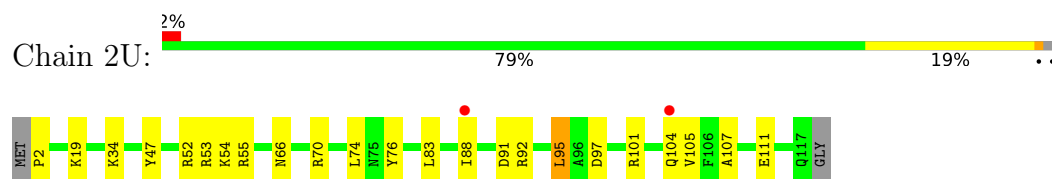
- Molecule 15: 50S ribosomal protein L19



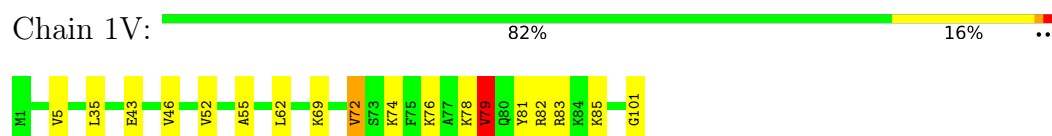
- Molecule 16: 50S ribosomal protein L20



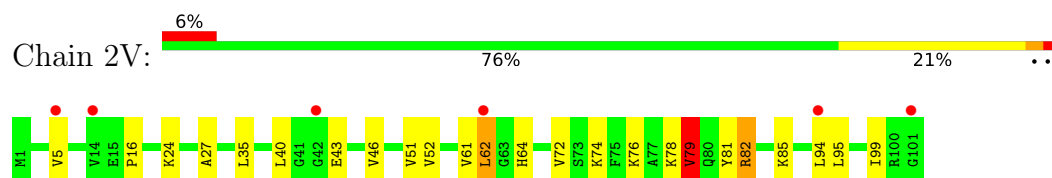
- Molecule 16: 50S ribosomal protein L20



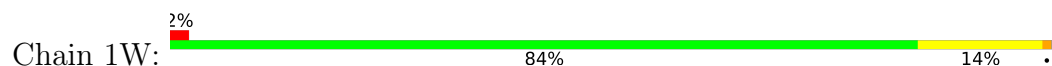
- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

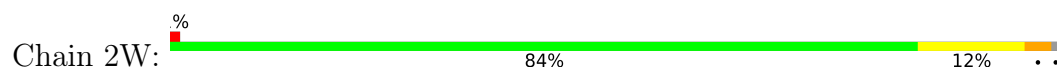


- Molecule 18: 50S ribosomal protein L22

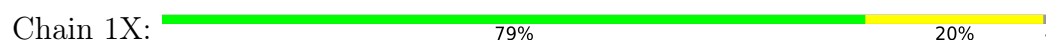




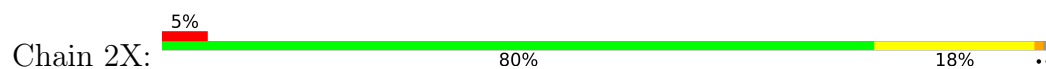
- Molecule 18: 50S ribosomal protein L22



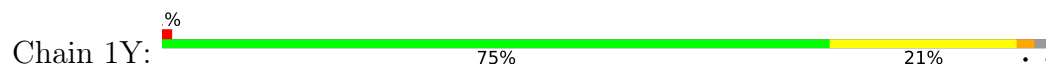
- Molecule 19: 50S ribosomal protein L23



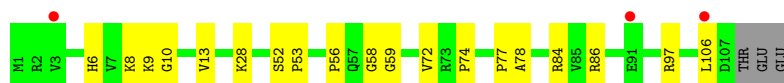
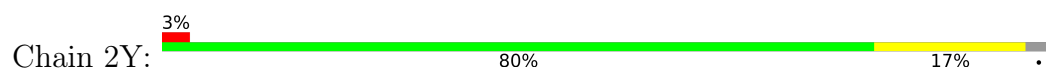
- Molecule 19: 50S ribosomal protein L23



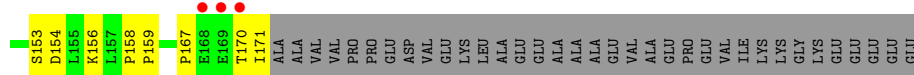
- Molecule 20: 50S ribosomal protein L24



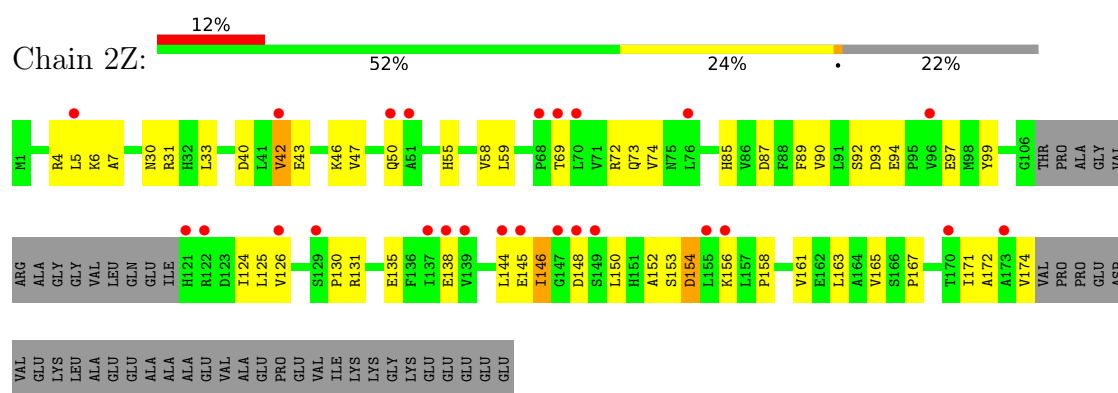
- Molecule 20: 50S ribosomal protein L24



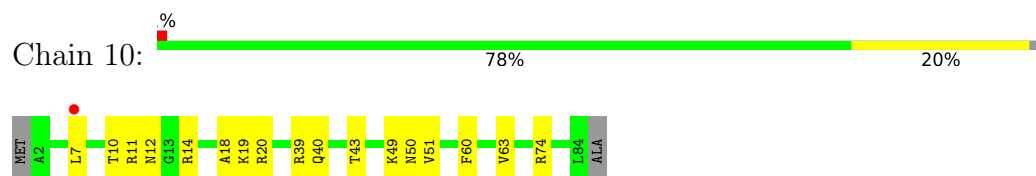
- Molecule 21: 50S ribosomal protein L25



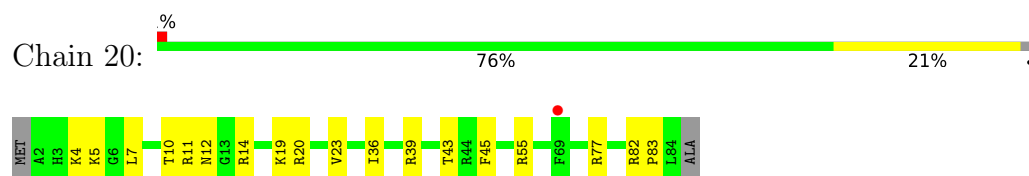
- Molecule 21: 50S ribosomal protein L25



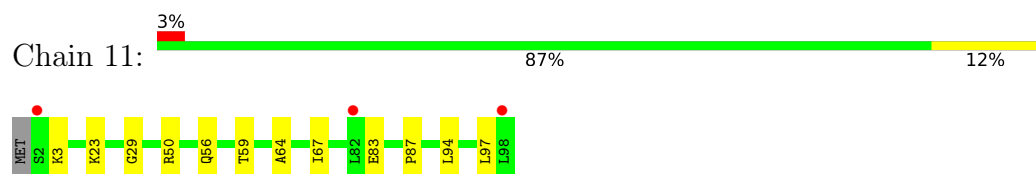
- Molecule 22: 50S ribosomal protein L27



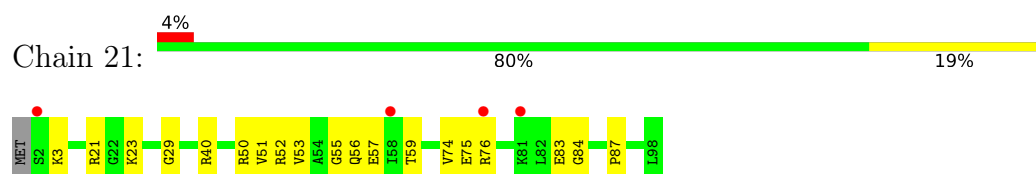
- Molecule 22: 50S ribosomal protein L27



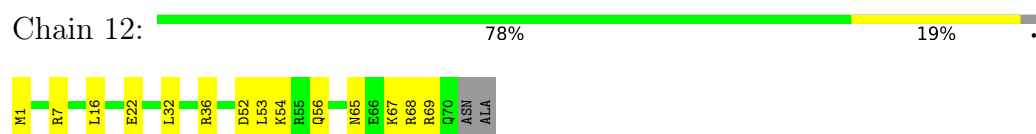
- Molecule 23: 50S ribosomal protein L28



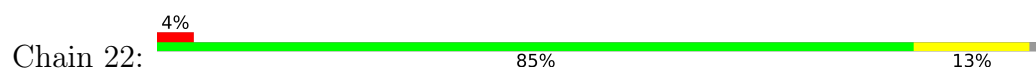
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

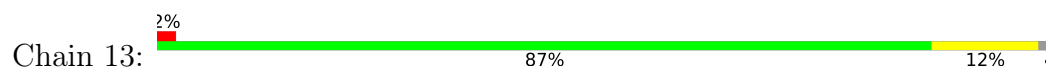


- Molecule 24: 50S ribosomal protein L29

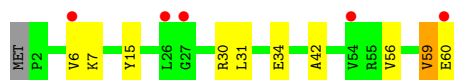
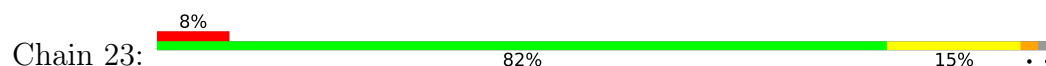




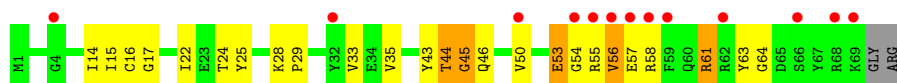
- Molecule 25: 50S ribosomal protein L30



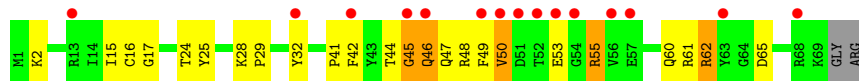
- Molecule 25: 50S ribosomal protein L30



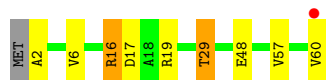
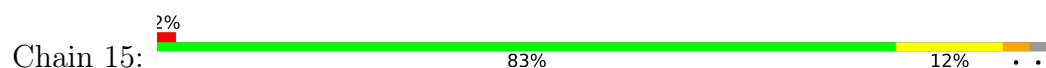
- Molecule 26: 50S ribosomal protein L31



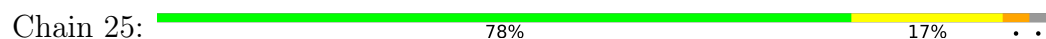
- Molecule 26: 50S ribosomal protein L31



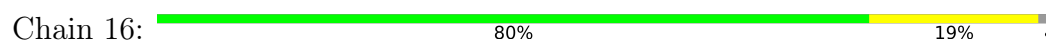
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

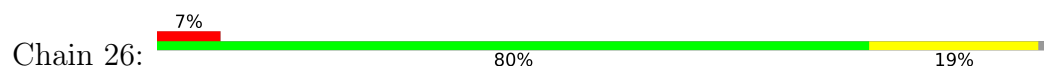


- Molecule 28: 50S ribosomal protein L33

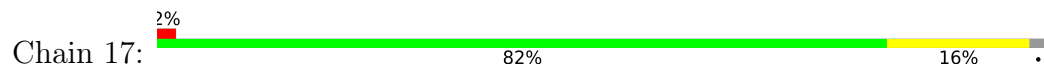




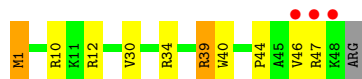
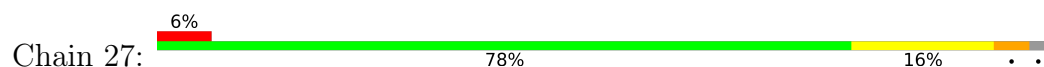
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



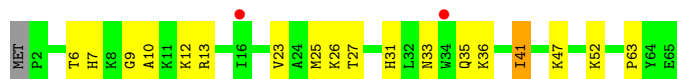
- Molecule 29: 50S ribosomal protein L34



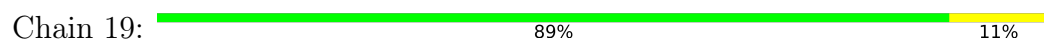
- Molecule 30: 50S ribosomal protein L35



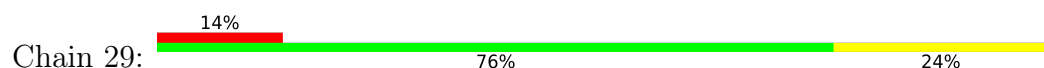
- Molecule 30: 50S ribosomal protein L35

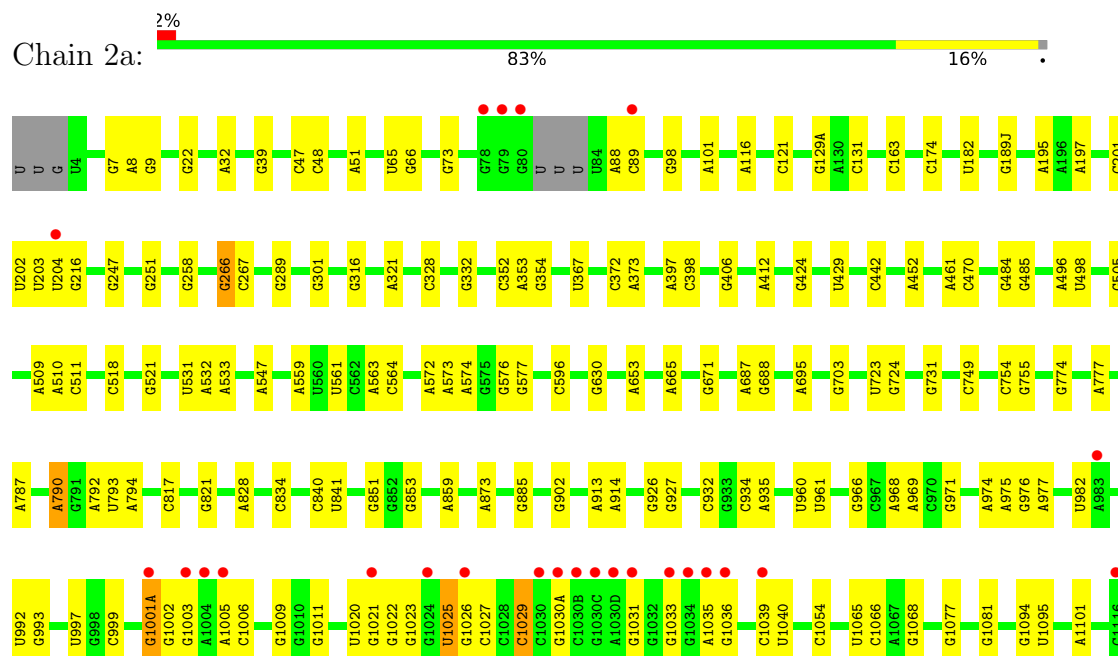


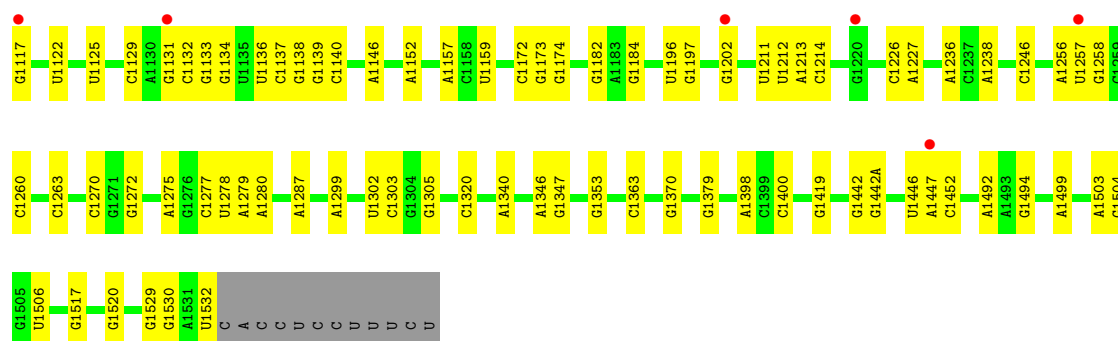
- Molecule 31: 50S ribosomal protein L36



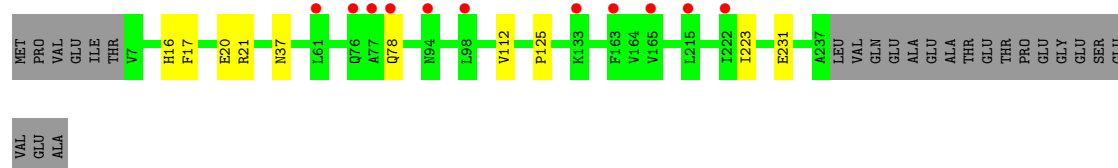
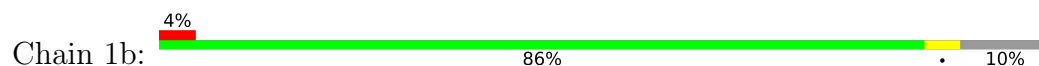
- Molecule 31: 50S ribosomal protein L36



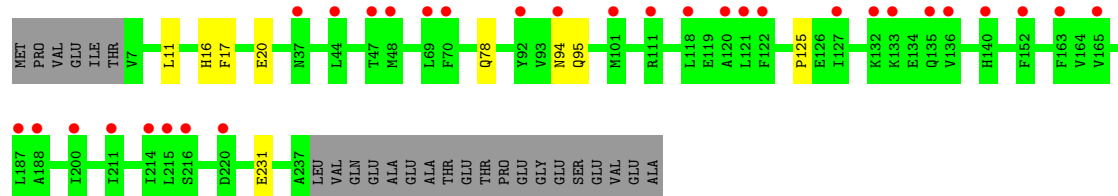
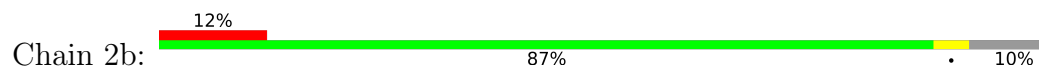




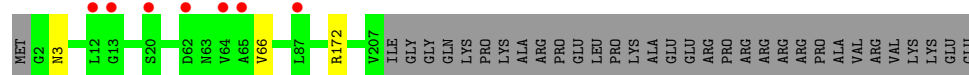
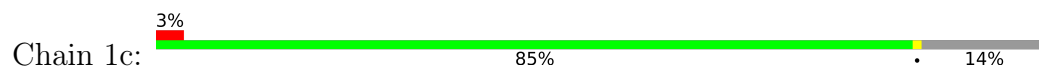
• Molecule 33: 30S ribosomal protein S2



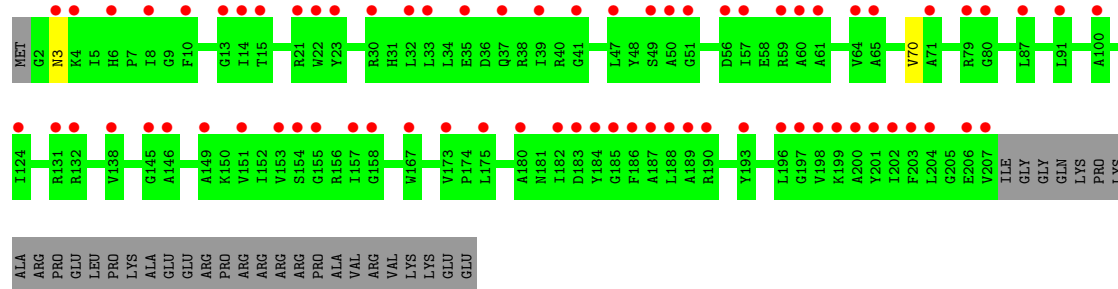
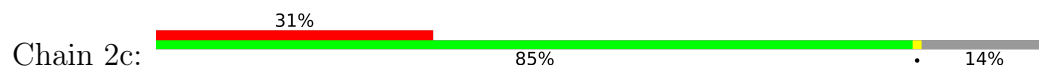
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3

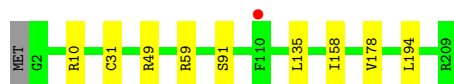


• Molecule 34: 30S ribosomal protein S3



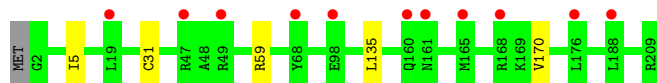
- Molecule 35: 30S ribosomal protein S4

Chain 1d:  95% .



- Molecule 35: 30S ribosomal protein S4

Chain 2d:  97% .



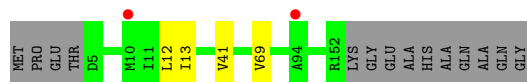
- Molecule 36: 30S ribosomal protein S5

Chain 1e:  87% . 9%



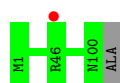
- Molecule 36: 30S ribosomal protein S5

Chain 2e:  89% . 9%



- Molecule 37: 30S ribosomal protein S6

Chain 1f:  99% .



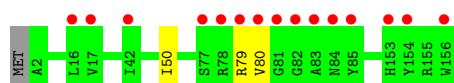
- Molecule 37: 30S ribosomal protein S6

Chain 2f:  98% ..



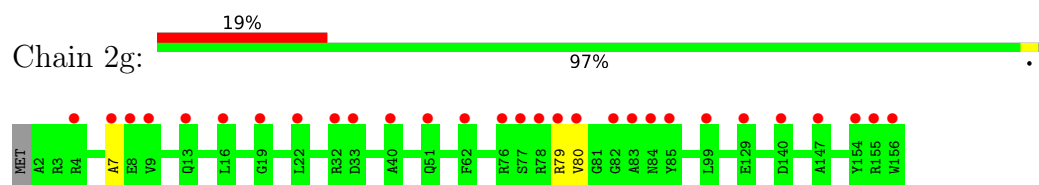
- Molecule 38: 30S ribosomal protein S7

Chain 1g:  97% ..

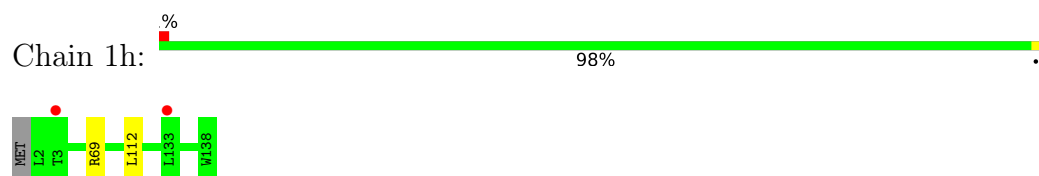




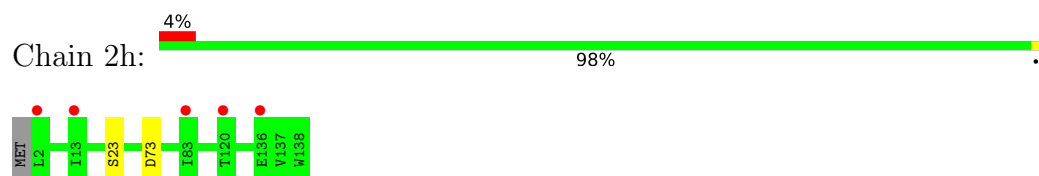
- Molecule 38: 30S ribosomal protein S7



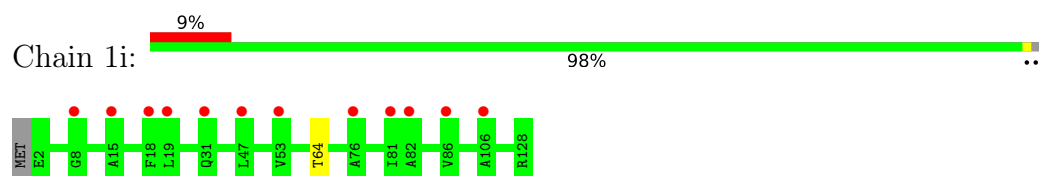
- Molecule 39: 30S ribosomal protein S8



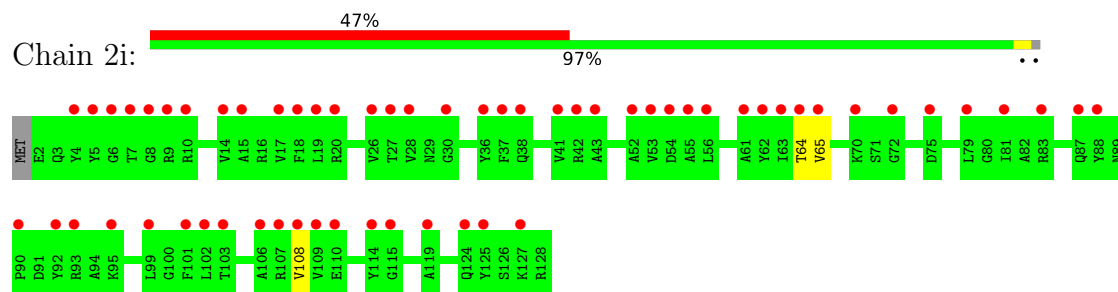
- Molecule 39: 30S ribosomal protein S8



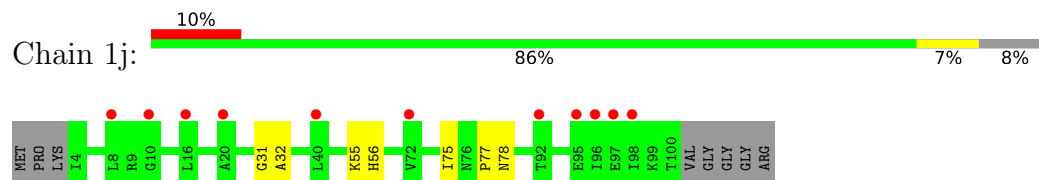
- Molecule 40: 30S ribosomal protein S9



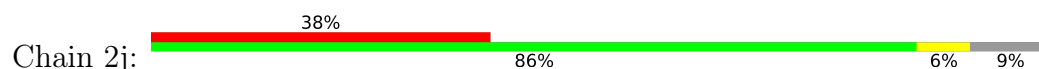
- Molecule 40: 30S ribosomal protein S9

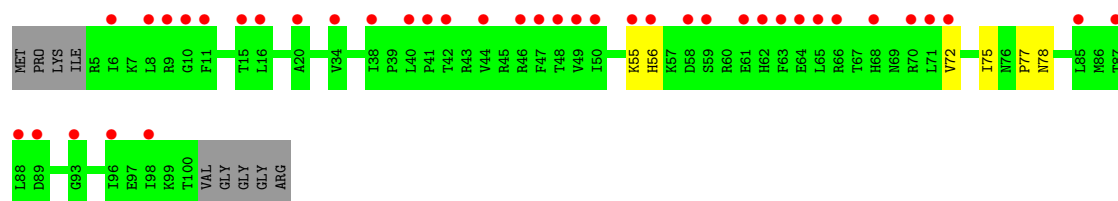


- Molecule 41: 30S ribosomal protein S10

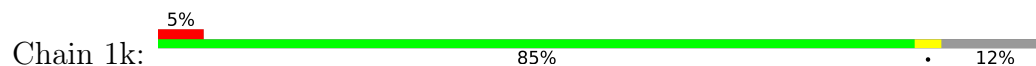


- Molecule 41: 30S ribosomal protein S10

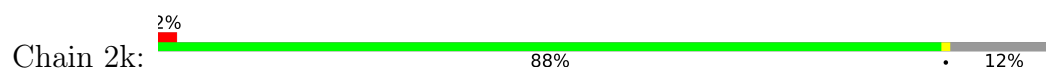




- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12



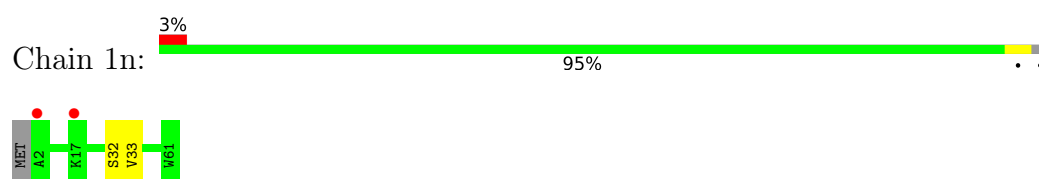
- Molecule 44: 30S ribosomal protein S13



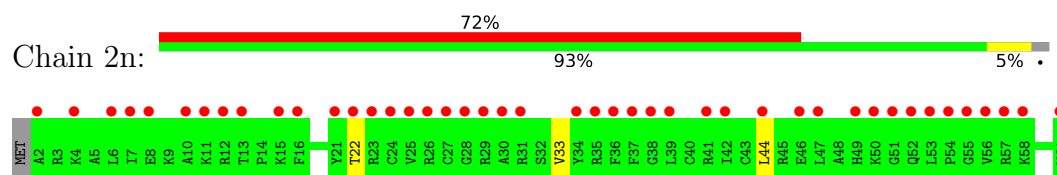
- Molecule 44: 30S ribosomal protein S13



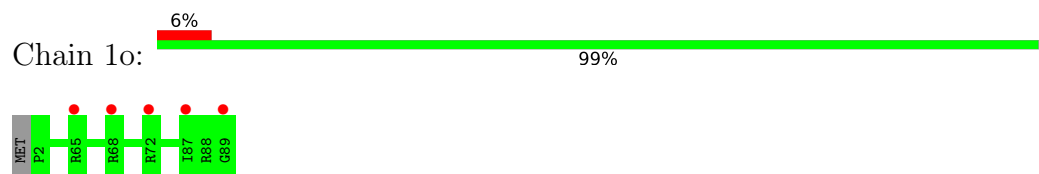
- Molecule 45: 30S ribosomal protein S14 type Z



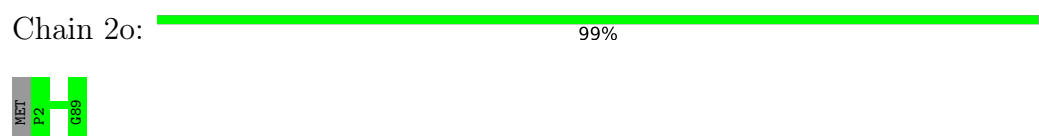
- Molecule 45: 30S ribosomal protein S14 type Z



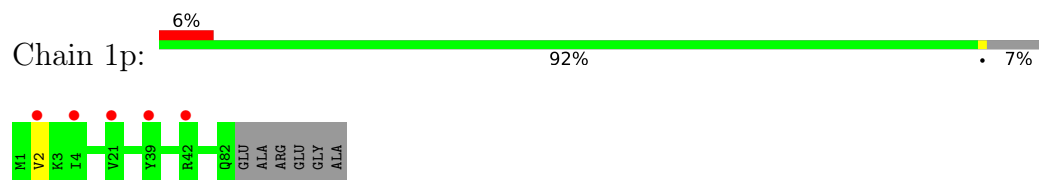
- Molecule 46: 30S ribosomal protein S15



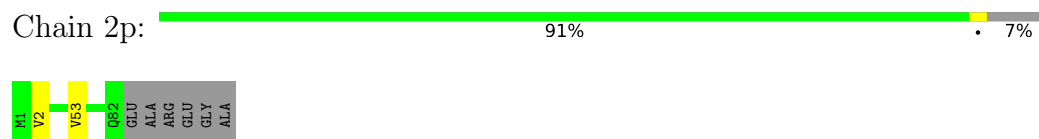
- Molecule 46: 30S ribosomal protein S15



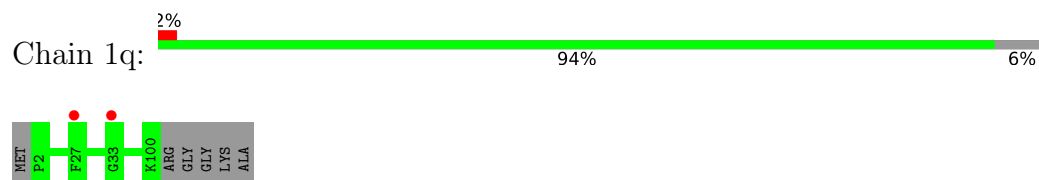
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16




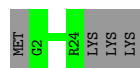
- Molecule 48: 30S ribosomal protein S17




- Molecule 48: 30S ribosomal protein S17

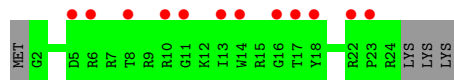


Chain 1u:  85% 15%



- Molecule 52: 30S ribosomal protein Thx

Chain 2u:  44% 85% 15%



- Molecule 53: mRNA

Chain 1v:  4% 46% 8% 46%



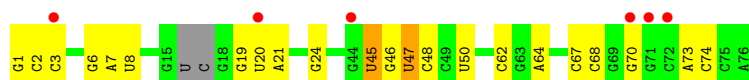
- Molecule 53: mRNA

Chain 2v:  4% 46% 8% 46%



- Molecule 54: A-site and E-site tRNAs

Chain 1w:  8% 68% 26% . .



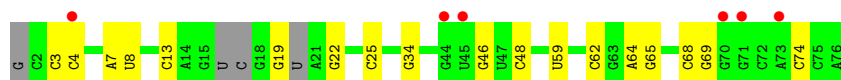
- Molecule 54: A-site and E-site tRNAs

Chain 1y:  4% 68% 29% .



- Molecule 54: A-site and E-site tRNAs

Chain 2w:  8% 71% 24% 5%

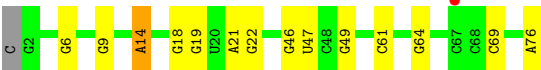
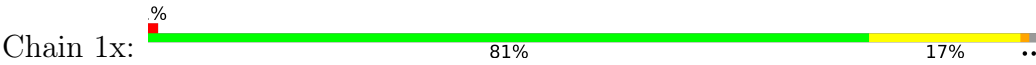


- Molecule 54: A-site and E-site tRNAs

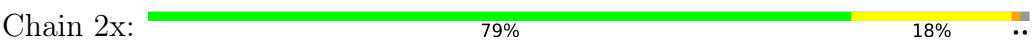
Chain 2y:  0% 66% 28% . .



● Molecule 55: P-site tRNA



● Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.98Å 446.99Å 621.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.65 – 2.80 152.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (152.65-2.80) 98.3 (152.64-2.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.219 , 0.268 0.219 , 0.268	Depositor DCC
$R_{free}$ test set	69488 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	301288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, M2G, OMG, 2MU, MIA, CPT, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, K, 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	0.51	2/69009 (0.0%)	0.91	44/107712 (0.0%)
1	2A	0.41	2/67293 (0.0%)	0.90	25/105034 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.83	0/4494
2	2B	0.49	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.38	0/2186	0.58	0/2944
3	2D	0.33	0/2186	0.58	1/2944 (0.0%)
4	1E	0.36	0/1592	0.54	0/2149
4	2E	0.33	0/1592	0.57	1/2149 (0.0%)
5	1F	0.35	0/1619	0.52	0/2193
5	2F	0.33	0/1615	0.54	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.31	0/1453	0.54	0/1963
7	1H	0.32	0/1347	0.51	0/1823
7	2H	0.29	0/1347	0.52	1/1823 (0.1%)
8	1I	0.29	0/1112	0.52	0/1514
8	2I	0.27	0/1079	0.50	0/1475
9	1N	0.35	0/1144	0.49	0/1543
9	2N	0.31	0/1144	0.50	0/1543
10	1O	0.37	0/943	0.53	0/1269
10	2O	0.30	0/943	0.48	0/1269
11	1P	0.35	0/1152	0.56	0/1533
11	2P	0.31	0/1152	0.58	0/1533
12	1Q	0.36	0/1143	0.50	0/1527
12	2Q	0.32	0/1143	0.55	0/1527
13	1R	0.35	0/982	0.54	0/1312
13	2R	0.31	0/982	0.53	0/1312
14	1S	0.32	0/883	0.51	0/1176
14	2S	0.32	0/880	0.51	0/1172
15	1T	0.34	0/1105	0.50	0/1477
15	2T	0.31	0/1097	0.50	0/1468
16	1U	0.39	0/977	0.52	0/1301



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.32	0/977	0.50	0/1301
17	1V	0.35	0/782	0.51	0/1049
17	2V	0.32	0/782	0.52	0/1049
18	1W	0.38	0/897	0.52	0/1205
18	2W	0.33	0/897	0.52	0/1205
19	1X	0.38	0/764	0.57	0/1025
19	2X	0.31	0/764	0.49	0/1025
20	1Y	0.36	0/819	0.55	0/1095
20	2Y	0.32	0/819	0.51	0/1095
21	1Z	0.30	0/1267	0.52	0/1717
21	2Z	0.31	0/1299	0.54	0/1763
22	10	0.36	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.34	0/762	0.51	0/1014
23	21	0.31	0/762	0.52	0/1014
24	12	0.34	0/590	0.51	0/781
24	22	0.31	0/590	0.43	0/781
25	13	0.35	0/474	0.52	0/635
25	23	0.29	0/469	0.48	0/630
26	14	0.36	0/565	0.64	0/761
26	24	0.32	0/545	0.50	0/737
27	15	0.33	0/469	0.52	0/635
27	25	0.31	0/469	0.50	0/635
28	16	0.35	0/460	0.48	0/613
28	26	0.33	0/456	0.48	0/608
29	17	0.36	0/426	0.52	0/561
29	27	0.33	0/426	0.58	0/561
30	18	0.36	0/525	0.53	0/691
30	28	0.31	0/525	0.51	0/691
31	19	0.39	0/310	0.53	0/407
31	29	0.29	0/310	0.49	0/407
32	1a	0.37	1/35795 (0.0%)	0.86	23/55864 (0.0%)
32	2a	0.35	3/35886 (0.0%)	0.86	30/56005 (0.1%)
33	1b	0.29	0/1881	0.53	0/2542
33	2b	0.31	0/1860	0.52	0/2518
34	1c	0.28	0/1572	0.47	0/2126
34	2c	0.30	0/1566	0.50	0/2119
35	1d	0.30	0/1685	0.50	0/2262
35	2d	0.29	0/1704	0.50	0/2284
36	1e	0.31	0/1145	0.52	0/1543
36	2e	0.31	0/1149	0.54	0/1548
37	1f	0.30	0/823	0.50	0/1115
37	2f	0.30	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.29	0/1250	0.47	0/1679
38	2g	0.28	0/1254	0.49	0/1683
39	1h	0.28	0/1108	0.49	0/1494
39	2h	0.27	0/1108	0.50	0/1494
40	1i	0.29	0/1002	0.52	0/1346
40	2i	0.28	0/997	0.50	0/1343
41	1j	0.27	0/722	0.53	0/982
41	2j	0.30	0/727	0.53	0/988
42	1k	0.28	0/844	0.49	0/1145
42	2k	0.29	0/848	0.49	0/1149
43	1l	0.32	0/937	0.53	0/1260
43	2l	0.28	0/937	0.57	1/1260 (0.1%)
44	1m	0.29	0/969	0.53	0/1302
44	2m	0.29	0/961	0.56	0/1291
45	1n	0.32	0/501	0.54	0/664
45	2n	0.29	0/501	0.52	0/664
46	1o	0.28	0/739	0.46	0/985
46	2o	0.28	0/739	0.50	0/985
47	1p	0.29	0/697	0.51	0/939
47	2p	0.29	0/693	0.50	0/935
48	1q	0.30	0/836	0.49	0/1117
48	2q	0.28	0/836	0.49	0/1117
49	1r	0.30	0/560	0.53	0/746
49	2r	0.30	0/560	0.47	0/746
50	1s	0.27	0/667	0.52	0/900
50	2s	0.32	0/661	0.61	0/893
51	1t	0.27	0/730	0.49	0/965
51	2t	0.27	0/729	0.48	0/965
52	1u	0.26	0/203	0.47	0/266
52	2u	0.26	0/203	0.49	0/266
53	1v	0.35	0/310	0.82	0/480
53	2v	0.34	0/310	0.78	0/480
54	1w	0.53	1/1606 (0.1%)	1.07	5/2497 (0.2%)
54	1y	0.48	1/1606 (0.1%)	1.02	4/2497 (0.2%)
54	2w	0.44	0/1556	1.03	0/2418
54	2y	0.51	1/1583 (0.1%)	1.06	3/2459 (0.1%)
55	1x	0.54	2/1725 (0.1%)	1.14	16/2689 (0.6%)
55	2x	0.46	0/1725	1.08	16/2689 (0.6%)
All	All	0.40	15/316668 (0.0%)	0.82	172/474091 (0.0%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.24	1.48	1.61
2	2B	1	U	OP3-P	-10.23	1.48	1.61
54	1y	1	G	OP3-P	-10.13	1.49	1.61
2	1B	1	U	OP3-P	-10.08	1.49	1.61
54	1w	1	G	OP3-P	-9.91	1.49	1.61

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	16.43	138.46	128.60
32	2a	1272	G	N3-C2-N2	14.39	129.97	119.90
32	2a	1263	C	N1-C2-O2	14.28	127.47	118.90
32	2a	1272	G	N1-C2-N2	-14.21	103.41	116.20
32	2a	1272	G	N1-C6-O6	-12.06	112.66	119.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31191	646	0
1	2A	60322	0	30423	856	0
2	1B	2577	0	1305	22	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	47	0
3	2D	2136	0	2218	55	0
4	1E	1559	0	1618	32	0
4	2E	1559	0	1618	31	0
5	1F	1584	0	1625	41	0
5	2F	1580	0	1619	49	0
6	1G	1423	0	1436	28	0
6	2G	1428	0	1438	36	0
7	1H	1321	0	1394	22	0
7	2H	1321	0	1394	41	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	22	0
10	1O	933	0	996	11	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	24	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	41	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	17	0
14	1S	873	0	927	17	0
14	2S	870	0	923	22	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	14	0
16	1U	959	0	1019	13	0
16	2U	959	0	1018	18	0
17	1V	771	0	830	10	0
17	2V	771	0	830	17	0
18	1W	886	0	940	14	0
18	2W	886	0	940	11	0
19	1X	750	0	814	12	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	13	0
21	1Z	1240	0	1240	16	0
21	2Z	1271	0	1273	35	0
22	10	653	0	674	22	0
22	20	653	0	674	16	0
23	11	755	0	826	11	0
23	21	755	0	826	17	0
24	12	588	0	643	11	0
24	22	588	0	643	8	0
25	13	469	0	518	3	0
25	23	464	0	514	8	0
26	14	552	0	533	18	0
26	24	532	0	503	20	0
27	15	455	0	465	7	0
27	25	455	0	465	10	0
28	16	453	0	473	6	0
28	26	449	0	469	6	0
29	17	418	0	467	5	0
29	27	418	0	467	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	18	517	0	582	19	0
30	28	517	0	582	16	0
31	19	307	0	335	2	0
31	29	307	0	335	8	0
32	1a	32246	0	16296	0	0
32	2a	32327	0	16338	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	828	0	0
56	10	7	0	0	0	0
56	11	3	0	0	0	0
56	12	2	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	4	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1254	0	0	0	0
56	1B	36	0	0	0	0
56	1D	12	0	0	0	0
56	1E	13	0	0	0	0
56	1F	10	0	0	0	0
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	7	0	0	0	0
56	1O	5	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1a	330	0	0	0	0
56	1b	2	0	0	0	0
56	1c	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1l	4	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	18	0	0	0	0
56	1y	5	0	0	0	0
56	20	3	0	0	0	0
56	23	3	0	0	0	0
56	25	4	0	0	0	0
56	27	1	0	0	0	0
56	28	3	0	0	0	0
56	2A	919	0	0	0	0
56	2B	21	0	0	0	0
56	2D	3	0	0	0	0
56	2E	8	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	1	0	0	0	0
56	2U	6	0	0	0	0
56	2V	1	0	0	0	0
56	2W	4	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	236	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2j	2	0	0	0	0
56	2l	4	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	4	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	6	0	0	0	0
56	2w	7	0	0	0	0
56	2x	6	0	0	0	0
56	2y	7	0	0	0	0
57	1A	8	0	0	1	0
57	1I	4	0	0	0	0
57	1a	4	0	0	0	0
57	2A	8	0	0	1	0
57	2I	4	0	0	1	0
57	2a	4	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	12	0	0	1	0
61	11	14	0	0	0	0
61	12	3	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	7	0	0	0	0
61	16	2	0	0	0	0
61	17	7	0	0	0	0
61	18	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1A	2273	0	0	110	0
61	1B	70	0	0	2	0
61	1D	28	0	0	0	0
61	1E	27	0	0	5	0
61	1F	15	0	0	0	0
61	1G	7	0	0	0	0
61	1H	1	0	0	0	0
61	1I	1	0	0	0	0
61	1N	3	0	0	0	0
61	1O	6	0	0	0	0
61	1P	23	0	0	1	0
61	1Q	12	0	0	0	0
61	1R	15	0	0	1	0
61	1S	5	0	0	0	0
61	1T	10	0	0	1	0
61	1U	16	0	0	0	0
61	1V	11	0	0	0	0
61	1W	13	0	0	2	0
61	1X	6	0	0	0	0
61	1Y	5	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	520	0	0	0	0
61	1b	1	0	0	0	0
61	1d	2	0	0	0	0
61	1e	1	0	0	0	0
61	1g	2	0	0	0	0
61	1i	1	0	0	0	0
61	1l	10	0	0	0	0
61	1m	2	0	0	0	0
61	1n	1	0	0	0	0
61	1o	2	0	0	0	0
61	1p	2	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	0	0
61	1v	5	0	0	0	0
61	1w	19	0	0	0	0
61	1x	15	0	0	0	0
61	1y	2	0	0	0	0
61	20	4	0	0	0	0
61	21	11	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	25	3	0	0	0	0
61	27	3	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	1393	0	0	97	0
61	2B	28	0	0	0	0
61	2D	29	0	0	0	0
61	2E	18	0	0	0	0
61	2F	17	0	0	0	0
61	2I	4	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	16	0	0	2	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	7	0	0	0	0
61	2U	3	0	0	0	0
61	2V	2	0	0	0	0
61	2W	4	0	0	0	0
61	2X	2	0	0	0	0
61	2Y	1	0	0	0	0
61	2Z	2	0	0	0	0
61	2a	373	0	0	0	0
61	2d	2	0	0	0	0
61	2e	2	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0
61	2l	6	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	4	0	0	0	0
61	2v	2	0	0	0	0
61	2w	3	0	0	0	0
61	2x	9	0	0	0	0
61	2y	20	0	0	0	0
All	All	301288	0	196660	2326	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 8.

The worst 5 of 2326 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:2138:C:N4	1:2A:2153:G:H1	1.49	1.10
1:1A:1740:U:H1'	3:1D:14:ARG:HH22	1.24	1.02
1:1A:2149:G:H1	1:1A:2183:C:N4	1.56	1.01
1:2A:79:G:H1	1:2A:90:U:H3	29.43	0.98
1:1A:2146:G:H1	1:1A:2196:C:H42	0.99	0.98

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%)	263 (96%)	10 (4%)	0	100	100
3	2D	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	36	70
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	31	65
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	31	65
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	31	65
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	17	48
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	27	60
6	2G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	27	60
7	1H	171/180 (95%)	161 (94%)	8 (5%)	2 (1%)	14	42
7	2H	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	27	60
8	1I	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
8	2I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	24	57
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	24	57
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	1P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
11	2P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	24	57
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	19	50
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	17	48
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	17	48
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%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	16	45
20	1Y	105/110 (96%)	100 (95%)	3 (3%)	2 (2%)	9	28
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	17	48
21	1Z	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
21	2Z	156/206 (76%)	139 (89%)	16 (10%)	1 (1%)	27	60
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	14	42
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	9	30
26	14	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	24	67/71 (94%)	53 (79%)	8 (12%)	6 (9%)	1	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%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	7	25
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	201 (88%)	20 (9%)	8 (4%)	4	13
33	2b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	15
34	1c	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	17	48
34	2c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	31	65
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	31	65
35	2d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	31	65
36	1e	146/162 (90%)	141 (97%)	2 (1%)	3 (2%)	8	26
36	2e	146/162 (90%)	139 (95%)	6 (4%)	1 (1%)	24	57
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	6 (4%)	2 (1%)	13	40
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	8	27
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	24	57
40	1i	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	2i	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
41	1j	95/105 (90%)	82 (86%)	6 (6%)	7 (7%)	1	2
41	2j	94/105 (90%)	84 (89%)	5 (5%)	5 (5%)	2	6
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	9	30
42	2k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	19	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	21	53
44	2m	120/126 (95%)	112 (93%)	7 (6%)	1 (1%)	21	53
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	13	40
48	1q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
48	2q	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
49	1r	66/88 (75%)	66 (100%)	0	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	14	42
50	2s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	6	21
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	3	9
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	3	9
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10766 (95%)	507 (4%)	95 (1%)	21	53

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	53	GLU
26	14	61	ARG
33	1b	17	PHE
38	1g	79	ARG

### 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%)	209 (97%)	6 (3%)	47	80
3	2D	215/218 (99%)	211 (98%)	4 (2%)	60	87
4	1E	164/166 (99%)	156 (95%)	8 (5%)	27	60
4	2E	164/166 (99%)	153 (93%)	11 (7%)	18	46
5	1F	160/166 (96%)	153 (96%)	7 (4%)	31	64
5	2F	159/166 (96%)	150 (94%)	9 (6%)	23	54
6	1G	143/156 (92%)	140 (98%)	3 (2%)	56	86
6	2G	143/156 (92%)	139 (97%)	4 (3%)	47	80
7	1H	143/148 (97%)	140 (98%)	3 (2%)	56	86
7	2H	143/148 (97%)	140 (98%)	3 (2%)	56	86
8	1I	113/124 (91%)	108 (96%)	5 (4%)	31	64
8	2I	105/124 (85%)	103 (98%)	2 (2%)	60	87
9	1N	118/119 (99%)	114 (97%)	4 (3%)	40	74
9	2N	118/119 (99%)	115 (98%)	3 (2%)	50	82
10	1O	100/100 (100%)	99 (99%)	1 (1%)	78	94
10	2O	100/100 (100%)	99 (99%)	1 (1%)	78	94
11	1P	115/116 (99%)	113 (98%)	2 (2%)	63	89
11	2P	115/116 (99%)	113 (98%)	2 (2%)	63	89
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	81	95
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	38	72
13	1R	101/101 (100%)	95 (94%)	6 (6%)	21	52
13	2R	101/101 (100%)	95 (94%)	6 (6%)	21	52
14	1S	86/88 (98%)	85 (99%)	1 (1%)	74	93
14	2S	85/88 (97%)	84 (99%)	1 (1%)	74	93
15	1T	115/127 (91%)	113 (98%)	2 (2%)	63	89
15	2T	113/127 (89%)	111 (98%)	2 (2%)	62	88
16	1U	93/94 (99%)	91 (98%)	2 (2%)	55	85
16	2U	93/94 (99%)	91 (98%)	2 (2%)	55	85
17	1V	80/82 (98%)	74 (92%)	6 (8%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	76 (95%)	4 (5%)	27	60
18	1W	90/92 (98%)	87 (97%)	3 (3%)	41	75
18	2W	90/92 (98%)	85 (94%)	5 (6%)	23	54
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	39	73
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	52	83
21	1Z	135/179 (75%)	130 (96%)	5 (4%)	37	71
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	55	85
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	80 (100%)	0	100	100
23	21	80/83 (96%)	79 (99%)	1 (1%)	71	92
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	50 (98%)	1 (2%)	58	86
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	57 (97%)	2 (3%)	40	74
26	24	53/63 (84%)	52 (98%)	1 (2%)	60	87
27	15	50/52 (96%)	47 (94%)	3 (6%)	21	52
27	25	50/52 (96%)	47 (94%)	3 (6%)	21	52
28	16	51/52 (98%)	50 (98%)	1 (2%)	58	86
28	26	50/52 (96%)	49 (98%)	1 (2%)	58	86
29	17	41/42 (98%)	40 (98%)	1 (2%)	52	83
29	27	41/42 (98%)	39 (95%)	2 (5%)	27	60
30	18	54/55 (98%)	52 (96%)	2 (4%)	37	71
30	28	54/55 (98%)	51 (94%)	3 (6%)	23	54
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	190 (99%)	2 (1%)	78	94
33	2b	187/220 (85%)	185 (99%)	2 (1%)	76	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	141 (99%)	1 (1%)	85	96
34	2c	140/188 (74%)	139 (99%)	1 (1%)	85	96
35	1d	169/181 (93%)	161 (95%)	8 (5%)	29	62
35	2d	173/181 (96%)	169 (98%)	4 (2%)	53	84
36	1e	113/123 (92%)	109 (96%)	4 (4%)	39	73
36	2e	114/123 (93%)	111 (97%)	3 (3%)	49	81
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	84 (99%)	1 (1%)	74	93
38	1g	119/127 (94%)	118 (99%)	1 (1%)	83	95
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	112 (98%)	2 (2%)	62	88
39	2h	114/119 (96%)	113 (99%)	1 (1%)	81	95
40	1i	90/99 (91%)	89 (99%)	1 (1%)	76	93
40	2i	89/99 (90%)	86 (97%)	3 (3%)	40	74
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	68 (99%)	1 (1%)	69	91
42	1k	82/99 (83%)	80 (98%)	2 (2%)	52	83
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	95 (99%)	1 (1%)	78	94
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	92 (99%)	1 (1%)	76	93
44	2m	92/101 (91%)	89 (97%)	3 (3%)	41	75
45	1n	49/50 (98%)	47 (96%)	2 (4%)	33	67
45	2n	49/50 (98%)	46 (94%)	3 (6%)	20	51
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	68 (99%)	1 (1%)	69	91
47	2p	68/74 (92%)	67 (98%)	1 (2%)	67	91
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	56	86
49	1r	59/77 (77%)	57 (97%)	2 (3%)	40	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	45	79
50	2s	67/80 (84%)	66 (98%)	1 (2%)	67	91
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9301/10064 (92%)	9088 (98%)	213 (2%)	53	84

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	1i	64	THR
4	2E	119	ARG
36	2e	41	VAL
43	1l	36	VAL
3	2D	94	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
47	1p	13	HIS
11	2P	27	HIS
40	2i	124	GLN
49	1r	63	GLN
51	1t	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	427 (14%)	30 (1%)
1	2A	2788/2915 (95%)	455 (16%)	22 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	22 (18%)	0
32	1a	1494/1521 (98%)	217 (14%)	0
32	2a	1498/1521 (98%)	239 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	1y	71/76 (93%)	20 (28%)	0
54	2w	68/76 (89%)	18 (26%)	0
54	2y	69/76 (90%)	22 (31%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9332/9620 (97%)	1480 (15%)	53 (0%)

5 of 1480 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	17	G
1	1A	34	C
1	1A	45	C
1	1A	70	A

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2156	A
1	1A	2769	U
1	2A	2119	A
1	1A	2203	G
1	1A	2442	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PSU	1A	1933	1	16,21,22	1.25	1 (6%)	20,30,33	3.13	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	1A	1937	1	13,22,23	0.76	0	14,32,35	1.82	1 (7%)
1	PSU	1A	1939	1	16,21,22	1.26	1 (6%)	20,30,33	3.01	6 (30%)
1	4OC	1A	1942	1	15,22,24	0.88	1 (6%)	20,31,35	1.58	2 (10%)
1	5MU	1A	1961	1,56	13,22,23	0.73	0	14,32,35	2.03	2 (14%)
1	5MC	1A	1964	1	14,22,23	1.44	1 (7%)	17,32,35	1.56	4 (23%)
1	5MC	1A	1984	1	14,22,23	1.38	1 (7%)	17,32,35	1.45	3 (17%)
1	OMG	1A	2263	1,55,56	18,26,27	1.32	2 (11%)	22,38,41	2.10	6 (27%)
1	2MA	1A	2515	1,56	16,25,26	1.32	2 (12%)	17,37,40	2.20	3 (17%)
1	2MU	1A	2564	1,56	14,22,24	1.03	1 (7%)	17,31,36	0.83	1 (5%)
1	PSU	1A	2617	1,56	16,21,22	1.72	5 (31%)	20,30,33	3.04	6 (30%)
32	2MG	1a	1207	32	18,26,27	1.37	2 (11%)	19,38,41	2.63	9 (47%)
32	5MC	1a	1400	32	14,22,23	1.40	1 (7%)	17,32,35	1.59	3 (17%)
32	4OC	1a	1402	32	16,23,24	0.81	0	20,32,35	1.13	1 (5%)
32	5MC	1a	1404	32	14,22,23	1.59	2 (14%)	17,32,35	1.44	2 (11%)
32	5MC	1a	1407	32	14,22,23	1.40	1 (7%)	17,32,35	1.40	3 (17%)
32	UR3	1a	1498	32	13,22,23	0.90	1 (7%)	15,32,35	0.72	0
32	MA6	1a	1518	32	16,26,27	1.11	1 (6%)	16,38,41	1.75	5 (31%)
32	MA6	1a	1519	32	16,26,27	1.11	1 (6%)	16,38,41	1.72	4 (25%)
32	PSU	1a	516	32	16,21,22	1.49	4 (25%)	20,30,33	3.00	6 (30%)
32	7MG	1a	527	32	20,26,27	1.99	4 (20%)	24,39,42	2.58	7 (29%)
32	M2G	1a	966	32	19,27,28	1.55	3 (15%)	20,40,43	2.28	6 (30%)
32	5MC	1a	967	32	14,22,23	1.42	1 (7%)	17,32,35	1.34	2 (11%)
43	0TD	1l	92	43	5,9,10	3.21	2 (40%)	4,11,13	2.44	1 (25%)
54	PSU	1w	32	54	16,21,22	1.33	1 (6%)	20,30,33	3.23	6 (30%)
54	MIA	1w	37	54	22,31,32	2.41	3 (13%)	26,44,47	2.50	10 (38%)
54	PSU	1w	39	54	16,21,22	1.43	2 (12%)	20,30,33	2.91	5 (25%)
54	7MG	1w	46	54	20,26,27	1.93	3 (15%)	24,39,42	2.67	6 (25%)
54	5MU	1w	54	54	13,22,23	0.84	0	14,32,35	2.09	1 (7%)
54	PSU	1w	55	54	16,21,22	1.23	1 (6%)	20,30,33	3.34	6 (30%)
54	4SU	1w	8	54	13,21,22	1.44	2 (15%)	14,30,33	1.49	2 (14%)
55	5MC	1x	32	55	14,22,23	1.46	2 (14%)	17,32,35	1.64	4 (23%)
55	5MU	1x	54	55	13,22,23	0.83	0	14,32,35	2.10	1 (7%)
55	PSU	1x	55	55,56	16,21,22	1.40	1 (6%)	20,30,33	3.28	6 (30%)
55	4SU	1x	8	55	13,21,22	1.56	2 (15%)	14,30,33	2.83	2 (14%)
54	PSU	1y	32	54	16,21,22	1.29	1 (6%)	20,30,33	3.23	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	MIA	1y	37	54	17,24,32	1.29	2 (11%)	16,35,47	1.29	2 (12%)
54	PSU	1y	39	54	16,21,22	1.26	1 (6%)	20,30,33	3.25	5 (25%)
54	7MG	1y	46	54	20,26,27	2.02	4 (20%)	24,39,42	3.03	9 (37%)
54	5MU	1y	54	54	13,22,23	0.83	1 (7%)	14,32,35	2.27	2 (14%)
54	PSU	1y	55	54	16,21,22	1.29	2 (12%)	20,30,33	3.18	5 (25%)
54	4SU	1y	8	54	13,21,22	1.24	1 (7%)	14,30,33	1.74	2 (14%)
1	PSU	2A	1911	1	16,21,22	1.62	1 (6%)	20,30,33	3.22	6 (30%)
1	5MU	2A	1915	1	13,22,23	0.77	0	14,32,35	2.02	2 (14%)
1	PSU	2A	1917	1	16,21,22	1.34	1 (6%)	20,30,33	3.17	6 (30%)
1	4OC	2A	1920	1	15,22,24	0.76	0	20,31,35	1.39	2 (10%)
1	5MU	2A	1939	1,56	13,22,23	0.76	0	14,32,35	1.94	2 (14%)
1	5MC	2A	1942	1	14,22,23	1.50	1 (7%)	17,32,35	1.41	2 (11%)
1	5MC	2A	1962	1,56	14,22,23	1.45	1 (7%)	17,32,35	1.52	3 (17%)
1	OMG	2A	2251	1,55,56	18,26,27	1.33	2 (11%)	22,38,41	1.93	6 (27%)
1	2MA	2A	2503	1,56	16,25,26	1.34	2 (12%)	17,37,40	2.02	3 (17%)
1	2MU	2A	2552	1,56	14,22,24	1.01	1 (7%)	17,31,36	0.91	2 (11%)
1	PSU	2A	2605	1	16,21,22	1.43	2 (12%)	20,30,33	3.12	6 (30%)
32	2MG	2a	1207	32,56	18,26,27	1.32	2 (11%)	19,38,41	2.50	8 (42%)
32	5MC	2a	1400	32	14,22,23	1.53	2 (14%)	17,32,35	1.54	3 (17%)
32	4OC	2a	1402	32	16,23,24	0.77	0	20,32,35	1.29	1 (5%)
32	5MC	2a	1404	32	14,22,23	1.54	1 (7%)	17,32,35	1.47	3 (17%)
32	5MC	2a	1407	32,56	14,22,23	1.51	2 (14%)	17,32,35	1.52	3 (17%)
32	UR3	2a	1498	32	13,22,23	0.93	1 (7%)	15,32,35	0.72	1 (6%)
32	MA6	2a	1518	32	16,26,27	1.13	1 (6%)	16,38,41	1.74	4 (25%)
32	MA6	2a	1519	32	16,26,27	1.08	1 (6%)	16,38,41	1.67	4 (25%)
32	PSU	2a	516	32	16,21,22	1.33	1 (6%)	20,30,33	3.17	7 (35%)
32	7MG	2a	527	32,56	20,26,27	1.98	3 (15%)	24,39,42	2.61	7 (29%)
32	M2G	2a	966	32	19,27,28	1.48	3 (15%)	20,40,43	2.13	6 (30%)
32	5MC	2a	967	32	14,22,23	1.55	1 (7%)	17,32,35	1.35	3 (17%)
43	0TD	2l	92	43	5,9,10	3.09	2 (40%)	4,11,13	4.55	1 (25%)
54	PSU	2w	32	54	16,21,22	1.21	1 (6%)	20,30,33	3.21	5 (25%)
54	MIA	2w	37	54	19,27,32	1.93	2 (10%)	21,39,47	1.87	7 (33%)
54	PSU	2w	39	54	16,21,22	1.19	1 (6%)	20,30,33	3.44	6 (30%)
54	7MG	2w	46	54	20,26,27	1.99	3 (15%)	24,39,42	2.61	7 (29%)
54	5MU	2w	54	54	13,22,23	0.76	0	14,32,35	2.02	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	PSU	2w	55	54	16,21,22	1.21	1 (6%)	20,30,33	3.22	6 (30%)
54	4SU	2w	8	54	13,21,22	1.33	1 (7%)	14,30,33	1.27	2 (14%)
55	5MC	2x	32	55	14,22,23	1.42	1 (7%)	17,32,35	1.51	2 (11%)
55	5MU	2x	54	55	13,22,23	0.77	0	14,32,35	1.81	2 (14%)
55	PSU	2x	55	55	16,21,22	1.44	1 (6%)	20,30,33	3.13	6 (30%)
55	4SU	2x	8	55,56	13,21,22	1.50	2 (15%)	14,30,33	2.32	2 (14%)
54	PSU	2y	32	54	16,21,22	1.24	1 (6%)	20,30,33	3.18	6 (30%)
54	MIA	2y	37	54	17,24,32	1.31	2 (11%)	16,35,47	1.38	2 (12%)
54	PSU	2y	39	54	16,21,22	1.36	1 (6%)	20,30,33	3.55	6 (30%)
54	7MG	2y	46	54	20,26,27	1.97	2 (10%)	24,39,42	3.00	7 (29%)
54	5MU	2y	54	54	13,22,23	0.71	0	14,32,35	1.83	1 (7%)
54	PSU	2y	55	54	16,21,22	1.38	1 (6%)	20,30,33	3.15	6 (30%)
54	4SU	2y	8	54	13,21,22	1.39	1 (7%)	14,30,33	1.38	2 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	2/3/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/5/27/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
1	2MU	1A	2564	1,56	-	0/5/27/28	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	2/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/2/12/14	-
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/3/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/3/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	4/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	2/3/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
1	2MU	2A	2552	1,56	-	1/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/2/12/14	-
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
54	5MU	2w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/3/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	0/3/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	1/3/25/26	0/2/2/2
54	PSU	2y	55	54	-	6/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/3/25/26	0/2/2/2

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.13	1.53	1.32
54	1w	37	MIA	C2-S10	-7.09	1.69	1.75
54	2w	37	MIA	C2-S10	-6.79	1.70	1.75
43	1l	92	0TD	CB-SB	-6.16	1.69	1.84
32	2a	527	7MG	C6-C5	6.06	1.48	1.41

The worst 5 of 336 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	9.74	139.76	126.94
54	2w	39	PSU	N1-C2-N3	-9.71	120.71	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N3-C4-N9	9.63	139.61	126.94
54	2y	39	PSU	N1-C2-N3	-9.28	121.05	128.43
55	1x	8	4SU	C2-N3-C4	9.22	128.52	115.15

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	PSU	1	0
1	1A	1961	5MU	1	0
1	1A	2263	OMG	1	0
1	1A	2564	2MU	1	0
1	2A	1917	PSU	1	0
1	2A	1920	4OC	2	0
1	2A	1939	5MU	1	0
1	2A	2503	2MA	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3095 ligands modelled in this entry, 3085 are monoatomic - leaving 10 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	$\# Z  > 2$
57	CPT	1A	4209	1	0,3,4	0.00	-	-		
57	CPT	1A	4210	1	0,3,4	0.00	-	-		
57	CPT	1I	3002	8	0,3,4	0.00	-	-		
57	CPT	1a	1930	32	0,3,4	0.00	-	-		
60	SF4	1d	501	35	0,12,12	0.00	-	-		
57	CPT	2A	3903	1	0,3,4	0.00	-	-		
57	CPT	2A	3904	1	0,3,4	0.00	-	-		
57	CPT	2I	201	8	0,3,4	0.00	-	-		
57	CPT	2a	3235	32	0,3,4	0.00	-	-		
60	SF4	2d	501	35	0,12,12	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
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

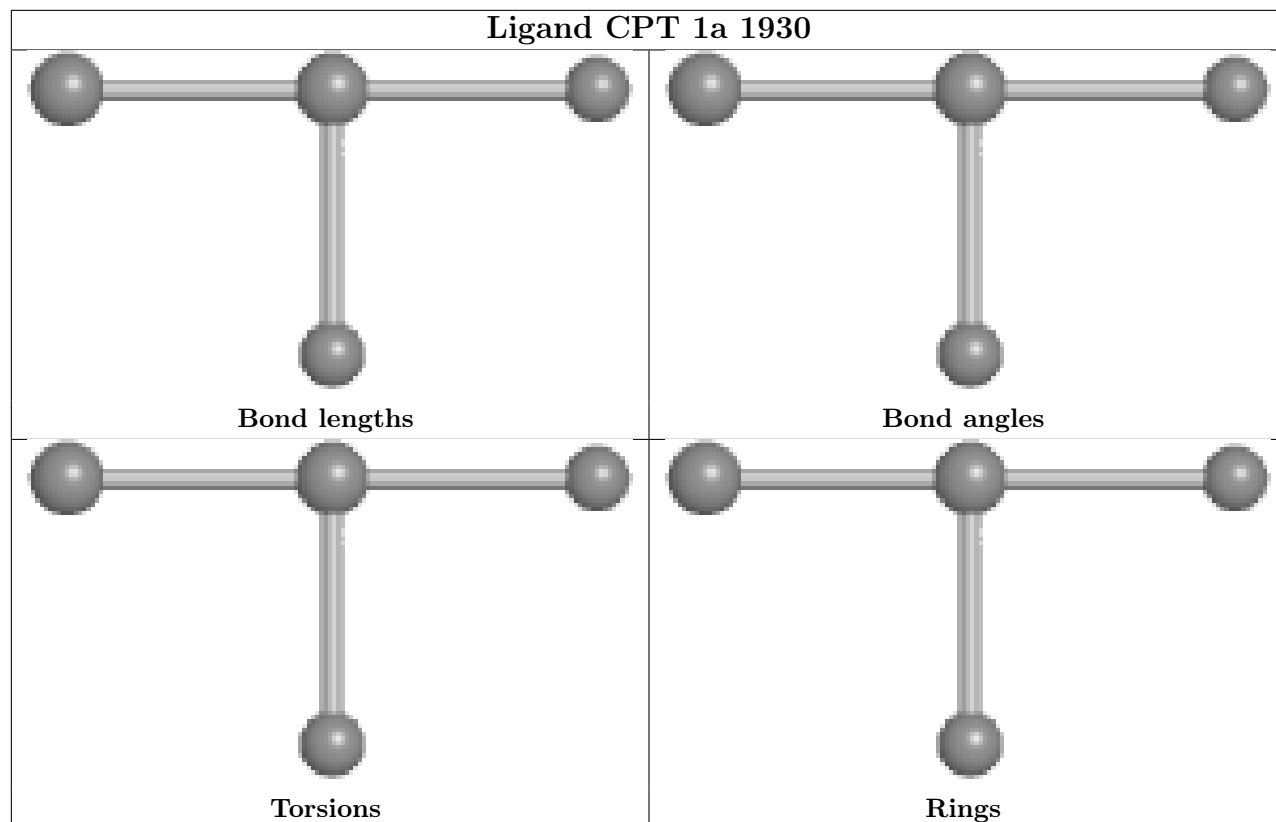
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



## 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	2860/2915 (98%)	0.29	49 (1%) 70 63	24, 45, 94, 107	0
1	2A	2789/2915 (95%)	-0.12	33 (1%) 79 72	27, 48, 92, 107	0
2	1B	120/121 (99%)	-0.05	0 100 100	40, 60, 72, 93	0
2	2B	120/121 (99%)	-0.23	1 (0%) 86 81	46, 65, 75, 93	0
3	1D	275/276 (99%)	0.21	2 (0%) 87 83	23, 43, 59, 79	0
3	2D	275/276 (99%)	0.01	0 100 100	24, 44, 61, 79	0
4	1E	204/206 (99%)	0.20	0 100 100	25, 50, 66, 82	0
4	2E	204/206 (99%)	0.29	4 (1%) 65 56	27, 52, 68, 85	0
5	1F	203/210 (96%)	0.24	2 (0%) 82 77	26, 54, 77, 90	0
5	2F	203/210 (96%)	0.34	9 (4%) 34 24	28, 57, 79, 89	0
6	1G	181/182 (99%)	0.32	5 (2%) 53 43	49, 69, 80, 95	0
6	2G	181/182 (99%)	0.90	33 (18%) 1 1	52, 72, 83, 98	0
7	1H	173/180 (96%)	0.04	1 (0%) 89 86	54, 68, 77, 85	0
7	2H	173/180 (96%)	1.91	76 (43%) 0 0	57, 72, 81, 86	0
8	1I	146/148 (98%)	0.33	3 (2%) 63 54	51, 75, 85, 90	0
8	2I	146/148 (98%)	0.26	10 (6%) 17 10	53, 74, 86, 92	0
9	1N	140/140 (100%)	0.16	0 100 100	34, 51, 73, 78	0
9	2N	140/140 (100%)	0.24	1 (0%) 87 83	37, 55, 75, 81	0
10	1O	122/122 (100%)	-0.12	0 100 100	25, 41, 58, 68	0
10	2O	122/122 (100%)	0.48	4 (3%) 46 36	45, 62, 74, 80	0
11	1P	149/150 (99%)	0.22	1 (0%) 87 83	27, 57, 78, 87	0
11	2P	149/150 (99%)	0.87	23 (15%) 2 1	29, 60, 79, 88	0
12	1Q	141/141 (100%)	0.37	2 (1%) 75 69	36, 53, 69, 84	0
12	2Q	141/141 (100%)	0.50	11 (7%) 13 7	38, 57, 73, 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%)	0.05	0 100 100	32, 42, 57, 67	0
13	2R	118/118 (100%)	0.19	2 (1%) 70 63	35, 45, 58, 69	0
14	1S	110/112 (98%)	0.12	0 100 100	45, 60, 73, 77	0
14	2S	110/112 (98%)	0.58	7 (6%) 19 12	49, 64, 76, 79	0
15	1T	131/146 (89%)	0.15	0 100 100	42, 54, 76, 86	0
15	2T	131/146 (89%)	0.55	5 (3%) 40 30	46, 57, 76, 86	0
16	1U	116/118 (98%)	0.29	1 (0%) 84 79	28, 45, 61, 75	0
16	2U	116/118 (98%)	0.09	2 (1%) 70 63	34, 49, 65, 77	0
17	1V	101/101 (100%)	0.13	0 100 100	31, 54, 70, 82	0
17	2V	101/101 (100%)	0.57	6 (5%) 22 14	34, 58, 73, 81	0
18	1W	112/113 (99%)	0.17	2 (1%) 68 61	30, 40, 64, 88	0
18	2W	112/113 (99%)	-0.05	1 (0%) 84 79	33, 42, 65, 90	0
19	1X	95/96 (98%)	-0.21	0 100 100	24, 38, 64, 78	0
19	2X	95/96 (98%)	0.63	5 (5%) 26 17	43, 61, 75, 87	0
20	1Y	107/110 (97%)	0.12	1 (0%) 84 79	47, 61, 74, 84	0
20	2Y	107/110 (97%)	0.37	3 (2%) 53 43	51, 64, 76, 86	0
21	1Z	154/206 (74%)	0.49	6 (3%) 39 29	55, 73, 89, 97	0
21	2Z	160/206 (77%)	1.09	25 (15%) 2 1	58, 76, 91, 98	0
22	10	83/85 (97%)	0.27	1 (1%) 79 72	23, 40, 62, 71	0
22	20	83/85 (97%)	0.41	1 (1%) 79 72	46, 65, 76, 84	0
23	11	97/98 (98%)	0.19	3 (3%) 49 38	27, 45, 72, 79	0
23	21	97/98 (98%)	0.45	4 (4%) 37 27	41, 56, 79, 88	0
24	12	70/72 (97%)	0.05	0 100 100	43, 58, 71, 82	0
24	22	70/72 (97%)	0.64	3 (4%) 35 25	46, 61, 75, 82	0
25	13	59/60 (98%)	0.29	1 (1%) 70 63	36, 50, 70, 83	0
25	23	59/60 (98%)	0.62	5 (8%) 11 5	41, 53, 74, 84	0
26	14	69/71 (97%)	0.79	13 (18%) 1 1	68, 82, 92, 97	0
26	24	69/71 (97%)	1.13	15 (21%) 0 0	72, 83, 92, 95	0
27	15	59/60 (98%)	0.05	1 (1%) 70 63	27, 41, 66, 71	0
27	25	59/60 (98%)	-0.08	0 100 100	29, 45, 67, 71	0
28	16	53/54 (98%)	0.18	0 100 100	41, 50, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.34	4 (7%) 14 7	42, 53, 67, 73	0
29	17	48/49 (97%)	0.21	1 (2%) 63 54	26, 32, 62, 71	0
29	27	48/49 (97%)	0.08	3 (6%) 20 12	28, 35, 62, 70	0
30	18	64/65 (98%)	0.20	0 100 100	35, 44, 55, 68	0
30	28	64/65 (98%)	0.46	2 (3%) 49 38	38, 47, 58, 67	0
31	19	37/37 (100%)	0.11	0 100 100	31, 40, 58, 65	0
31	29	37/37 (100%)	0.97	5 (13%) 3 1	52, 71, 80, 81	0
32	1a	1488/1521 (97%)	0.03	22 (1%) 73 67	35, 63, 92, 109	0
32	2a	1491/1521 (98%)	0.11	31 (2%) 63 54	47, 77, 96, 107	0
33	1b	231/256 (90%)	0.29	11 (4%) 30 21	65, 82, 89, 96	0
33	2b	231/256 (90%)	0.88	31 (13%) 3 1	68, 83, 90, 98	0
34	1c	206/239 (86%)	0.32	7 (3%) 45 35	63, 76, 84, 91	0
34	2c	206/239 (86%)	1.63	73 (35%) 0 0	67, 78, 86, 91	0
35	1d	208/209 (99%)	0.14	1 (0%) 90 88	59, 71, 82, 87	0
35	2d	208/209 (99%)	0.61	11 (5%) 26 17	60, 72, 83, 88	0
36	1e	148/162 (91%)	0.17	0 100 100	57, 70, 79, 87	0
36	2e	148/162 (91%)	0.37	2 (1%) 75 69	60, 72, 81, 88	0
37	1f	100/101 (99%)	0.00	1 (1%) 82 77	48, 65, 77, 82	0
37	2f	100/101 (99%)	-0.05	1 (1%) 82 77	53, 70, 79, 86	0
38	1g	155/156 (99%)	0.60	15 (9%) 8 4	63, 72, 83, 95	0
38	2g	155/156 (99%)	1.09	29 (18%) 1 1	64, 74, 84, 95	0
39	1h	137/138 (99%)	0.19	2 (1%) 73 67	59, 72, 79, 88	0
39	2h	137/138 (99%)	0.70	5 (3%) 42 32	63, 74, 81, 88	0
40	1i	127/128 (99%)	0.66	12 (9%) 8 4	49, 73, 85, 91	0
40	2i	127/128 (99%)	2.02	60 (47%) 0 0	69, 83, 91, 93	0
41	1j	97/105 (92%)	0.65	11 (11%) 5 2	60, 80, 90, 93	0
41	2j	96/105 (91%)	2.08	40 (41%) 0 0	63, 81, 91, 97	0
42	1k	114/129 (88%)	0.66	7 (6%) 21 13	53, 68, 78, 85	0
42	2k	114/129 (88%)	0.24	3 (2%) 56 45	53, 69, 79, 85	0
43	1l	121/132 (91%)	0.04	1 (0%) 86 81	45, 58, 70, 84	0
43	2l	121/132 (91%)	0.02	0 100 100	46, 61, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.30	5 (4%) 37 27	50, 67, 80, 88	0
44	2m	122/126 (96%)	1.28	34 (27%) 0 0	67, 83, 89, 93	0
45	1n	60/61 (98%)	0.44	2 (3%) 46 36	62, 71, 76, 81	0
45	2n	60/61 (98%)	2.76	44 (73%) 0 0	67, 74, 80, 85	0
46	1o	88/89 (98%)	0.49	5 (5%) 24 15	55, 68, 79, 83	0
46	2o	88/89 (98%)	0.20	0 100 100	58, 70, 80, 83	0
47	1p	82/88 (93%)	0.69	5 (6%) 21 13	57, 68, 79, 81	0
47	2p	82/88 (93%)	0.38	0 100 100	60, 68, 78, 84	0
48	1q	99/105 (94%)	0.56	2 (2%) 65 56	57, 70, 79, 83	0
48	2q	99/105 (94%)	0.97	10 (10%) 7 3	58, 71, 81, 84	0
49	1r	68/88 (77%)	0.68	4 (5%) 22 14	58, 68, 80, 83	0
49	2r	68/88 (77%)	0.01	2 (2%) 51 41	59, 69, 80, 85	0
50	1s	83/93 (89%)	0.52	3 (3%) 42 32	67, 76, 85, 92	0
50	2s	83/93 (89%)	1.20	19 (22%) 0 0	71, 79, 86, 93	0
51	1t	96/106 (90%)	1.40	25 (26%) 0 0	59, 70, 82, 89	0
51	2t	96/106 (90%)	1.32	21 (21%) 0 0	59, 70, 82, 89	0
52	1u	23/27 (85%)	0.63	0 100 100	64, 71, 77, 82	0
52	2u	23/27 (85%)	2.00	12 (52%) 0 0	67, 73, 79, 83	0
53	1v	13/24 (54%)	0.39	1 (7%) 13 7	43, 51, 74, 97	0
53	2v	13/24 (54%)	0.48	1 (7%) 13 7	63, 82, 98, 100	0
54	1w	67/76 (88%)	0.38	6 (8%) 9 5	49, 84, 99, 106	0
54	1y	67/76 (88%)	0.46	3 (4%) 33 23	39, 91, 99, 103	0
54	2w	65/76 (85%)	0.41	6 (9%) 9 5	62, 95, 102, 105	0
54	2y	66/76 (86%)	0.61	1 (1%) 73 67	49, 97, 101, 102	0
55	1x	72/77 (93%)	0.07	1 (1%) 75 69	33, 66, 82, 91	0
55	2x	72/77 (93%)	-0.01	0 100 100	50, 79, 88, 95	0
All	All	20873/21748 (95%)	0.31	986 (4%) 31 21	23, 63, 89, 109	0

The worst 5 of 986 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.0
41	2j	47	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	7.8
38	2g	82	GLY	7.6
21	2Z	144	LEU	7.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	PSU	2y	55	20/21	0.73	0.29	92,98,114,119	0
54	5MU	1y	54	21/22	0.78	0.22	73,89,102,120	0
54	7MG	2w	46	24/25	0.79	0.23	86,100,114,145	0
54	PSU	1y	55	20/21	0.79	0.26	86,98,106,123	0
54	4SU	1y	8	20/21	0.81	0.18	87,98,107,113	0
54	7MG	2y	46	24/25	0.82	0.18	93,98,105,125	0
54	5MU	2y	54	21/22	0.83	0.25	82,92,106,130	0
54	4SU	2w	8	20/21	0.84	0.17	84,95,110,123	0
54	4SU	2y	8	20/21	0.84	0.13	89,98,109,120	0
54	PSU	2y	32	20/21	0.85	0.20	74,90,101,111	0
54	MIA	2y	37	22/30	0.85	0.20	71,86,96,112	0
54	7MG	1y	46	24/25	0.87	0.21	83,94,107,126	0
54	4SU	1w	8	20/21	0.87	0.15	75,82,99,108	0
54	7MG	1w	46	24/25	0.87	0.15	74,87,111,126	0
54	PSU	2w	55	20/21	0.88	0.18	66,88,96,96	0
54	PSU	2y	39	20/21	0.90	0.20	74,86,97,100	0
54	PSU	1y	39	20/21	0.90	0.19	69,80,87,89	0
54	MIA	1y	37	22/30	0.91	0.12	65,81,88,93	0
55	4SU	2x	8	20/21	0.91	0.19	66,79,93,93	0
55	PSU	1x	55	20/21	0.91	0.17	62,72,91,96	0
54	PSU	1w	55	20/21	0.91	0.15	67,77,89,95	0
54	PSU	1y	32	20/21	0.92	0.18	68,86,94,94	0
54	PSU	2w	39	20/21	0.92	0.18	61,81,86,87	0
55	PSU	2x	55	20/21	0.92	0.15	73,79,92,97	0
55	5MU	2x	54	21/22	0.93	0.17	74,83,90,105	0
54	PSU	2w	32	20/21	0.93	0.19	67,83,98,106	0
54	5MU	2w	54	21/22	0.93	0.14	62,80,88,92	0
32	2MG	2a	1207	24/25	0.94	0.13	70,80,89,102	0
32	M2G	2a	966	25/26	0.94	0.21	53,67,78,82	0
32	5MC	2a	967	21/22	0.94	0.17	57,71,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	5MU	1x	54	21/22	0.94	0.15	56,73,78,85	0
43	0TD	2l	92	10/11	0.94	0.19	53,60,64,85	0
32	4OC	2a	1402	22/23	0.94	0.17	52,64,71,74	0
32	PSU	2a	516	20/21	0.95	0.16	54,68,81,87	0
1	PSU	1A	1939	20/21	0.95	0.20	50,57,64,65	0
1	PSU	2A	1911	20/21	0.95	0.17	42,57,65,65	0
1	5MC	2A	1962	21/22	0.95	0.22	37,42,53,60	0
55	5MC	2x	32	21/22	0.95	0.21	65,72,77,83	0
1	PSU	2A	1917	20/21	0.95	0.15	52,62,66,70	0
1	5MU	2A	1915	21/22	0.95	0.14	52,64,68,68	0
43	0TD	1l	92	10/11	0.95	0.22	47,57,60,73	0
54	MIA	2w	37	25/30	0.95	0.16	66,79,88,95	0
55	4SU	1x	8	20/21	0.95	0.18	50,61,71,83	0
32	7MG	2a	527	24/25	0.95	0.16	52,64,75,87	0
32	MA6	2a	1518	24/25	0.96	0.18	50,65,75,80	0
32	5MC	2a	1407	21/22	0.96	0.20	40,55,59,68	0
1	5MU	1A	1937	21/22	0.96	0.19	49,62,65,68	0
1	5MC	2A	1942	21/22	0.96	0.19	42,53,59,66	0
54	PSU	1w	32	20/21	0.96	0.13	58,66,79,81	0
32	7MG	1a	527	24/25	0.96	0.16	37,48,54,61	0
32	5MC	2a	1400	21/22	0.96	0.20	50,68,78,89	0
32	MA6	2a	1519	24/25	0.96	0.20	44,61,71,73	0
32	2MG	1a	1207	24/25	0.96	0.14	56,65,69,76	0
32	5MC	2a	1404	21/22	0.96	0.17	47,56,60,67	0
1	4OC	2A	1920	21/23	0.97	0.15	43,52,58,61	0
32	5MC	1a	1407	21/22	0.97	0.19	31,42,48,51	0
32	UR3	2a	1498	21/22	0.97	0.17	49,56,60,69	0
32	PSU	1a	516	20/21	0.97	0.15	39,51,60,64	0
1	PSU	1A	1933	20/21	0.97	0.19	38,55,63,65	0
1	5MC	1A	1984	21/22	0.97	0.22	33,39,46,58	0
55	5MC	1x	32	21/22	0.97	0.18	42,47,58,59	0
1	PSU	2A	2605	20/21	0.97	0.18	25,32,38,38	0
54	5MU	1w	54	21/22	0.97	0.17	48,62,67,73	0
1	2MU	1A	2564	21/23	0.97	0.22	29,36,42,46	0
32	5MC	1a	1400	21/22	0.97	0.17	31,45,56,63	0
54	MIA	1w	37	29/30	0.97	0.17	31,47,60,67	0
54	PSU	1w	39	20/21	0.97	0.15	35,56,64,66	0
32	5MC	1a	1404	21/22	0.97	0.19	30,36,44,47	0
32	MA6	1a	1519	24/25	0.98	0.20	35,39,47,51	0
1	2MU	2A	2552	21/23	0.98	0.15	29,38,45,51	0
1	2MA	2A	2503	23/24	0.98	0.18	22,28,37,40	0
32	5MC	1a	967	21/22	0.98	0.16	45,53,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	OMG	1A	2263	24/25	0.98	0.19	24,33,37,37	0
1	4OC	1A	1942	21/23	0.98	0.21	37,48,53,57	0
32	M2G	1a	966	25/26	0.98	0.18	46,54,60,69	0
1	PSU	1A	2617	20/21	0.98	0.20	25,30,34,35	0
32	MA6	1a	1518	24/25	0.98	0.19	30,41,47,50	0
1	5MU	1A	1961	21/22	0.98	0.21	25,31,36,41	0
1	5MC	1A	1964	21/22	0.98	0.20	39,51,57,64	0
32	4OC	1a	1402	22/23	0.98	0.18	34,43,56,68	0
1	OMG	2A	2251	24/25	0.98	0.17	29,36,40,41	0
1	5MU	2A	1939	21/22	0.98	0.19	28,34,38,40	0
32	UR3	1a	1498	21/22	0.99	0.19	29,37,45,49	0
1	2MA	1A	2515	23/24	0.99	0.19	20,27,33,37	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2B	3011	1/1	0.01	0.58	95,95,95,95	0
56	MG	1A	4085	1/1	0.16	0.27	99,99,99,99	0
56	MG	1a	1871	1/1	0.26	0.18	79,79,79,79	0
56	MG	2a	3146	1/1	0.27	0.13	114,114,114,114	0
56	MG	2l	3001	1/1	0.28	0.69	62,62,62,62	0
56	MG	2a	3031	1/1	0.28	0.55	76,76,76,76	0
56	MG	2A	3792	1/1	0.32	0.44	61,61,61,61	0
56	MG	1A	4054	1/1	0.33	0.26	73,73,73,73	0
56	MG	2a	3109	1/1	0.35	0.38	89,89,89,89	0
56	MG	2a	3173	1/1	0.37	0.29	104,104,104,104	0
56	MG	2y	3006	1/1	0.41	0.10	106,106,106,106	0
56	MG	1A	4048	1/1	0.41	0.11	68,68,68,68	0
56	MG	2v	102	1/1	0.41	0.49	93,93,93,93	0
56	MG	1B	227	1/1	0.42	0.63	106,106,106,106	0
56	MG	1w	103	1/1	0.42	0.57	80,80,80,80	0
56	MG	2a	3064	1/1	0.44	0.48	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	2A	3360	1/1	0.44	0.14	70,70,70,70	0
56	MG	2a	3131	1/1	0.44	0.18	90,90,90,90	0
56	MG	2a	3056	1/1	0.45	0.21	71,71,71,71	0
56	MG	2a	3162	1/1	0.45	0.24	100,100,100,100	0
56	MG	1A	3351	1/1	0.45	0.55	72,72,72,72	0
56	MG	1l	203	1/1	0.46	0.11	75,75,75,75	0
56	MG	1A	4068	1/1	0.47	0.28	83,83,83,83	0
56	MG	2a	3029	1/1	0.48	1.16	90,90,90,90	0
56	MG	1x	110	1/1	0.49	0.20	75,75,75,75	0
56	MG	1A	4083	1/1	0.50	0.15	63,63,63,63	0
56	MG	1A	4141	1/1	0.50	0.11	63,63,63,63	0
56	MG	2A	3816	1/1	0.50	0.32	75,75,75,75	0
56	MG	2A	3665	1/1	0.50	0.25	53,53,53,53	0
56	MG	1A	3357	1/1	0.51	0.30	69,69,69,69	0
56	MG	1A	3366	1/1	0.53	0.78	60,60,60,60	0
56	MG	2A	3411	1/1	0.53	0.75	52,52,52,52	0
56	MG	1a	1615	1/1	0.53	0.53	87,87,87,87	0
56	MG	2a	3003	1/1	0.54	0.20	75,75,75,75	0
56	MG	1a	1710	1/1	0.55	0.22	79,79,79,79	0
56	MG	2A	3382	1/1	0.55	0.43	55,55,55,55	0
56	MG	2a	3026	1/1	0.56	1.04	88,88,88,88	0
56	MG	1A	4116	1/1	0.56	0.35	85,85,85,85	0
56	MG	2a	3140	1/1	0.56	0.21	95,95,95,95	0
56	MG	2A	3872	1/1	0.57	0.33	63,63,63,63	0
56	MG	10	102	1/1	0.57	0.59	77,77,77,77	0
56	MG	2A	3798	1/1	0.57	0.21	75,75,75,75	0
56	MG	1A	3417	1/1	0.57	0.76	67,67,67,67	0
56	MG	1A	4166	1/1	0.58	0.18	70,70,70,70	0
56	MG	1A	4180	1/1	0.58	0.39	62,62,62,62	0
56	MG	1A	3369	1/1	0.58	1.00	66,66,66,66	0
56	MG	2a	3182	1/1	0.58	0.16	74,74,74,74	0
56	MG	1A	3260	1/1	0.59	0.33	57,57,57,57	0
56	MG	1A	4014	1/1	0.59	0.08	81,81,81,81	0
56	MG	2a	3222	1/1	0.60	0.43	94,94,94,94	0
56	MG	2A	3059	1/1	0.61	0.24	57,57,57,57	0
56	MG	1x	102	1/1	0.61	0.55	74,74,74,74	0
56	MG	2A	3831	1/1	0.61	0.10	57,57,57,57	0
56	MG	1A	4099	1/1	0.61	0.10	82,82,82,82	0
56	MG	2A	3284	1/1	0.62	0.23	56,56,56,56	0
56	MG	1A	3646	1/1	0.63	0.29	49,49,49,49	0
56	MG	1A	3540	1/1	0.63	0.34	60,60,60,60	0
56	MG	1A	3222	1/1	0.63	0.60	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3864	1/1	0.63	0.12	73,73,73,73	0
56	MG	1B	228	1/1	0.63	0.32	80,80,80,80	0
56	MG	2A	3343	1/1	0.63	1.04	63,63,63,63	0
56	MG	1a	1725	1/1	0.63	0.12	62,62,62,62	0
56	MG	1A	4009	1/1	0.64	0.14	81,81,81,81	0
56	MG	1A	3756	1/1	0.64	0.15	67,67,67,67	0
56	MG	2A	3332	1/1	0.64	0.38	53,53,53,53	0
56	MG	1a	1914	1/1	0.64	0.13	84,84,84,84	0
56	MG	2A	3410	1/1	0.64	0.36	71,71,71,71	0
56	MG	2A	3683	1/1	0.64	0.18	49,49,49,49	0
56	MG	1G	3002	1/1	0.64	0.17	63,63,63,63	0
56	MG	2a	3204	1/1	0.64	0.18	90,90,90,90	0
56	MG	1A	3915	1/1	0.65	0.20	51,51,51,51	0
56	MG	1A	4050	1/1	0.65	0.08	57,57,57,57	0
56	MG	1x	113	1/1	0.65	0.24	48,48,48,48	0
56	MG	2A	3894	1/1	0.65	0.24	60,60,60,60	0
56	MG	2A	3832	1/1	0.65	0.20	69,69,69,69	0
56	MG	2A	3837	1/1	0.65	0.17	48,48,48,48	0
56	MG	2a	3116	1/1	0.66	0.17	73,73,73,73	0
56	MG	1a	1658	1/1	0.66	0.25	84,84,84,84	0
56	MG	1A	4162	1/1	0.66	0.16	68,68,68,68	0
56	MG	2A	3823	1/1	0.66	0.49	79,79,79,79	0
56	MG	1A	3386	1/1	0.66	0.20	63,63,63,63	0
56	MG	2A	3527	1/1	0.67	0.13	38,38,38,38	0
56	MG	2A	3868	1/1	0.67	0.23	71,71,71,71	0
56	MG	2A	3874	1/1	0.67	0.12	74,74,74,74	0
56	MG	1a	1915	1/1	0.67	0.07	68,68,68,68	0
56	MG	2a	3169	1/1	0.67	0.14	80,80,80,80	0
56	MG	2A	3617	1/1	0.67	0.20	47,47,47,47	0
56	MG	2a	3054	1/1	0.67	0.20	61,61,61,61	0
56	MG	1a	1881	1/1	0.67	0.09	73,73,73,73	0
56	MG	1A	3600	1/1	0.67	0.14	64,64,64,64	0
56	MG	1A	3007	1/1	0.68	0.35	52,52,52,52	0
56	MG	1A	4087	1/1	0.68	0.36	79,79,79,79	0
56	MG	1a	1874	1/1	0.68	0.11	82,82,82,82	0
56	MG	1A	4146	1/1	0.68	0.88	80,80,80,80	0
56	MG	2A	3734	1/1	0.68	0.27	67,67,67,67	0
56	MG	2A	3090	1/1	0.68	0.10	71,71,71,71	0
56	MG	1a	1607	1/1	0.68	0.14	71,71,71,71	0
56	MG	1w	108	1/1	0.68	0.20	63,63,63,63	0
56	MG	1l	102	1/1	0.68	0.35	58,58,58,58	0
56	MG	2A	3388	1/1	0.68	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3066	1/1	0.68	0.30	77,77,77,77	0
56	MG	1A	3383	1/1	0.68	0.53	72,72,72,72	0
56	MG	1A	3890	1/1	0.68	0.12	65,65,65,65	0
56	MG	2A	3362	1/1	0.68	0.29	61,61,61,61	0
56	MG	1a	1751	1/1	0.68	0.12	78,78,78,78	0
56	MG	2a	3034	1/1	0.68	0.40	64,64,64,64	0
56	MG	2A	3068	1/1	0.69	0.19	56,56,56,56	0
56	MG	1A	3987	1/1	0.69	0.09	71,71,71,71	0
56	MG	1a	1861	1/1	0.69	0.31	102,102,102,102	0
56	MG	2a	3007	1/1	0.69	0.16	70,70,70,70	0
56	MG	1a	1693	1/1	0.69	0.16	66,66,66,66	0
56	MG	1A	4123	1/1	0.69	0.17	78,78,78,78	0
56	MG	1A	3358	1/1	0.69	0.35	64,64,64,64	0
56	MG	2A	3713	1/1	0.69	0.12	63,63,63,63	0
56	MG	2A	3495	1/1	0.69	0.58	66,66,66,66	0
56	MG	1A	4063	1/1	0.70	0.38	63,63,63,63	0
56	MG	1A	4111	1/1	0.70	0.21	92,92,92,92	0
56	MG	2a	3086	1/1	0.70	0.60	81,81,81,81	0
56	MG	1A	4151	1/1	0.70	0.28	59,59,59,59	0
56	MG	1a	1887	1/1	0.70	0.16	57,57,57,57	0
56	MG	1A	3464	1/1	0.70	0.19	50,50,50,50	0
56	MG	1A	4015	1/1	0.70	0.22	73,73,73,73	0
56	MG	2a	3044	1/1	0.70	0.17	70,70,70,70	0
56	MG	1A	4038	1/1	0.70	0.15	71,71,71,71	0
56	MG	2a	3170	1/1	0.70	0.13	79,79,79,79	0
56	MG	1A	3981	1/1	0.70	0.17	41,41,41,41	0
56	MG	1A	3265	1/1	0.70	0.19	64,64,64,64	0
56	MG	2A	3265	1/1	0.70	0.34	61,61,61,61	0
56	MG	1A	3091	1/1	0.70	0.57	72,72,72,72	0
56	MG	1A	3112	1/1	0.70	0.48	54,54,54,54	0
56	MG	1A	3634	1/1	0.70	0.21	68,68,68,68	0
56	MG	1A	3370	1/1	0.70	0.84	55,55,55,55	0
56	MG	1I	3001	1/1	0.70	0.34	76,76,76,76	0
56	MG	1A	4207	1/1	0.70	0.28	60,60,60,60	0
56	MG	1A	4135	1/1	0.71	0.11	67,67,67,67	0
56	MG	2A	3888	1/1	0.71	0.13	42,42,42,42	0
56	MG	2A	3380	1/1	0.71	0.14	67,67,67,67	0
56	MG	2A	3271	1/1	0.71	0.21	59,59,59,59	0
56	MG	2A	3113	1/1	0.71	0.23	71,71,71,71	0
56	MG	1A	3255	1/1	0.71	0.24	60,60,60,60	0
56	MG	1a	1750	1/1	0.71	0.11	75,75,75,75	0
56	MG	1A	3312	1/1	0.71	0.41	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1814	1/1	0.71	0.15	71,71,71,71	0
56	MG	1A	3730	1/1	0.71	0.18	44,44,44,44	0
56	MG	2a	3174	1/1	0.71	0.12	88,88,88,88	0
56	MG	2A	3058	1/1	0.71	0.37	68,68,68,68	0
56	MG	2A	3326	1/1	0.71	0.27	57,57,57,57	0
56	MG	2A	3057	1/1	0.72	0.40	68,68,68,68	0
56	MG	2A	3757	1/1	0.72	0.19	54,54,54,54	0
56	MG	2A	3476	1/1	0.72	0.22	63,63,63,63	0
56	MG	1A	4024	1/1	0.72	0.10	48,48,48,48	0
57	CPT	1a	1930	4/5	0.72	0.45	60,62,73,353	0
56	MG	1a	1649	1/1	0.72	0.09	62,62,62,62	0
56	MG	2A	3672	1/1	0.72	0.12	68,68,68,68	0
56	MG	1A	3227	1/1	0.72	0.29	65,65,65,65	0
56	MG	2a	3060	1/1	0.72	0.51	82,82,82,82	0
56	MG	1A	3934	1/1	0.72	0.12	64,64,64,64	0
56	MG	2B	3009	1/1	0.72	0.14	61,61,61,61	0
56	MG	1a	1723	1/1	0.72	0.71	69,69,69,69	0
56	MG	2a	3047	1/1	0.72	0.15	72,72,72,72	0
56	MG	1A	3397	1/1	0.72	0.36	44,44,44,44	0
56	MG	2A	3593	1/1	0.72	0.30	71,71,71,71	0
56	MG	1a	1867	1/1	0.73	0.11	83,83,83,83	0
56	MG	1t	3001	1/1	0.73	0.35	65,65,65,65	0
56	MG	2A	3797	1/1	0.73	0.26	50,50,50,50	0
56	MG	2A	3835	1/1	0.73	0.13	32,32,32,32	0
56	MG	1A	3274	1/1	0.73	0.38	71,71,71,71	0
56	MG	1A	4179	1/1	0.73	0.22	51,51,51,51	0
56	MG	2A	3688	1/1	0.73	0.24	68,68,68,68	0
56	MG	2A	3377	1/1	0.73	0.75	64,64,64,64	0
56	MG	2a	3143	1/1	0.73	0.16	82,82,82,82	0
56	MG	2x	103	1/1	0.73	0.33	83,83,83,83	0
56	MG	1A	4121	1/1	0.73	0.14	91,91,91,91	0
56	MG	1A	3246	1/1	0.73	0.19	54,54,54,54	0
56	MG	2A	3329	1/1	0.73	0.21	58,58,58,58	0
56	MG	2a	3020	1/1	0.73	0.27	61,61,61,61	0
56	MG	1A	4066	1/1	0.73	0.44	82,82,82,82	0
56	MG	2a	3234	1/1	0.73	0.15	76,76,76,76	0
56	MG	1A	4138	1/1	0.73	0.20	76,76,76,76	0
56	MG	1a	1754	1/1	0.73	0.18	63,63,63,63	0
56	MG	1A	3406	1/1	0.73	0.25	54,54,54,54	0
56	MG	1A	4008	1/1	0.73	0.07	84,84,84,84	0
56	MG	2A	3479	1/1	0.73	0.57	58,58,58,58	0
56	MG	1A	3352	1/1	0.73	0.27	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1899	1/1	0.74	0.20	86,86,86,86	0
56	MG	1A	4153	1/1	0.74	0.15	90,90,90,90	0
56	MG	1A	3251	1/1	0.74	0.66	57,57,57,57	0
56	MG	2a	3148	1/1	0.74	0.10	75,75,75,75	0
56	MG	1A	3960	1/1	0.74	0.13	50,50,50,50	0
56	MG	2A	3725	1/1	0.74	0.12	52,52,52,52	0
56	MG	2A	3261	1/1	0.74	0.31	65,65,65,65	0
56	MG	2a	3191	1/1	0.74	0.19	65,65,65,65	0
56	MG	2A	3769	1/1	0.74	0.14	54,54,54,54	0
56	MG	1a	1679	1/1	0.74	0.14	75,75,75,75	0
56	MG	1A	3215	1/1	0.74	0.20	56,56,56,56	0
56	MG	1A	3151	1/1	0.74	0.86	54,54,54,54	0
56	MG	2a	3152	1/1	0.74	0.20	69,69,69,69	0
56	MG	2a	3057	1/1	0.74	0.79	97,97,97,97	0
56	MG	2A	3387	1/1	0.74	0.58	64,64,64,64	0
56	MG	20	101	1/1	0.74	0.21	60,60,60,60	0
56	MG	1A	4053	1/1	0.74	0.17	41,41,41,41	0
56	MG	1A	3560	1/1	0.74	0.44	55,55,55,55	0
56	MG	2A	3810	1/1	0.74	0.10	59,59,59,59	0
56	MG	1A	3575	1/1	0.74	0.43	54,54,54,54	0
56	MG	1A	4124	1/1	0.74	0.07	67,67,67,67	0
56	MG	1a	1602	1/1	0.74	0.44	83,83,83,83	0
56	MG	2A	3756	1/1	0.74	0.18	40,40,40,40	0
56	MG	1A	3403	1/1	0.74	0.39	53,53,53,53	0
56	MG	1A	3375	1/1	0.75	0.94	60,60,60,60	0
56	MG	1A	4037	1/1	0.75	0.11	64,64,64,64	0
56	MG	1A	3059	1/1	0.75	0.24	63,63,63,63	0
56	MG	2A	3165	1/1	0.75	0.19	72,72,72,72	0
56	MG	1a	1878	1/1	0.75	0.07	70,70,70,70	0
56	MG	2a	3055	1/1	0.75	0.30	67,67,67,67	0
56	MG	2A	3303	1/1	0.75	0.24	45,45,45,45	0
56	MG	1A	3392	1/1	0.75	0.59	55,55,55,55	0
56	MG	2A	3334	1/1	0.75	0.34	54,54,54,54	0
56	MG	2A	3373	1/1	0.75	0.17	72,72,72,72	0
56	MG	2w	103	1/1	0.75	0.52	83,83,83,83	0
56	MG	1G	3003	1/1	0.75	0.28	67,67,67,67	0
56	MG	2A	3394	1/1	0.75	0.59	61,61,61,61	0
56	MG	1A	3297	1/1	0.75	0.26	67,67,67,67	0
56	MG	1A	3384	1/1	0.75	0.24	51,51,51,51	0
56	MG	1A	4125	1/1	0.75	0.09	77,77,77,77	0
56	MG	1a	1781	1/1	0.75	0.22	58,58,58,58	0
56	MG	1Z	302	1/1	0.75	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3460	1/1	0.75	0.24	62,62,62,62	0
56	MG	2A	3297	1/1	0.75	0.18	54,54,54,54	0
56	MG	1A	3331	1/1	0.75	0.17	67,67,67,67	0
56	MG	2A	3719	1/1	0.75	0.25	55,55,55,55	0
56	MG	2a	3100	1/1	0.75	0.12	67,67,67,67	0
56	MG	1A	4186	1/1	0.75	0.47	66,66,66,66	0
56	MG	2a	3025	1/1	0.75	0.17	68,68,68,68	0
56	MG	2a	3192	1/1	0.75	0.10	74,74,74,74	0
56	MG	2A	3092	1/1	0.75	0.58	34,34,34,34	0
56	MG	1A	3296	1/1	0.76	0.17	53,53,53,53	0
56	MG	1A	3372	1/1	0.76	0.37	74,74,74,74	0
56	MG	2A	3214	1/1	0.76	0.64	64,64,64,64	0
56	MG	1A	4114	1/1	0.76	0.50	87,87,87,87	0
56	MG	2A	3408	1/1	0.76	0.24	60,60,60,60	0
56	MG	1Q	204	1/1	0.76	0.10	33,33,33,33	0
56	MG	10	105	1/1	0.76	0.16	66,66,66,66	0
56	MG	1A	3367	1/1	0.76	0.51	56,56,56,56	0
56	MG	15	102	1/1	0.76	0.51	42,42,42,42	0
56	MG	1A	3256	1/1	0.76	0.15	73,73,73,73	0
56	MG	1A	4002	1/1	0.76	0.26	45,45,45,45	0
56	MG	1A	3496	1/1	0.76	0.33	57,57,57,57	0
56	MG	1A	4113	1/1	0.76	0.11	60,60,60,60	0
56	MG	1A	3192	1/1	0.76	0.18	57,57,57,57	0
56	MG	1A	4072	1/1	0.76	0.37	95,95,95,95	0
56	MG	1a	1690	1/1	0.76	0.26	71,71,71,71	0
56	MG	1A	3639	1/1	0.76	0.22	56,56,56,56	0
56	MG	1a	1673	1/1	0.76	0.29	69,69,69,69	0
56	MG	1a	1726	1/1	0.76	0.15	85,85,85,85	0
56	MG	1A	3212	1/1	0.76	0.26	53,53,53,53	0
56	MG	2A	3288	1/1	0.76	0.20	56,56,56,56	0
56	MG	2A	3671	1/1	0.76	0.34	57,57,57,57	0
56	MG	2A	3188	1/1	0.76	0.13	57,57,57,57	0
56	MG	2A	3296	1/1	0.76	0.34	55,55,55,55	0
56	MG	1a	1659	1/1	0.76	0.09	68,68,68,68	0
56	MG	1A	4154	1/1	0.76	0.23	88,88,88,88	0
56	MG	2A	3274	1/1	0.76	0.25	52,52,52,52	0
56	MG	1A	3633	1/1	0.76	0.29	55,55,55,55	0
56	MG	2A	3029	1/1	0.76	0.12	51,51,51,51	0
56	MG	1A	3270	1/1	0.76	0.14	64,64,64,64	0
56	MG	1A	3468	1/1	0.76	0.25	68,68,68,68	0
56	MG	23	3001	1/1	0.76	0.69	56,56,56,56	0
56	MG	1a	1742	1/1	0.76	0.16	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	1A	3978	1/1	0.76	0.21	35,35,35,35	0
56	MG	2A	3548	1/1	0.76	0.13	49,49,49,49	0
56	MG	1a	1732	1/1	0.76	0.18	57,57,57,57	0
56	MG	2v	103	1/1	0.76	0.41	67,67,67,67	0
56	MG	2A	3301	1/1	0.76	0.43	64,64,64,64	0
56	MG	2A	3460	1/1	0.76	0.27	66,66,66,66	0
56	MG	1A	3002	1/1	0.76	0.31	59,59,59,59	0
56	MG	2A	3875	1/1	0.77	0.25	48,48,48,48	0
56	MG	2A	3550	1/1	0.77	0.15	41,41,41,41	0
56	MG	2A	3152	1/1	0.77	0.16	53,53,53,53	0
56	MG	2A	3089	1/1	0.77	0.17	60,60,60,60	0
56	MG	1A	3467	1/1	0.77	0.26	65,65,65,65	0
56	MG	1A	3363	1/1	0.77	0.34	58,58,58,58	0
56	MG	2A	3073	1/1	0.77	0.24	43,43,43,43	0
56	MG	2A	3521	1/1	0.77	0.09	53,53,53,53	0
56	MG	2A	3858	1/1	0.77	0.24	52,52,52,52	0
56	MG	2A	3200	1/1	0.77	0.38	73,73,73,73	0
56	MG	2A	3255	1/1	0.77	0.24	60,60,60,60	0
56	MG	1A	3601	1/1	0.77	0.12	70,70,70,70	0
56	MG	2A	3879	1/1	0.77	0.08	91,91,91,91	0
56	MG	1A	4119	1/1	0.77	0.29	73,73,73,73	0
56	MG	2E	303	1/1	0.77	0.14	51,51,51,51	0
56	MG	1A	3862	1/1	0.77	0.24	31,31,31,31	0
56	MG	1A	3745	1/1	0.77	0.28	49,49,49,49	0
56	MG	1A	3817	1/1	0.77	0.15	67,67,67,67	0
56	MG	2A	3516	1/1	0.77	0.06	57,57,57,57	0
56	MG	1x	118	1/1	0.77	0.35	66,66,66,66	0
56	MG	1a	1872	1/1	0.77	0.10	85,85,85,85	0
56	MG	1A	4199	1/1	0.77	0.22	36,36,36,36	0
56	MG	1a	1755	1/1	0.77	0.13	62,62,62,62	0
56	MG	2A	3312	1/1	0.77	0.24	60,60,60,60	0
56	MG	2A	3400	1/1	0.77	0.22	77,77,77,77	0
56	MG	2A	3251	1/1	0.77	0.44	68,68,68,68	0
56	MG	2A	3201	1/1	0.77	0.17	61,61,61,61	0
56	MG	2A	3064	1/1	0.77	0.09	64,64,64,64	0
56	MG	1A	3688	1/1	0.77	0.45	53,53,53,53	0
56	MG	2A	3173	1/1	0.77	0.08	61,61,61,61	0
56	MG	1A	3984	1/1	0.77	0.27	49,49,49,49	0
56	MG	1A	4208	1/1	0.77	0.30	79,79,79,79	0
56	MG	2A	3393	1/1	0.77	0.15	67,67,67,67	0
56	MG	1a	1917	1/1	0.77	0.17	55,55,55,55	0
56	MG	1A	3506	1/1	0.77	0.34	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3073	1/1	0.78	0.13	58,58,58,58	0
56	MG	2A	3210	1/1	0.78	0.38	61,61,61,61	0
56	MG	1A	3519	1/1	0.78	0.11	71,71,71,71	0
56	MG	2A	3355	1/1	0.78	0.35	73,73,73,73	0
56	MG	2A	3195	1/1	0.78	0.45	53,53,53,53	0
56	MG	1a	1798	1/1	0.78	0.15	66,66,66,66	0
56	MG	2A	3687	1/1	0.78	0.16	53,53,53,53	0
56	MG	2p	3001	1/1	0.78	0.22	63,63,63,63	0
56	MG	1A	3720	1/1	0.78	0.15	37,37,37,37	0
56	MG	1B	204	1/1	0.78	0.27	61,61,61,61	0
56	MG	2A	3803	1/1	0.78	0.15	64,64,64,64	0
56	MG	1A	3457	1/1	0.78	0.25	63,63,63,63	0
56	MG	1A	3024	1/1	0.78	0.18	53,53,53,53	0
56	MG	1A	3409	1/1	0.78	0.21	64,64,64,64	0
56	MG	2A	3177	1/1	0.78	0.31	46,46,46,46	0
56	MG	2A	3582	1/1	0.78	0.10	76,76,76,76	0
56	MG	2A	3270	1/1	0.78	0.46	65,65,65,65	0
56	MG	1a	1612	1/1	0.78	0.18	62,62,62,62	0
56	MG	1a	1851	1/1	0.78	0.16	76,76,76,76	0
56	MG	1a	1805	1/1	0.78	0.17	63,63,63,63	0
56	MG	1a	1880	1/1	0.78	0.17	51,51,51,51	0
56	MG	1A	4065	1/1	0.78	0.09	64,64,64,64	0
56	MG	2A	3243	1/1	0.78	0.40	60,60,60,60	0
56	MG	2A	3456	1/1	0.78	0.56	52,52,52,52	0
56	MG	2A	3589	1/1	0.78	0.20	65,65,65,65	0
56	MG	2A	3358	1/1	0.78	0.18	78,78,78,78	0
56	MG	2B	3020	1/1	0.78	0.14	75,75,75,75	0
56	MG	1A	3888	1/1	0.78	0.19	54,54,54,54	0
56	MG	1A	3695	1/1	0.79	0.16	37,37,37,37	0
56	MG	2A	3222	1/1	0.79	0.27	72,72,72,72	0
56	MG	16	102	1/1	0.79	0.62	68,68,68,68	0
56	MG	2A	3800	1/1	0.79	0.15	67,67,67,67	0
56	MG	1a	1902	1/1	0.79	0.10	77,77,77,77	0
56	MG	2a	3142	1/1	0.79	0.14	86,86,86,86	0
56	MG	2B	3002	1/1	0.79	0.30	60,60,60,60	0
56	MG	1A	4201	1/1	0.79	0.19	51,51,51,51	0
56	MG	2A	3342	1/1	0.79	0.37	53,53,53,53	0
56	MG	2B	3015	1/1	0.79	0.19	62,62,62,62	0
56	MG	1A	3327	1/1	0.79	0.33	56,56,56,56	0
56	MG	2a	3059	1/1	0.79	0.17	61,61,61,61	0
56	MG	2A	3551	1/1	0.79	0.14	44,44,44,44	0
56	MG	1a	1677	1/1	0.79	0.27	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3649	1/1	0.79	0.39	79,79,79,79	0
56	MG	2a	3167	1/1	0.79	0.08	75,75,75,75	0
56	MG	2F	303	1/1	0.79	0.31	52,52,52,52	0
56	MG	1A	4147	1/1	0.79	0.13	79,79,79,79	0
56	MG	1B	234	1/1	0.79	0.27	78,78,78,78	0
56	MG	1A	4013	1/1	0.79	0.09	50,50,50,50	0
56	MG	2v	105	1/1	0.79	0.17	76,76,76,76	0
56	MG	1a	1919	1/1	0.79	0.10	54,54,54,54	0
56	MG	1A	3484	1/1	0.79	0.23	58,58,58,58	0
56	MG	2a	3023	1/1	0.79	0.28	72,72,72,72	0
56	MG	1a	1793	1/1	0.79	0.26	65,65,65,65	0
56	MG	1A	3321	1/1	0.79	0.21	57,57,57,57	0
56	MG	2a	3139	1/1	0.79	0.19	85,85,85,85	0
56	MG	1x	117	1/1	0.79	0.17	78,78,78,78	0
56	MG	1A	3359	1/1	0.79	0.22	53,53,53,53	0
56	MG	1A	4255	1/1	0.79	0.19	48,48,48,48	0
56	MG	2a	3004	1/1	0.79	0.12	68,68,68,68	0
56	MG	2A	3604	1/1	0.79	0.22	34,34,34,34	0
56	MG	1A	3425	1/1	0.79	0.20	54,54,54,54	0
56	MG	2a	3137	1/1	0.79	0.06	87,87,87,87	0
56	MG	2y	3002	1/1	0.79	0.20	58,58,58,58	0
56	MG	1A	3517	1/1	0.80	0.38	53,53,53,53	0
56	MG	1a	1776	1/1	0.80	0.42	69,69,69,69	0
56	MG	2a	3048	1/1	0.80	0.11	58,58,58,58	0
56	MG	2A	3726	1/1	0.80	0.09	64,64,64,64	0
56	MG	2A	3352	1/1	0.80	0.25	47,47,47,47	0
56	MG	1A	3684	1/1	0.80	0.24	67,67,67,67	0
56	MG	2a	3078	1/1	0.80	0.15	50,50,50,50	0
56	MG	1a	1728	1/1	0.80	0.09	62,62,62,62	0
56	MG	2A	3422	1/1	0.80	0.20	56,56,56,56	0
56	MG	1A	3797	1/1	0.80	0.20	49,49,49,49	0
56	MG	1A	3374	1/1	0.80	0.29	53,53,53,53	0
56	MG	1A	3472	1/1	0.80	0.20	59,59,59,59	0
56	MG	2a	3134	1/1	0.80	0.15	74,74,74,74	0
56	MG	1A	3595	1/1	0.80	0.26	49,49,49,49	0
56	MG	1a	1620	1/1	0.80	0.13	54,54,54,54	0
56	MG	1A	4168	1/1	0.80	0.11	66,66,66,66	0
56	MG	1A	3308	1/1	0.80	0.79	62,62,62,62	0
56	MG	1a	1864	1/1	0.80	0.10	94,94,94,94	0
56	MG	2A	3247	1/1	0.80	0.47	56,56,56,56	0
56	MG	2a	3216	1/1	0.80	0.18	66,66,66,66	0
56	MG	1A	3512	1/1	0.80	0.43	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3107	1/1	0.80	0.30	75,75,75,75	0
56	MG	1A	3049	1/1	0.80	0.29	45,45,45,45	0
56	MG	1A	4011	1/1	0.80	0.20	73,73,73,73	0
56	MG	2l	3002	1/1	0.80	0.17	62,62,62,62	0
56	MG	2a	3157	1/1	0.80	0.09	79,79,79,79	0
56	MG	1A	3995	1/1	0.80	0.20	51,51,51,51	0
56	MG	1E	309	1/1	0.80	0.14	54,54,54,54	0
56	MG	2A	3727	1/1	0.80	0.15	53,53,53,53	0
56	MG	2A	3248	1/1	0.80	0.41	66,66,66,66	0
56	MG	2A	3824	1/1	0.80	0.21	80,80,80,80	0
56	MG	1A	3615	1/1	0.80	0.18	33,33,33,33	0
56	MG	1F	308	1/1	0.80	0.11	45,45,45,45	0
56	MG	2A	3290	1/1	0.80	0.28	62,62,62,62	0
56	MG	2a	3006	1/1	0.80	0.17	65,65,65,65	0
56	MG	1a	1709	1/1	0.80	0.07	73,73,73,73	0
56	MG	2A	3339	1/1	0.80	0.24	56,56,56,56	0
56	MG	2A	3431	1/1	0.80	0.24	58,58,58,58	0
56	MG	1A	3941	1/1	0.80	0.23	29,29,29,29	0
56	MG	1a	1891	1/1	0.80	0.13	91,91,91,91	0
56	MG	1A	4205	1/1	0.80	0.18	46,46,46,46	0
56	MG	2a	3188	1/1	0.80	0.19	78,78,78,78	0
56	MG	1A	4193	1/1	0.80	0.15	49,49,49,49	0
56	MG	1w	111	1/1	0.80	0.29	84,84,84,84	0
56	MG	2a	3133	1/1	0.80	0.15	94,94,94,94	0
56	MG	2a	3214	1/1	0.80	0.14	63,63,63,63	0
56	MG	1A	4240	1/1	0.80	0.25	51,51,51,51	0
56	MG	2A	3809	1/1	0.80	0.23	67,67,67,67	0
56	MG	2A	3146	1/1	0.80	0.21	56,56,56,56	0
56	MG	2v	106	1/1	0.80	0.22	68,68,68,68	0
56	MG	1a	1694	1/1	0.80	0.40	62,62,62,62	0
56	MG	2A	3853	1/1	0.80	0.13	63,63,63,63	0
56	MG	1A	4118	1/1	0.81	0.09	66,66,66,66	0
56	MG	1A	3599	1/1	0.81	0.25	64,64,64,64	0
56	MG	2A	3414	1/1	0.81	0.32	52,52,52,52	0
56	MG	1A	4007	1/1	0.81	0.13	51,51,51,51	0
56	MG	2A	3761	1/1	0.81	0.51	47,47,47,47	0
56	MG	1A	3801	1/1	0.81	0.15	60,60,60,60	0
56	MG	1a	1641	1/1	0.81	0.17	73,73,73,73	0
56	MG	1A	3800	1/1	0.81	0.13	57,57,57,57	0
56	MG	2N	8001	1/1	0.81	0.14	53,53,53,53	0
56	MG	1G	3005	1/1	0.81	0.11	65,65,65,65	0
56	MG	2a	3024	1/1	0.81	0.17	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1X	106	1/1	0.81	0.24	56,56,56,56	0
56	MG	1E	302	1/1	0.81	0.19	51,51,51,51	0
56	MG	1A	4046	1/1	0.81	0.17	69,69,69,69	0
56	MG	1A	4051	1/1	0.81	0.15	55,55,55,55	0
56	MG	1A	3315	1/1	0.81	0.23	51,51,51,51	0
56	MG	1a	1705	1/1	0.81	0.15	65,65,65,65	0
56	MG	2A	3645	1/1	0.81	0.19	40,40,40,40	0
56	MG	2a	3018	1/1	0.81	0.17	62,62,62,62	0
56	MG	1A	3757	1/1	0.81	0.14	51,51,51,51	0
56	MG	2A	3005	1/1	0.81	0.15	56,56,56,56	0
56	MG	2a	3221	1/1	0.81	0.10	81,81,81,81	0
56	MG	2A	3489	1/1	0.81	0.51	82,82,82,82	0
56	MG	2A	3783	1/1	0.81	0.15	42,42,42,42	0
56	MG	1y	3005	1/1	0.81	0.44	83,83,83,83	0
56	MG	2A	3885	1/1	0.81	0.26	50,50,50,50	0
56	MG	2A	3340	1/1	0.81	0.47	75,75,75,75	0
56	MG	1A	4078	1/1	0.81	0.19	24,24,24,24	0
56	MG	1W	3002	1/1	0.81	0.21	51,51,51,51	0
56	MG	1A	3904	1/1	0.81	0.11	57,57,57,57	0
56	MG	1A	4100	1/1	0.81	0.08	95,95,95,95	0
56	MG	1a	1832	1/1	0.81	0.15	59,59,59,59	0
56	MG	2f	3002	1/1	0.81	0.22	63,63,63,63	0
56	MG	1A	4034	1/1	0.81	0.16	24,24,24,24	0
56	MG	2a	3058	1/1	0.81	0.54	76,76,76,76	0
56	MG	1A	3480	1/1	0.81	0.24	53,53,53,53	0
56	MG	1A	4165	1/1	0.81	0.09	45,45,45,45	0
56	MG	1B	215	1/1	0.81	0.09	45,45,45,45	0
56	MG	1A	4115	1/1	0.81	0.13	86,86,86,86	0
56	MG	2A	3313	1/1	0.81	0.42	71,71,71,71	0
56	MG	1B	210	1/1	0.81	0.92	62,62,62,62	0
56	MG	1A	3431	1/1	0.81	0.46	47,47,47,47	0
56	MG	1A	3152	1/1	0.81	0.24	51,51,51,51	0
56	MG	2a	3196	1/1	0.81	0.24	71,71,71,71	0
56	MG	2A	3540	1/1	0.81	0.10	54,54,54,54	0
56	MG	1A	3626	1/1	0.81	0.11	64,64,64,64	0
56	MG	1A	3643	1/1	0.81	0.14	51,51,51,51	0
56	MG	2A	3229	1/1	0.81	0.27	55,55,55,55	0
56	MG	2A	3287	1/1	0.81	0.25	60,60,60,60	0
56	MG	1a	1713	1/1	0.81	0.61	79,79,79,79	0
56	MG	1A	3662	1/1	0.81	0.27	59,59,59,59	0
56	MG	1A	3354	1/1	0.81	0.24	55,55,55,55	0
56	MG	1A	4091	1/1	0.81	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1809	1/1	0.82	0.13	64,64,64,64	0
56	MG	1D	312	1/1	0.82	0.21	63,63,63,63	0
56	MG	2A	3050	1/1	0.82	0.46	47,47,47,47	0
56	MG	2a	3156	1/1	0.82	0.10	77,77,77,77	0
56	MG	2a	3187	1/1	0.82	0.22	78,78,78,78	0
56	MG	1A	3538	1/1	0.82	0.20	50,50,50,50	0
56	MG	2A	3420	1/1	0.82	0.16	61,61,61,61	0
56	MG	1A	3677	1/1	0.82	0.22	57,57,57,57	0
56	MG	2A	3359	1/1	0.82	0.15	73,73,73,73	0
56	MG	2a	3075	1/1	0.82	0.20	70,70,70,70	0
56	MG	1A	3611	1/1	0.82	0.20	59,59,59,59	0
56	MG	2A	3309	1/1	0.82	0.15	66,66,66,66	0
56	MG	2A	3262	1/1	0.82	0.36	55,55,55,55	0
56	MG	1A	3364	1/1	0.82	0.21	52,52,52,52	0
56	MG	1A	3879	1/1	0.82	0.10	57,57,57,57	0
56	MG	1A	3330	1/1	0.82	0.15	67,67,67,67	0
56	MG	2a	3113	1/1	0.82	0.55	73,73,73,73	0
56	MG	1a	1665	1/1	0.82	0.12	67,67,67,67	0
56	MG	2A	3258	1/1	0.82	0.20	55,55,55,55	0
56	MG	1A	3804	1/1	0.82	0.14	66,66,66,66	0
56	MG	1A	3149	1/1	0.82	0.55	42,42,42,42	0
56	MG	2a	3027	1/1	0.82	0.20	69,69,69,69	0
56	MG	1A	3690	1/1	0.82	0.14	52,52,52,52	0
56	MG	1A	3648	1/1	0.82	0.23	53,53,53,53	0
56	MG	1A	3430	1/1	0.82	0.15	50,50,50,50	0
56	MG	1a	1875	1/1	0.82	0.13	55,55,55,55	0
56	MG	1A	3518	1/1	0.82	0.11	81,81,81,81	0
56	MG	1A	4171	1/1	0.82	0.17	74,74,74,74	0
56	MG	1A	3269	1/1	0.82	0.28	57,57,57,57	0
56	MG	1a	1759	1/1	0.82	0.19	53,53,53,53	0
56	MG	2A	3354	1/1	0.82	0.10	69,69,69,69	0
56	MG	2A	3202	1/1	0.82	0.16	53,53,53,53	0
56	MG	1a	1618	1/1	0.82	0.16	51,51,51,51	0
56	MG	1A	3692	1/1	0.82	0.27	73,73,73,73	0
56	MG	2A	3066	1/1	0.82	0.17	55,55,55,55	0
56	MG	1A	3947	1/1	0.82	0.11	47,47,47,47	0
56	MG	1A	3225	1/1	0.82	0.41	53,53,53,53	0
56	MG	1a	1876	1/1	0.82	0.12	65,65,65,65	0
56	MG	1A	3081	1/1	0.82	0.31	44,44,44,44	0
56	MG	2A	3618	1/1	0.82	0.12	46,46,46,46	0
56	MG	1A	4145	1/1	0.82	0.23	35,35,35,35	0
56	MG	2a	3052	1/1	0.82	0.31	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3298	1/1	0.82	0.16	67,67,67,67	0
56	MG	1A	3469	1/1	0.82	0.19	60,60,60,60	0
56	MG	1A	4084	1/1	0.82	0.21	78,78,78,78	0
56	MG	2A	3001	1/1	0.82	0.35	49,49,49,49	0
56	MG	1A	3226	1/1	0.82	0.40	51,51,51,51	0
56	MG	2U	203	1/1	0.82	0.63	57,57,57,57	0
56	MG	2a	3068	1/1	0.82	0.13	71,71,71,71	0
56	MG	1a	1784	1/1	0.82	0.11	59,59,59,59	0
56	MG	1A	3244	1/1	0.83	0.19	55,55,55,55	0
56	MG	2x	102	1/1	0.83	0.55	71,71,71,71	0
56	MG	2A	3198	1/1	0.83	0.26	48,48,48,48	0
56	MG	1a	1691	1/1	0.83	0.29	79,79,79,79	0
56	MG	2E	304	1/1	0.83	0.18	55,55,55,55	0
56	MG	2A	3363	1/1	0.83	0.27	65,65,65,65	0
56	MG	2A	3820	1/1	0.83	0.23	75,75,75,75	0
56	MG	1A	3793	1/1	0.83	0.17	36,36,36,36	0
56	MG	1A	3373	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3029	1/1	0.83	0.20	41,41,41,41	0
56	MG	1A	3336	1/1	0.83	0.29	59,59,59,59	0
56	MG	2A	3676	1/1	0.83	0.22	55,55,55,55	0
56	MG	2a	3036	1/1	0.83	0.30	60,60,60,60	0
56	MG	1A	3791	1/1	0.83	0.34	61,61,61,61	0
56	MG	1A	3952	1/1	0.83	0.22	52,52,52,52	0
56	MG	1A	3683	1/1	0.83	0.15	76,76,76,76	0
56	MG	1A	3867	1/1	0.83	0.10	62,62,62,62	0
56	MG	1A	4184	1/1	0.83	0.21	33,33,33,33	0
56	MG	1a	1792	1/1	0.83	0.21	51,51,51,51	0
56	MG	2A	3376	1/1	0.83	0.20	59,59,59,59	0
56	MG	2g	8001	1/1	0.83	0.08	61,61,61,61	0
56	MG	1A	3577	1/1	0.83	0.17	69,69,69,69	0
56	MG	1a	1868	1/1	0.83	0.17	75,75,75,75	0
56	MG	1B	208	1/1	0.83	0.13	71,71,71,71	0
56	MG	1A	3678	1/1	0.83	0.30	50,50,50,50	0
56	MG	1A	3053	1/1	0.83	0.12	62,62,62,62	0
56	MG	2A	3900	1/1	0.83	0.29	53,53,53,53	0
56	MG	1A	3189	1/1	0.83	0.20	43,43,43,43	0
56	MG	1A	4157	1/1	0.83	0.11	61,61,61,61	0
56	MG	2Q	3003	1/1	0.83	0.15	41,41,41,41	0
56	MG	2a	3200	1/1	0.83	0.14	71,71,71,71	0
56	MG	2A	3026	1/1	0.83	0.92	56,56,56,56	0
56	MG	2a	3127	1/1	0.83	0.25	67,67,67,67	0
56	MG	1B	209	1/1	0.83	0.46	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1782	1/1	0.83	0.12	58,58,58,58	0
56	MG	1a	1707	1/1	0.83	0.24	59,59,59,59	0
56	MG	2A	3321	1/1	0.83	0.32	62,62,62,62	0
56	MG	1A	3515	1/1	0.83	0.50	55,55,55,55	0
56	MG	1A	4137	1/1	0.83	0.20	72,72,72,72	0
56	MG	1A	3299	1/1	0.83	0.22	54,54,54,54	0
56	MG	1A	3343	1/1	0.83	0.39	60,60,60,60	0
56	MG	2B	3001	1/1	0.83	0.15	66,66,66,66	0
56	MG	2A	3158	1/1	0.83	0.32	58,58,58,58	0
56	MG	1A	3631	1/1	0.83	0.20	57,57,57,57	0
56	MG	2A	3644	1/1	0.83	0.17	46,46,46,46	0
56	MG	2A	3920	1/1	0.83	0.72	60,60,60,60	0
56	MG	1A	3713	1/1	0.83	0.14	50,50,50,50	0
56	MG	2A	3765	1/1	0.83	0.18	62,62,62,62	0
56	MG	1A	3997	1/1	0.83	0.18	68,68,68,68	0
56	MG	1l	202	1/1	0.83	0.23	63,63,63,63	0
56	MG	1a	1909	1/1	0.83	0.07	64,64,64,64	0
56	MG	1A	4159	1/1	0.83	0.16	60,60,60,60	0
56	MG	2a	3013	1/1	0.83	0.20	66,66,66,66	0
56	MG	1A	3026	1/1	0.83	0.23	56,56,56,56	0
56	MG	2A	3815	1/1	0.83	0.13	69,69,69,69	0
56	MG	2A	3722	1/1	0.83	0.17	48,48,48,48	0
56	MG	2A	3266	1/1	0.83	0.20	62,62,62,62	0
56	MG	1A	3185	1/1	0.83	0.18	41,41,41,41	0
56	MG	1A	4017	1/1	0.83	0.20	29,29,29,29	0
56	MG	1A	3805	1/1	0.83	0.23	62,62,62,62	0
56	MG	2a	3155	1/1	0.83	0.11	91,91,91,91	0
56	MG	2A	3085	1/1	0.83	0.25	55,55,55,55	0
56	MG	1A	4139	1/1	0.83	0.13	34,34,34,34	0
56	MG	2A	3204	1/1	0.83	0.14	58,58,58,58	0
56	MG	2A	3454	1/1	0.83	0.19	48,48,48,48	0
56	MG	2A	3865	1/1	0.83	0.16	57,57,57,57	0
56	MG	2A	3771	1/1	0.83	0.14	47,47,47,47	0
56	MG	1w	104	1/1	0.83	0.13	54,54,54,54	0
56	MG	1a	1811	1/1	0.83	0.33	68,68,68,68	0
56	MG	1a	1859	1/1	0.83	0.21	77,77,77,77	0
56	MG	1A	3605	1/1	0.83	0.16	48,48,48,48	0
56	MG	2a	3194	1/1	0.84	0.12	77,77,77,77	0
56	MG	2a	3132	1/1	0.84	0.10	59,59,59,59	0
56	MG	2A	3241	1/1	0.84	0.76	44,44,44,44	0
56	MG	1F	302	1/1	0.84	0.58	66,66,66,66	0
56	MG	1A	3489	1/1	0.84	0.42	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4140	1/1	0.84	0.31	74,74,74,74	0
56	MG	1A	4128	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3514	1/1	0.84	0.16	48,48,48,48	0
56	MG	1a	1749	1/1	0.84	0.19	62,62,62,62	0
56	MG	1A	4074	1/1	0.84	0.12	58,58,58,58	0
56	MG	2A	3866	1/1	0.84	0.11	63,63,63,63	0
56	MG	2a	3080	1/1	0.84	0.42	62,62,62,62	0
56	MG	2A	3206	1/1	0.84	0.18	59,59,59,59	0
56	MG	1a	1688	1/1	0.84	0.29	71,71,71,71	0
56	MG	2A	3375	1/1	0.84	0.44	59,59,59,59	0
56	MG	10	104	1/1	0.84	0.74	53,53,53,53	0
56	MG	1A	3598	1/1	0.84	0.22	54,54,54,54	0
56	MG	1A	3455	1/1	0.84	0.41	41,41,41,41	0
56	MG	2A	3109	1/1	0.84	0.09	58,58,58,58	0
56	MG	2a	3168	1/1	0.84	0.09	68,68,68,68	0
56	MG	2A	3086	1/1	0.84	0.13	51,51,51,51	0
56	MG	2a	3225	1/1	0.84	0.17	68,68,68,68	0
56	MG	2A	3753	1/1	0.84	0.13	66,66,66,66	0
56	MG	1A	3318	1/1	0.84	0.31	57,57,57,57	0
56	MG	2A	3179	1/1	0.84	0.26	55,55,55,55	0
56	MG	2A	3870	1/1	0.84	0.11	45,45,45,45	0
56	MG	1A	3082	1/1	0.84	0.61	50,50,50,50	0
56	MG	1A	3580	1/1	0.84	0.14	57,57,57,57	0
56	MG	1A	4088	1/1	0.84	0.14	62,62,62,62	0
56	MG	1a	1663	1/1	0.84	0.10	73,73,73,73	0
56	MG	2A	3854	1/1	0.84	0.28	42,42,42,42	0
56	MG	2A	3311	1/1	0.84	0.58	59,59,59,59	0
56	MG	2y	3003	1/1	0.84	0.30	71,71,71,71	0
56	MG	2A	3227	1/1	0.84	0.20	62,62,62,62	0
56	MG	1x	107	1/1	0.84	0.14	66,66,66,66	0
56	MG	1O	3001	1/1	0.84	0.48	82,82,82,82	0
56	MG	28	103	1/1	0.84	0.24	63,63,63,63	0
56	MG	1a	1714	1/1	0.84	0.34	75,75,75,75	0
56	MG	1A	3247	1/1	0.84	1.13	71,71,71,71	0
56	MG	2A	3169	1/1	0.84	0.15	49,49,49,49	0
56	MG	2A	3447	1/1	0.84	0.34	51,51,51,51	0
56	MG	1a	1711	1/1	0.84	0.11	54,54,54,54	0
56	MG	2A	3423	1/1	0.84	0.13	61,61,61,61	0
56	MG	1a	1639	1/1	0.84	0.07	56,56,56,56	0
56	MG	2A	3682	1/1	0.84	0.18	56,56,56,56	0
56	MG	2A	3383	1/1	0.84	0.37	59,59,59,59	0
56	MG	1A	3865	1/1	0.84	0.20	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3113	1/1	0.84	0.15	61,61,61,61	0
56	MG	1A	3475	1/1	0.84	0.33	48,48,48,48	0
56	MG	1A	3220	1/1	0.84	0.18	47,47,47,47	0
56	MG	2A	3172	1/1	0.84	0.40	55,55,55,55	0
56	MG	2a	3177	1/1	0.84	0.13	69,69,69,69	0
56	MG	1a	1683	1/1	0.84	0.14	80,80,80,80	0
56	MG	1A	4098	1/1	0.84	0.09	81,81,81,81	0
56	MG	2a	3083	1/1	0.84	0.13	62,62,62,62	0
56	MG	2a	3121	1/1	0.84	0.07	78,78,78,78	0
56	MG	1x	116	1/1	0.84	0.13	65,65,65,65	0
56	MG	1a	1644	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3102	1/1	0.84	0.20	42,42,42,42	0
56	MG	1A	4059	1/1	0.84	0.15	65,65,65,65	0
56	MG	2A	3892	1/1	0.84	0.45	52,52,52,52	0
56	MG	1A	3557	1/1	0.84	0.20	59,59,59,59	0
56	MG	1a	1763	1/1	0.84	0.37	65,65,65,65	0
56	MG	1a	1605	1/1	0.84	0.49	72,72,72,72	0
56	MG	1a	1834	1/1	0.84	0.25	60,60,60,60	0
56	MG	1B	230	1/1	0.84	0.10	82,82,82,82	0
56	MG	1A	3052	1/1	0.84	0.39	59,59,59,59	0
56	MG	1A	3132	1/1	0.84	0.36	58,58,58,58	0
56	MG	1a	1604	1/1	0.84	0.37	63,63,63,63	0
56	MG	1A	3320	1/1	0.84	0.12	55,55,55,55	0
56	MG	1A	3338	1/1	0.84	0.21	50,50,50,50	0
56	MG	1a	1854	1/1	0.84	0.25	68,68,68,68	0
56	MG	2A	3112	1/1	0.84	0.11	60,60,60,60	0
56	MG	1A	3644	1/1	0.84	0.19	44,44,44,44	0
56	MG	2A	3452	1/1	0.84	0.20	60,60,60,60	0
56	MG	1A	3316	1/1	0.85	0.17	51,51,51,51	0
56	MG	1a	1900	1/1	0.85	0.08	62,62,62,62	0
56	MG	1A	4195	1/1	0.85	0.73	59,59,59,59	0
56	MG	2A	3714	1/1	0.85	0.16	58,58,58,58	0
56	MG	2A	3855	1/1	0.85	0.17	47,47,47,47	0
56	MG	1A	3647	1/1	0.85	0.20	40,40,40,40	0
56	MG	1a	1715	1/1	0.85	0.25	62,62,62,62	0
56	MG	1a	1802	1/1	0.85	0.10	63,63,63,63	0
56	MG	1A	3881	1/1	0.85	0.09	78,78,78,78	0
56	MG	1a	1734	1/1	0.85	0.16	67,67,67,67	0
56	MG	2A	3470	1/1	0.85	0.50	60,60,60,60	0
56	MG	1B	207	1/1	0.85	0.11	65,65,65,65	0
56	MG	1A	3034	1/1	0.85	0.78	51,51,51,51	0
56	MG	1A	3273	1/1	0.85	0.41	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3988	1/1	0.85	0.14	58,58,58,58	0
56	MG	1A	3292	1/1	0.85	0.23	62,62,62,62	0
56	MG	1A	3333	1/1	0.85	0.13	55,55,55,55	0
56	MG	1A	3441	1/1	0.85	0.26	48,48,48,48	0
56	MG	2A	3395	1/1	0.85	0.08	61,61,61,61	0
56	MG	1A	3079	1/1	0.85	0.17	46,46,46,46	0
56	MG	2A	3503	1/1	0.85	0.10	45,45,45,45	0
56	MG	1A	4232	1/1	0.85	1.31	62,62,62,62	0
56	MG	2A	3230	1/1	0.85	0.33	58,58,58,58	0
56	MG	2A	3549	1/1	0.85	0.14	52,52,52,52	0
56	MG	1A	3231	1/1	0.85	0.16	54,54,54,54	0
56	MG	2A	3384	1/1	0.85	0.30	70,70,70,70	0
56	MG	10	106	1/1	0.85	0.13	70,70,70,70	0
56	MG	2A	3002	1/1	0.85	0.41	61,61,61,61	0
56	MG	2A	3361	1/1	0.85	0.12	57,57,57,57	0
56	MG	2A	3091	1/1	0.85	0.26	55,55,55,55	0
56	MG	1A	3930	1/1	0.85	0.14	44,44,44,44	0
56	MG	1a	1818	1/1	0.85	0.42	45,45,45,45	0
56	MG	2A	3344	1/1	0.85	1.10	71,71,71,71	0
56	MG	2A	3244	1/1	0.85	0.25	46,46,46,46	0
56	MG	1A	3826	1/1	0.85	0.21	61,61,61,61	0
56	MG	2A	3409	1/1	0.85	0.37	51,51,51,51	0
56	MG	1B	205	1/1	0.85	0.19	48,48,48,48	0
56	MG	1a	1700	1/1	0.85	0.16	55,55,55,55	0
56	MG	1A	4133	1/1	0.85	0.14	57,57,57,57	0
56	MG	1A	3974	1/1	0.85	0.20	35,35,35,35	0
56	MG	2a	3237	1/1	0.85	0.18	61,61,61,61	0
56	MG	1A	4010	1/1	0.85	0.45	85,85,85,85	0
56	MG	1x	111	1/1	0.85	0.10	61,61,61,61	0
56	MG	2w	104	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	3483	1/1	0.85	0.15	43,43,43,43	0
56	MG	1A	3492	1/1	0.85	0.29	47,47,47,47	0
56	MG	1A	3208	1/1	0.85	0.28	52,52,52,52	0
56	MG	2A	3902	1/1	0.85	0.30	61,61,61,61	0
56	MG	1A	3783	1/1	0.85	0.22	37,37,37,37	0
56	MG	2a	3120	1/1	0.85	0.11	77,77,77,77	0
56	MG	2A	3793	1/1	0.85	0.19	56,56,56,56	0
56	MG	1A	4220	1/1	0.85	0.28	48,48,48,48	0
56	MG	2A	3746	1/1	0.85	0.11	76,76,76,76	0
56	MG	1A	4117	1/1	0.85	0.09	83,83,83,83	0
56	MG	25	101	1/1	0.85	0.34	57,57,57,57	0
56	MG	1A	3371	1/1	0.85	0.34	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1S	3002	1/1	0.85	0.58	63,63,63,63	0
56	MG	1a	1804	1/1	0.85	0.16	67,67,67,67	0
56	MG	1a	1611	1/1	0.85	0.17	63,63,63,63	0
56	MG	1A	3776	1/1	0.85	0.20	43,43,43,43	0
56	MG	2a	3123	1/1	0.85	0.09	61,61,61,61	0
56	MG	2A	3328	1/1	0.85	0.48	58,58,58,58	0
56	MG	1A	3340	1/1	0.85	0.16	65,65,65,65	0
56	MG	2A	3077	1/1	0.85	0.16	46,46,46,46	0
56	MG	1y	3003	1/1	0.85	0.18	85,85,85,85	0
56	MG	2A	3685	1/1	0.85	0.11	44,44,44,44	0
56	MG	1A	3958	1/1	0.85	0.18	48,48,48,48	0
56	MG	2A	3246	1/1	0.85	0.28	59,59,59,59	0
56	MG	2A	3335	1/1	0.85	0.10	52,52,52,52	0
56	MG	2a	3219	1/1	0.85	0.19	81,81,81,81	0
56	MG	1A	3899	1/1	0.85	0.17	35,35,35,35	0
56	MG	2A	3404	1/1	0.85	0.25	55,55,55,55	0
56	MG	1A	3337	1/1	0.85	0.26	48,48,48,48	0
56	MG	1A	3573	1/1	0.85	0.27	51,51,51,51	0
56	MG	1A	3587	1/1	0.85	0.16	54,54,54,54	0
56	MG	1A	3399	1/1	0.85	0.36	72,72,72,72	0
56	MG	2A	3154	1/1	0.85	0.17	50,50,50,50	0
56	MG	1A	3501	1/1	0.85	0.35	62,62,62,62	0
56	MG	1A	4222	1/1	0.85	0.31	45,45,45,45	0
56	MG	1a	1704	1/1	0.85	0.41	67,67,67,67	0
56	MG	2A	3207	1/1	0.85	0.12	38,38,38,38	0
56	MG	2A	3203	1/1	0.85	0.21	48,48,48,48	0
56	MG	1A	3413	1/1	0.85	0.20	54,54,54,54	0
56	MG	1B	202	1/1	0.85	0.26	56,56,56,56	0
56	MG	1A	3640	1/1	0.86	0.20	40,40,40,40	0
56	MG	1A	3555	1/1	0.86	0.21	72,72,72,72	0
56	MG	1a	1682	1/1	0.86	0.14	69,69,69,69	0
56	MG	2A	3429	1/1	0.86	0.19	55,55,55,55	0
56	MG	1A	3860	1/1	0.86	0.21	36,36,36,36	0
56	MG	2A	3159	1/1	0.86	0.38	44,44,44,44	0
56	MG	2A	3424	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3726	1/1	0.86	0.19	30,30,30,30	0
56	MG	1A	4149	1/1	0.86	0.10	61,61,61,61	0
56	MG	2A	3132	1/1	0.86	0.08	53,53,53,53	0
56	MG	1A	3680	1/1	0.86	0.14	64,64,64,64	0
56	MG	2A	3642	1/1	0.86	0.27	44,44,44,44	0
56	MG	1a	1762	1/1	0.86	0.23	60,60,60,60	0
56	MG	1A	3169	1/1	0.86	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1D	305	1/1	0.86	0.24	48,48,48,48	0
56	MG	1A	3660	1/1	0.86	0.29	61,61,61,61	0
56	MG	1A	3931	1/1	0.86	0.31	59,59,59,59	0
56	MG	1a	1916	1/1	0.86	0.12	79,79,79,79	0
56	MG	2A	3240	1/1	0.86	0.38	41,41,41,41	0
56	MG	1A	3849	1/1	0.86	0.16	55,55,55,55	0
56	MG	1A	3237	1/1	0.86	0.60	39,39,39,39	0
56	MG	1A	3544	1/1	0.86	0.17	65,65,65,65	0
56	MG	2W	204	1/1	0.86	0.43	51,51,51,51	0
56	MG	2a	3032	1/1	0.86	0.42	65,65,65,65	0
56	MG	1a	1654	1/1	0.86	0.23	52,52,52,52	0
56	MG	1a	1743	1/1	0.86	0.23	66,66,66,66	0
56	MG	1a	1858	1/1	0.86	0.15	74,74,74,74	0
56	MG	1A	3243	1/1	0.86	0.58	47,47,47,47	0
56	MG	2A	3385	1/1	0.86	0.23	55,55,55,55	0
56	MG	2A	3127	1/1	0.86	0.10	48,48,48,48	0
56	MG	1A	3140	1/1	0.86	0.33	37,37,37,37	0
56	MG	1a	1866	1/1	0.86	0.09	62,62,62,62	0
56	MG	2A	3324	1/1	0.86	0.35	57,57,57,57	0
56	MG	1A	4197	1/1	0.86	0.33	59,59,59,59	0
56	MG	1B	229	1/1	0.86	0.20	66,66,66,66	0
56	MG	2W	203	1/1	0.86	0.11	49,49,49,49	0
56	MG	2B	3017	1/1	0.86	0.10	68,68,68,68	0
56	MG	2T	3001	1/1	0.86	0.70	74,74,74,74	0
56	MG	1A	4093	1/1	0.86	0.21	39,39,39,39	0
56	MG	2A	3294	1/1	0.86	0.70	59,59,59,59	0
56	MG	1a	1729	1/1	0.86	0.16	47,47,47,47	0
56	MG	1A	3463	1/1	0.86	0.31	59,59,59,59	0
56	MG	2A	3785	1/1	0.86	0.37	57,57,57,57	0
56	MG	2a	3090	1/1	0.86	0.13	64,64,64,64	0
56	MG	1A	3288	1/1	0.86	0.23	54,54,54,54	0
56	MG	2A	3755	1/1	0.86	0.21	47,47,47,47	0
56	MG	1a	1667	1/1	0.86	0.12	59,59,59,59	0
56	MG	1A	3604	1/1	0.86	0.13	42,42,42,42	0
56	MG	2a	3112	1/1	0.86	0.18	70,70,70,70	0
56	MG	1a	1842	1/1	0.86	0.19	61,61,61,61	0
56	MG	1a	1813	1/1	0.86	0.13	76,76,76,76	0
56	MG	2W	202	1/1	0.86	0.39	66,66,66,66	0
56	MG	2A	3104	1/1	0.86	0.17	60,60,60,60	0
56	MG	2a	3105	1/1	0.86	0.09	57,57,57,57	0
56	MG	2A	3106	1/1	0.86	0.09	52,52,52,52	0
56	MG	2A	3126	1/1	0.86	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4090	1/1	0.86	0.18	54,54,54,54	0
56	MG	1A	3728	1/1	0.86	0.10	60,60,60,60	0
56	MG	2a	3038	1/1	0.86	0.28	58,58,58,58	0
56	MG	1A	3971	1/1	0.86	0.16	31,31,31,31	0
56	MG	1a	1897	1/1	0.86	0.31	95,95,95,95	0
56	MG	1A	3624	1/1	0.86	0.25	60,60,60,60	0
56	MG	1A	3618	1/1	0.86	0.33	53,53,53,53	0
56	MG	2A	3100	1/1	0.86	0.10	72,72,72,72	0
56	MG	1A	3565	1/1	0.86	0.16	67,67,67,67	0
56	MG	2A	3819	1/1	0.86	0.07	64,64,64,64	0
56	MG	2A	3913	1/1	0.86	0.76	46,46,46,46	0
56	MG	2A	3677	1/1	0.86	0.13	44,44,44,44	0
56	MG	2A	3427	1/1	0.86	0.36	58,58,58,58	0
56	MG	2A	3056	1/1	0.86	0.41	46,46,46,46	0
56	MG	2A	3055	1/1	0.86	0.18	55,55,55,55	0
56	MG	1a	1817	1/1	0.86	0.31	56,56,56,56	0
56	MG	1A	4081	1/1	0.86	0.18	99,99,99,99	0
56	MG	1A	3632	1/1	0.86	0.35	60,60,60,60	0
56	MG	1m	201	1/1	0.86	0.14	59,59,59,59	0
56	MG	1A	4150	1/1	0.86	0.13	36,36,36,36	0
56	MG	1A	3248	1/1	0.86	0.13	67,67,67,67	0
56	MG	1A	3442	1/1	0.86	0.55	40,40,40,40	0
56	MG	1A	3721	1/1	0.86	0.12	37,37,37,37	0
56	MG	2a	3069	1/1	0.86	0.23	65,65,65,65	0
56	MG	1a	1901	1/1	0.86	0.10	70,70,70,70	0
56	MG	1A	3535	1/1	0.86	0.28	56,56,56,56	0
56	MG	1a	1907	1/1	0.87	0.14	58,58,58,58	0
56	MG	2a	3149	1/1	0.87	0.11	86,86,86,86	0
56	MG	1w	107	1/1	0.87	0.27	70,70,70,70	0
56	MG	1F	309	1/1	0.87	0.16	62,62,62,62	0
56	MG	1A	4132	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3218	1/1	0.87	0.12	63,63,63,63	0
56	MG	2A	3213	1/1	0.87	0.27	54,54,54,54	0
56	MG	2A	3245	1/1	0.87	0.29	51,51,51,51	0
56	MG	2A	3223	1/1	0.87	0.21	50,50,50,50	0
56	MG	2A	3692	1/1	0.87	0.36	65,65,65,65	0
56	MG	1A	3448	1/1	0.87	0.24	59,59,59,59	0
56	MG	1A	3636	1/1	0.87	0.18	66,66,66,66	0
56	MG	2A	3374	1/1	0.87	0.15	76,76,76,76	0
56	MG	2A	3087	1/1	0.87	0.39	57,57,57,57	0
56	MG	1N	3005	1/1	0.87	0.19	69,69,69,69	0
56	MG	1A	3205	1/1	0.87	0.24	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3825	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3759	1/1	0.87	0.24	34,34,34,34	0
56	MG	2A	3621	1/1	0.87	0.19	32,32,32,32	0
56	MG	2A	3863	1/1	0.87	0.26	68,68,68,68	0
56	MG	1A	3671	1/1	0.87	0.22	49,49,49,49	0
56	MG	1A	3967	1/1	0.87	0.40	61,61,61,61	0
56	MG	1A	3084	1/1	0.87	0.23	42,42,42,42	0
56	MG	28	101	1/1	0.87	0.15	75,75,75,75	0
56	MG	1A	3491	1/1	0.87	0.51	58,58,58,58	0
56	MG	1E	313	1/1	0.87	0.29	47,47,47,47	0
56	MG	1A	3629	1/1	0.87	0.26	62,62,62,62	0
56	MG	1a	1927	1/1	0.87	0.07	71,71,71,71	0
56	MG	1A	3405	1/1	0.87	0.27	51,51,51,51	0
56	MG	2A	3346	1/1	0.87	0.34	55,55,55,55	0
56	MG	1a	1722	1/1	0.87	0.28	58,58,58,58	0
56	MG	2A	3861	1/1	0.87	0.09	67,67,67,67	0
56	MG	2j	8001	1/1	0.87	0.12	80,80,80,80	0
56	MG	1A	3586	1/1	0.87	0.19	44,44,44,44	0
56	MG	1A	3504	1/1	0.87	0.31	51,51,51,51	0
56	MG	1Z	301	1/1	0.87	0.19	50,50,50,50	0
56	MG	1A	3252	1/1	0.87	0.17	66,66,66,66	0
56	MG	1A	3342	1/1	0.87	0.20	54,54,54,54	0
56	MG	1a	1671	1/1	0.87	0.23	53,53,53,53	0
56	MG	1A	3040	1/1	0.87	0.20	43,43,43,43	0
56	MG	2A	3181	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3024	1/1	0.87	0.12	42,42,42,42	0
56	MG	1A	3616	1/1	0.87	0.41	69,69,69,69	0
56	MG	2A	3449	1/1	0.87	0.39	57,57,57,57	0
56	MG	1A	3812	1/1	0.87	0.15	39,39,39,39	0
56	MG	1a	1921	1/1	0.87	0.33	55,55,55,55	0
56	MG	1A	3582	1/1	0.87	0.21	37,37,37,37	0
56	MG	2a	3128	1/1	0.87	0.15	60,60,60,60	0
56	MG	2A	3848	1/1	0.87	0.12	79,79,79,79	0
56	MG	1a	1840	1/1	0.87	0.17	50,50,50,50	0
56	MG	2A	3253	1/1	0.87	0.23	57,57,57,57	0
56	MG	1a	1633	1/1	0.87	0.23	62,62,62,62	0
56	MG	1A	3802	1/1	0.87	0.15	58,58,58,58	0
56	MG	1a	1800	1/1	0.87	0.19	56,56,56,56	0
56	MG	1A	3576	1/1	0.87	0.23	54,54,54,54	0
56	MG	2A	3176	1/1	0.87	0.09	62,62,62,62	0
56	MG	1B	226	1/1	0.87	0.10	54,54,54,54	0
56	MG	1A	3365	1/1	0.87	0.60	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3889	1/1	0.87	0.17	49,49,49,49	0
56	MG	1E	307	1/1	0.87	0.16	67,67,67,67	0
56	MG	1a	1774	1/1	0.87	0.13	51,51,51,51	0
56	MG	2A	3033	1/1	0.87	0.13	53,53,53,53	0
56	MG	2j	8002	1/1	0.87	0.43	79,79,79,79	0
56	MG	1A	3837	1/1	0.87	0.18	29,29,29,29	0
56	MG	2A	3189	1/1	0.87	0.19	51,51,51,51	0
56	MG	1a	1906	1/1	0.87	0.13	50,50,50,50	0
56	MG	2A	3773	1/1	0.87	0.20	67,67,67,67	0
56	MG	2A	3317	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	3539	1/1	0.87	0.12	57,57,57,57	0
56	MG	1A	3858	1/1	0.87	0.22	34,34,34,34	0
56	MG	1A	3172	1/1	0.87	0.18	60,60,60,60	0
56	MG	1A	3380	1/1	0.87	0.22	50,50,50,50	0
56	MG	1A	3686	1/1	0.87	0.25	52,52,52,52	0
56	MG	2a	3039	1/1	0.87	0.17	45,45,45,45	0
56	MG	1x	103	1/1	0.87	0.24	59,59,59,59	0
56	MG	1A	3533	1/1	0.87	0.42	53,53,53,53	0
56	MG	1A	4058	1/1	0.87	0.57	65,65,65,65	0
56	MG	2A	3724	1/1	0.87	0.10	48,48,48,48	0
56	MG	1a	1812	1/1	0.87	0.14	58,58,58,58	0
56	MG	1x	104	1/1	0.87	0.26	68,68,68,68	0
56	MG	1A	3253	1/1	0.87	0.26	48,48,48,48	0
56	MG	1A	3975	1/1	0.87	0.27	48,48,48,48	0
56	MG	2A	3442	1/1	0.87	0.35	48,48,48,48	0
56	MG	1A	3486	1/1	0.87	0.17	52,52,52,52	0
56	MG	1a	1724	1/1	0.87	0.24	52,52,52,52	0
56	MG	2a	3061	1/1	0.87	0.10	69,69,69,69	0
56	MG	2A	3466	1/1	0.87	0.26	50,50,50,50	0
56	MG	1A	3707	1/1	0.87	0.20	43,43,43,43	0
56	MG	1a	1778	1/1	0.87	0.45	65,65,65,65	0
56	MG	1A	3295	1/1	0.87	0.18	55,55,55,55	0
56	MG	2A	3293	1/1	0.87	1.25	64,64,64,64	0
56	MG	2A	3040	1/1	0.87	0.35	42,42,42,42	0
56	MG	1A	3487	1/1	0.87	0.36	62,62,62,62	0
56	MG	2A	3499	1/1	0.87	0.32	41,41,41,41	0
56	MG	2A	3080	1/1	0.87	0.22	57,57,57,57	0
56	MG	2A	3263	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3153	1/1	0.87	0.07	63,63,63,63	0
56	MG	2A	3366	1/1	0.87	0.46	52,52,52,52	0
56	MG	1A	3069	1/1	0.87	0.14	45,45,45,45	0
56	MG	2A	3232	1/1	0.87	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3350	1/1	0.87	0.11	44,44,44,44	0
56	MG	2A	3194	1/1	0.87	0.20	63,63,63,63	0
56	MG	1a	1849	1/1	0.87	0.09	54,54,54,54	0
56	MG	1A	3520	1/1	0.87	0.21	52,52,52,52	0
56	MG	2A	3813	1/1	0.87	0.25	39,39,39,39	0
56	MG	25	103	1/1	0.87	0.31	61,61,61,61	0
56	MG	2A	3457	1/1	0.87	0.41	66,66,66,66	0
56	MG	2a	3144	1/1	0.87	0.08	88,88,88,88	0
56	MG	1A	3402	1/1	0.87	0.30	53,53,53,53	0
56	MG	1A	3553	1/1	0.87	0.26	76,76,76,76	0
56	MG	2a	3129	1/1	0.87	0.30	65,65,65,65	0
56	MG	2A	3817	1/1	0.87	0.18	63,63,63,63	0
56	MG	1a	1795	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3446	1/1	0.87	0.19	49,49,49,49	0
56	MG	2A	3357	1/1	0.87	0.39	66,66,66,66	0
56	MG	2A	3733	1/1	0.88	0.15	38,38,38,38	0
56	MG	2A	3276	1/1	0.88	0.29	49,49,49,49	0
56	MG	2A	3657	1/1	0.88	0.12	65,65,65,65	0
56	MG	1A	4156	1/1	0.88	0.08	54,54,54,54	0
56	MG	1A	3681	1/1	0.88	0.21	73,73,73,73	0
56	MG	1a	1753	1/1	0.88	0.15	74,74,74,74	0
56	MG	1A	3909	1/1	0.88	0.10	50,50,50,50	0
56	MG	2A	3696	1/1	0.88	0.16	50,50,50,50	0
56	MG	1A	3725	1/1	0.88	0.09	53,53,53,53	0
56	MG	1A	3437	1/1	0.88	0.47	59,59,59,59	0
56	MG	1a	1810	1/1	0.88	0.10	64,64,64,64	0
56	MG	1a	1664	1/1	0.88	0.09	62,62,62,62	0
56	MG	2A	3545	1/1	0.88	0.19	30,30,30,30	0
56	MG	2A	3292	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	4104	1/1	0.88	0.07	32,32,32,32	0
56	MG	2a	3145	1/1	0.88	0.13	71,71,71,71	0
56	MG	2A	3367	1/1	0.88	0.09	59,59,59,59	0
56	MG	1A	3548	1/1	0.88	0.31	37,37,37,37	0
56	MG	2a	3082	1/1	0.88	0.12	64,64,64,64	0
56	MG	1A	3188	1/1	0.88	0.18	61,61,61,61	0
56	MG	2A	3841	1/1	0.88	0.14	66,66,66,66	0
56	MG	1A	3196	1/1	0.88	0.57	44,44,44,44	0
56	MG	2A	3628	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3807	1/1	0.88	0.09	50,50,50,50	0
56	MG	1a	1609	1/1	0.88	0.09	64,64,64,64	0
56	MG	2D	303	1/1	0.88	1.02	51,51,51,51	0
56	MG	1A	4248	1/1	0.88	0.29	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3128	1/1	0.88	0.18	56,56,56,56	0
56	MG	1A	3874	1/1	0.88	0.20	29,29,29,29	0
56	MG	2A	3748	1/1	0.88	0.08	61,61,61,61	0
56	MG	1A	3267	1/1	0.88	0.23	57,57,57,57	0
56	MG	1A	3085	1/1	0.88	0.30	48,48,48,48	0
56	MG	1A	3204	1/1	0.88	0.18	48,48,48,48	0
56	MG	1B	223	1/1	0.88	0.12	75,75,75,75	0
56	MG	1a	1672	1/1	0.88	0.19	61,61,61,61	0
56	MG	1A	3957	1/1	0.88	0.10	57,57,57,57	0
56	MG	1A	3574	1/1	0.88	0.26	49,49,49,49	0
56	MG	2A	3403	1/1	0.88	0.20	54,54,54,54	0
56	MG	2A	3706	1/1	0.88	0.19	60,60,60,60	0
56	MG	1A	3532	1/1	0.88	0.21	51,51,51,51	0
56	MG	2a	3195	1/1	0.88	0.28	85,85,85,85	0
56	MG	1a	1787	1/1	0.88	0.10	61,61,61,61	0
56	MG	1l	101	1/1	0.88	0.16	44,44,44,44	0
56	MG	1A	3583	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3097	1/1	0.88	0.12	64,64,64,64	0
56	MG	2x	105	1/1	0.88	0.38	59,59,59,59	0
56	MG	2A	3775	1/1	0.88	0.18	40,40,40,40	0
56	MG	1A	3875	1/1	0.88	0.06	69,69,69,69	0
56	MG	1A	3735	1/1	0.88	0.16	61,61,61,61	0
56	MG	2A	3537	1/1	0.88	0.09	50,50,50,50	0
56	MG	1A	3378	1/1	0.88	0.17	63,63,63,63	0
56	MG	1A	3663	1/1	0.88	0.17	39,39,39,39	0
56	MG	2A	3228	1/1	0.88	0.64	53,53,53,53	0
56	MG	2A	3264	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3379	1/1	0.88	0.31	58,58,58,58	0
56	MG	1A	3317	1/1	0.88	0.16	53,53,53,53	0
56	MG	2a	3037	1/1	0.88	0.55	92,92,92,92	0
56	MG	1A	3314	1/1	0.88	0.26	53,53,53,53	0
56	MG	2A	3139	1/1	0.88	0.26	45,45,45,45	0
56	MG	2A	3076	1/1	0.88	0.33	39,39,39,39	0
56	MG	2A	3318	1/1	0.88	0.35	61,61,61,61	0
56	MG	2A	3014	1/1	0.88	0.35	40,40,40,40	0
56	MG	2a	3124	1/1	0.88	0.11	81,81,81,81	0
56	MG	2A	3883	1/1	0.88	0.41	44,44,44,44	0
56	MG	2A	3160	1/1	0.88	0.26	42,42,42,42	0
56	MG	2A	3721	1/1	0.88	0.19	45,45,45,45	0
56	MG	2A	3897	1/1	0.88	0.31	71,71,71,71	0
56	MG	1a	1716	1/1	0.88	0.39	53,53,53,53	0
56	MG	2a	3008	1/1	0.88	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3426	1/1	0.88	0.07	47,47,47,47	0
56	MG	1a	1757	1/1	0.88	0.17	71,71,71,71	0
56	MG	1A	3356	1/1	0.88	0.34	76,76,76,76	0
56	MG	1A	3458	1/1	0.88	0.33	55,55,55,55	0
56	MG	1a	1780	1/1	0.88	0.22	70,70,70,70	0
56	MG	1A	3067	1/1	0.88	0.15	44,44,44,44	0
56	MG	2A	3138	1/1	0.88	0.38	40,40,40,40	0
59	ZN	29	501	1/1	0.88	0.06	79,79,79,79	0
56	MG	2A	3814	1/1	0.88	0.28	56,56,56,56	0
56	MG	2a	3166	1/1	0.88	0.06	81,81,81,81	0
56	MG	2A	3208	1/1	0.88	0.29	50,50,50,50	0
56	MG	2A	3370	1/1	0.88	0.52	62,62,62,62	0
56	MG	1A	3500	1/1	0.88	0.62	50,50,50,50	0
56	MG	2A	3042	1/1	0.88	0.20	59,59,59,59	0
56	MG	1N	3007	1/1	0.88	0.57	56,56,56,56	0
56	MG	12	3001	1/1	0.88	0.24	56,56,56,56	0
56	MG	2a	3085	1/1	0.88	0.31	57,57,57,57	0
56	MG	1A	3513	1/1	0.88	0.60	36,36,36,36	0
56	MG	1a	1624	1/1	0.88	0.08	60,60,60,60	0
56	MG	1a	1806	1/1	0.88	0.20	53,53,53,53	0
56	MG	1A	3073	1/1	0.88	0.31	52,52,52,52	0
56	MG	2A	3796	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3121	1/1	0.88	0.47	54,54,54,54	0
56	MG	2A	3226	1/1	0.88	0.39	51,51,51,51	0
56	MG	1A	3554	1/1	0.88	0.16	53,53,53,53	0
56	MG	1A	3768	1/1	0.88	0.21	28,28,28,28	0
56	MG	1a	1839	1/1	0.88	0.15	69,69,69,69	0
56	MG	1A	4057	1/1	0.88	0.23	47,47,47,47	0
56	MG	2A	3211	1/1	0.88	0.37	56,56,56,56	0
56	MG	1A	3853	1/1	0.88	0.20	24,24,24,24	0
56	MG	1a	1646	1/1	0.88	0.09	59,59,59,59	0
56	MG	1B	221	1/1	0.88	0.16	65,65,65,65	0
56	MG	1A	3263	1/1	0.88	0.21	61,61,61,61	0
56	MG	1A	3920	1/1	0.88	0.17	60,60,60,60	0
56	MG	2A	3878	1/1	0.88	0.17	64,64,64,64	0
56	MG	1E	303	1/1	0.88	0.45	46,46,46,46	0
56	MG	2a	3224	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3778	1/1	0.88	0.09	66,66,66,66	0
56	MG	2a	3099	1/1	0.88	0.10	60,60,60,60	0
56	MG	2A	3065	1/1	0.88	0.10	59,59,59,59	0
56	MG	2A	3279	1/1	0.88	0.14	60,60,60,60	0
56	MG	1A	3679	1/1	0.88	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3043	1/1	0.88	0.23	61,61,61,61	0
56	MG	1A	3545	1/1	0.88	0.14	62,62,62,62	0
56	MG	2w	107	1/1	0.88	0.11	63,63,63,63	0
56	MG	1A	3106	1/1	0.88	0.52	47,47,47,47	0
56	MG	2A	3101	1/1	0.88	0.14	51,51,51,51	0
56	MG	2A	3405	1/1	0.88	0.10	72,72,72,72	0
56	MG	1O	3003	1/1	0.88	0.21	50,50,50,50	0
56	MG	1U	206	1/1	0.88	0.45	41,41,41,41	0
56	MG	2A	3205	1/1	0.88	0.18	45,45,45,45	0
56	MG	2A	3304	1/1	0.88	0.12	52,52,52,52	0
56	MG	2A	3416	1/1	0.88	0.27	52,52,52,52	0
56	MG	1A	3921	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3423	1/1	0.88	0.47	61,61,61,61	0
56	MG	2A	3560	1/1	0.88	0.21	41,41,41,41	0
56	MG	1A	4045	1/1	0.88	0.06	57,57,57,57	0
56	MG	2a	3164	1/1	0.88	0.06	88,88,88,88	0
56	MG	1a	1873	1/1	0.89	0.05	90,90,90,90	0
56	MG	1A	3788	1/1	0.89	0.15	27,27,27,27	0
56	MG	1Q	203	1/1	0.89	0.16	53,53,53,53	0
56	MG	2a	3103	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3456	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3147	1/1	0.89	0.21	45,45,45,45	0
56	MG	1a	1708	1/1	0.89	0.18	48,48,48,48	0
56	MG	1A	3928	1/1	0.89	0.14	47,47,47,47	0
56	MG	2a	3077	1/1	0.89	0.15	59,59,59,59	0
56	MG	1A	4108	1/1	0.89	0.07	44,44,44,44	0
56	MG	1A	3219	1/1	0.89	0.10	51,51,51,51	0
56	MG	1A	3650	1/1	0.89	0.25	45,45,45,45	0
56	MG	1A	3011	1/1	0.89	0.19	42,42,42,42	0
56	MG	2A	3436	1/1	0.89	0.19	54,54,54,54	0
56	MG	2A	3475	1/1	0.89	0.24	49,49,49,49	0
56	MG	1a	1740	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3768	1/1	0.89	0.25	66,66,66,66	0
56	MG	1A	3348	1/1	0.89	0.26	53,53,53,53	0
56	MG	2A	3717	1/1	0.89	0.46	55,55,55,55	0
56	MG	1x	115	1/1	0.89	0.28	49,49,49,49	0
56	MG	1A	3645	1/1	0.89	0.25	59,59,59,59	0
56	MG	2A	3281	1/1	0.89	0.22	34,34,34,34	0
56	MG	1s	3001	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3635	1/1	0.89	0.25	59,59,59,59	0
56	MG	1A	3526	1/1	0.89	0.25	46,46,46,46	0
56	MG	1A	3828	1/1	0.89	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1892	1/1	0.89	0.09	66,66,66,66	0
56	MG	1A	3774	1/1	0.89	0.19	75,75,75,75	0
56	MG	2A	3579	1/1	0.89	0.14	39,39,39,39	0
56	MG	1c	301	1/1	0.89	0.19	66,66,66,66	0
56	MG	2A	3030	1/1	0.89	0.12	35,35,35,35	0
56	MG	1A	4136	1/1	0.89	0.10	59,59,59,59	0
56	MG	1A	3180	1/1	0.89	0.33	52,52,52,52	0
56	MG	2A	3701	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3926	1/1	0.89	0.20	62,62,62,62	0
56	MG	1F	304	1/1	0.89	0.12	44,44,44,44	0
56	MG	2A	3592	1/1	0.89	0.14	52,52,52,52	0
56	MG	2a	3022	1/1	0.89	0.32	67,67,67,67	0
56	MG	2a	3011	1/1	0.89	0.06	69,69,69,69	0
56	MG	1A	3422	1/1	0.89	0.25	56,56,56,56	0
56	MG	1a	1797	1/1	0.89	0.24	66,66,66,66	0
56	MG	2A	3779	1/1	0.89	0.14	73,73,73,73	0
56	MG	1A	3514	1/1	0.89	0.18	51,51,51,51	0
56	MG	2A	3555	1/1	0.89	0.14	36,36,36,36	0
56	MG	2A	3061	1/1	0.89	0.15	51,51,51,51	0
56	MG	2A	3842	1/1	0.89	0.18	35,35,35,35	0
56	MG	1A	3353	1/1	0.89	0.12	69,69,69,69	0
56	MG	2A	3882	1/1	0.89	0.27	51,51,51,51	0
56	MG	1a	1852	1/1	0.89	0.13	66,66,66,66	0
56	MG	2A	3300	1/1	0.89	0.30	63,63,63,63	0
56	MG	1A	4006	1/1	0.89	0.22	57,57,57,57	0
56	MG	2A	3471	1/1	0.89	0.33	59,59,59,59	0
56	MG	1A	3325	1/1	0.89	0.33	47,47,47,47	0
56	MG	1A	3209	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3458	1/1	0.89	0.44	57,57,57,57	0
56	MG	1A	3433	1/1	0.89	0.26	57,57,57,57	0
56	MG	1A	3672	1/1	0.89	0.17	40,40,40,40	0
56	MG	1a	1745	1/1	0.89	0.36	58,58,58,58	0
56	MG	2A	3557	1/1	0.89	0.08	51,51,51,51	0
56	MG	1a	1879	1/1	0.89	0.17	49,49,49,49	0
56	MG	1A	3239	1/1	0.89	0.15	55,55,55,55	0
56	MG	17	102	1/1	0.89	0.33	62,62,62,62	0
56	MG	2a	3229	1/1	0.89	0.23	81,81,81,81	0
56	MG	2A	3918	1/1	0.89	0.95	52,52,52,52	0
56	MG	1a	1636	1/1	0.89	0.12	66,66,66,66	0
56	MG	2A	3506	1/1	0.89	0.11	38,38,38,38	0
56	MG	2a	3141	1/1	0.89	0.14	57,57,57,57	0
56	MG	1A	3394	1/1	0.89	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3805	1/1	0.89	0.12	64,64,64,64	0
56	MG	2A	3668	1/1	0.89	0.12	41,41,41,41	0
56	MG	1a	1766	1/1	0.89	0.37	62,62,62,62	0
56	MG	20	102	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3345	1/1	0.89	0.36	58,58,58,58	0
56	MG	1A	3444	1/1	0.89	0.24	45,45,45,45	0
56	MG	2A	3583	1/1	0.89	0.07	56,56,56,56	0
56	MG	2A	3529	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3585	1/1	0.89	0.13	49,49,49,49	0
56	MG	1A	3361	1/1	0.89	0.27	63,63,63,63	0
56	MG	1A	3412	1/1	0.89	0.27	56,56,56,56	0
56	MG	2a	3115	1/1	0.89	0.22	61,61,61,61	0
56	MG	1a	1662	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3487	1/1	0.89	0.19	45,45,45,45	0
56	MG	2A	3553	1/1	0.89	0.11	42,42,42,42	0
56	MG	1a	1718	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3360	1/1	0.89	0.31	54,54,54,54	0
56	MG	1A	3642	1/1	0.89	0.28	53,53,53,53	0
56	MG	1A	3285	1/1	0.89	0.93	43,43,43,43	0
56	MG	2A	3744	1/1	0.89	0.13	71,71,71,71	0
56	MG	2a	3181	1/1	0.89	0.19	62,62,62,62	0
56	MG	1A	3382	1/1	0.89	0.32	53,53,53,53	0
56	MG	2A	3772	1/1	0.89	0.10	59,59,59,59	0
56	MG	1A	3436	1/1	0.89	0.37	47,47,47,47	0
56	MG	1a	1894	1/1	0.89	0.05	71,71,71,71	0
56	MG	1A	3401	1/1	0.89	0.20	46,46,46,46	0
56	MG	1A	3980	1/1	0.89	0.21	33,33,33,33	0
56	MG	1A	3495	1/1	0.89	0.44	48,48,48,48	0
56	MG	1A	3741	1/1	0.89	0.07	58,58,58,58	0
56	MG	1A	3830	1/1	0.89	0.15	53,53,53,53	0
56	MG	1A	3474	1/1	0.89	0.17	51,51,51,51	0
56	MG	2A	3280	1/1	0.89	0.48	59,59,59,59	0
56	MG	2A	3415	1/1	0.89	0.24	59,59,59,59	0
56	MG	1a	1756	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3592	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3381	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	4004	1/1	0.89	0.21	56,56,56,56	0
56	MG	1A	3302	1/1	0.89	0.32	33,33,33,33	0
56	MG	2A	3093	1/1	0.89	0.70	48,48,48,48	0
56	MG	2A	3739	1/1	0.89	0.13	52,52,52,52	0
56	MG	1a	1670	1/1	0.89	0.34	56,56,56,56	0
56	MG	1A	3065	1/1	0.89	0.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4082	1/1	0.89	0.14	90,90,90,90	0
56	MG	1A	3498	1/1	0.89	0.22	64,64,64,64	0
56	MG	2A	3482	1/1	0.89	0.67	48,48,48,48	0
56	MG	1O	3005	1/1	0.89	0.35	68,68,68,68	0
56	MG	1A	3850	1/1	0.89	0.23	25,25,25,25	0
56	MG	2a	3159	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3860	1/1	0.89	0.08	70,70,70,70	0
56	MG	2A	3552	1/1	0.89	0.20	34,34,34,34	0
56	MG	2A	3759	1/1	0.89	0.17	37,37,37,37	0
56	MG	2a	3017	1/1	0.89	0.07	71,71,71,71	0
56	MG	1A	3956	1/1	0.89	0.20	55,55,55,55	0
56	MG	1A	3445	1/1	0.89	0.37	59,59,59,59	0
56	MG	2A	3192	1/1	0.89	0.46	52,52,52,52	0
56	MG	18	101	1/1	0.89	0.37	77,77,77,77	0
56	MG	1N	3002	1/1	0.89	0.13	46,46,46,46	0
56	MG	1A	3485	1/1	0.89	0.11	51,51,51,51	0
56	MG	2A	3512	1/1	0.89	0.14	53,53,53,53	0
56	MG	2A	3498	1/1	0.89	0.16	62,62,62,62	0
56	MG	1A	3322	1/1	0.89	0.36	50,50,50,50	0
56	MG	1A	3446	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3571	1/1	0.89	0.16	36,36,36,36	0
56	MG	1A	3459	1/1	0.89	0.35	53,53,53,53	0
56	MG	1A	3945	1/1	0.89	0.20	35,35,35,35	0
56	MG	1B	236	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3185	1/1	0.89	0.27	60,60,60,60	0
56	MG	2A	3330	1/1	0.89	0.21	69,69,69,69	0
56	MG	2A	3580	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3393	1/1	0.89	0.31	67,67,67,67	0
56	MG	1F	303	1/1	0.89	0.15	57,57,57,57	0
56	MG	2W	201	1/1	0.89	0.11	61,61,61,61	0
56	MG	2A	3098	1/1	0.89	0.15	51,51,51,51	0
56	MG	2A	3417	1/1	0.89	0.16	60,60,60,60	0
56	MG	1a	1748	1/1	0.89	0.05	53,53,53,53	0
56	MG	2a	3089	1/1	0.89	0.20	70,70,70,70	0
56	MG	1A	3913	1/1	0.89	0.24	45,45,45,45	0
56	MG	1a	1632	1/1	0.89	0.22	62,62,62,62	0
56	MG	1A	3542	1/1	0.89	0.28	50,50,50,50	0
56	MG	1A	3451	1/1	0.89	0.26	63,63,63,63	0
56	MG	1A	3224	1/1	0.89	0.22	50,50,50,50	0
56	MG	1F	307	1/1	0.89	0.12	35,35,35,35	0
56	MG	1A	3704	1/1	0.89	0.19	38,38,38,38	0
56	MG	2A	3212	1/1	0.89	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3217	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3979	1/1	0.89	0.18	46,46,46,46	0
56	MG	1A	4043	1/1	0.89	0.13	38,38,38,38	0
56	MG	2A	3131	1/1	0.89	0.20	56,56,56,56	0
56	MG	1x	109	1/1	0.90	0.30	74,74,74,74	0
56	MG	1A	3164	1/1	0.90	0.30	66,66,66,66	0
56	MG	1A	3018	1/1	0.90	0.30	50,50,50,50	0
56	MG	1A	4204	1/1	0.90	0.23	50,50,50,50	0
56	MG	2A	3191	1/1	0.90	0.27	52,52,52,52	0
56	MG	2A	3268	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3450	1/1	0.90	0.18	56,56,56,56	0
56	MG	2a	3209	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3094	1/1	0.90	0.09	52,52,52,52	0
56	MG	2A	3622	1/1	0.90	0.15	47,47,47,47	0
56	MG	2A	3908	1/1	0.90	0.23	43,43,43,43	0
56	MG	1f	3002	1/1	0.90	0.27	61,61,61,61	0
56	MG	2A	3603	1/1	0.90	0.06	44,44,44,44	0
56	MG	2a	3189	1/1	0.90	0.12	54,54,54,54	0
56	MG	1A	3814	1/1	0.90	0.16	64,64,64,64	0
56	MG	1A	4172	1/1	0.90	0.18	46,46,46,46	0
56	MG	1a	1844	1/1	0.90	0.14	52,52,52,52	0
56	MG	1A	3502	1/1	0.90	0.19	55,55,55,55	0
56	MG	2A	3216	1/1	0.90	0.24	54,54,54,54	0
56	MG	2A	3365	1/1	0.90	0.18	58,58,58,58	0
56	MG	1A	3567	1/1	0.90	0.18	38,38,38,38	0
56	MG	1A	3465	1/1	0.90	0.46	53,53,53,53	0
56	MG	1A	4071	1/1	0.90	0.20	71,71,71,71	0
56	MG	1A	3603	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	4218	1/1	0.90	0.17	36,36,36,36	0
56	MG	1A	3466	1/1	0.90	0.25	58,58,58,58	0
56	MG	2A	3469	1/1	0.90	0.41	61,61,61,61	0
56	MG	1A	4221	1/1	0.90	0.23	35,35,35,35	0
56	MG	1A	3588	1/1	0.90	0.13	50,50,50,50	0
56	MG	1a	1856	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3233	1/1	0.90	0.27	65,65,65,65	0
56	MG	2A	3215	1/1	0.90	0.20	61,61,61,61	0
56	MG	2A	3474	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3345	1/1	0.90	0.28	57,57,57,57	0
56	MG	2a	3201	1/1	0.90	0.06	70,70,70,70	0
56	MG	2q	204	1/1	0.90	0.10	68,68,68,68	0
56	MG	1A	3471	1/1	0.90	0.50	65,65,65,65	0
56	MG	2A	3877	1/1	0.90	0.07	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3324	1/1	0.90	0.18	62,62,62,62	0
56	MG	1A	3737	1/1	0.90	0.13	35,35,35,35	0
56	MG	2A	3766	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3016	1/1	0.90	0.15	50,50,50,50	0
56	MG	1A	3613	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	4211	1/1	0.90	0.23	61,61,61,61	0
56	MG	1a	1822	1/1	0.90	0.17	45,45,45,45	0
56	MG	2A	3121	1/1	0.90	0.25	53,53,53,53	0
56	MG	2A	3371	1/1	0.90	0.15	53,53,53,53	0
56	MG	25	104	1/1	0.90	0.17	51,51,51,51	0
56	MG	1A	4021	1/1	0.90	0.14	36,36,36,36	0
56	MG	2A	3219	1/1	0.90	0.26	56,56,56,56	0
56	MG	1A	3278	1/1	0.90	0.22	55,55,55,55	0
56	MG	2A	3536	1/1	0.90	0.12	60,60,60,60	0
56	MG	2A	3282	1/1	0.90	0.34	64,64,64,64	0
56	MG	1A	3884	1/1	0.90	0.23	63,63,63,63	0
56	MG	2F	302	1/1	0.90	0.21	63,63,63,63	0
56	MG	1A	4019	1/1	0.90	0.11	47,47,47,47	0
56	MG	1A	4105	1/1	0.90	0.15	33,33,33,33	0
56	MG	1A	3499	1/1	0.90	0.20	62,62,62,62	0
56	MG	2A	3062	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3703	1/1	0.90	0.08	64,64,64,64	0
56	MG	1A	3562	1/1	0.90	0.15	45,45,45,45	0
56	MG	2A	3069	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3693	1/1	0.90	0.22	57,57,57,57	0
56	MG	1a	1767	1/1	0.90	0.16	51,51,51,51	0
56	MG	1a	1747	1/1	0.90	0.07	60,60,60,60	0
56	MG	1a	1845	1/1	0.90	0.13	75,75,75,75	0
56	MG	1a	1826	1/1	0.90	0.14	68,68,68,68	0
56	MG	1A	4174	1/1	0.90	0.12	83,83,83,83	0
56	MG	2a	3104	1/1	0.90	0.18	81,81,81,81	0
56	MG	1A	4086	1/1	0.90	0.33	57,57,57,57	0
56	MG	2A	3627	1/1	0.90	0.23	43,43,43,43	0
56	MG	2A	3822	1/1	0.90	0.06	78,78,78,78	0
56	MG	2A	3072	1/1	0.90	0.15	47,47,47,47	0
56	MG	1f	3001	1/1	0.90	0.15	44,44,44,44	0
56	MG	1a	1603	1/1	0.90	0.18	87,87,87,87	0
56	MG	1A	4076	1/1	0.90	0.19	30,30,30,30	0
56	MG	1A	3706	1/1	0.90	0.16	23,23,23,23	0
56	MG	2A	3273	1/1	0.90	0.17	58,58,58,58	0
56	MG	1A	3493	1/1	0.90	0.31	33,33,33,33	0
56	MG	1A	4219	1/1	0.90	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3703	1/1	0.90	0.26	47,47,47,47	0
56	MG	2A	3801	1/1	0.90	0.14	59,59,59,59	0
56	MG	2A	3433	1/1	0.90	0.19	46,46,46,46	0
56	MG	1A	3685	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3019	1/1	0.90	0.14	40,40,40,40	0
56	MG	2A	3675	1/1	0.90	0.22	42,42,42,42	0
56	MG	2a	3053	1/1	0.90	0.27	82,82,82,82	0
56	MG	1A	3429	1/1	0.90	0.35	48,48,48,48	0
56	MG	2A	3652	1/1	0.90	0.55	45,45,45,45	0
56	MG	2A	3448	1/1	0.90	0.33	61,61,61,61	0
56	MG	1a	1853	1/1	0.90	0.09	48,48,48,48	0
56	MG	1A	3056	1/1	0.90	0.21	50,50,50,50	0
56	MG	1a	1619	1/1	0.90	0.08	55,55,55,55	0
56	MG	2E	307	1/1	0.90	0.07	61,61,61,61	0
56	MG	2A	3740	1/1	0.90	0.18	73,73,73,73	0
56	MG	2A	3610	1/1	0.90	0.10	62,62,62,62	0
56	MG	2a	3117	1/1	0.90	0.15	63,63,63,63	0
56	MG	1T	202	1/1	0.90	0.50	59,59,59,59	0
56	MG	1A	4169	1/1	0.90	0.13	77,77,77,77	0
56	MG	2A	3310	1/1	0.90	0.20	49,49,49,49	0
56	MG	1A	3803	1/1	0.90	0.27	48,48,48,48	0
56	MG	2A	3308	1/1	0.90	0.11	56,56,56,56	0
56	MG	1A	3996	1/1	0.90	0.14	48,48,48,48	0
56	MG	2A	3425	1/1	0.90	0.41	73,73,73,73	0
56	MG	1a	1684	1/1	0.90	0.22	55,55,55,55	0
56	MG	2A	3840	1/1	0.90	0.10	49,49,49,49	0
56	MG	2w	106	1/1	0.90	0.10	71,71,71,71	0
56	MG	2A	3811	1/1	0.90	0.11	34,34,34,34	0
56	MG	1a	1650	1/1	0.90	0.22	54,54,54,54	0
56	MG	2A	3561	1/1	0.90	0.07	37,37,37,37	0
56	MG	2A	3283	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3396	1/1	0.90	0.42	43,43,43,43	0
56	MG	2A	3004	1/1	0.90	0.38	44,44,44,44	0
56	MG	2A	3237	1/1	0.90	0.22	48,48,48,48	0
56	MG	2A	3609	1/1	0.90	0.20	60,60,60,60	0
56	MG	2r	3001	1/1	0.90	0.27	75,75,75,75	0
59	ZN	2Y	501	1/1	0.90	0.07	101,101,101,101	0
56	MG	1A	4257	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	4244	1/1	0.90	0.15	39,39,39,39	0
56	MG	1a	1824	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3421	1/1	0.90	0.25	46,46,46,46	0
56	MG	1A	3339	1/1	0.90	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3115	1/1	0.90	0.25	44,44,44,44	0
56	MG	1a	1825	1/1	0.90	0.21	57,57,57,57	0
56	MG	2A	3530	1/1	0.90	0.11	45,45,45,45	0
56	MG	1a	1627	1/1	0.90	0.09	46,46,46,46	0
56	MG	1A	3427	1/1	0.90	0.19	44,44,44,44	0
56	MG	1a	1629	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3762	1/1	0.90	0.16	54,54,54,54	0
56	MG	2a	3208	1/1	0.90	0.17	70,70,70,70	0
56	MG	1A	3617	1/1	0.90	0.18	48,48,48,48	0
56	MG	2A	3102	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3766	1/1	0.90	0.26	26,26,26,26	0
56	MG	1A	3846	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3961	1/1	0.90	0.52	60,60,60,60	0
56	MG	2a	3093	1/1	0.90	0.14	55,55,55,55	0
56	MG	1a	1816	1/1	0.90	0.54	59,59,59,59	0
56	MG	1A	3202	1/1	0.90	0.15	46,46,46,46	0
56	MG	2A	3455	1/1	0.90	0.29	44,44,44,44	0
56	MG	2A	3220	1/1	0.90	0.21	46,46,46,46	0
56	MG	1A	3497	1/1	0.90	0.14	59,59,59,59	0
56	MG	1Q	205	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	3620	1/1	0.90	0.60	59,59,59,59	0
56	MG	2a	3212	1/1	0.90	0.12	71,71,71,71	0
56	MG	2x	101	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3387	1/1	0.90	0.41	63,63,63,63	0
56	MG	1A	4129	1/1	0.90	0.07	56,56,56,56	0
56	MG	2A	3899	1/1	0.90	0.38	61,61,61,61	0
56	MG	1A	3893	1/1	0.90	0.15	33,33,33,33	0
56	MG	1a	1630	1/1	0.90	0.16	57,57,57,57	0
56	MG	2a	3050	1/1	0.90	0.09	69,69,69,69	0
56	MG	2a	3110	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3257	1/1	0.90	0.26	49,49,49,49	0
56	MG	2A	3186	1/1	0.90	0.29	54,54,54,54	0
56	MG	1A	4040	1/1	0.90	0.12	74,74,74,74	0
56	MG	1A	3841	1/1	0.90	0.19	42,42,42,42	0
56	MG	1N	3003	1/1	0.90	0.17	53,53,53,53	0
56	MG	2A	3481	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	3782	1/1	0.90	0.24	26,26,26,26	0
56	MG	1a	1877	1/1	0.90	0.07	72,72,72,72	0
56	MG	12	3002	1/1	0.90	0.42	48,48,48,48	0
56	MG	2B	3004	1/1	0.90	0.08	79,79,79,79	0
56	MG	2A	3782	1/1	0.90	0.10	44,44,44,44	0
56	MG	1E	312	1/1	0.90	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3723	1/1	0.90	0.16	37,37,37,37	0
56	MG	2a	3074	1/1	0.90	0.12	63,63,63,63	0
56	MG	1A	3898	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3585	1/1	0.90	0.28	49,49,49,49	0
56	MG	1A	3856	1/1	0.90	0.37	56,56,56,56	0
56	MG	1B	211	1/1	0.90	0.20	62,62,62,62	0
56	MG	1A	3857	1/1	0.90	0.21	29,29,29,29	0
56	MG	1A	3181	1/1	0.90	0.23	53,53,53,53	0
56	MG	1B	225	1/1	0.90	0.12	42,42,42,42	0
56	MG	1A	3408	1/1	0.90	0.30	48,48,48,48	0
56	MG	1a	1885	1/1	0.90	0.12	78,78,78,78	0
56	MG	1A	3385	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	4079	1/1	0.90	0.17	36,36,36,36	0
56	MG	2A	3921	1/1	0.90	0.28	65,65,65,65	0
56	MG	2w	102	1/1	0.90	0.28	60,60,60,60	0
56	MG	2A	3235	1/1	0.90	0.21	52,52,52,52	0
56	MG	1E	308	1/1	0.91	0.19	34,34,34,34	0
56	MG	2a	3096	1/1	0.91	0.06	70,70,70,70	0
56	MG	1a	1896	1/1	0.91	0.07	77,77,77,77	0
56	MG	19	101	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3051	1/1	0.91	0.30	43,43,43,43	0
56	MG	2A	3118	1/1	0.91	0.17	52,52,52,52	0
56	MG	2a	3175	1/1	0.91	0.09	58,58,58,58	0
56	MG	1A	3148	1/1	0.91	0.39	40,40,40,40	0
56	MG	1A	3651	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3025	1/1	0.91	1.40	55,55,55,55	0
56	MG	2A	3178	1/1	0.91	0.31	49,49,49,49	0
56	MG	2a	3063	1/1	0.91	0.30	64,64,64,64	0
56	MG	2A	3821	1/1	0.91	0.09	76,76,76,76	0
56	MG	1a	1889	1/1	0.91	0.08	77,77,77,77	0
56	MG	2v	104	1/1	0.91	0.13	61,61,61,61	0
56	MG	1a	1614	1/1	0.91	0.19	63,63,63,63	0
56	MG	2A	3569	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	3870	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3440	1/1	0.91	0.38	38,38,38,38	0
56	MG	1A	3807	1/1	0.91	0.14	44,44,44,44	0
56	MG	1x	114	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3109	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3184	1/1	0.91	0.10	61,61,61,61	0
56	MG	1A	3276	1/1	0.91	0.19	55,55,55,55	0
56	MG	1A	3117	1/1	0.91	0.36	46,46,46,46	0
56	MG	2A	3764	1/1	0.91	0.11	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3105	1/1	0.91	0.12	31,31,31,31	0
56	MG	1A	4075	1/1	0.91	0.19	21,21,21,21	0
56	MG	2A	3502	1/1	0.91	0.10	54,54,54,54	0
56	MG	2D	301	1/1	0.91	0.27	51,51,51,51	0
56	MG	2A	3036	1/1	0.91	0.14	50,50,50,50	0
56	MG	2a	3183	1/1	0.91	0.21	39,39,39,39	0
56	MG	1X	102	1/1	0.91	0.23	45,45,45,45	0
56	MG	2a	3227	1/1	0.91	0.15	68,68,68,68	0
56	MG	2a	3206	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3047	1/1	0.91	0.10	44,44,44,44	0
56	MG	1a	1883	1/1	0.91	0.15	47,47,47,47	0
56	MG	2A	3286	1/1	0.91	0.28	52,52,52,52	0
56	MG	1A	3481	1/1	0.91	0.35	52,52,52,52	0
56	MG	1A	3609	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	1791	1/1	0.91	0.29	71,71,71,71	0
56	MG	2A	3567	1/1	0.91	0.16	33,33,33,33	0
56	MG	2A	3486	1/1	0.91	0.47	46,46,46,46	0
56	MG	1a	1642	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3503	1/1	0.91	0.36	56,56,56,56	0
56	MG	1A	3627	1/1	0.91	0.26	55,55,55,55	0
56	MG	1A	3159	1/1	0.91	0.36	35,35,35,35	0
56	MG	2A	3053	1/1	0.91	0.10	55,55,55,55	0
56	MG	1a	1913	1/1	0.91	0.09	80,80,80,80	0
56	MG	2A	3910	1/1	0.91	0.65	58,58,58,58	0
56	MG	2q	202	1/1	0.91	0.28	74,74,74,74	0
56	MG	1A	3282	1/1	0.91	0.61	51,51,51,51	0
56	MG	1A	3344	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3573	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3998	1/1	0.91	0.42	48,48,48,48	0
56	MG	1a	1621	1/1	0.91	0.25	59,59,59,59	0
56	MG	1a	1706	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3190	1/1	0.91	0.30	40,40,40,40	0
56	MG	1A	4164	1/1	0.91	0.11	55,55,55,55	0
56	MG	2a	3193	1/1	0.91	0.22	63,63,63,63	0
56	MG	1a	1739	1/1	0.91	0.11	49,49,49,49	0
56	MG	2a	3213	1/1	0.91	0.20	60,60,60,60	0
56	MG	1A	3198	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3134	1/1	0.91	0.10	39,39,39,39	0
56	MG	1a	1720	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3610	1/1	0.91	0.29	61,61,61,61	0
56	MG	1A	3155	1/1	0.91	0.32	47,47,47,47	0
56	MG	1a	1821	1/1	0.91	0.15	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1R	201	1/1	0.91	0.18	54,54,54,54	0
57	CPT	1A	4210	4/5	0.91	0.10	77,103,121,207	0
56	MG	2a	3016	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3722	1/1	0.91	0.16	21,21,21,21	0
56	MG	1A	3966	1/1	0.91	0.81	45,45,45,45	0
56	MG	1A	3400	1/1	0.91	0.17	56,56,56,56	0
56	MG	1a	1730	1/1	0.91	0.11	57,57,57,57	0
56	MG	1A	3473	1/1	0.91	0.15	59,59,59,59	0
56	MG	1a	1869	1/1	0.91	0.34	101,101,101,101	0
56	MG	2A	3291	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3670	1/1	0.91	0.18	42,42,42,42	0
56	MG	1a	1912	1/1	0.91	0.15	69,69,69,69	0
56	MG	2A	3463	1/1	0.91	0.18	59,59,59,59	0
56	MG	1A	4130	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3390	1/1	0.91	0.41	55,55,55,55	0
56	MG	1A	3570	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3774	1/1	0.91	0.07	57,57,57,57	0
56	MG	1A	3004	1/1	0.91	0.26	35,35,35,35	0
56	MG	1A	3479	1/1	0.91	0.32	57,57,57,57	0
56	MG	2A	3162	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	3232	1/1	0.91	0.40	55,55,55,55	0
56	MG	2A	3743	1/1	0.91	0.10	79,79,79,79	0
56	MG	2A	3389	1/1	0.91	0.22	52,52,52,52	0
56	MG	1A	4243	1/1	0.91	0.59	40,40,40,40	0
56	MG	1A	3559	1/1	0.91	0.50	35,35,35,35	0
56	MG	1a	1865	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3170	1/1	0.91	0.22	47,47,47,47	0
56	MG	1A	4234	1/1	0.91	0.69	46,46,46,46	0
56	MG	2A	3319	1/1	0.91	0.39	57,57,57,57	0
56	MG	2A	3697	1/1	0.91	0.05	42,42,42,42	0
56	MG	2A	3325	1/1	0.91	0.58	47,47,47,47	0
56	MG	2A	3323	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3348	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3802	1/1	0.91	0.18	43,43,43,43	0
56	MG	1A	3777	1/1	0.91	0.17	33,33,33,33	0
56	MG	2a	3076	1/1	0.91	0.10	64,64,64,64	0
56	MG	2A	3869	1/1	0.91	0.07	54,54,54,54	0
56	MG	1A	3218	1/1	0.91	0.44	55,55,55,55	0
56	MG	1A	3878	1/1	0.91	0.05	63,63,63,63	0
56	MG	2a	3065	1/1	0.91	0.45	47,47,47,47	0
56	MG	1A	3739	1/1	0.91	0.16	30,30,30,30	0
56	MG	1a	1771	1/1	0.91	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3507	1/1	0.91	0.12	49,49,49,49	0
56	MG	1a	1815	1/1	0.91	0.17	57,57,57,57	0
56	MG	1a	1789	1/1	0.91	0.20	69,69,69,69	0
56	MG	2A	3174	1/1	0.91	0.11	66,66,66,66	0
56	MG	2x	104	1/1	0.91	0.26	58,58,58,58	0
56	MG	2A	3067	1/1	0.91	0.37	56,56,56,56	0
56	MG	2y	3004	1/1	0.91	0.18	69,69,69,69	0
56	MG	2A	3081	1/1	0.91	0.29	51,51,51,51	0
56	MG	2A	3599	1/1	0.91	0.22	55,55,55,55	0
56	MG	2y	3005	1/1	0.91	0.13	79,79,79,79	0
56	MG	2A	3616	1/1	0.91	0.26	31,31,31,31	0
56	MG	1A	3751	1/1	0.91	0.14	40,40,40,40	0
56	MG	1a	1777	1/1	0.91	0.38	51,51,51,51	0
56	MG	2a	3005	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3378	1/1	0.91	0.18	58,58,58,58	0
56	MG	1a	1928	1/1	0.91	0.12	57,57,57,57	0
56	MG	2U	201	1/1	0.91	0.28	56,56,56,56	0
56	MG	2A	3209	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3760	1/1	0.91	0.18	64,64,64,64	0
56	MG	2A	3901	1/1	0.91	0.20	77,77,77,77	0
56	MG	1A	3795	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3322	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3258	1/1	0.91	0.11	53,53,53,53	0
56	MG	1H	201	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3859	1/1	0.91	0.18	37,37,37,37	0
56	MG	1A	3834	1/1	0.91	0.25	28,28,28,28	0
56	MG	2a	3176	1/1	0.91	0.09	74,74,74,74	0
56	MG	2A	3285	1/1	0.91	0.32	55,55,55,55	0
56	MG	2A	3018	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3754	1/1	0.91	0.12	71,71,71,71	0
56	MG	1A	3937	1/1	0.91	0.33	56,56,56,56	0
56	MG	2a	3021	1/1	0.91	0.12	72,72,72,72	0
56	MG	1U	201	1/1	0.91	0.45	53,53,53,53	0
56	MG	2a	3019	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3404	1/1	0.91	0.56	69,69,69,69	0
56	MG	1A	3300	1/1	0.91	0.28	52,52,52,52	0
56	MG	1y	3004	1/1	0.91	0.26	78,78,78,78	0
56	MG	1A	4064	1/1	0.91	0.16	39,39,39,39	0
56	MG	2A	3522	1/1	0.91	0.07	63,63,63,63	0
56	MG	1A	3259	1/1	0.91	0.23	61,61,61,61	0
56	MG	1a	1687	1/1	0.91	0.20	73,73,73,73	0
56	MG	2a	3072	1/1	0.91	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3854	1/1	0.91	0.15	49,49,49,49	0
56	MG	1a	1783	1/1	0.91	0.06	88,88,88,88	0
56	MG	1A	3906	1/1	0.91	0.11	55,55,55,55	0
56	MG	1A	3831	1/1	0.91	0.11	46,46,46,46	0
56	MG	2w	105	1/1	0.91	0.32	71,71,71,71	0
56	MG	2A	3123	1/1	0.91	0.21	50,50,50,50	0
56	MG	1A	3536	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	3279	1/1	0.91	0.21	40,40,40,40	0
56	MG	1A	3088	1/1	0.91	0.30	54,54,54,54	0
56	MG	2A	3032	1/1	0.91	0.20	57,57,57,57	0
56	MG	2A	3108	1/1	0.91	0.20	39,39,39,39	0
56	MG	2x	106	1/1	0.91	0.23	57,57,57,57	0
56	MG	2A	3168	1/1	0.91	0.19	50,50,50,50	0
56	MG	1a	1746	1/1	0.91	0.07	66,66,66,66	0
56	MG	1A	3391	1/1	0.91	0.50	71,71,71,71	0
56	MG	2a	3071	1/1	0.91	0.09	71,71,71,71	0
56	MG	1A	3291	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3329	1/1	0.91	0.19	54,54,54,54	0
59	ZN	24	501	1/1	0.91	0.04	114,114,114,114	0
56	MG	2A	3461	1/1	0.91	0.33	47,47,47,47	0
56	MG	2A	3401	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	4215	1/1	0.91	0.48	73,73,73,73	0
56	MG	1A	4206	1/1	0.91	0.42	45,45,45,45	0
56	MG	1A	4163	1/1	0.91	0.13	70,70,70,70	0
56	MG	2a	3030	1/1	0.91	0.14	52,52,52,52	0
56	MG	2a	3185	1/1	0.91	0.13	87,87,87,87	0
56	MG	1A	4067	1/1	0.91	0.06	53,53,53,53	0
56	MG	1A	3516	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3862	1/1	0.91	0.08	62,62,62,62	0
56	MG	2A	3135	1/1	0.91	0.54	51,51,51,51	0
56	MG	2a	3231	1/1	0.91	0.07	77,77,77,77	0
56	MG	1A	3275	1/1	0.91	0.59	45,45,45,45	0
56	MG	2A	3911	1/1	0.91	0.19	43,43,43,43	0
56	MG	1a	1648	1/1	0.91	0.08	53,53,53,53	0
56	MG	18	103	1/1	0.91	0.45	57,57,57,57	0
56	MG	1A	3044	1/1	0.91	0.45	48,48,48,48	0
56	MG	2A	3795	1/1	0.91	0.23	63,63,63,63	0
56	MG	1a	1846	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	4106	1/1	0.91	0.15	28,28,28,28	0
56	MG	1A	3505	1/1	0.91	0.40	44,44,44,44	0
56	MG	1A	3418	1/1	0.91	0.25	49,49,49,49	0
56	MG	1A	3779	1/1	0.91	0.22	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3574	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	4194	1/1	0.91	0.20	55,55,55,55	0
56	MG	2A	3659	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3490	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3411	1/1	0.91	0.22	58,58,58,58	0
56	MG	1a	1773	1/1	0.91	0.15	53,53,53,53	0
56	MG	1a	1827	1/1	0.92	0.10	66,66,66,66	0
56	MG	1a	1870	1/1	0.92	0.35	81,81,81,81	0
56	MG	1A	3395	1/1	0.92	0.89	46,46,46,46	0
56	MG	1A	3428	1/1	0.92	0.21	46,46,46,46	0
56	MG	1A	3699	1/1	0.92	0.18	24,24,24,24	0
56	MG	1a	1920	1/1	0.92	0.25	59,59,59,59	0
56	MG	2A	3008	1/1	0.92	0.15	41,41,41,41	0
56	MG	2A	3681	1/1	0.92	0.20	66,66,66,66	0
56	MG	2A	3881	1/1	0.92	0.14	71,71,71,71	0
56	MG	2A	3689	1/1	0.92	0.17	53,53,53,53	0
56	MG	1A	3482	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3520	1/1	0.92	0.18	55,55,55,55	0
56	MG	2A	3338	1/1	0.92	1.03	64,64,64,64	0
56	MG	1A	3135	1/1	0.92	0.29	39,39,39,39	0
56	MG	1A	4188	1/1	0.92	0.18	37,37,37,37	0
56	MG	1A	4052	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3031	1/1	0.92	0.15	46,46,46,46	0
56	MG	2A	3392	1/1	0.92	0.18	72,72,72,72	0
56	MG	2a	3009	1/1	0.92	0.13	72,72,72,72	0
56	MG	2A	3439	1/1	0.92	0.26	38,38,38,38	0
56	MG	2A	3843	1/1	0.92	0.13	27,27,27,27	0
56	MG	2A	3465	1/1	0.92	0.22	52,52,52,52	0
56	MG	2A	3347	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3134	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3829	1/1	0.92	0.08	54,54,54,54	0
56	MG	1a	1882	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3239	1/1	0.92	0.82	54,54,54,54	0
56	MG	1A	3199	1/1	0.92	0.74	56,56,56,56	0
56	MG	2a	3091	1/1	0.92	0.12	62,62,62,62	0
56	MG	1w	106	1/1	0.92	0.10	63,63,63,63	0
56	MG	2A	3133	1/1	0.92	0.16	63,63,63,63	0
56	MG	2A	3851	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	4035	1/1	0.92	0.16	39,39,39,39	0
56	MG	1A	3851	1/1	0.92	0.19	45,45,45,45	0
56	MG	1A	4213	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3145	1/1	0.92	0.29	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3074	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3543	1/1	0.92	0.20	71,71,71,71	0
56	MG	2A	3484	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	3811	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3673	1/1	0.92	0.11	50,50,50,50	0
56	MG	17	103	1/1	0.92	0.18	48,48,48,48	0
56	MG	2Q	3001	1/1	0.92	0.08	59,59,59,59	0
56	MG	13	101	1/1	0.92	0.32	50,50,50,50	0
56	MG	1a	1926	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	4003	1/1	0.92	0.17	57,57,57,57	0
56	MG	2A	3640	1/1	0.92	0.25	45,45,45,45	0
56	MG	1A	3083	1/1	0.92	0.14	41,41,41,41	0
56	MG	1A	3341	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3519	1/1	0.92	0.24	57,57,57,57	0
56	MG	1a	1758	1/1	0.92	0.18	49,49,49,49	0
56	MG	1A	3160	1/1	0.92	0.64	49,49,49,49	0
56	MG	2A	3023	1/1	0.92	0.14	57,57,57,57	0
56	MG	2A	3626	1/1	0.92	0.29	48,48,48,48	0
56	MG	1A	3063	1/1	0.92	0.29	51,51,51,51	0
56	MG	1A	3355	1/1	0.92	0.22	60,60,60,60	0
56	MG	1A	3838	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3912	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3955	1/1	0.92	0.26	37,37,37,37	0
56	MG	1a	1847	1/1	0.92	0.13	51,51,51,51	0
56	MG	2D	302	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	3993	1/1	0.92	0.28	55,55,55,55	0
56	MG	1A	3416	1/1	0.92	0.24	65,65,65,65	0
56	MG	1A	3447	1/1	0.92	0.42	58,58,58,58	0
56	MG	1A	3420	1/1	0.92	0.31	50,50,50,50	0
56	MG	2a	3150	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3122	1/1	0.92	0.19	47,47,47,47	0
56	MG	2A	3459	1/1	0.92	0.30	46,46,46,46	0
56	MG	1a	1931	1/1	0.92	0.10	49,49,49,49	0
56	MG	2A	3509	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3158	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3376	1/1	0.92	0.15	48,48,48,48	0
56	MG	1A	4103	1/1	0.92	0.15	26,26,26,26	0
56	MG	1a	1765	1/1	0.92	0.34	53,53,53,53	0
56	MG	1a	1692	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3449	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	4077	1/1	0.92	0.24	26,26,26,26	0
56	MG	1A	3579	1/1	0.92	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3844	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3587	1/1	0.92	0.16	46,46,46,46	0
56	MG	2A	3827	1/1	0.92	0.20	64,64,64,64	0
56	MG	2a	3002	1/1	0.92	0.42	72,72,72,72	0
56	MG	1A	3596	1/1	0.92	0.22	44,44,44,44	0
56	MG	2A	3224	1/1	0.92	0.21	55,55,55,55	0
56	MG	1A	4227	1/1	0.92	0.37	38,38,38,38	0
56	MG	1A	3200	1/1	0.92	0.21	49,49,49,49	0
56	MG	2A	3784	1/1	0.92	0.23	48,48,48,48	0
56	MG	1A	3767	1/1	0.92	0.15	24,24,24,24	0
56	MG	1A	3558	1/1	0.92	0.18	48,48,48,48	0
56	MG	2A	3559	1/1	0.92	0.20	38,38,38,38	0
56	MG	1A	3240	1/1	0.92	0.29	39,39,39,39	0
56	MG	2B	3016	1/1	0.92	0.15	63,63,63,63	0
56	MG	2A	3413	1/1	0.92	0.28	61,61,61,61	0
56	MG	2a	3035	1/1	0.92	0.13	81,81,81,81	0
56	MG	1A	3946	1/1	0.92	0.16	34,34,34,34	0
56	MG	1A	3214	1/1	0.92	0.24	58,58,58,58	0
56	MG	1a	1929	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3730	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3217	1/1	0.92	0.34	59,59,59,59	0
56	MG	2A	3257	1/1	0.92	0.28	70,70,70,70	0
56	MG	23	3002	1/1	0.92	0.19	53,53,53,53	0
56	MG	1A	3792	1/1	0.92	0.18	30,30,30,30	0
56	MG	2a	3062	1/1	0.92	0.20	85,85,85,85	0
56	MG	2A	3063	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3445	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3586	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	3900	1/1	0.92	0.08	64,64,64,64	0
56	MG	1a	1622	1/1	0.92	0.18	55,55,55,55	0
56	MG	2a	3158	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3731	1/1	0.92	0.19	57,57,57,57	0
56	MG	1A	3943	1/1	0.92	0.10	68,68,68,68	0
56	MG	2A	3651	1/1	0.92	0.07	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.20	65,65,65,65	0
56	MG	1A	3625	1/1	0.92	0.27	66,66,66,66	0
56	MG	2A	3751	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	3202	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3847	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	4018	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3785	1/1	0.92	0.23	33,33,33,33	0
56	MG	2A	3543	1/1	0.92	0.14	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3896	1/1	0.92	0.39	53,53,53,53	0
56	MG	1A	3334	1/1	0.92	0.32	54,54,54,54	0
56	MG	1T	201	1/1	0.92	0.14	57,57,57,57	0
56	MG	1w	110	1/1	0.92	0.16	78,78,78,78	0
56	MG	2A	3912	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	3319	1/1	0.92	0.33	58,58,58,58	0
56	MG	1A	3568	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3715	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3036	1/1	0.92	0.32	43,43,43,43	0
56	MG	2A	3873	1/1	0.92	0.23	57,57,57,57	0
56	MG	1A	3326	1/1	0.92	0.14	53,53,53,53	0
56	MG	13	102	1/1	0.92	0.17	46,46,46,46	0
56	MG	2A	3735	1/1	0.92	0.09	49,49,49,49	0
56	MG	1a	1675	1/1	0.92	0.17	53,53,53,53	0
56	MG	2a	3151	1/1	0.92	0.09	74,74,74,74	0
56	MG	1A	3983	1/1	0.92	0.20	73,73,73,73	0
56	MG	1A	4177	1/1	0.92	0.12	36,36,36,36	0
56	MG	1B	222	1/1	0.92	0.14	59,59,59,59	0
56	MG	2a	3014	1/1	0.92	0.21	70,70,70,70	0
56	MG	2A	3421	1/1	0.92	0.23	60,60,60,60	0
56	MG	2A	3758	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3781	1/1	0.92	0.10	47,47,47,47	0
56	MG	2A	3045	1/1	0.92	0.09	48,48,48,48	0
58	K	1A	4256	1/1	0.92	0.18	65,65,65,65	0
56	MG	1a	1785	1/1	0.92	0.07	71,71,71,71	0
56	MG	1a	1808	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3143	1/1	0.92	0.13	44,44,44,44	0
56	MG	23	3003	1/1	0.92	0.21	48,48,48,48	0
56	MG	1A	3968	1/1	0.92	0.08	63,63,63,63	0
56	MG	1a	1635	1/1	0.92	0.33	62,62,62,62	0
56	MG	1A	3156	1/1	0.92	0.97	47,47,47,47	0
56	MG	2A	3602	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3732	1/1	0.92	0.16	35,35,35,35	0
56	MG	1A	4062	1/1	0.92	0.08	76,76,76,76	0
56	MG	1A	3746	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3424	1/1	0.92	0.21	75,75,75,75	0
56	MG	2A	3705	1/1	0.92	0.22	58,58,58,58	0
56	MG	1x	101	1/1	0.92	0.25	45,45,45,45	0
56	MG	1A	3589	1/1	0.92	0.26	53,53,53,53	0
56	MG	1A	3944	1/1	0.92	0.09	69,69,69,69	0
56	MG	2a	3108	1/1	0.92	0.05	57,57,57,57	0
56	MG	2A	3505	1/1	0.92	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3533	1/1	0.92	0.09	44,44,44,44	0
56	MG	1A	3552	1/1	0.92	0.21	34,34,34,34	0
56	MG	2A	3558	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3652	1/1	0.92	0.16	52,52,52,52	0
56	MG	2a	3236	1/1	0.92	0.10	65,65,65,65	0
56	MG	1A	3717	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	4120	1/1	0.92	0.12	76,76,76,76	0
56	MG	2A	3674	1/1	0.92	0.16	49,49,49,49	0
56	MG	2G	3001	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3799	1/1	0.92	0.06	58,58,58,58	0
56	MG	1A	3929	1/1	0.92	0.16	62,62,62,62	0
56	MG	2A	3595	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3828	1/1	0.92	0.09	64,64,64,64	0
56	MG	2A	3419	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3182	1/1	0.92	0.14	62,62,62,62	0
56	MG	1A	3950	1/1	0.92	0.15	68,68,68,68	0
56	MG	2A	3022	1/1	0.92	0.17	37,37,37,37	0
56	MG	2A	3906	1/1	0.92	0.18	64,64,64,64	0
56	MG	2A	3249	1/1	0.92	0.34	64,64,64,64	0
56	MG	1A	3019	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	4126	1/1	0.92	0.16	67,67,67,67	0
56	MG	1A	3245	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3903	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3593	1/1	0.92	0.13	50,50,50,50	0
56	MG	1A	3781	1/1	0.92	0.20	26,26,26,26	0
56	MG	1A	3933	1/1	0.92	0.14	81,81,81,81	0
56	MG	2A	3790	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3544	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	4202	1/1	0.92	0.20	39,39,39,39	0
56	MG	1a	1848	1/1	0.92	0.29	44,44,44,44	0
56	MG	2a	3226	1/1	0.93	0.16	79,79,79,79	0
56	MG	1A	3691	1/1	0.93	0.22	55,55,55,55	0
56	MG	2A	3480	1/1	0.93	0.37	50,50,50,50	0
56	MG	1A	3836	1/1	0.93	0.20	42,42,42,42	0
56	MG	2a	3136	1/1	0.93	0.24	83,83,83,83	0
56	MG	1A	3949	1/1	0.93	0.50	41,41,41,41	0
56	MG	2A	3488	1/1	0.93	0.31	53,53,53,53	0
56	MG	2A	3196	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	4189	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3676	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3546	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3629	1/1	0.93	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3228	1/1	0.93	0.17	37,37,37,37	0
56	MG	2A	3699	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3062	1/1	0.93	0.32	56,56,56,56	0
56	MG	2a	3102	1/1	0.93	0.25	63,63,63,63	0
56	MG	1A	4246	1/1	0.93	0.43	40,40,40,40	0
56	MG	2A	3812	1/1	0.93	0.19	48,48,48,48	0
56	MG	1A	4047	1/1	0.93	0.14	58,58,58,58	0
56	MG	2a	3211	1/1	0.93	0.10	71,71,71,71	0
56	MG	1A	3103	1/1	0.93	0.84	47,47,47,47	0
58	K	2A	3922	1/1	0.93	0.13	72,72,72,72	0
56	MG	1X	101	1/1	0.93	0.15	38,38,38,38	0
56	MG	2A	3594	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3349	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1769	1/1	0.93	0.14	44,44,44,44	0
56	MG	1a	1661	1/1	0.93	0.18	73,73,73,73	0
56	MG	1E	304	1/1	0.93	0.19	51,51,51,51	0
56	MG	2A	3631	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	4056	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3076	1/1	0.93	0.51	43,43,43,43	0
56	MG	1A	3435	1/1	0.93	0.43	53,53,53,53	0
56	MG	1A	3138	1/1	0.93	0.87	49,49,49,49	0
56	MG	1a	1843	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3939	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	4198	1/1	0.93	0.08	45,45,45,45	0
56	MG	1A	3549	1/1	0.93	0.83	50,50,50,50	0
56	MG	2A	3336	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	4028	1/1	0.93	0.08	46,46,46,46	0
56	MG	1A	4032	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3621	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3163	1/1	0.93	0.34	55,55,55,55	0
56	MG	2E	305	1/1	0.93	0.19	53,53,53,53	0
56	MG	1a	1638	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3320	1/1	0.93	0.21	55,55,55,55	0
56	MG	1a	1626	1/1	0.93	0.21	48,48,48,48	0
56	MG	2A	3260	1/1	0.93	0.10	73,73,73,73	0
56	MG	1a	1904	1/1	0.93	0.08	56,56,56,56	0
56	MG	2A	3107	1/1	0.93	0.40	50,50,50,50	0
56	MG	2Z	8001	1/1	0.93	0.06	65,65,65,65	0
59	ZN	2n	102	1/1	0.93	0.04	85,85,85,85	0
56	MG	1D	308	1/1	0.93	0.51	56,56,56,56	0
56	MG	1A	4102	1/1	0.93	0.12	32,32,32,32	0
56	MG	2a	3220	1/1	0.93	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3137	1/1	0.93	0.19	52,52,52,52	0
56	MG	2A	3391	1/1	0.93	0.11	58,58,58,58	0
56	MG	2A	3635	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3833	1/1	0.93	0.14	37,37,37,37	0
56	MG	2t	3001	1/1	0.93	0.07	63,63,63,63	0
56	MG	2A	3577	1/1	0.93	0.20	35,35,35,35	0
56	MG	1A	4101	1/1	0.93	0.07	61,61,61,61	0
56	MG	2A	3406	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1717	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	4142	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3233	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3581	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3982	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	4231	1/1	0.93	0.40	55,55,55,55	0
56	MG	25	105	1/1	0.93	0.10	55,55,55,55	0
56	MG	1a	1637	1/1	0.93	0.34	56,56,56,56	0
56	MG	1A	3187	1/1	0.93	0.61	51,51,51,51	0
56	MG	1a	1850	1/1	0.93	0.12	59,59,59,59	0
56	MG	1R	203	1/1	0.93	0.12	36,36,36,36	0
56	MG	2E	308	1/1	0.93	0.96	59,59,59,59	0
56	MG	1A	4230	1/1	0.93	0.60	45,45,45,45	0
56	MG	2A	3576	1/1	0.93	0.14	29,29,29,29	0
56	MG	1A	3578	1/1	0.93	0.23	61,61,61,61	0
56	MG	1A	3092	1/1	0.93	0.15	53,53,53,53	0
56	MG	1a	1652	1/1	0.93	0.24	41,41,41,41	0
56	MG	1a	1884	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	4005	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3491	1/1	0.93	0.34	37,37,37,37	0
56	MG	1A	3197	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3611	1/1	0.93	0.05	60,60,60,60	0
56	MG	2A	3524	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3101	1/1	0.93	0.10	66,66,66,66	0
56	MG	2A	3095	1/1	0.93	0.19	48,48,48,48	0
56	MG	2B	3008	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3275	1/1	0.93	0.14	67,67,67,67	0
56	MG	1A	3954	1/1	0.93	0.24	62,62,62,62	0
56	MG	1A	3098	1/1	0.93	0.22	57,57,57,57	0
56	MG	1U	203	1/1	0.93	0.62	46,46,46,46	0
56	MG	1A	3347	1/1	0.93	0.51	42,42,42,42	0
56	MG	2A	3661	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3120	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3638	1/1	0.93	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3095	1/1	0.93	0.26	50,50,50,50	0
56	MG	2A	3052	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3753	1/1	0.93	0.16	32,32,32,32	0
56	MG	1a	1863	1/1	0.93	0.12	76,76,76,76	0
56	MG	1A	3349	1/1	0.93	0.21	41,41,41,41	0
56	MG	2a	3138	1/1	0.93	0.12	83,83,83,83	0
56	MG	10	103	1/1	0.93	1.00	54,54,54,54	0
56	MG	1a	1601	1/1	0.93	0.23	50,50,50,50	0
56	MG	2A	3070	1/1	0.93	0.16	34,34,34,34	0
56	MG	2A	3256	1/1	0.93	0.15	58,58,58,58	0
56	MG	2A	3856	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3594	1/1	0.93	0.24	40,40,40,40	0
56	MG	1A	4196	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3163	1/1	0.93	0.26	49,49,49,49	0
56	MG	1a	1886	1/1	0.93	0.08	54,54,54,54	0
56	MG	2A	3694	1/1	0.93	0.07	60,60,60,60	0
56	MG	1N	3006	1/1	0.93	0.14	46,46,46,46	0
56	MG	1R	202	1/1	0.93	0.21	36,36,36,36	0
56	MG	1A	3005	1/1	0.93	0.22	53,53,53,53	0
56	MG	1F	301	1/1	0.93	0.27	68,68,68,68	0
56	MG	1F	305	1/1	0.93	0.55	39,39,39,39	0
56	MG	2A	3660	1/1	0.93	0.16	57,57,57,57	0
56	MG	1a	1608	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	4027	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3210	1/1	0.93	0.08	67,67,67,67	0
56	MG	1a	1922	1/1	0.93	0.16	52,52,52,52	0
56	MG	2A	3167	1/1	0.93	0.31	41,41,41,41	0
56	MG	1A	3335	1/1	0.93	0.32	56,56,56,56	0
56	MG	1a	1761	1/1	0.93	0.23	55,55,55,55	0
57	CPT	2A	3904	4/5	0.93	0.13	79,102,124,194	4
56	MG	1D	309	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3507	1/1	0.93	0.29	72,72,72,72	0
56	MG	2A	3171	1/1	0.93	0.13	61,61,61,61	0
56	MG	1A	3133	1/1	0.93	0.35	36,36,36,36	0
56	MG	2a	3230	1/1	0.93	0.11	66,66,66,66	0
56	MG	1a	1779	1/1	0.93	0.16	56,56,56,56	0
56	MG	2A	3221	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3141	1/1	0.93	0.28	43,43,43,43	0
56	MG	2A	3269	1/1	0.93	0.20	50,50,50,50	0
56	MG	1B	231	1/1	0.93	0.18	56,56,56,56	0
56	MG	1A	3765	1/1	0.93	0.21	28,28,28,28	0
56	MG	2A	3017	1/1	0.93	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1772	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3054	1/1	0.93	0.17	53,53,53,53	0
56	MG	1U	204	1/1	0.93	0.90	66,66,66,66	0
56	MG	1A	3277	1/1	0.93	0.46	47,47,47,47	0
56	MG	1A	3045	1/1	0.93	0.15	38,38,38,38	0
56	MG	1A	3799	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3948	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3659	1/1	0.93	0.31	41,41,41,41	0
56	MG	1A	3193	1/1	0.93	0.44	44,44,44,44	0
56	MG	1A	4229	1/1	0.93	0.44	45,45,45,45	0
56	MG	1A	3940	1/1	0.93	0.33	47,47,47,47	0
56	MG	1A	3716	1/1	0.93	0.11	44,44,44,44	0
56	MG	1a	1678	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3494	1/1	0.93	0.09	45,45,45,45	0
56	MG	2y	3007	1/1	0.93	0.14	84,84,84,84	0
56	MG	2A	3142	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3454	1/1	0.93	0.25	51,51,51,51	0
56	MG	1A	3414	1/1	0.93	0.37	62,62,62,62	0
56	MG	2A	3277	1/1	0.93	0.56	63,63,63,63	0
56	MG	1A	3241	1/1	0.93	0.22	37,37,37,37	0
56	MG	2A	3054	1/1	0.93	0.11	44,44,44,44	0
56	MG	2a	3070	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3119	1/1	0.93	0.16	41,41,41,41	0
56	MG	1A	3932	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3808	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3328	1/1	0.93	0.34	53,53,53,53	0
56	MG	1a	1645	1/1	0.93	0.20	53,53,53,53	0
56	MG	1A	3655	1/1	0.93	0.21	50,50,50,50	0
56	MG	2a	3232	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3571	1/1	0.93	0.29	58,58,58,58	0
56	MG	1A	3478	1/1	0.93	0.20	47,47,47,47	0
56	MG	1A	4109	1/1	0.93	0.12	40,40,40,40	0
56	MG	2A	3048	1/1	0.93	0.18	53,53,53,53	0
56	MG	2Q	3002	1/1	0.93	0.38	47,47,47,47	0
56	MG	1A	3511	1/1	0.93	0.44	44,44,44,44	0
56	MG	2a	3203	1/1	0.93	0.25	50,50,50,50	0
56	MG	2A	3523	1/1	0.93	0.11	31,31,31,31	0
56	MG	1A	3798	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3508	1/1	0.93	0.35	41,41,41,41	0
56	MG	2a	3033	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	3045	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3658	1/1	0.93	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3003	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3496	1/1	0.93	0.21	51,51,51,51	0
56	MG	2A	3250	1/1	0.93	0.69	62,62,62,62	0
56	MG	1A	3379	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3887	1/1	0.93	0.21	29,29,29,29	0
56	MG	1A	3527	1/1	0.93	0.17	55,55,55,55	0
56	MG	2A	3193	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3075	1/1	0.93	0.15	32,32,32,32	0
56	MG	2A	3710	1/1	0.93	0.19	28,28,28,28	0
56	MG	1A	3790	1/1	0.93	0.18	46,46,46,46	0
56	MG	2A	3356	1/1	0.93	0.15	53,53,53,53	0
56	MG	2A	3238	1/1	0.93	0.29	43,43,43,43	0
56	MG	1a	1696	1/1	0.93	0.13	55,55,55,55	0
56	MG	1a	1703	1/1	0.93	0.27	51,51,51,51	0
56	MG	2A	3418	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	4239	1/1	0.94	0.64	33,33,33,33	0
56	MG	1A	3990	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3236	1/1	0.94	0.26	61,61,61,61	0
56	MG	2A	3563	1/1	0.94	0.29	41,41,41,41	0
56	MG	1A	3021	1/1	0.94	0.16	43,43,43,43	0
56	MG	1S	3003	1/1	0.94	0.17	72,72,72,72	0
56	MG	1A	3666	1/1	0.94	0.22	43,43,43,43	0
56	MG	1A	3419	1/1	0.94	0.33	61,61,61,61	0
56	MG	2A	3650	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3012	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3157	1/1	0.94	0.24	45,45,45,45	0
56	MG	2a	3186	1/1	0.94	0.16	62,62,62,62	0
56	MG	1v	3001	1/1	0.94	0.20	64,64,64,64	0
56	MG	1E	310	1/1	0.94	0.69	49,49,49,49	0
56	MG	1a	1701	1/1	0.94	0.41	46,46,46,46	0
56	MG	1A	3368	1/1	0.94	0.51	62,62,62,62	0
56	MG	1a	1888	1/1	0.94	0.07	58,58,58,58	0
56	MG	1a	1712	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3959	1/1	0.94	0.31	46,46,46,46	0
56	MG	1A	3426	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3923	1/1	0.94	0.14	67,67,67,67	0
56	MG	1A	4112	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3223	1/1	0.94	0.65	43,43,43,43	0
56	MG	2A	3295	1/1	0.94	0.40	43,43,43,43	0
56	MG	2A	3252	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3836	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3902	1/1	0.94	0.07	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3839	1/1	0.94	0.08	50,50,50,50	0
56	MG	1a	1764	1/1	0.94	0.19	36,36,36,36	0
56	MG	2U	202	1/1	0.94	0.49	46,46,46,46	0
56	MG	1a	1760	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	4080	1/1	0.94	0.15	26,26,26,26	0
56	MG	1A	3911	1/1	0.94	0.09	36,36,36,36	0
56	MG	2A	3606	1/1	0.94	0.14	56,56,56,56	0
56	MG	2a	3163	1/1	0.94	0.13	46,46,46,46	0
56	MG	1a	1685	1/1	0.94	0.31	53,53,53,53	0
56	MG	2A	3225	1/1	0.94	0.23	54,54,54,54	0
56	MG	2B	3005	1/1	0.94	0.11	64,64,64,64	0
56	MG	1A	4158	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3055	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3368	1/1	0.94	0.36	65,65,65,65	0
56	MG	2A	3568	1/1	0.94	0.14	31,31,31,31	0
56	MG	1x	108	1/1	0.94	0.23	73,73,73,73	0
56	MG	2A	3151	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3855	1/1	0.94	0.15	34,34,34,34	0
56	MG	2A	3886	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3693	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3623	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1623	1/1	0.94	0.16	56,56,56,56	0
56	MG	2y	3001	1/1	0.94	0.10	58,58,58,58	0
56	MG	1a	1925	1/1	0.94	0.14	52,52,52,52	0
56	MG	2a	3233	1/1	0.94	0.19	60,60,60,60	0
56	MG	1A	3770	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	3010	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3415	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3039	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3816	1/1	0.94	0.20	58,58,58,58	0
56	MG	1A	3523	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3438	1/1	0.94	0.40	41,41,41,41	0
56	MG	1a	1737	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4127	1/1	0.94	0.07	38,38,38,38	0
56	MG	2a	3199	1/1	0.94	0.31	62,62,62,62	0
56	MG	1A	3630	1/1	0.94	0.30	39,39,39,39	0
56	MG	1a	1676	1/1	0.94	0.21	60,60,60,60	0
56	MG	2A	3051	1/1	0.94	0.30	54,54,54,54	0
56	MG	1V	201	1/1	0.94	0.22	41,41,41,41	0
59	ZN	14	501	1/1	0.94	0.08	104,104,104,104	0
56	MG	2A	3525	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3020	1/1	0.94	0.24	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3264	1/1	0.94	0.43	57,57,57,57	0
56	MG	1a	1631	1/1	0.94	0.07	51,51,51,51	0
56	MG	2A	3857	1/1	0.94	0.16	56,56,56,56	0
56	MG	2B	3012	1/1	0.94	0.12	58,58,58,58	0
56	MG	2a	3207	1/1	0.94	0.12	71,71,71,71	0
56	MG	2A	3718	1/1	0.94	0.14	30,30,30,30	0
56	MG	1a	1681	1/1	0.94	0.28	60,60,60,60	0
56	MG	1A	4251	1/1	0.94	0.52	49,49,49,49	0
56	MG	1A	3935	1/1	0.94	0.20	58,58,58,58	0
56	MG	1A	3668	1/1	0.94	0.17	48,48,48,48	0
56	MG	2A	3656	1/1	0.94	0.15	58,58,58,58	0
56	MG	1A	4012	1/1	0.94	0.08	68,68,68,68	0
56	MG	2A	3613	1/1	0.94	0.17	62,62,62,62	0
56	MG	1W	3001	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3918	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3090	1/1	0.94	0.40	62,62,62,62	0
56	MG	1A	3488	1/1	0.94	0.26	45,45,45,45	0
56	MG	1A	3877	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3749	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3893	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3916	1/1	0.94	0.11	53,53,53,53	0
56	MG	1B	219	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3372	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3682	1/1	0.94	0.14	40,40,40,40	0
56	MG	2a	3125	1/1	0.94	0.22	48,48,48,48	0
56	MG	2A	3564	1/1	0.94	0.16	70,70,70,70	0
56	MG	1l	204	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3752	1/1	0.94	0.30	45,45,45,45	0
56	MG	1A	3122	1/1	0.94	0.23	53,53,53,53	0
56	MG	2E	302	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3100	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1674	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3922	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3542	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	4042	1/1	0.94	0.06	51,51,51,51	0
56	MG	1P	202	1/1	0.94	0.31	39,39,39,39	0
56	MG	2A	3620	1/1	0.94	0.21	40,40,40,40	0
56	MG	2A	3143	1/1	0.94	0.27	35,35,35,35	0
56	MG	2A	3510	1/1	0.94	0.22	26,26,26,26	0
56	MG	1a	1803	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4070	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3157	1/1	0.94	0.48	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3541	1/1	0.94	0.19	48,48,48,48	0
56	MG	1a	1799	1/1	0.94	0.09	62,62,62,62	0
56	MG	1x	112	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3638	1/1	0.94	0.34	44,44,44,44	0
56	MG	2a	3001	1/1	0.94	0.20	62,62,62,62	0
56	MG	1A	3528	1/1	0.94	0.20	35,35,35,35	0
56	MG	2A	3020	1/1	0.94	0.28	50,50,50,50	0
56	MG	2a	3126	1/1	0.94	0.13	49,49,49,49	0
56	MG	2F	304	1/1	0.94	0.62	52,52,52,52	0
56	MG	2A	3156	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	4190	1/1	0.94	0.14	58,58,58,58	0
56	MG	1a	1640	1/1	0.94	0.16	52,52,52,52	0
56	MG	2U	206	1/1	0.94	0.39	49,49,49,49	0
56	MG	1A	4250	1/1	0.94	0.14	38,38,38,38	0
56	MG	2a	3084	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3118	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3166	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3845	1/1	0.94	0.09	53,53,53,53	0
56	MG	2B	3007	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3006	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3839	1/1	0.94	0.19	33,33,33,33	0
56	MG	1A	3674	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	3529	1/1	0.94	0.24	45,45,45,45	0
56	MG	2A	3909	1/1	0.94	0.21	51,51,51,51	0
56	MG	2A	3649	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3515	1/1	0.94	0.18	25,25,25,25	0
56	MG	1A	3763	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3653	1/1	0.94	0.18	34,34,34,34	0
56	MG	2a	3049	1/1	0.94	0.22	50,50,50,50	0
56	MG	1A	4073	1/1	0.94	0.25	68,68,68,68	0
56	MG	2A	3402	1/1	0.94	0.26	47,47,47,47	0
56	MG	2A	3124	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3718	1/1	0.94	0.17	35,35,35,35	0
56	MG	2A	3305	1/1	0.94	0.25	55,55,55,55	0
56	MG	2A	3190	1/1	0.94	0.24	64,64,64,64	0
56	MG	1A	3173	1/1	0.94	0.46	50,50,50,50	0
59	ZN	26	501	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3331	1/1	0.94	0.20	64,64,64,64	0
56	MG	2A	3534	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3670	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3478	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3826	1/1	0.94	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3302	1/1	0.94	0.37	57,57,57,57	0
56	MG	1A	3410	1/1	0.94	0.28	40,40,40,40	0
56	MG	1A	3825	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3510	1/1	0.94	0.45	50,50,50,50	0
56	MG	1A	3027	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3412	1/1	0.94	0.31	53,53,53,53	0
56	MG	1a	1735	1/1	0.94	0.07	47,47,47,47	0
56	MG	2B	3013	1/1	0.94	0.15	72,72,72,72	0
56	MG	2a	3223	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4181	1/1	0.94	0.34	47,47,47,47	0
56	MG	2A	3890	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3591	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3600	1/1	0.94	0.16	62,62,62,62	0
56	MG	1A	3293	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3144	1/1	0.94	0.39	50,50,50,50	0
56	MG	1A	3124	1/1	0.94	0.43	39,39,39,39	0
56	MG	1A	3398	1/1	0.94	0.18	41,41,41,41	0
56	MG	2P	201	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3938	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3664	1/1	0.94	0.19	51,51,51,51	0
56	MG	1N	3004	1/1	0.94	1.17	60,60,60,60	0
56	MG	1A	3346	1/1	0.94	0.44	57,57,57,57	0
56	MG	1A	3590	1/1	0.94	0.21	44,44,44,44	0
56	MG	2a	3051	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3646	1/1	0.94	0.18	50,50,50,50	0
56	MG	1A	4253	1/1	0.94	0.66	45,45,45,45	0
56	MG	1A	3114	1/1	0.94	0.23	48,48,48,48	0
56	MG	1D	311	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3473	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	4185	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3554	1/1	0.94	0.22	33,33,33,33	0
56	MG	2A	3528	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3333	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3780	1/1	0.94	0.12	57,57,57,57	0
56	MG	1a	1666	1/1	0.94	0.38	49,49,49,49	0
56	MG	1A	4089	1/1	0.94	0.15	64,64,64,64	0
56	MG	1a	1731	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3114	1/1	0.94	0.11	51,51,51,51	0
56	MG	2a	3165	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3942	1/1	0.94	0.21	49,49,49,49	0
56	MG	1D	304	1/1	0.94	0.13	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3452	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3155	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3787	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3665	1/1	0.94	0.12	40,40,40,40	0
56	MG	2A	3905	1/1	0.94	0.22	33,33,33,33	0
56	MG	2A	3636	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3655	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3662	1/1	0.94	0.33	52,52,52,52	0
56	MG	1a	1794	1/1	0.94	0.34	52,52,52,52	0
56	MG	1A	3131	1/1	0.94	0.25	45,45,45,45	0
56	MG	2A	3578	1/1	0.94	0.12	29,29,29,29	0
56	MG	2a	3179	1/1	0.94	0.09	80,80,80,80	0
56	MG	1A	4216	1/1	0.94	0.15	28,28,28,28	0
56	MG	1A	3290	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3490	1/1	0.94	0.09	49,49,49,49	0
56	MG	2E	301	1/1	0.94	0.19	53,53,53,53	0
56	MG	2A	3041	1/1	0.94	0.18	39,39,39,39	0
56	MG	1a	1836	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3648	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3231	1/1	0.94	0.43	49,49,49,49	0
56	MG	2a	3178	1/1	0.94	0.13	64,64,64,64	0
56	MG	1c	302	1/1	0.94	0.15	71,71,71,71	0
56	MG	1N	3001	1/1	0.94	0.44	56,56,56,56	0
56	MG	1A	3842	1/1	0.94	0.13	58,58,58,58	0
56	MG	2l	3004	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3470	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3747	1/1	0.94	0.16	32,32,32,32	0
56	MG	1G	3001	1/1	0.94	0.07	41,41,41,41	0
56	MG	2R	201	1/1	0.94	0.44	57,57,57,57	0
56	MG	1A	3780	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	3736	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3272	1/1	0.94	0.33	55,55,55,55	0
56	MG	2A	3741	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3530	1/1	0.94	0.27	43,43,43,43	0
56	MG	1A	3761	1/1	0.94	0.15	26,26,26,26	0
56	MG	1A	3657	1/1	0.94	0.17	49,49,49,49	0
56	MG	2A	3777	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3508	1/1	0.94	0.05	35,35,35,35	0
56	MG	2A	3110	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3313	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3201	1/1	0.94	0.17	28,28,28,28	0
56	MG	2A	3472	1/1	0.94	0.34	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3736	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3986	1/1	0.94	0.21	39,39,39,39	0
56	MG	1a	1770	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3915	1/1	0.94	0.26	54,54,54,54	0
56	MG	1A	3962	1/1	0.94	0.82	58,58,58,58	0
56	MG	2A	3396	1/1	0.94	0.12	50,50,50,50	0
56	MG	1B	213	1/1	0.94	0.13	80,80,80,80	0
56	MG	2A	3667	1/1	0.94	0.17	36,36,36,36	0
56	MG	15	101	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3719	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3924	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3992	1/1	0.95	0.10	73,73,73,73	0
56	MG	1A	3848	1/1	0.95	0.21	57,57,57,57	0
56	MG	2a	3046	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1835	1/1	0.95	0.09	39,39,39,39	0
56	MG	1a	1788	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3859	1/1	0.95	0.26	41,41,41,41	0
56	MG	1A	3281	1/1	0.95	0.34	53,53,53,53	0
56	MG	1A	3891	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3742	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3547	1/1	0.95	0.32	40,40,40,40	0
56	MG	1A	3017	1/1	0.95	0.32	44,44,44,44	0
56	MG	2A	3889	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	3116	1/1	0.95	0.29	33,33,33,33	0
56	MG	1A	3999	1/1	0.95	0.42	32,32,32,32	0
56	MG	1P	203	1/1	0.95	0.38	44,44,44,44	0
56	MG	1A	3669	1/1	0.95	0.31	48,48,48,48	0
56	MG	1A	3303	1/1	0.95	0.39	40,40,40,40	0
56	MG	2A	3919	1/1	0.95	0.12	39,39,39,39	0
56	MG	17	104	1/1	0.95	0.17	41,41,41,41	0
56	MG	2A	3084	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3511	1/1	0.95	0.25	52,52,52,52	0
56	MG	2a	3154	1/1	0.95	0.14	48,48,48,48	0
56	MG	2e	3001	1/1	0.95	0.07	66,66,66,66	0
56	MG	2w	101	1/1	0.95	0.22	65,65,65,65	0
56	MG	1a	1733	1/1	0.95	0.23	41,41,41,41	0
56	MG	1x	106	1/1	0.95	0.35	50,50,50,50	0
56	MG	1a	1697	1/1	0.95	0.18	45,45,45,45	0
56	MG	1S	3001	1/1	0.95	0.36	52,52,52,52	0
56	MG	2A	3307	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3829	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3369	1/1	0.95	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3661	1/1	0.95	0.47	61,61,61,61	0
56	MG	1A	3022	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3591	1/1	0.95	0.26	48,48,48,48	0
56	MG	1A	3066	1/1	0.95	0.17	46,46,46,46	0
56	MG	2A	3398	1/1	0.95	0.18	48,48,48,48	0
56	MG	2A	3500	1/1	0.95	0.37	33,33,33,33	0
56	MG	1A	3917	1/1	0.95	0.18	36,36,36,36	0
56	MG	2A	3147	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3846	1/1	0.95	0.12	31,31,31,31	0
56	MG	1a	1719	1/1	0.95	0.06	60,60,60,60	0
56	MG	1A	3820	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3972	1/1	0.95	0.15	34,34,34,34	0
56	MG	2A	3170	1/1	0.95	0.13	38,38,38,38	0
56	MG	1a	1689	1/1	0.95	0.13	65,65,65,65	0
56	MG	1A	4203	1/1	0.95	0.71	50,50,50,50	0
56	MG	1A	3332	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3033	1/1	0.95	0.62	39,39,39,39	0
56	MG	1A	3230	1/1	0.95	0.26	39,39,39,39	0
56	MG	1A	3970	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3186	1/1	0.95	0.24	50,50,50,50	0
56	MG	1A	3183	1/1	0.95	0.18	54,54,54,54	0
56	MG	1W	3005	1/1	0.95	0.16	29,29,29,29	0
56	MG	2A	3289	1/1	0.95	0.39	52,52,52,52	0
56	MG	1A	3964	1/1	0.95	0.49	37,37,37,37	0
56	MG	2a	3088	1/1	0.95	0.13	63,63,63,63	0
56	MG	1A	3250	1/1	0.95	0.08	58,58,58,58	0
56	MG	2A	3103	1/1	0.95	0.20	28,28,28,28	0
56	MG	2A	3105	1/1	0.95	0.08	44,44,44,44	0
56	MG	1a	1617	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3440	1/1	0.95	0.18	42,42,42,42	0
56	MG	1A	3111	1/1	0.95	0.30	38,38,38,38	0
56	MG	1A	4092	1/1	0.95	0.15	57,57,57,57	0
56	MG	2A	3254	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3057	1/1	0.95	0.11	38,38,38,38	0
56	MG	1a	1807	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3130	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3919	1/1	0.95	0.23	47,47,47,47	0
56	MG	2A	3129	1/1	0.95	0.23	56,56,56,56	0
56	MG	2A	3111	1/1	0.95	0.13	34,34,34,34	0
56	MG	2A	3663	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3390	1/1	0.95	0.23	43,43,43,43	0
56	MG	2A	3849	1/1	0.95	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3041	1/1	0.95	0.14	33,33,33,33	0
56	MG	1A	3301	1/1	0.95	0.31	58,58,58,58	0
56	MG	2a	3010	1/1	0.95	0.17	76,76,76,76	0
56	MG	1A	4023	1/1	0.95	0.15	19,19,19,19	0
56	MG	1A	3755	1/1	0.95	0.20	26,26,26,26	0
56	MG	2U	205	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3014	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3399	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3985	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3071	1/1	0.95	0.31	38,38,38,38	0
56	MG	1A	3089	1/1	0.95	0.20	48,48,48,48	0
56	MG	2B	3006	1/1	0.95	0.17	54,54,54,54	0
56	MG	2A	3314	1/1	0.95	0.12	48,48,48,48	0
56	MG	2a	3198	1/1	0.95	0.18	68,68,68,68	0
56	MG	2A	3654	1/1	0.95	0.27	54,54,54,54	0
56	MG	1A	3407	1/1	0.95	0.21	61,61,61,61	0
56	MG	1A	4000	1/1	0.95	0.18	29,29,29,29	0
56	MG	2A	3485	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	4029	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3009	1/1	0.95	0.16	33,33,33,33	0
56	MG	2A	3917	1/1	0.95	0.19	52,52,52,52	0
56	MG	2a	3180	1/1	0.95	0.11	70,70,70,70	0
56	MG	1X	105	1/1	0.95	0.31	62,62,62,62	0
56	MG	1A	3058	1/1	0.95	0.15	60,60,60,60	0
56	MG	1A	3167	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3364	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3794	1/1	0.95	0.14	32,32,32,32	0
56	MG	1a	1905	1/1	0.95	0.08	56,56,56,56	0
56	MG	1w	109	1/1	0.95	0.05	61,61,61,61	0
56	MG	1A	3242	1/1	0.95	0.84	40,40,40,40	0
56	MG	1A	3936	1/1	0.95	0.13	64,64,64,64	0
56	MG	1a	1830	1/1	0.95	0.19	36,36,36,36	0
56	MG	15	105	1/1	0.95	0.17	62,62,62,62	0
56	MG	11	103	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3976	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3030	1/1	0.95	0.25	40,40,40,40	0
56	MG	1O	3002	1/1	0.95	0.46	59,59,59,59	0
56	MG	1G	3004	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3377	1/1	0.95	0.45	50,50,50,50	0
56	MG	2A	3088	1/1	0.95	0.13	55,55,55,55	0
56	MG	2E	306	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3712	1/1	0.95	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2n	101	1/1	0.95	0.18	70,70,70,70	0
56	MG	2A	3669	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3602	1/1	0.95	0.27	56,56,56,56	0
56	MG	1A	4173	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3607	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3569	1/1	0.95	0.49	43,43,43,43	0
56	MG	2A	3184	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3597	1/1	0.95	0.50	49,49,49,49	0
56	MG	1A	3306	1/1	0.95	0.22	40,40,40,40	0
56	MG	1l	201	1/1	0.95	0.22	49,49,49,49	0
56	MG	1a	1890	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3477	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3694	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3687	1/1	0.95	0.49	39,39,39,39	0
56	MG	2A	3637	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3521	1/1	0.95	0.30	71,71,71,71	0
56	MG	1w	101	1/1	0.95	0.16	87,87,87,87	0
56	MG	1a	1643	1/1	0.95	0.15	57,57,57,57	0
56	MG	2A	3492	1/1	0.95	0.16	58,58,58,58	0
56	MG	1A	3216	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3871	1/1	0.95	0.27	37,37,37,37	0
56	MG	2a	3028	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	4228	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3350	1/1	0.95	0.74	39,39,39,39	0
56	MG	2a	3210	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	3546	1/1	0.95	0.17	50,50,50,50	0
56	MG	1B	220	1/1	0.95	0.14	51,51,51,51	0
56	MG	2A	3767	1/1	0.95	0.25	52,52,52,52	0
56	MG	1A	3821	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3572	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	4161	1/1	0.95	0.13	23,23,23,23	0
56	MG	2A	3539	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3266	1/1	0.95	0.17	54,54,54,54	0
56	MG	1a	1680	1/1	0.95	0.51	48,48,48,48	0
56	MG	1A	3061	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3236	1/1	0.95	0.11	64,64,64,64	0
56	MG	2A	3612	1/1	0.95	0.19	41,41,41,41	0
56	MG	2B	3018	1/1	0.95	0.17	42,42,42,42	0
56	MG	2B	3019	1/1	0.95	0.20	66,66,66,66	0
56	MG	2A	3493	1/1	0.95	0.39	45,45,45,45	0
56	MG	2A	3451	1/1	0.95	0.19	54,54,54,54	0
56	MG	1a	1628	1/1	0.95	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3710	1/1	0.95	0.22	44,44,44,44	0
56	MG	2A	3532	1/1	0.95	0.15	49,49,49,49	0
56	MG	2A	3441	1/1	0.95	0.28	36,36,36,36	0
56	MG	1A	4022	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3011	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	4237	1/1	0.95	0.66	48,48,48,48	0
56	MG	1A	3551	1/1	0.95	0.28	33,33,33,33	0
56	MG	2A	3643	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3830	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	4254	1/1	0.95	0.60	49,49,49,49	0
56	MG	1a	1911	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3038	1/1	0.95	0.22	36,36,36,36	0
56	MG	2a	3092	1/1	0.95	0.18	77,77,77,77	0
56	MG	2A	3501	1/1	0.95	0.07	72,72,72,72	0
56	MG	2A	3679	1/1	0.95	0.10	51,51,51,51	0
56	MG	1a	1752	1/1	0.95	0.04	63,63,63,63	0
56	MG	1A	3969	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1647	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3362	1/1	0.95	0.12	54,54,54,54	0
56	MG	2a	3160	1/1	0.95	0.07	77,77,77,77	0
56	MG	1A	4226	1/1	0.95	0.43	38,38,38,38	0
56	MG	2A	3634	1/1	0.95	0.16	39,39,39,39	0
56	MG	1A	4192	1/1	0.95	0.47	52,52,52,52	0
56	MG	1A	3139	1/1	0.95	0.20	42,42,42,42	0
56	MG	1E	306	1/1	0.95	0.18	50,50,50,50	0
56	MG	2A	3150	1/1	0.95	0.21	38,38,38,38	0
56	MG	1A	3843	1/1	0.95	0.09	50,50,50,50	0
56	MG	2a	3094	1/1	0.95	0.20	61,61,61,61	0
56	MG	1A	4183	1/1	0.95	0.36	33,33,33,33	0
56	MG	1A	3104	1/1	0.95	0.50	54,54,54,54	0
56	MG	1A	4217	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3925	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3729	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3443	1/1	0.95	0.12	42,42,42,42	0
56	MG	1D	303	1/1	0.95	0.50	45,45,45,45	0
56	MG	1A	4061	1/1	0.95	0.08	72,72,72,72	0
56	MG	1A	3653	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3770	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3895	1/1	0.95	0.36	41,41,41,41	0
56	MG	2A	3078	1/1	0.95	0.28	41,41,41,41	0
56	MG	2a	3147	1/1	0.95	0.07	78,78,78,78	0
56	MG	1A	3434	1/1	0.95	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3633	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	3612	1/1	0.95	0.22	41,41,41,41	0
56	MG	2B	3014	1/1	0.95	0.13	81,81,81,81	0
56	MG	2A	3116	1/1	0.95	0.36	40,40,40,40	0
56	MG	1D	310	1/1	0.95	0.34	27,27,27,27	0
56	MG	2A	3723	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3108	1/1	0.95	0.52	42,42,42,42	0
56	MG	1a	1910	1/1	0.95	0.07	61,61,61,61	0
56	MG	2A	3789	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3910	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3680	1/1	0.95	0.10	51,51,51,51	0
56	MG	1x	105	1/1	0.95	0.19	62,62,62,62	0
56	MG	1a	1855	1/1	0.95	0.12	49,49,49,49	0
56	MG	2a	3184	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3304	1/1	0.95	0.18	55,55,55,55	0
56	MG	2A	3916	1/1	0.95	0.50	41,41,41,41	0
56	MG	2A	3566	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3598	1/1	0.95	0.12	46,46,46,46	0
56	MG	2A	3788	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3852	1/1	0.95	0.07	72,72,72,72	0
56	MG	1A	4175	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3242	1/1	0.95	0.16	46,46,46,46	0
56	MG	2B	3021	1/1	0.95	0.79	74,74,74,74	0
56	MG	2A	3483	1/1	0.95	0.20	52,52,52,52	0
56	MG	1A	3705	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3007	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3153	1/1	0.95	0.25	39,39,39,39	0
56	MG	1A	3136	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3720	1/1	0.95	0.21	57,57,57,57	0
56	MG	2a	3111	1/1	0.95	0.23	67,67,67,67	0
56	MG	2A	3467	1/1	0.95	0.26	56,56,56,56	0
56	MG	1a	1837	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3566	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3711	1/1	0.95	0.23	73,73,73,73	0
56	MG	1A	3120	1/1	0.95	0.61	41,41,41,41	0
56	MG	1A	3709	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3175	1/1	0.96	0.46	43,43,43,43	0
56	MG	1A	3087	1/1	0.96	0.43	38,38,38,38	0
56	MG	2A	3695	1/1	0.96	0.09	43,43,43,43	0
56	MG	2q	201	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3818	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3714	1/1	0.96	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3294	1/1	0.96	0.26	32,32,32,32	0
56	MG	1A	3046	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3137	1/1	0.96	0.44	38,38,38,38	0
56	MG	1A	4182	1/1	0.96	0.27	57,57,57,57	0
56	MG	2A	3513	1/1	0.96	0.16	28,28,28,28	0
56	MG	2A	3316	1/1	0.96	0.38	52,52,52,52	0
56	MG	1a	1744	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3809	1/1	0.96	0.09	56,56,56,56	0
56	MG	1a	1860	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3667	1/1	0.96	0.16	44,44,44,44	0
56	MG	1B	233	1/1	0.96	0.16	82,82,82,82	0
56	MG	1a	1796	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3696	1/1	0.96	0.13	49,49,49,49	0
56	MG	1a	1820	1/1	0.96	0.29	46,46,46,46	0
56	MG	2A	3615	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3207	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	4131	1/1	0.96	0.12	24,24,24,24	0
56	MG	2A	3684	1/1	0.96	0.13	63,63,63,63	0
56	MG	2A	3074	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	3254	1/1	0.96	0.24	56,56,56,56	0
56	MG	1A	3206	1/1	0.96	0.32	39,39,39,39	0
56	MG	1A	3827	1/1	0.96	0.13	56,56,56,56	0
56	MG	1a	1741	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3550	1/1	0.96	0.28	34,34,34,34	0
56	MG	1A	3733	1/1	0.96	0.18	21,21,21,21	0
56	MG	1a	1841	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3140	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3238	1/1	0.96	0.47	39,39,39,39	0
56	MG	1F	306	1/1	0.96	0.69	47,47,47,47	0
56	MG	1A	3128	1/1	0.96	0.25	49,49,49,49	0
56	MG	1A	4212	1/1	0.96	0.16	32,32,32,32	0
56	MG	2A	3891	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3211	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3476	1/1	0.96	0.52	53,53,53,53	0
56	MG	2A	3547	1/1	0.96	0.12	28,28,28,28	0
56	MG	1a	1895	1/1	0.96	0.06	58,58,58,58	0
56	MG	1a	1721	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3747	1/1	0.96	0.34	47,47,47,47	0
56	MG	2A	3898	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3656	1/1	0.96	0.28	53,53,53,53	0
56	MG	1A	3622	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3035	1/1	0.96	0.34	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3205	1/1	0.96	0.18	59,59,59,59	0
56	MG	1A	3738	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3873	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	3129	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	1625	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3896	1/1	0.96	0.18	38,38,38,38	0
56	MG	2a	3098	1/1	0.96	0.23	61,61,61,61	0
56	MG	1a	1829	1/1	0.96	0.18	27,27,27,27	0
56	MG	1A	3840	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3117	1/1	0.96	0.10	54,54,54,54	0
56	MG	1a	1924	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3563	1/1	0.96	0.57	44,44,44,44	0
56	MG	1A	3522	1/1	0.96	0.44	51,51,51,51	0
56	MG	1A	3861	1/1	0.96	0.17	31,31,31,31	0
56	MG	2a	3081	1/1	0.96	0.16	52,52,52,52	0
56	MG	1a	1768	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3712	1/1	0.96	0.31	39,39,39,39	0
56	MG	1A	3235	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	3822	1/1	0.96	0.20	34,34,34,34	0
56	MG	2R	202	1/1	0.96	0.34	50,50,50,50	0
56	MG	1A	3032	1/1	0.96	0.86	47,47,47,47	0
56	MG	1A	3883	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3742	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	4242	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	4016	1/1	0.96	0.16	58,58,58,58	0
56	MG	2A	3731	1/1	0.96	0.24	62,62,62,62	0
56	MG	2A	3584	1/1	0.96	0.27	25,25,25,25	0
56	MG	1A	3885	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3704	1/1	0.96	0.13	50,50,50,50	0
56	MG	27	101	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	3715	1/1	0.96	0.10	44,44,44,44	0
56	MG	2a	3106	1/1	0.96	0.19	66,66,66,66	0
56	MG	1X	103	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3123	1/1	0.96	0.55	41,41,41,41	0
56	MG	1A	3864	1/1	0.96	0.18	24,24,24,24	0
56	MG	1A	4096	1/1	0.96	0.19	17,17,17,17	0
56	MG	1A	3832	1/1	0.96	0.05	48,48,48,48	0
56	MG	1a	1790	1/1	0.96	0.06	78,78,78,78	0
56	MG	1B	203	1/1	0.96	0.20	45,45,45,45	0
56	MG	2A	3834	1/1	0.96	0.13	65,65,65,65	0
56	MG	1A	3762	1/1	0.96	0.11	29,29,29,29	0
56	MG	1n	502	1/1	0.96	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3078	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3702	1/1	0.96	0.15	45,45,45,45	0
56	MG	2U	204	1/1	0.96	0.37	42,42,42,42	0
56	MG	1A	4033	1/1	0.96	0.17	49,49,49,49	0
56	MG	1a	1918	1/1	0.96	0.12	75,75,75,75	0
56	MG	2A	3658	1/1	0.96	0.31	36,36,36,36	0
56	MG	2A	3183	1/1	0.96	0.11	54,54,54,54	0
56	MG	1Q	201	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3287	1/1	0.96	0.13	51,51,51,51	0
56	MG	2A	3161	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3080	1/1	0.96	0.36	44,44,44,44	0
56	MG	1A	4095	1/1	0.96	0.29	51,51,51,51	0
56	MG	1A	3171	1/1	0.96	0.67	50,50,50,50	0
56	MG	1A	4152	1/1	0.96	0.15	24,24,24,24	0
56	MG	1a	1660	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3608	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3234	1/1	0.96	0.17	62,62,62,62	0
56	MG	1A	4236	1/1	0.96	0.20	37,37,37,37	0
56	MG	2A	3044	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3744	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3012	1/1	0.96	0.12	32,32,32,32	0
56	MG	1D	301	1/1	0.96	0.18	46,46,46,46	0
56	MG	1A	3013	1/1	0.96	0.55	34,34,34,34	0
56	MG	1A	3953	1/1	0.96	0.10	54,54,54,54	0
56	MG	2A	3119	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3565	1/1	0.96	0.13	53,53,53,53	0
56	MG	2A	3125	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3641	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3001	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3050	1/1	0.96	0.25	24,24,24,24	0
56	MG	1A	3808	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3504	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3537	1/1	0.96	0.18	33,33,33,33	0
56	MG	2A	3049	1/1	0.96	0.25	21,21,21,21	0
56	MG	1A	3097	1/1	0.96	0.20	31,31,31,31	0
56	MG	2A	3136	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	4235	1/1	0.96	0.55	37,37,37,37	0
56	MG	1a	1857	1/1	0.96	0.17	64,64,64,64	0
56	MG	1A	3754	1/1	0.96	0.18	21,21,21,21	0
56	MG	2A	3341	1/1	0.96	0.13	56,56,56,56	0
56	MG	2A	3844	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3810	1/1	0.96	0.17	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	212	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3006	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3077	1/1	0.96	0.50	39,39,39,39	0
56	MG	2A	3327	1/1	0.96	0.20	54,54,54,54	0
56	MG	2A	3686	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3518	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3619	1/1	0.96	0.31	41,41,41,41	0
56	MG	1A	4148	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3572	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	4069	1/1	0.96	0.13	89,89,89,89	0
56	MG	1A	3286	1/1	0.96	0.36	62,62,62,62	0
56	MG	2A	3750	1/1	0.96	0.30	44,44,44,44	0
56	MG	1A	3581	1/1	0.96	0.08	39,39,39,39	0
56	MG	2A	3013	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3125	1/1	0.96	0.85	47,47,47,47	0
56	MG	2A	3698	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3435	1/1	0.96	0.23	44,44,44,44	0
56	MG	2A	3082	1/1	0.96	0.06	49,49,49,49	0
56	MG	2a	3197	1/1	0.96	0.14	63,63,63,63	0
56	MG	1A	3628	1/1	0.96	0.16	49,49,49,49	0
56	MG	1A	4223	1/1	0.96	0.23	39,39,39,39	0
56	MG	2A	3306	1/1	0.96	0.14	44,44,44,44	0
56	MG	20	103	1/1	0.96	0.16	55,55,55,55	0
56	MG	1A	3110	1/1	0.96	0.28	40,40,40,40	0
56	MG	1a	1801	1/1	0.96	0.05	59,59,59,59	0
56	MG	1A	4191	1/1	0.96	0.16	25,25,25,25	0
56	MG	2A	3043	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3614	1/1	0.96	0.09	40,40,40,40	0
56	MG	1a	1775	1/1	0.96	0.29	60,60,60,60	0
56	MG	1A	3093	1/1	0.96	0.23	26,26,26,26	0
56	MG	1A	3194	1/1	0.96	0.22	49,49,49,49	0
56	MG	2A	3806	1/1	0.96	0.20	55,55,55,55	0
56	MG	1E	305	1/1	0.96	0.34	57,57,57,57	0
56	MG	1a	1833	1/1	0.96	0.38	70,70,70,70	0
56	MG	1a	1898	1/1	0.96	0.20	43,43,43,43	0
56	MG	2A	3871	1/1	0.96	0.28	67,67,67,67	0
56	MG	1A	3989	1/1	0.96	0.10	49,49,49,49	0
56	MG	2B	3003	1/1	0.96	0.11	58,58,58,58	0
56	MG	1a	1656	1/1	0.96	0.20	40,40,40,40	0
56	MG	1a	1634	1/1	0.96	0.21	14,14,14,14	0
56	MG	1A	4178	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3025	1/1	0.96	0.35	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3165	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3606	1/1	0.96	0.15	54,54,54,54	0
56	MG	2A	3778	1/1	0.96	0.16	53,53,53,53	0
56	MG	2a	3041	1/1	0.96	0.34	43,43,43,43	0
56	MG	2A	3732	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3305	1/1	0.96	0.24	35,35,35,35	0
56	MG	1A	3389	1/1	0.96	0.35	43,43,43,43	0
56	MG	1A	3637	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3095	1/1	0.96	0.27	47,47,47,47	0
56	MG	1A	4160	1/1	0.96	0.16	72,72,72,72	0
59	ZN	1Y	501	1/1	0.96	0.11	79,79,79,79	0
56	MG	2a	3015	1/1	0.96	0.13	63,63,63,63	0
56	MG	1A	3750	1/1	0.96	0.15	45,45,45,45	0
56	MG	1a	1831	1/1	0.96	0.18	29,29,29,29	0
56	MG	1A	3743	1/1	0.96	0.25	43,43,43,43	0
56	MG	1A	3381	1/1	0.96	0.26	38,38,38,38	0
56	MG	1A	3009	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	1738	1/1	0.96	0.09	51,51,51,51	0
56	MG	2a	3067	1/1	0.96	0.05	62,62,62,62	0
56	MG	2A	3130	1/1	0.96	0.20	47,47,47,47	0
56	MG	2a	3172	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3107	1/1	0.96	0.56	47,47,47,47	0
56	MG	2A	3096	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3804	1/1	0.96	0.22	74,74,74,74	0
56	MG	1a	1655	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3819	1/1	0.96	0.15	58,58,58,58	0
56	MG	2a	3040	1/1	0.96	0.25	44,44,44,44	0
56	MG	1A	3003	1/1	0.96	0.20	30,30,30,30	0
56	MG	2X	102	1/1	0.96	0.23	66,66,66,66	0
56	MG	2A	3607	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3698	1/1	0.96	0.21	48,48,48,48	0
56	MG	2A	3664	1/1	0.96	0.13	62,62,62,62	0
56	MG	1A	3043	1/1	0.96	0.28	34,34,34,34	0
56	MG	2A	3083	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3015	1/1	0.96	0.14	30,30,30,30	0
56	MG	1Q	202	1/1	0.96	0.34	35,35,35,35	0
56	MG	1a	1606	1/1	0.96	0.09	68,68,68,68	0
56	MG	2A	3094	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3907	1/1	0.96	0.12	38,38,38,38	0
56	MG	2a	3119	1/1	0.96	0.30	63,63,63,63	0
56	MG	2a	3130	1/1	0.96	0.14	67,67,67,67	0
56	MG	1A	3221	1/1	0.96	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	18	102	1/1	0.96	0.27	45,45,45,45	0
56	MG	2A	3386	1/1	0.96	0.55	68,68,68,68	0
56	MG	2A	3666	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3866	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	4247	1/1	0.96	0.15	34,34,34,34	0
56	MG	1A	3772	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	4020	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	3869	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3623	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3175	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3461	1/1	0.96	0.38	45,45,45,45	0
56	MG	2a	3161	1/1	0.96	0.08	70,70,70,70	0
56	MG	1F	310	1/1	0.96	0.53	66,66,66,66	0
56	MG	2A	3428	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3213	1/1	0.96	0.44	53,53,53,53	0
56	MG	1A	3775	1/1	0.96	0.28	30,30,30,30	0
56	MG	1A	3174	1/1	0.97	0.40	47,47,47,47	0
56	MG	2A	3353	1/1	0.97	0.42	73,73,73,73	0
56	MG	1A	4039	1/1	0.97	0.14	51,51,51,51	0
56	MG	2A	3673	1/1	0.97	0.17	33,33,33,33	0
56	MG	2A	3608	1/1	0.97	0.09	57,57,57,57	0
56	MG	1w	102	1/1	0.97	0.22	77,77,77,77	0
56	MG	1a	1727	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3880	1/1	0.97	0.21	32,32,32,32	0
56	MG	2a	3228	1/1	0.97	0.29	66,66,66,66	0
56	MG	1Z	303	1/1	0.97	0.14	62,62,62,62	0
56	MG	2A	3575	1/1	0.97	0.06	45,45,45,45	0
56	MG	1U	205	1/1	0.97	0.34	42,42,42,42	0
56	MG	1a	1828	1/1	0.97	0.14	67,67,67,67	0
56	MG	1A	3179	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3311	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3689	1/1	0.97	0.34	30,30,30,30	0
56	MG	1A	4225	1/1	0.97	0.35	35,35,35,35	0
56	MG	1A	3991	1/1	0.97	0.45	53,53,53,53	0
56	MG	1A	3697	1/1	0.97	0.24	34,34,34,34	0
56	MG	1A	3048	1/1	0.97	0.15	34,34,34,34	0
56	MG	2A	3562	1/1	0.97	0.16	23,23,23,23	0
56	MG	1B	201	1/1	0.97	0.11	24,24,24,24	0
56	MG	16	103	1/1	0.97	0.10	53,53,53,53	0
56	MG	2A	3729	1/1	0.97	0.10	48,48,48,48	0
56	MG	1W	3003	1/1	0.97	0.53	45,45,45,45	0
56	MG	2A	3464	1/1	0.97	0.04	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3150	1/1	0.97	0.19	43,43,43,43	0
56	MG	2A	3015	1/1	0.97	0.13	34,34,34,34	0
56	MG	2A	3700	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3760	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3298	1/1	0.97	0.24	49,49,49,49	0
56	MG	2A	3075	1/1	0.97	0.33	46,46,46,46	0
56	MG	1A	4044	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3588	1/1	0.97	0.26	36,36,36,36	0
56	MG	1A	3178	1/1	0.97	0.16	18,18,18,18	0
56	MG	1A	3145	1/1	0.97	0.42	45,45,45,45	0
56	MG	1A	3654	1/1	0.97	0.28	52,52,52,52	0
56	MG	1A	4055	1/1	0.97	0.12	47,47,47,47	0
56	MG	2A	3497	1/1	0.97	0.45	58,58,58,58	0
56	MG	1A	3907	1/1	0.97	0.27	35,35,35,35	0
56	MG	1A	3161	1/1	0.97	0.21	46,46,46,46	0
56	MG	2a	3122	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3914	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3641	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3764	1/1	0.97	0.10	40,40,40,40	0
56	MG	2B	3010	1/1	0.97	0.12	59,59,59,59	0
56	MG	2A	3786	1/1	0.97	0.05	42,42,42,42	0
56	MG	1a	1823	1/1	0.97	0.21	51,51,51,51	0
56	MG	1A	3784	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3039	1/1	0.97	0.52	33,33,33,33	0
56	MG	2A	3624	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3882	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	4214	1/1	0.97	0.21	47,47,47,47	0
56	MG	1a	1699	1/1	0.97	0.33	38,38,38,38	0
56	MG	1Y	502	1/1	0.97	0.08	50,50,50,50	0
56	MG	1P	201	1/1	0.97	0.56	34,34,34,34	0
56	MG	2A	3763	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3284	1/1	0.97	0.34	40,40,40,40	0
56	MG	1A	4155	1/1	0.97	0.15	19,19,19,19	0
56	MG	1B	218	1/1	0.97	0.28	22,22,22,22	0
56	MG	1A	4224	1/1	0.97	0.41	49,49,49,49	0
56	MG	2A	3535	1/1	0.97	0.20	37,37,37,37	0
56	MG	1e	3001	1/1	0.97	0.14	61,61,61,61	0
56	MG	2A	3099	1/1	0.97	0.29	44,44,44,44	0
56	MG	2A	3267	1/1	0.97	0.12	56,56,56,56	0
56	MG	1A	4049	1/1	0.97	0.13	63,63,63,63	0
56	MG	1A	3727	1/1	0.97	0.12	26,26,26,26	0
56	MG	2A	3601	1/1	0.97	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1y	3001	1/1	0.97	0.60	42,42,42,42	0
56	MG	1d	502	1/1	0.97	0.34	55,55,55,55	0
56	MG	2F	301	1/1	0.97	0.21	44,44,44,44	0
56	MG	1B	235	1/1	0.97	0.12	52,52,52,52	0
56	MG	2A	3034	1/1	0.97	0.16	41,41,41,41	0
56	MG	1U	202	1/1	0.97	0.43	35,35,35,35	0
57	CPT	1A	4209	4/5	0.97	0.21	75,78,104,121	4
56	MG	1A	3166	1/1	0.97	0.64	42,42,42,42	0
56	MG	1E	311	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3709	1/1	0.97	0.06	59,59,59,59	0
56	MG	1B	217	1/1	0.97	0.08	28,28,28,28	0
56	MG	2a	3218	1/1	0.97	0.09	49,49,49,49	0
56	MG	2A	3187	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3462	1/1	0.97	0.25	42,42,42,42	0
56	MG	2V	201	1/1	0.97	0.13	50,50,50,50	0
56	MG	1A	3824	1/1	0.97	0.09	65,65,65,65	0
56	MG	1A	3509	1/1	0.97	0.25	38,38,38,38	0
56	MG	1A	3531	1/1	0.97	0.28	34,34,34,34	0
56	MG	1A	4249	1/1	0.97	0.29	46,46,46,46	0
56	MG	1B	206	1/1	0.97	0.37	51,51,51,51	0
56	MG	1a	1923	1/1	0.97	0.15	69,69,69,69	0
56	MG	2O	8001	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3734	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	4134	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3047	1/1	0.97	0.13	30,30,30,30	0
56	MG	2A	3787	1/1	0.97	0.04	51,51,51,51	0
56	MG	1A	3927	1/1	0.97	0.07	65,65,65,65	0
56	MG	2A	3884	1/1	0.97	0.29	32,32,32,32	0
56	MG	2A	3477	1/1	0.97	0.36	44,44,44,44	0
56	MG	2l	3003	1/1	0.97	0.12	68,68,68,68	0
56	MG	1D	306	1/1	0.97	0.23	35,35,35,35	0
56	MG	2A	3199	1/1	0.97	0.44	55,55,55,55	0
56	MG	1A	3835	1/1	0.97	0.20	37,37,37,37	0
56	MG	2A	3716	1/1	0.97	0.14	29,29,29,29	0
56	MG	2A	3010	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3584	1/1	0.97	0.26	57,57,57,57	0
56	MG	1B	224	1/1	0.97	0.16	76,76,76,76	0
56	MG	1A	3868	1/1	0.97	0.18	38,38,38,38	0
56	MG	1a	1686	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3462	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3786	1/1	0.97	0.21	48,48,48,48	0
56	MG	2A	3880	1/1	0.97	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3806	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3708	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3259	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	4107	1/1	0.97	0.09	36,36,36,36	0
56	MG	2A	3468	1/1	0.97	0.35	62,62,62,62	0
56	MG	2A	3494	1/1	0.97	0.17	59,59,59,59	0
56	MG	1A	3064	1/1	0.97	0.11	37,37,37,37	0
56	MG	2A	3556	1/1	0.97	0.12	59,59,59,59	0
56	MG	1A	3702	1/1	0.97	0.15	56,56,56,56	0
56	MG	1a	1702	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3745	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3773	1/1	0.97	0.13	54,54,54,54	0
56	MG	2A	3351	1/1	0.97	0.29	48,48,48,48	0
56	MG	1a	1653	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3453	1/1	0.97	0.25	42,42,42,42	0
56	MG	2A	3430	1/1	0.97	0.34	57,57,57,57	0
56	MG	2A	3630	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	3439	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3740	1/1	0.97	0.09	42,42,42,42	0
56	MG	2A	3833	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3796	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3008	1/1	0.97	0.20	26,26,26,26	0
56	MG	2A	3776	1/1	0.97	0.20	33,33,33,33	0
56	MG	2A	3887	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3675	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3450	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	4167	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3647	1/1	0.97	0.25	39,39,39,39	0
56	MG	2A	3728	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3164	1/1	0.97	0.50	43,43,43,43	0
56	MG	1A	4122	1/1	0.97	0.12	48,48,48,48	0
56	MG	1a	1698	1/1	0.97	0.17	36,36,36,36	0
56	MG	1a	1908	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3149	1/1	0.97	0.26	35,35,35,35	0
56	MG	2A	3079	1/1	0.97	0.15	47,47,47,47	0
56	MG	1a	1903	1/1	0.97	0.16	49,49,49,49	0
56	MG	2A	3337	1/1	0.97	0.15	53,53,53,53	0
56	MG	2a	3118	1/1	0.97	0.15	70,70,70,70	0
56	MG	1A	3771	1/1	0.97	0.17	25,25,25,25	0
56	MG	2A	3570	1/1	0.97	0.10	41,41,41,41	0
56	MG	2a	3190	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3758	1/1	0.97	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1y	3002	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3605	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3154	1/1	0.97	0.23	49,49,49,49	0
56	MG	1A	3963	1/1	0.97	0.41	38,38,38,38	0
56	MG	2X	101	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	4060	1/1	0.97	0.09	52,52,52,52	0
56	MG	2A	3678	1/1	0.97	0.11	29,29,29,29	0
56	MG	2A	3625	1/1	0.97	0.12	53,53,53,53	0
56	MG	2a	3215	1/1	0.97	0.18	69,69,69,69	0
56	MG	2a	3012	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3556	1/1	0.97	0.53	45,45,45,45	0
56	MG	1A	4252	1/1	0.97	0.29	24,24,24,24	0
56	MG	1A	3564	1/1	0.97	0.35	40,40,40,40	0
56	MG	1A	3561	1/1	0.97	0.72	42,42,42,42	0
56	MG	1A	3168	1/1	0.97	0.27	36,36,36,36	0
56	MG	1A	3748	1/1	0.97	0.13	56,56,56,56	0
56	MG	1A	4238	1/1	0.97	0.45	39,39,39,39	0
56	MG	1A	3769	1/1	0.97	0.23	27,27,27,27	0
56	MG	1A	3323	1/1	0.97	0.23	43,43,43,43	0
56	MG	28	102	1/1	0.97	0.16	55,55,55,55	0
56	MG	1A	3534	1/1	0.97	0.25	19,19,19,19	0
56	MG	1a	1819	1/1	0.97	0.12	46,46,46,46	0
56	MG	2A	3614	1/1	0.97	0.17	54,54,54,54	0
56	MG	2A	3538	1/1	0.97	0.15	48,48,48,48	0
56	MG	2a	3171	1/1	0.97	0.10	71,71,71,71	0
57	CPT	2I	201	4/5	0.97	0.13	67,68,96,140	4
56	MG	1V	202	1/1	0.97	0.18	65,65,65,65	0
56	MG	2a	3101	1/1	0.97	0.23	40,40,40,40	0
56	MG	2A	3144	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3162	1/1	0.97	0.79	40,40,40,40	0
56	MG	2A	3517	1/1	0.97	0.10	28,28,28,28	0
56	MG	1A	4176	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3068	1/1	0.97	0.08	55,55,55,55	0
56	MG	2A	3407	1/1	0.97	0.14	62,62,62,62	0
56	MG	1D	302	1/1	0.97	0.42	44,44,44,44	0
56	MG	1A	3261	1/1	0.97	0.08	56,56,56,56	0
56	MG	10	107	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3268	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3525	1/1	0.97	0.48	47,47,47,47	0
56	MG	1A	3789	1/1	0.97	0.29	39,39,39,39	0
56	MG	1A	3177	1/1	0.97	0.12	42,42,42,42	0
56	MG	1a	1610	1/1	0.97	0.45	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3195	1/1	0.97	0.61	39,39,39,39	0
56	MG	2a	3217	1/1	0.97	0.27	45,45,45,45	0
56	MG	1A	4026	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3023	1/1	0.98	0.29	46,46,46,46	0
56	MG	1a	1651	1/1	0.98	0.23	39,39,39,39	0
56	MG	1a	1613	1/1	0.98	0.17	18,18,18,18	0
56	MG	1A	4025	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3737	1/1	0.98	0.11	58,58,58,58	0
56	MG	1A	3035	1/1	0.98	0.08	54,54,54,54	0
56	MG	2A	3818	1/1	0.98	0.08	55,55,55,55	0
57	CPT	2A	3903	4/5	0.98	0.13	70,73,87,100	4
56	MG	2A	3071	1/1	0.98	0.28	31,31,31,31	0
56	MG	1a	1616	1/1	0.98	0.14	36,36,36,36	0
56	MG	1a	1862	1/1	0.98	0.10	49,49,49,49	0
56	MG	2v	101	1/1	0.98	0.27	55,55,55,55	0
56	MG	1A	3701	1/1	0.98	0.13	31,31,31,31	0
56	MG	1A	3994	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3283	1/1	0.98	0.27	42,42,42,42	0
56	MG	1a	1736	1/1	0.98	0.23	44,44,44,44	0
56	MG	1A	3307	1/1	0.98	0.16	53,53,53,53	0
60	SF4	2d	501	8/8	0.98	0.12	58,66,75,87	0
56	MG	1B	216	1/1	0.98	0.14	37,37,37,37	0
56	MG	2a	3087	1/1	0.98	0.11	64,64,64,64	0
56	MG	1A	3249	1/1	0.98	0.20	44,44,44,44	0
56	MG	2P	202	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3060	1/1	0.98	0.16	50,50,50,50	0
56	MG	1A	3070	1/1	0.98	0.20	25,25,25,25	0
56	MG	2A	3749	1/1	0.98	0.11	49,49,49,49	0
56	MG	1b	3001	1/1	0.98	0.07	62,62,62,62	0
56	MG	2A	3914	1/1	0.98	0.49	38,38,38,38	0
56	MG	1A	3977	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3180	1/1	0.98	0.18	22,22,22,22	0
56	MG	19	103	1/1	0.98	0.16	41,41,41,41	0
56	MG	1A	4200	1/1	0.98	0.06	55,55,55,55	0
56	MG	2A	3867	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	4030	1/1	0.98	0.07	29,29,29,29	0
56	MG	2A	3526	1/1	0.98	0.10	48,48,48,48	0
57	CPT	1I	3002	4/5	0.98	0.11	70,77,97,175	0
56	MG	1A	3271	1/1	0.98	0.31	47,47,47,47	0
56	MG	2A	3278	1/1	0.98	0.14	57,57,57,57	0
56	MG	1A	3289	1/1	0.98	0.41	59,59,59,59	0
56	MG	2A	3632	1/1	0.98	0.20	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3524	1/1	0.98	0.39	43,43,43,43	0
56	MG	1A	3700	1/1	0.98	0.07	55,55,55,55	0
56	MG	2A	3791	1/1	0.98	0.10	46,46,46,46	0
56	MG	2A	3434	1/1	0.98	0.32	46,46,46,46	0
56	MG	1A	3072	1/1	0.98	0.18	15,15,15,15	0
56	MG	1A	3028	1/1	0.98	0.37	28,28,28,28	0
56	MG	1B	214	1/1	0.98	0.14	46,46,46,46	0
56	MG	1A	3711	1/1	0.98	0.19	51,51,51,51	0
56	MG	1A	3176	1/1	0.98	0.18	42,42,42,42	0
56	MG	1A	3965	1/1	0.98	0.16	45,45,45,45	0
56	MG	2a	3135	1/1	0.98	0.22	95,95,95,95	0
56	MG	1A	3191	1/1	0.98	0.54	48,48,48,48	0
56	MG	1B	232	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3037	1/1	0.98	0.18	33,33,33,33	0
56	MG	1a	1893	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3872	1/1	0.98	0.12	55,55,55,55	0
56	MG	1A	3897	1/1	0.98	0.41	44,44,44,44	0
56	MG	10	101	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3850	1/1	0.98	0.13	68,68,68,68	0
57	CPT	2a	3235	4/5	0.98	0.12	85,87,90,125	0
56	MG	2d	502	1/1	0.98	0.09	58,58,58,58	0
56	MG	2A	3597	1/1	0.98	0.09	28,28,28,28	0
56	MG	1a	1668	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3182	1/1	0.98	0.19	58,58,58,58	0
56	MG	2A	3438	1/1	0.98	0.35	44,44,44,44	0
56	MG	2A	3541	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3127	1/1	0.98	0.38	46,46,46,46	0
56	MG	1A	3146	1/1	0.98	0.25	32,32,32,32	0
56	MG	17	101	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	4144	1/1	0.98	0.18	34,34,34,34	0
56	MG	2A	3838	1/1	0.98	0.17	31,31,31,31	0
56	MG	1e	3002	1/1	0.98	0.53	65,65,65,65	0
56	MG	1A	4031	1/1	0.98	0.05	34,34,34,34	0
56	MG	2A	3690	1/1	0.98	0.06	43,43,43,43	0
56	MG	1Y	503	1/1	0.98	0.68	54,54,54,54	0
56	MG	1A	4233	1/1	0.98	0.32	47,47,47,47	0
56	MG	1A	3388	1/1	0.98	0.41	45,45,45,45	0
56	MG	2A	3453	1/1	0.98	0.24	53,53,53,53	0
56	MG	1A	4041	1/1	0.98	0.07	71,71,71,71	0
56	MG	1A	3142	1/1	0.98	0.21	22,22,22,22	0
56	MG	2A	3707	1/1	0.98	0.10	50,50,50,50	0
56	MG	1W	3004	1/1	0.98	0.28	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1786	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3031	1/1	0.98	0.17	27,27,27,27	0
56	MG	1A	3895	1/1	0.98	0.07	48,48,48,48	0
56	MG	1A	3852	1/1	0.98	0.18	48,48,48,48	0
56	MG	2A	3531	1/1	0.98	0.20	21,21,21,21	0
56	MG	1A	3905	1/1	0.98	0.12	27,27,27,27	0
56	MG	2A	3596	1/1	0.98	0.14	29,29,29,29	0
56	MG	1A	3086	1/1	0.98	0.39	56,56,56,56	0
59	ZN	15	103	1/1	0.98	0.17	46,46,46,46	0
56	MG	1A	3038	1/1	0.98	0.42	46,46,46,46	0
56	MG	2a	3042	1/1	0.98	0.10	81,81,81,81	0
56	MG	2A	3046	1/1	0.98	0.04	37,37,37,37	0
56	MG	2q	203	1/1	0.98	0.24	72,72,72,72	0
56	MG	2A	3148	1/1	0.98	0.15	45,45,45,45	0
56	MG	1A	3752	1/1	0.98	0.10	34,34,34,34	0
56	MG	1b	3002	1/1	0.98	0.06	65,65,65,65	0
56	MG	1A	3096	1/1	0.98	0.15	46,46,46,46	0
56	MG	1A	3901	1/1	0.98	0.13	60,60,60,60	0
56	MG	2A	3639	1/1	0.98	0.30	49,49,49,49	0
56	MG	1a	1657	1/1	0.98	0.19	48,48,48,48	0
56	MG	1a	1838	1/1	0.98	0.14	39,39,39,39	0
56	MG	2a	3079	1/1	0.98	0.13	40,40,40,40	0
56	MG	2A	3794	1/1	0.98	0.08	74,74,74,74	0
56	MG	1A	3037	1/1	0.98	0.19	21,21,21,21	0
56	MG	2f	3001	1/1	0.98	0.20	41,41,41,41	0
56	MG	2A	3299	1/1	0.98	0.13	58,58,58,58	0
56	MG	1X	104	1/1	0.98	0.50	48,48,48,48	0
56	MG	1A	4170	1/1	0.98	0.21	13,13,13,13	0
56	MG	1O	3004	1/1	0.98	0.21	54,54,54,54	0
56	MG	1A	3724	1/1	0.98	0.20	31,31,31,31	0
56	MG	2A	3590	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3973	1/1	0.98	0.16	41,41,41,41	0
56	MG	2A	3315	1/1	0.98	0.33	62,62,62,62	0
56	MG	1A	4143	1/1	0.98	0.20	36,36,36,36	0
56	MG	1a	1669	1/1	0.98	0.05	47,47,47,47	0
56	MG	2A	3432	1/1	0.98	0.17	38,38,38,38	0
56	MG	1A	3042	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	4187	1/1	0.98	0.17	28,28,28,28	0
56	MG	1D	307	1/1	0.98	0.21	25,25,25,25	0
56	MG	1A	4110	1/1	0.98	0.12	36,36,36,36	0
56	MG	2A	3197	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3021	1/1	0.98	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3894	1/1	0.99	0.20	34,34,34,34	0
59	ZN	25	102	1/1	0.99	0.13	61,61,61,61	0
56	MG	1A	3951	1/1	0.99	0.08	43,43,43,43	0
56	MG	1A	4245	1/1	0.99	0.19	46,46,46,46	0
56	MG	2A	3397	1/1	0.99	0.06	36,36,36,36	0
56	MG	2a	3097	1/1	0.99	0.24	48,48,48,48	0
59	ZN	1n	501	1/1	0.99	0.15	59,59,59,59	0
56	MG	2A	3016	1/1	0.99	0.12	52,52,52,52	0
56	MG	1w	105	1/1	0.99	0.11	58,58,58,58	0
56	MG	1A	3886	1/1	0.99	0.21	26,26,26,26	0
56	MG	1E	301	1/1	0.99	0.18	14,14,14,14	0
56	MG	1A	3823	1/1	0.99	0.18	28,28,28,28	0
56	MG	2A	3028	1/1	0.99	0.45	47,47,47,47	0
56	MG	1A	3229	1/1	0.99	0.17	47,47,47,47	0
60	SF4	1d	501	8/8	0.99	0.18	55,59,67,69	0
56	MG	1A	3815	1/1	0.99	0.13	44,44,44,44	0
56	MG	1A	4036	1/1	0.99	0.06	71,71,71,71	0
56	MG	2a	3153	1/1	0.99	0.13	43,43,43,43	0
56	MG	2A	3060	1/1	0.99	0.26	50,50,50,50	0
56	MG	1A	3280	1/1	0.99	0.21	29,29,29,29	0
56	MG	1A	3908	1/1	0.99	0.08	47,47,47,47	0
56	MG	1A	3203	1/1	0.99	0.15	38,38,38,38	0
56	MG	1A	3126	1/1	0.99	0.19	40,40,40,40	0
56	MG	1A	3892	1/1	0.99	0.06	60,60,60,60	0
56	MG	1A	4001	1/1	0.99	0.16	32,32,32,32	0
56	MG	1A	3813	1/1	0.99	0.18	34,34,34,34	0
56	MG	1A	3432	1/1	0.99	0.36	40,40,40,40	0
56	MG	2A	3027	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3847	1/1	0.99	0.15	30,30,30,30	0
56	MG	1A	4094	1/1	0.99	0.09	22,22,22,22	0
56	MG	1A	3309	1/1	0.99	0.43	47,47,47,47	0
56	MG	2A	3443	1/1	0.99	0.19	43,43,43,43	0
56	MG	1W	3006	1/1	0.99	0.13	35,35,35,35	0
56	MG	1A	3708	1/1	0.99	0.27	16,16,16,16	0
56	MG	1A	3099	1/1	0.99	0.27	57,57,57,57	0
56	MG	1A	4241	1/1	0.99	0.15	23,23,23,23	0
56	MG	15	104	1/1	0.99	0.30	42,42,42,42	0
56	MG	1A	3863	1/1	0.99	0.12	59,59,59,59	0
56	MG	2A	3234	1/1	0.99	0.14	62,62,62,62	0
56	MG	1A	3310	1/1	0.99	0.18	42,42,42,42	0
56	MG	2A	3691	1/1	0.99	0.16	66,66,66,66	0
56	MG	1A	4097	1/1	0.99	0.08	23,23,23,23	0

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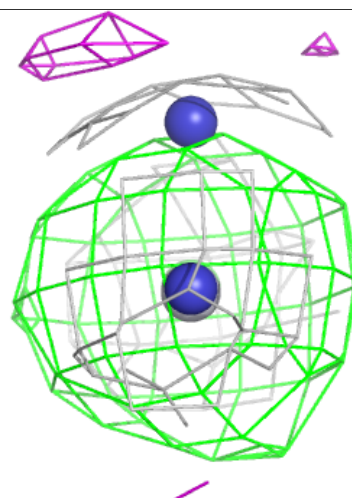
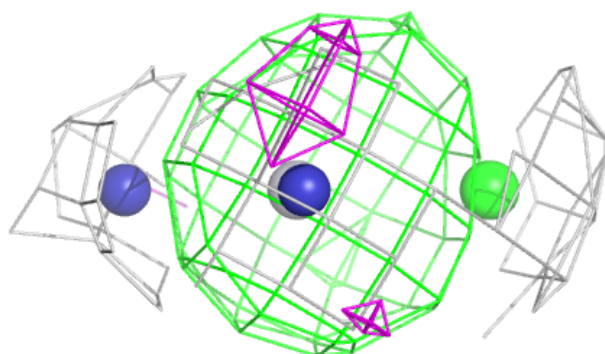
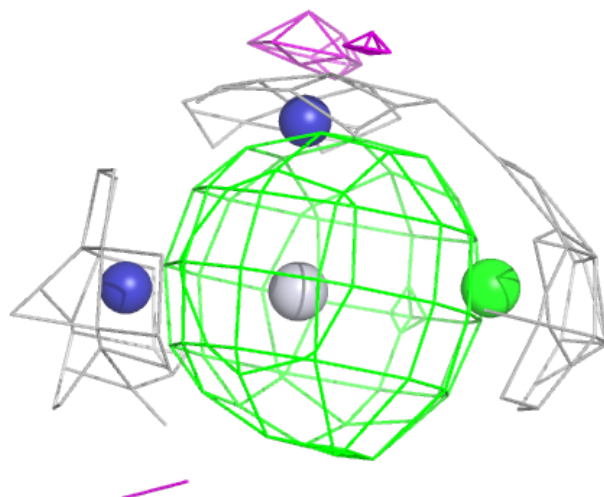
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3619	1/1	0.99	0.13	44,44,44,44	0
59	ZN	19	102	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3444	1/1	0.99	0.31	32,32,32,32	0
56	MG	2a	3114	1/1	0.99	0.10	69,69,69,69	0
56	MG	1A	3262	1/1	0.99	0.10	58,58,58,58	0
56	MG	2A	3141	1/1	0.99	0.24	35,35,35,35	0
56	MG	2A	3115	1/1	0.99	0.21	46,46,46,46	0
56	MG	2A	3437	1/1	0.99	0.24	45,45,45,45	0
56	MG	2A	3876	1/1	0.99	0.10	62,62,62,62	0
56	MG	1A	3845	1/1	0.99	0.20	25,25,25,25	0
56	MG	2A	3738	1/1	0.99	0.08	63,63,63,63	0
56	MG	1A	3876	1/1	0.99	0.22	48,48,48,48	0
59	ZN	16	101	1/1	1.00	0.16	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around CPT 1a 1930:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.