



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 2, 2020 – 08:46 am BST

PDB ID : 4V9Q
Title : Crystal Structure of Blasticidin S Bound to Thermus Thermophilus 70S Ribosome.
Authors : Svidritskiy, E.; Ling, C.; Ermolenko, D.N.; Korostelev, A.A.
Deposited on : 2013-06-12
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

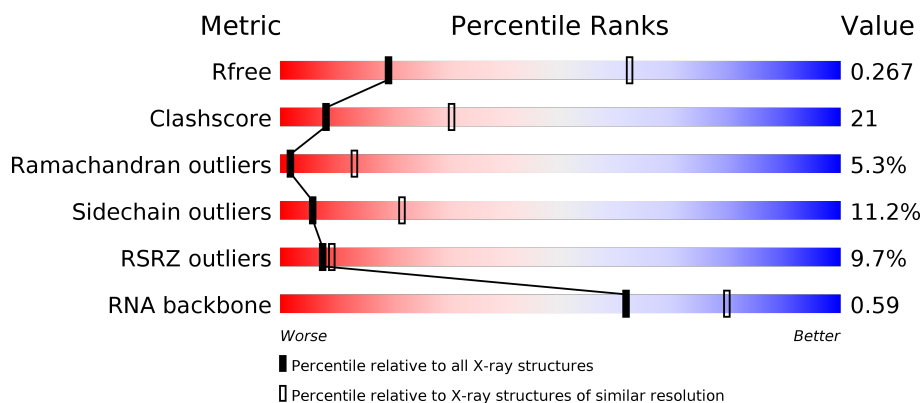
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



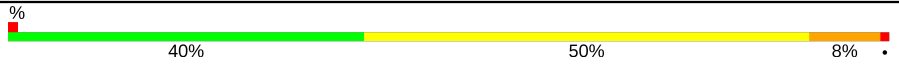
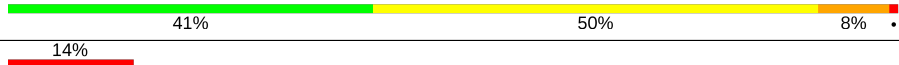

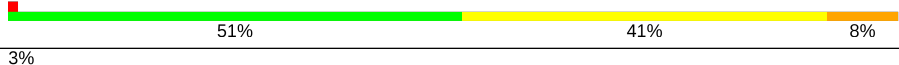
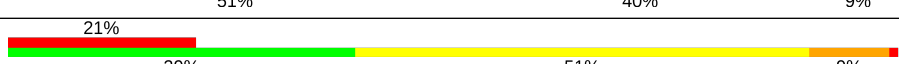
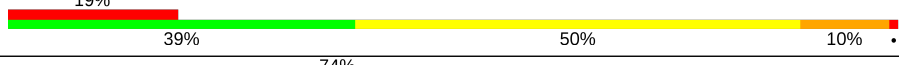



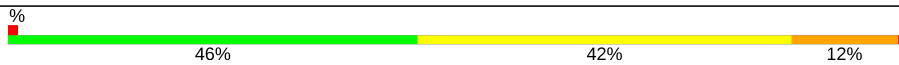

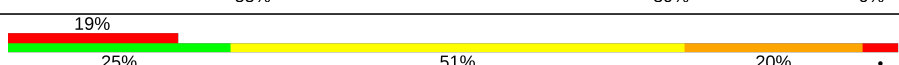
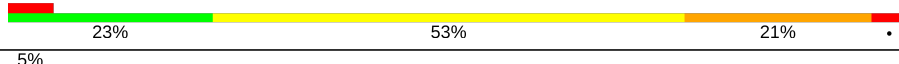
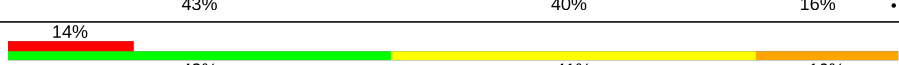
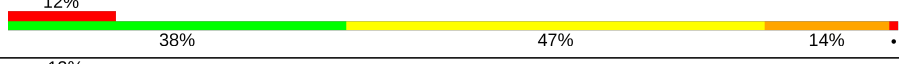
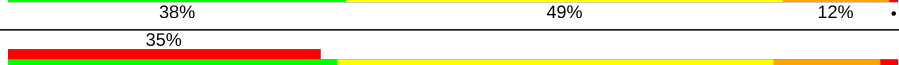




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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

Mol	Chain	Length	Quality of chain
1	AA	2879	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>10%</div> </div> </div>
1	CA	2879	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>39%</div> <div>10%</div> </div> </div>
2	AB	119	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>39%</div> <div>6%</div> </div> </div>
2	CB	119	<div> <div>0%</div> <div> <div></div> <div>52%</div> <div>42%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	271	
3	CD	271	
4	AE	204	
4	CE	204	
5	AF	202	
5	CF	202	
6	AG	181	
6	CG	181	
7	AH	159	
7	CH	159	
8	AI	145	
8	CI	145	
9	AJ	137	
9	CJ	137	
10	AK	122	
10	CK	122	
11	AL	146	
11	CL	146	
12	AM	134	
12	CM	134	
13	AN	117	
13	CN	117	
14	AO	98	
14	CO	98	
15	AP	137	

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Mol	Chain	Length	Quality of chain
15	CP	137	
16	AQ	117	
16	CQ	117	
17	AR	101	
17	CR	101	
18	AS	112	
18	CS	112	
19	AT	92	
19	CT	92	
20	AU	100	
20	CU	100	
21	AV	187	
21	CV	187	
22	AW	76	
22	CW	76	
23	AX	88	
23	CX	88	
24	AY	62	
24	CY	62	
25	AZ	59	
25	CZ	59	
26	A1	30	
26	C1	30	
27	A2	52	
27	C2	52	

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Mol	Chain	Length	Quality of chain
28	A3	44	
28	C3	44	
29	A4	48	
29	C4	48	
30	A5	63	
30	C5	63	
31	BA	1504	
31	DA	1504	
32	BB	234	
32	DB	234	
33	BC	206	
33	DC	206	
34	BD	208	
34	DD	208	
35	BE	151	
35	DE	151	
36	BF	101	
36	DF	101	
37	BG	155	
37	DG	155	
38	BH	138	
38	DH	138	
39	BI	127	
39	DI	127	
40	BJ	98	

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Mol	Chain	Length	Quality of chain
40	DJ	98	
41	BK	114	
41	DK	114	
42	BL	122	
42	DL	122	
43	BM	117	
43	DM	117	
44	BN	60	
44	DN	60	
45	BO	88	
45	DO	88	
46	BP	83	
46	DP	83	
47	BQ	99	
47	DQ	99	
48	BR	70	
48	DR	70	
49	BS	78	
49	DS	78	
50	BT	99	
50	DT	99	
51	BU	24	
51	DU	24	
52	BV	77	
52	BW	77	

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Mol	Chain	Length	Quality of chain
52	DV	77	
52	DW	77	
53	BX	5	
53	DX	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	4011	-	-	-	X
55	MG	AA	4017	-	-	-	X
55	MG	AA	4023	-	-	-	X
55	MG	AA	4025	-	-	-	X
55	MG	AA	4032	-	-	-	X
55	MG	AA	4035	-	-	-	X
55	MG	AA	4047	-	-	-	X
55	MG	AA	4054	-	-	-	X
55	MG	AA	4057	-	-	-	X
55	MG	AA	4067	-	-	-	X
55	MG	AA	4069	-	-	-	X
55	MG	AA	4074	-	-	-	X
55	MG	AA	4084	-	-	-	X
55	MG	AA	4086	-	-	-	X
55	MG	AA	4089	-	-	-	X
55	MG	AA	4096	-	-	-	X
55	MG	AA	4097	-	-	-	X
55	MG	AA	4099	-	-	-	X
55	MG	AA	4110	-	-	-	X
55	MG	AA	4113	-	-	-	X
55	MG	AA	4114	-	-	-	X
55	MG	AA	4120	-	-	-	X
55	MG	AA	4121	-	-	-	X
55	MG	AA	4123	-	-	-	X
55	MG	AA	4129	-	-	-	X
55	MG	AA	4130	-	-	-	X
55	MG	AA	4135	-	-	-	X
55	MG	AA	4150	-	-	-	X
55	MG	AA	4151	-	-	-	X
55	MG	AA	4159	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	4162	-	-	-	X
55	MG	AA	4169	-	-	-	X
55	MG	AA	4290	-	-	-	X
55	MG	AA	4293	-	-	-	X
55	MG	AA	4305	-	-	-	X
55	MG	AA	4310	-	-	-	X
55	MG	AA	4328	-	-	-	X
55	MG	AA	4342	-	-	-	X
55	MG	AA	4354	-	-	-	X
55	MG	AA	4355	-	-	-	X
55	MG	AA	4363	-	-	-	X
55	MG	AA	4375	-	-	-	X
55	MG	AA	4377	-	-	-	X
55	MG	AA	4391	-	-	-	X
55	MG	AA	4397	-	-	-	X
55	MG	AA	4421	-	-	-	X
55	MG	AA	4442	-	-	-	X
55	MG	AA	4447	-	-	-	X
55	MG	AA	4453	-	-	-	X
55	MG	AA	4473	-	-	-	X
55	MG	AA	4481	-	-	-	X
55	MG	AA	4499	-	-	-	X
55	MG	AA	4502	-	-	-	X
55	MG	AA	4510	-	-	-	X
55	MG	AA	4511	-	-	-	X
55	MG	AA	4514	-	-	-	X
55	MG	AA	4524	-	-	-	X
55	MG	AA	4529	-	-	-	X
55	MG	AA	4535	-	-	-	X
55	MG	AA	4539	-	-	-	X
55	MG	AA	4546	-	-	-	X
55	MG	AA	4549	-	-	-	X
55	MG	AA	4567	-	-	-	X
55	MG	AA	4584	-	-	-	X
55	MG	AA	4590	-	-	-	X
55	MG	AA	4593	-	-	-	X
55	MG	AA	4594	-	-	-	X
55	MG	AA	4606	-	-	-	X
55	MG	AA	4616	-	-	-	X
55	MG	AA	4625	-	-	-	X
55	MG	AA	4628	-	-	-	X
55	MG	AA	4635	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	4650	-	-	-	X
55	MG	AA	4653	-	-	-	X
55	MG	AA	4656	-	-	-	X
55	MG	AA	4664	-	-	-	X
55	MG	AA	4667	-	-	-	X
55	MG	AA	4678	-	-	-	X
55	MG	AA	4680	-	-	-	X
55	MG	AA	4684	-	-	-	X
55	MG	AA	4688	-	-	-	X
55	MG	AA	4696	-	-	-	X
55	MG	AA	4697	-	-	-	X
55	MG	AA	4702	-	-	-	X
55	MG	AA	4708	-	-	-	X
55	MG	AA	4715	-	-	-	X
55	MG	AA	4716	-	-	-	X
55	MG	AA	4723	-	-	-	X
55	MG	AA	4732	-	-	-	X
55	MG	AA	4737	-	-	-	X
55	MG	AA	4741	-	-	-	X
55	MG	AA	4749	-	-	-	X
55	MG	AA	4750	-	-	-	X
55	MG	AA	4755	-	-	-	X
55	MG	AA	4756	-	-	-	X
55	MG	AA	4759	-	-	-	X
55	MG	AA	4763	-	-	-	X
55	MG	AA	4767	-	-	-	X
55	MG	AA	4769	-	-	-	X
55	MG	AA	4770	-	-	-	X
55	MG	AA	4773	-	-	-	X
55	MG	AA	4779	-	-	-	X
55	MG	AA	4780	-	-	-	X
55	MG	AA	4788	-	-	-	X
55	MG	AA	4797	-	-	-	X
55	MG	AA	4798	-	-	-	X
55	MG	AA	4803	-	-	-	X
55	MG	AA	4804	-	-	-	X
55	MG	AA	4807	-	-	-	X
55	MG	AA	4809	-	-	-	X
55	MG	AA	4810	-	-	-	X
55	MG	AA	4818	-	-	-	X
55	MG	AA	4822	-	-	-	X
55	MG	AA	4826	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	4833	-	-	-	X
55	MG	AA	4835	-	-	-	X
55	MG	AA	4841	-	-	-	X
55	MG	AA	4842	-	-	-	X
55	MG	AA	4844	-	-	-	X
55	MG	AA	4865	-	-	-	X
55	MG	AA	4870	-	-	-	X
55	MG	AA	4874	-	-	-	X
55	MG	AA	4906	-	-	-	X
55	MG	AA	4918	-	-	-	X
55	MG	AA	4923	-	-	-	X
55	MG	AA	4945	-	-	-	X
55	MG	AA	4947	-	-	-	X
55	MG	AA	4958	-	-	-	X
55	MG	AA	4965	-	-	-	X
55	MG	AA	4972	-	-	-	X
55	MG	AA	4973	-	-	-	X
55	MG	AA	4979	-	-	-	X
55	MG	AA	4982	-	-	-	X
55	MG	AA	4986	-	-	-	X
55	MG	AA	4994	-	-	-	X
55	MG	AA	4997	-	-	-	X
55	MG	AA	5002	-	-	-	X
55	MG	AA	5010	-	-	-	X
55	MG	AA	5020	-	-	-	X
55	MG	AA	5023	-	-	-	X
55	MG	AA	5032	-	-	-	X
55	MG	AA	5037	-	-	-	X
55	MG	AA	5039	-	-	-	X
55	MG	AA	5044	-	-	-	X
55	MG	AA	5047	-	-	-	X
55	MG	AA	5059	-	-	-	X
55	MG	AA	5063	-	-	-	X
55	MG	AA	5075	-	-	-	X
55	MG	AA	5078	-	-	-	X
55	MG	AA	5086	-	-	-	X
55	MG	AA	5090	-	-	-	X
55	MG	AA	5100	-	-	-	X
55	MG	AA	5110	-	-	-	X
55	MG	AA	5117	-	-	-	X
55	MG	AA	5119	-	-	-	X
55	MG	AA	5137	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	5142	-	-	-	X
55	MG	AA	5143	-	-	-	X
55	MG	AA	5147	-	-	-	X
55	MG	AA	5154	-	-	-	X
55	MG	AA	5159	-	-	-	X
55	MG	AA	5160	-	-	-	X
55	MG	AA	5169	-	-	-	X
55	MG	AA	5177	-	-	-	X
55	MG	AA	5178	-	-	-	X
55	MG	AA	5179	-	-	-	X
55	MG	AA	5190	-	-	-	X
55	MG	AA	5200	-	-	-	X
55	MG	AA	5201	-	-	-	X
55	MG	AA	5202	-	-	-	X
55	MG	AA	5219	-	-	-	X
55	MG	AA	5223	-	-	-	X
55	MG	AA	5228	-	-	-	X
55	MG	AA	5229	-	-	-	X
55	MG	AA	5235	-	-	-	X
55	MG	AA	5236	-	-	-	X
55	MG	AA	5239	-	-	-	X
55	MG	AA	5240	-	-	-	X
55	MG	AA	5245	-	-	-	X
55	MG	AA	5247	-	-	-	X
55	MG	AA	5248	-	-	-	X
55	MG	AA	5249	-	-	-	X
55	MG	AA	5250	-	-	-	X
55	MG	AA	5251	-	-	-	X
55	MG	AA	5264	-	-	-	X
55	MG	AA	5265	-	-	-	X
55	MG	AA	5267	-	-	-	X
55	MG	AA	5268	-	-	-	X
55	MG	AA	5279	-	-	-	X
55	MG	AA	5292	-	-	-	X
55	MG	AA	5297	-	-	-	X
55	MG	AB	202	-	-	-	X
55	MG	AB	204	-	-	-	X
55	MG	AB	205	-	-	-	X
55	MG	AB	216	-	-	-	X
55	MG	AB	218	-	-	-	X
55	MG	AB	237	-	-	-	X
55	MG	AB	243	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AE	303	-	-	-	X
55	MG	AF	301	-	-	-	X
55	MG	AG	202	-	-	-	X
55	MG	AN	204	-	-	-	X
55	MG	AS	205	-	-	-	X
55	MG	BA	1604	-	-	-	X
55	MG	BA	1608	-	-	-	X
55	MG	BA	1610	-	-	-	X
55	MG	BA	1615	-	-	-	X
55	MG	BA	1624	-	-	-	X
55	MG	BA	1625	-	-	-	X
55	MG	BA	1626	-	-	-	X
55	MG	BA	1628	-	-	-	X
55	MG	BA	1634	-	-	-	X
55	MG	BA	1639	-	-	-	X
55	MG	BA	1641	-	-	-	X
55	MG	BA	1645	-	-	-	X
55	MG	BA	1647	-	-	-	X
55	MG	BA	1648	-	-	-	X
55	MG	BA	1649	-	-	-	X
55	MG	BA	1652	-	-	-	X
55	MG	BA	1653	-	-	-	X
55	MG	BA	1656	-	-	-	X
55	MG	BA	1659	-	-	-	X
55	MG	BA	1673	-	-	-	X
55	MG	BA	1680	-	-	-	X
55	MG	BA	1717	-	-	-	X
55	MG	BA	1724	-	-	-	X
55	MG	BA	1731	-	-	-	X
55	MG	BA	1739	-	-	-	X
55	MG	BA	1752	-	-	-	X
55	MG	BA	1761	-	-	-	X
55	MG	BA	1775	-	-	-	X
55	MG	BA	1781	-	-	-	X
55	MG	BA	1788	-	-	-	X
55	MG	BA	1792	-	-	-	X
55	MG	BA	1801	-	-	-	X
55	MG	BA	1803	-	-	-	X
55	MG	BA	1808	-	-	-	X
55	MG	BA	1810	-	-	-	X
55	MG	BA	1818	-	-	-	X
55	MG	BA	1827	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	1833	-	-	-	X
55	MG	BA	1840	-	-	-	X
55	MG	BA	1843	-	-	-	X
55	MG	BA	1852	-	-	-	X
55	MG	BA	1859	-	-	-	X
55	MG	BA	1863	-	-	-	X
55	MG	BA	1867	-	-	-	X
55	MG	BA	1875	-	-	-	X
55	MG	BA	1879	-	-	-	X
55	MG	BA	1898	-	-	-	X
55	MG	BA	1900	-	-	-	X
55	MG	BA	1901	-	-	-	X
55	MG	BA	1902	-	-	-	X
55	MG	BA	1904	-	-	-	X
55	MG	BA	1911	-	-	-	X
55	MG	BA	1913	-	-	-	X
55	MG	BA	1923	-	-	-	X
55	MG	BA	1925	-	-	-	X
55	MG	BA	1929	-	-	-	X
55	MG	BA	1931	-	-	-	X
55	MG	BA	1943	-	-	-	X
55	MG	BA	1945	-	-	-	X
55	MG	BA	1947	-	-	-	X
55	MG	BA	1949	-	-	-	X
55	MG	BA	1967	-	-	-	X
55	MG	BA	1972	-	-	-	X
55	MG	BA	1975	-	-	-	X
55	MG	BA	1992	-	-	-	X
55	MG	BA	2002	-	-	-	X
55	MG	BA	2008	-	-	-	X
55	MG	BA	2009	-	-	-	X
55	MG	BA	2010	-	-	-	X
55	MG	BA	2033	-	-	-	X
55	MG	BA	2046	-	-	-	X
55	MG	BA	2053	-	-	-	X
55	MG	BA	2057	-	-	-	X
55	MG	BA	2060	-	-	-	X
55	MG	BA	2082	-	-	-	X
55	MG	BA	2086	-	-	-	X
55	MG	BA	2093	-	-	-	X
55	MG	BA	2094	-	-	-	X
55	MG	BA	2097	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	2098	-	-	-	X
55	MG	BA	2099	-	-	-	X
55	MG	BA	2102	-	-	-	X
55	MG	BA	2103	-	-	-	X
55	MG	BA	2106	-	-	-	X
55	MG	BA	2109	-	-	-	X
55	MG	BA	2114	-	-	-	X
55	MG	BA	2123	-	-	-	X
55	MG	BA	2125	-	-	-	X
55	MG	BA	2126	-	-	-	X
55	MG	BA	2127	-	-	-	X
55	MG	BA	2129	-	-	-	X
55	MG	BA	2132	-	-	-	X
55	MG	BA	2133	-	-	-	X
55	MG	BA	2134	-	-	-	X
55	MG	BA	2137	-	-	-	X
55	MG	BA	2139	-	-	-	X
55	MG	BA	2140	-	-	-	X
55	MG	BA	2152	-	-	-	X
55	MG	BC	301	-	-	-	X
55	MG	BO	101	-	-	-	X
55	MG	BR	101	-	-	-	X
55	MG	BV	102	-	-	-	X
55	MG	BV	116	-	-	-	X
55	MG	BW	117	-	-	-	X
55	MG	BW	118	-	-	-	X
55	MG	C4	103	-	-	-	X
55	MG	CA	2902	-	-	-	X
55	MG	CA	2903	-	-	-	X
55	MG	CA	2907	-	-	-	X
55	MG	CA	2914	-	-	-	X
55	MG	CA	2919	-	-	-	X
55	MG	CA	2920	-	-	-	X
55	MG	CA	2926	-	-	-	X
55	MG	CA	2938	-	-	-	X
55	MG	CA	2941	-	-	-	X
55	MG	CA	2944	-	-	-	X
55	MG	CA	2950	-	-	-	X
55	MG	CA	2960	-	-	-	X
55	MG	CA	2972	-	-	-	X
55	MG	CA	2973	-	-	-	X
55	MG	CA	2977	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	2981	-	-	-	X
55	MG	CA	2984	-	-	-	X
55	MG	CA	2994	-	-	-	X
55	MG	CA	2996	-	-	-	X
55	MG	CA	3002	-	-	-	X
55	MG	CA	3004	-	-	-	X
55	MG	CA	3008	-	-	-	X
55	MG	CA	3010	-	-	-	X
55	MG	CA	3013	-	-	-	X
55	MG	CA	3022	-	-	-	X
55	MG	CA	3024	-	-	-	X
55	MG	CA	3054	-	-	-	X
55	MG	CA	3058	-	-	-	X
55	MG	CA	3059	-	-	-	X
55	MG	CA	3062	-	-	-	X
55	MG	CA	3065	-	-	-	X
55	MG	CA	3072	-	-	-	X
55	MG	CA	3075	-	-	-	X
55	MG	CA	3080	-	-	-	X
55	MG	CA	3082	-	-	-	X
55	MG	CA	3085	-	-	-	X
55	MG	CA	3090	-	-	-	X
55	MG	CA	3165	-	-	-	X
55	MG	CA	3166	-	-	-	X
55	MG	CA	3310	-	-	-	X
55	MG	CA	3321	-	-	-	X
55	MG	CA	3322	-	-	-	X
55	MG	CA	3326	-	-	-	X
55	MG	CA	3356	-	-	-	X
55	MG	CA	3382	-	-	-	X
55	MG	CA	3388	-	-	-	X
55	MG	CA	3399	-	-	-	X
55	MG	CA	3401	-	-	-	X
55	MG	CA	3435	-	-	-	X
55	MG	CA	3436	-	-	-	X
55	MG	CA	3450	-	-	-	X
55	MG	CA	3453	-	-	-	X
55	MG	CA	3455	-	-	-	X
55	MG	CA	3460	-	-	-	X
55	MG	CA	3462	-	-	-	X
55	MG	CA	3489	-	-	-	X
55	MG	CA	3493	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	3497	-	-	-	X
55	MG	CA	3499	-	-	-	X
55	MG	CA	3500	-	-	-	X
55	MG	CA	3517	-	-	-	X
55	MG	CA	3522	-	-	-	X
55	MG	CA	3525	-	-	-	X
55	MG	CA	3528	-	-	-	X
55	MG	CA	3532	-	-	-	X
55	MG	CA	3535	-	-	-	X
55	MG	CA	3540	-	-	-	X
55	MG	CA	3546	-	-	-	X
55	MG	CA	3551	-	-	-	X
55	MG	CA	3561	-	-	-	X
55	MG	CA	3583	-	-	-	X
55	MG	CA	3586	-	-	-	X
55	MG	CA	3593	-	-	-	X
55	MG	CA	3623	-	-	-	X
55	MG	CA	3626	-	-	-	X
55	MG	CA	3647	-	-	-	X
55	MG	CA	3649	-	-	-	X
55	MG	CA	3650	-	-	-	X
55	MG	CA	3653	-	-	-	X
55	MG	CA	3677	-	-	-	X
55	MG	CA	3686	-	-	-	X
55	MG	CA	3692	-	-	-	X
55	MG	CA	3706	-	-	-	X
55	MG	CA	3709	-	-	-	X
55	MG	CA	3713	-	-	-	X
55	MG	CA	3716	-	-	-	X
55	MG	CA	3718	-	-	-	X
55	MG	CA	3720	-	-	-	X
55	MG	CA	3727	-	-	-	X
55	MG	CA	3760	-	-	-	X
55	MG	CA	3764	-	-	-	X
55	MG	CA	3782	-	-	-	X
55	MG	CA	3786	-	-	-	X
55	MG	CA	3788	-	-	-	X
55	MG	CA	3789	-	-	-	X
55	MG	CA	3795	-	-	-	X
55	MG	CA	3797	-	-	-	X
55	MG	CA	3799	-	-	-	X
55	MG	CA	3800	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	3803	-	-	-	X
55	MG	CA	3804	-	-	-	X
55	MG	CA	3807	-	-	-	X
55	MG	CA	3824	-	-	-	X
55	MG	CA	3830	-	-	-	X
55	MG	CA	3844	-	-	-	X
55	MG	CA	3849	-	-	-	X
55	MG	CA	3857	-	-	-	X
55	MG	CA	3858	-	-	-	X
55	MG	CA	3859	-	-	-	X
55	MG	CA	3862	-	-	-	X
55	MG	CA	3864	-	-	-	X
55	MG	CA	3871	-	-	-	X
55	MG	CA	3877	-	-	-	X
55	MG	CA	3881	-	-	-	X
55	MG	CA	3883	-	-	-	X
55	MG	CA	3885	-	-	-	X
55	MG	CA	3888	-	-	-	X
55	MG	CA	3891	-	-	-	X
55	MG	CA	3892	-	-	-	X
55	MG	CA	3898	-	-	-	X
55	MG	CA	3915	-	-	-	X
55	MG	CA	3917	-	-	-	X
55	MG	CA	3920	-	-	-	X
55	MG	CA	3932	-	-	-	X
55	MG	CA	3935	-	-	-	X
55	MG	CA	3936	-	-	-	X
55	MG	CA	3938	-	-	-	X
55	MG	CA	3941	-	-	-	X
55	MG	CA	3942	-	-	-	X
55	MG	CA	3945	-	-	-	X
55	MG	CA	3948	-	-	-	X
55	MG	CA	3949	-	-	-	X
55	MG	CA	3958	-	-	-	X
55	MG	CA	3964	-	-	-	X
55	MG	CA	3986	-	-	-	X
55	MG	CA	3995	-	-	-	X
55	MG	CA	4004	-	-	-	X
55	MG	CA	4035	-	-	-	X
55	MG	CA	4041	-	-	-	X
55	MG	CA	4046	-	-	-	X
55	MG	CA	4050	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	4058	-	-	-	X
55	MG	CA	4063	-	-	-	X
55	MG	CA	4068	-	-	-	X
55	MG	CA	4070	-	-	-	X
55	MG	CA	4100	-	-	-	X
55	MG	CA	4102	-	-	-	X
55	MG	CA	4109	-	-	-	X
55	MG	CA	4117	-	-	-	X
55	MG	CA	4119	-	-	-	X
55	MG	CA	4122	-	-	-	X
55	MG	CA	4136	-	-	-	X
55	MG	CA	4137	-	-	-	X
55	MG	CA	4141	-	-	-	X
55	MG	CA	4144	-	-	-	X
55	MG	CA	4146	-	-	-	X
55	MG	CA	4147	-	-	-	X
55	MG	CA	4151	-	-	-	X
55	MG	CA	4157	-	-	-	X
55	MG	CA	4163	-	-	-	X
55	MG	CA	4183	-	-	-	X
55	MG	CA	4194	-	-	-	X
55	MG	CA	4195	-	-	-	X
55	MG	CA	4205	-	-	-	X
55	MG	CA	4209	-	-	-	X
55	MG	CA	4213	-	-	-	X
55	MG	CA	4221	-	-	-	X
55	MG	CA	4222	-	-	-	X
55	MG	CA	4228	-	-	-	X
55	MG	CA	4233	-	-	-	X
55	MG	CA	4235	-	-	-	X
55	MG	CA	4239	-	-	-	X
55	MG	CA	4248	-	-	-	X
55	MG	CA	4257	-	-	-	X
55	MG	CA	4263	-	-	-	X
55	MG	CA	4266	-	-	-	X
55	MG	CA	4273	-	-	-	X
55	MG	CA	4278	-	-	-	X
55	MG	CA	4280	-	-	-	X
55	MG	CA	4294	-	-	-	X
55	MG	CA	4300	-	-	-	X
55	MG	CA	4325	-	-	-	X
55	MG	CA	4326	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	4337	-	-	-	X
55	MG	CA	4339	-	-	-	X
55	MG	CA	4347	-	-	-	X
55	MG	CA	4348	-	-	-	X
55	MG	CA	4349	-	-	-	X
55	MG	CA	4352	-	-	-	X
55	MG	CA	4358	-	-	-	X
55	MG	CA	4359	-	-	-	X
55	MG	CA	4362	-	-	-	X
55	MG	CA	4367	-	-	-	X
55	MG	CA	4369	-	-	-	X
55	MG	CA	4373	-	-	-	X
55	MG	CA	4388	-	-	-	X
55	MG	CA	4394	-	-	-	X
55	MG	CA	4395	-	-	-	X
55	MG	CA	4404	-	-	-	X
55	MG	CB	212	-	-	-	X
55	MG	CB	237	-	-	-	X
55	MG	CB	257	-	-	-	X
55	MG	CB	262	-	-	-	X
55	MG	CD	306	-	-	-	X
55	MG	CF	303	-	-	-	X
55	MG	CQ	205	-	-	-	X
55	MG	CR	202	-	-	-	X
55	MG	CV	201	-	-	-	X
55	MG	CW	103	-	-	-	X
55	MG	CX	101	-	-	-	X
55	MG	DA	1602	-	-	-	X
55	MG	DA	1607	-	-	-	X
55	MG	DA	1611	-	-	-	X
55	MG	DA	1612	-	-	-	X
55	MG	DA	1619	-	-	-	X
55	MG	DA	1622	-	-	-	X
55	MG	DA	1626	-	-	-	X
55	MG	DA	1630	-	-	-	X
55	MG	DA	1638	-	-	-	X
55	MG	DA	1648	-	-	-	X
55	MG	DA	1649	-	-	-	X
55	MG	DA	1650	-	-	-	X
55	MG	DA	1651	-	-	-	X
55	MG	DA	1671	-	-	-	X
55	MG	DA	1672	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	1673	-	-	-	X
55	MG	DA	1676	-	-	-	X
55	MG	DA	1677	-	-	-	X
55	MG	DA	1678	-	-	-	X
55	MG	DA	1681	-	-	-	X
55	MG	DA	1682	-	-	-	X
55	MG	DA	1684	-	-	-	X
55	MG	DA	1690	-	-	-	X
55	MG	DA	1705	-	-	-	X
55	MG	DA	1717	-	-	-	X
55	MG	DA	1748	-	-	-	X
55	MG	DA	1752	-	-	-	X
55	MG	DA	1761	-	-	-	X
55	MG	DA	1763	-	-	-	X
55	MG	DA	1794	-	-	-	X
55	MG	DA	1795	-	-	-	X
55	MG	DA	1811	-	-	-	X
55	MG	DA	1818	-	-	-	X
55	MG	DA	1826	-	-	-	X
55	MG	DA	1841	-	-	-	X
55	MG	DA	1845	-	-	-	X
55	MG	DA	1863	-	-	-	X
55	MG	DA	1865	-	-	-	X
55	MG	DA	1872	-	-	-	X
55	MG	DA	1896	-	-	-	X
55	MG	DA	1898	-	-	-	X
55	MG	DA	1901	-	-	-	X
55	MG	DA	1907	-	-	-	X
55	MG	DA	1910	-	-	-	X
55	MG	DA	1913	-	-	-	X
55	MG	DA	1916	-	-	-	X
55	MG	DA	1921	-	-	-	X
55	MG	DA	1924	-	-	-	X
55	MG	DA	1928	-	-	-	X
55	MG	DA	1932	-	-	-	X
55	MG	DA	1933	-	-	-	X
55	MG	DA	1935	-	-	-	X
55	MG	DA	1937	-	-	-	X
55	MG	DA	1939	-	-	-	X
55	MG	DA	1949	-	-	-	X
55	MG	DA	1951	-	-	-	X
55	MG	DA	1952	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	1967	-	-	-	X
55	MG	DA	1973	-	-	-	X
55	MG	DA	1991	-	-	-	X
55	MG	DA	1995	-	-	-	X
55	MG	DA	1999	-	-	-	X
55	MG	DA	2028	-	-	-	X
55	MG	DA	2037	-	-	-	X
55	MG	DA	2051	-	-	-	X
55	MG	DA	2055	-	-	-	X
55	MG	DA	2066	-	-	-	X
55	MG	DA	2067	-	-	-	X
55	MG	DA	2069	-	-	-	X
55	MG	DA	2083	-	-	-	X
55	MG	DA	2087	-	-	-	X
55	MG	DA	2099	-	-	-	X
55	MG	DA	2117	-	-	-	X
55	MG	DA	2121	-	-	-	X
55	MG	DA	2123	-	-	-	X
55	MG	DA	2125	-	-	-	X
55	MG	DA	2127	-	-	-	X
55	MG	DA	2144	-	-	-	X
55	MG	DA	2150	-	-	-	X
55	MG	DA	2153	-	-	-	X
55	MG	DA	2169	-	-	-	X
55	MG	DA	2172	-	-	-	X
55	MG	DA	2180	-	-	-	X
55	MG	DA	2181	-	-	-	X
55	MG	DA	2184	-	-	-	X
55	MG	DA	2191	-	-	-	X
55	MG	DA	2192	-	-	-	X
55	MG	DA	2195	-	-	-	X
55	MG	DA	2198	-	-	-	X
55	MG	DA	2200	-	-	-	X
55	MG	DH	202	-	-	-	X
55	MG	DI	201	-	-	-	X
55	MG	DL	202	-	-	-	X
55	MG	DO	102	-	-	-	X

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 293113 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	AA	2832	Total	C	N	O	P	0	0	0
			60991	27143	11396	19620	2832			
1	CA	2832	Total	C	N	O	P	0	0	0
			60991	27143	11396	19620	2832			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	276	C	A	CONFLICT	GB AE017221.1
AA	277	A	C	CONFLICT	GB AE017221.1
AA	1142	U	C	CONFLICT	GB AE017221.1
AA	2825	U	G	CONFLICT	GB AE017221.1
CA	276	C	A	CONFLICT	GB AE017221.1
CA	277	A	C	CONFLICT	GB AE017221.1
CA	1142	U	C	CONFLICT	GB AE017221.1
CA	2825	U	G	CONFLICT	GB AE017221.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	119	Total	C	N	O	P	0	0	0
			2555	1136	471	829	119			
2	CB	119	Total	C	N	O	P	0	0	0
			2555	1136	471	829	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
3	CD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
4	CE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
5	CF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
6	CG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
7	CH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
8	CI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
9	CJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
10	CK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
11	CL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			
12	CM	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	117	Total	C	N	O		0	0	0
			960	599	202	159				
13	CN	117	Total	C	N	O		0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	98	Total	C	N	O		0	0	0
			771	486	154	131				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	CO	98	Total	C	N	O	0	0	0
			771	486	154	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			
15	CP	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	CQ	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	CR	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
18	CS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			726	471	131	124			
19	CT	92	Total	C	N	O	0	0	0
			726	471	131	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
20	CU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			
21	CV	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
22	CW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	AX	88	Total	C	N	O	0	0	0
			695	435	141	119			
23	CX	88	Total	C	N	O	0	0	0
			695	435	141	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
24	CY	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
25	CZ	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
26	C1	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
27	C2	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
28	C3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
29	C4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	C5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1504	Total	C	N	O	P	0	0	0
			32336	14391	5994	10447	1504			
31	DA	1504	Total	C	N	O	P	0	0	0
			32336	14391	5994	10447	1504			

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
32	DB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
33	DC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	DD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
35	DE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	DF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	DG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	DH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
39	DI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
40	DJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			
41	DK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			
42	DL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
43	DM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BM	118	ALA	-	EXPRESSION TAG	UNP P62655

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
44	DN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	DO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
46	DP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			
47	DQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BR	70	Total	C	N	O		0	0	0
			574	367	112	95				
48	DR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
49	DS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
50	DT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BU	24	Total	C	N	O		0	0	0
			209	128	50	31				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	DU	24	Total	C	N	O	0	0	0
			209	128	50	31			

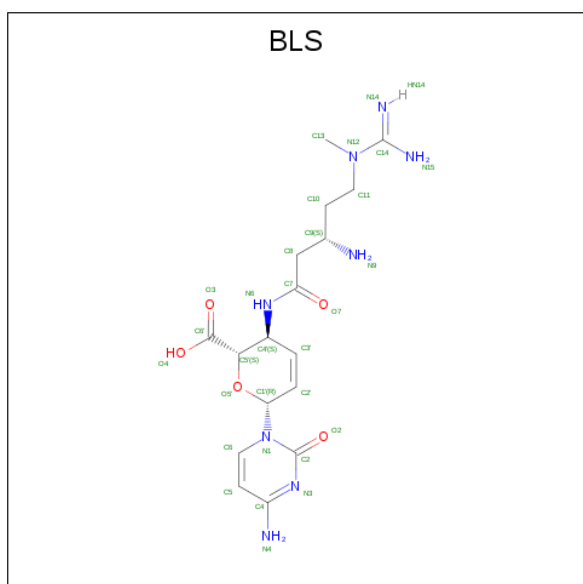
- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
52	BW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
52	DV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
52	DW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BX	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	DX	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is BLASTICIDIN S (three-letter code: BLS) (formula: C₁₇H₂₆N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
54	AA	1	Total	C	N	O	0	0
			30	17	8	5		
54	CA	1	Total	C	N	O	0	0
			30	17	8	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AP	2	Total	Mg	0	0
			2	2		
55	DX	1	Total	Mg	0	0
			1	1		
55	BA	570	Total	Mg	0	0
			570	570		
55	AK	2	Total	Mg	0	0
			2	2		
55	DQ	1	Total	Mg	0	0
			1	1		
55	C5	3	Total	Mg	0	0
			3	3		
55	AB	50	Total	Mg	0	0
			50	50		
55	BL	2	Total	Mg	0	0
			2	2		
55	CV	4	Total	Mg	0	0
			4	4		
55	C3	2	Total	Mg	0	0
			2	2		
55	BE	5	Total	Mg	0	0
			5	5		
55	CR	2	Total	Mg	0	0
			2	2		
55	AN	4	Total	Mg	0	0
			4	4		
55	BP	1	Total	Mg	0	0
			1	1		
55	AX	6	Total	Mg	0	0
			6	6		
55	CN	3	Total	Mg	0	0
			3	3		
55	DR	2	Total	Mg	0	0
			2	2		
55	BI	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AS	6	Total 6	Mg 6	0	0
55	CA	1504	Total 1504	Mg 1504	0	0
55	BB	2	Total 2	Mg 2	0	0
55	AJ	1	Total 1	Mg 1	0	0
55	BT	1	Total 1	Mg 1	0	0
55	C4	4	Total 4	Mg 4	0	0
55	AE	4	Total 4	Mg 4	0	0
55	DG	1	Total 1	Mg 1	0	0
55	CF	7	Total 7	Mg 7	0	0
55	DT	1	Total 1	Mg 1	0	0
55	DL	2	Total 2	Mg 2	0	0
55	AV	2	Total 2	Mg 2	0	0
55	CY	2	Total 2	Mg 2	0	0
55	AA	1296	Total 1296	Mg 1296	0	0
55	BQ	2	Total 2	Mg 2	0	0
55	CQ	5	Total 5	Mg 5	0	0
55	A5	2	Total 2	Mg 2	0	0
55	AR	5	Total 5	Mg 5	0	0
55	DV	24	Total 24	Mg 24	0	0
55	DM	1	Total 1	Mg 1	0	0
55	BC	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AM	3	Total 3	Mg 3	0	0
55	BU	1	Total 1	Mg 1	0	0
55	DK	1	Total 1	Mg 1	0	0
55	AD	4	Total 4	Mg 4	0	0
55	DD	2	Total 2	Mg 2	0	0
55	CT	1	Total 1	Mg 1	0	0
55	DH	3	Total 3	Mg 3	0	0
55	CG	1	Total 1	Mg 1	0	0
55	BG	2	Total 2	Mg 2	0	0
55	DE	2	Total 2	Mg 2	0	0
55	CJ	2	Total 2	Mg 2	0	0
55	BR	1	Total 1	Mg 1	0	0
55	CP	1	Total 1	Mg 1	0	0
55	A4	5	Total 5	Mg 5	0	0
55	DA	604	Total 604	Mg 604	0	0
55	CE	6	Total 6	Mg 6	0	0
55	DW	22	Total 22	Mg 22	0	0
55	CK	2	Total 2	Mg 2	0	0
55	AL	2	Total 2	Mg 2	0	0
55	BV	30	Total 30	Mg 30	0	0
55	AG	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BO	1	Total 1	Mg 1	0	0
55	CS	4	Total 4	Mg 4	0	0
55	CX	3	Total 3	Mg 3	0	0
55	DI	1	Total 1	Mg 1	0	0
55	CB	65	Total 65	Mg 65	0	0
55	DJ	1	Total 1	Mg 1	0	0
55	DO	2	Total 2	Mg 2	0	0
55	CO	1	Total 1	Mg 1	0	0
55	CI	1	Total 1	Mg 1	0	0
55	CW	4	Total 4	Mg 4	0	0
55	CD	6	Total 6	Mg 6	0	0
55	CL	7	Total 7	Mg 7	0	0
55	C2	2	Total 2	Mg 2	0	0
55	AO	1	Total 1	Mg 1	0	0
55	BW	19	Total 19	Mg 19	0	0
55	AY	1	Total 1	Mg 1	0	0
55	A3	3	Total 3	Mg 3	0	0
55	AF	6	Total 6	Mg 6	0	0
55	BH	1	Total 1	Mg 1	0	0

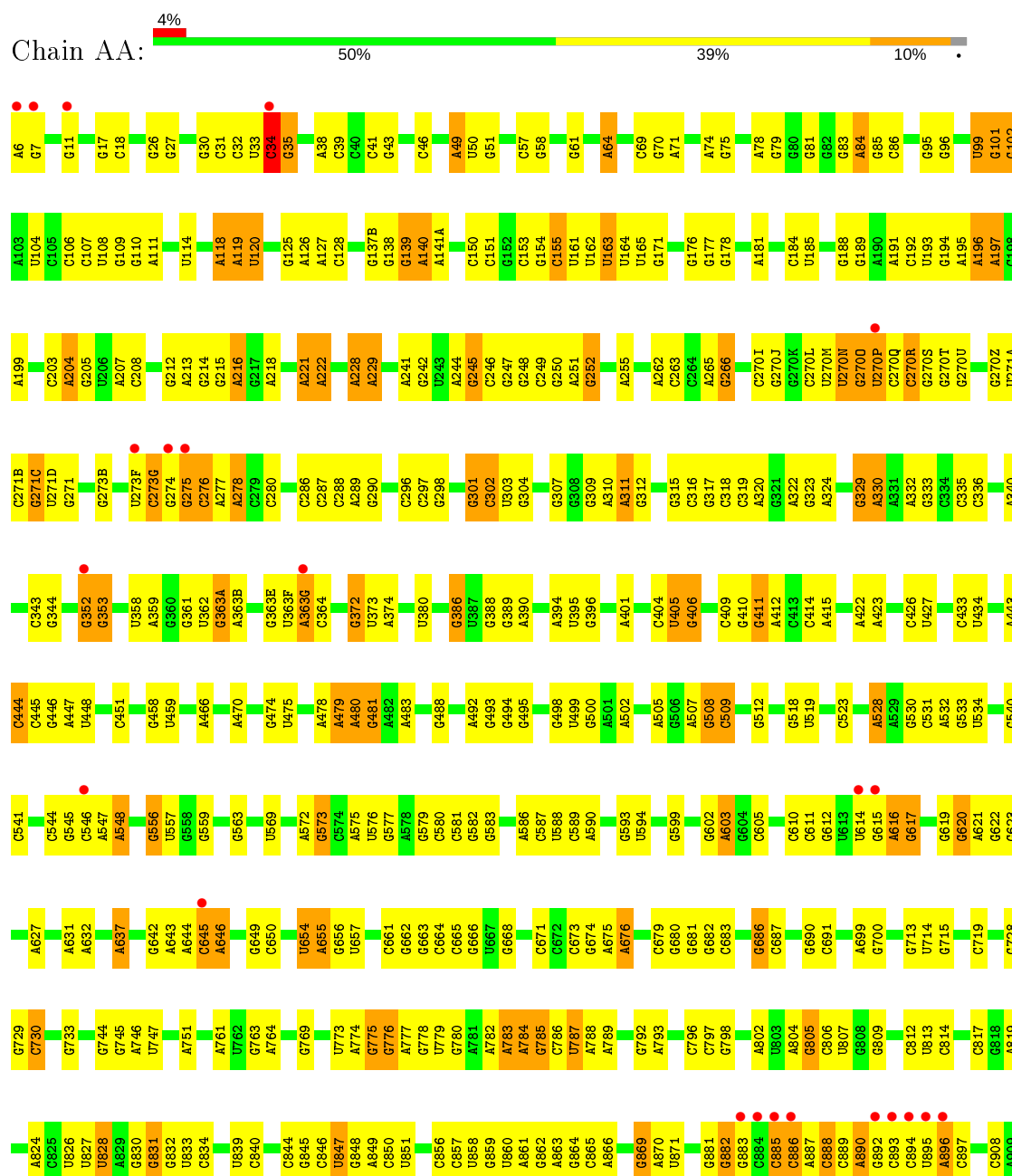
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DN	1	Total 1	Zn 1	0	0
56	BD	1	Total 1	Zn 1	0	0
56	BN	1	Total 1	Zn 1	0	0
56	DD	1	Total 1	Zn 1	0	0

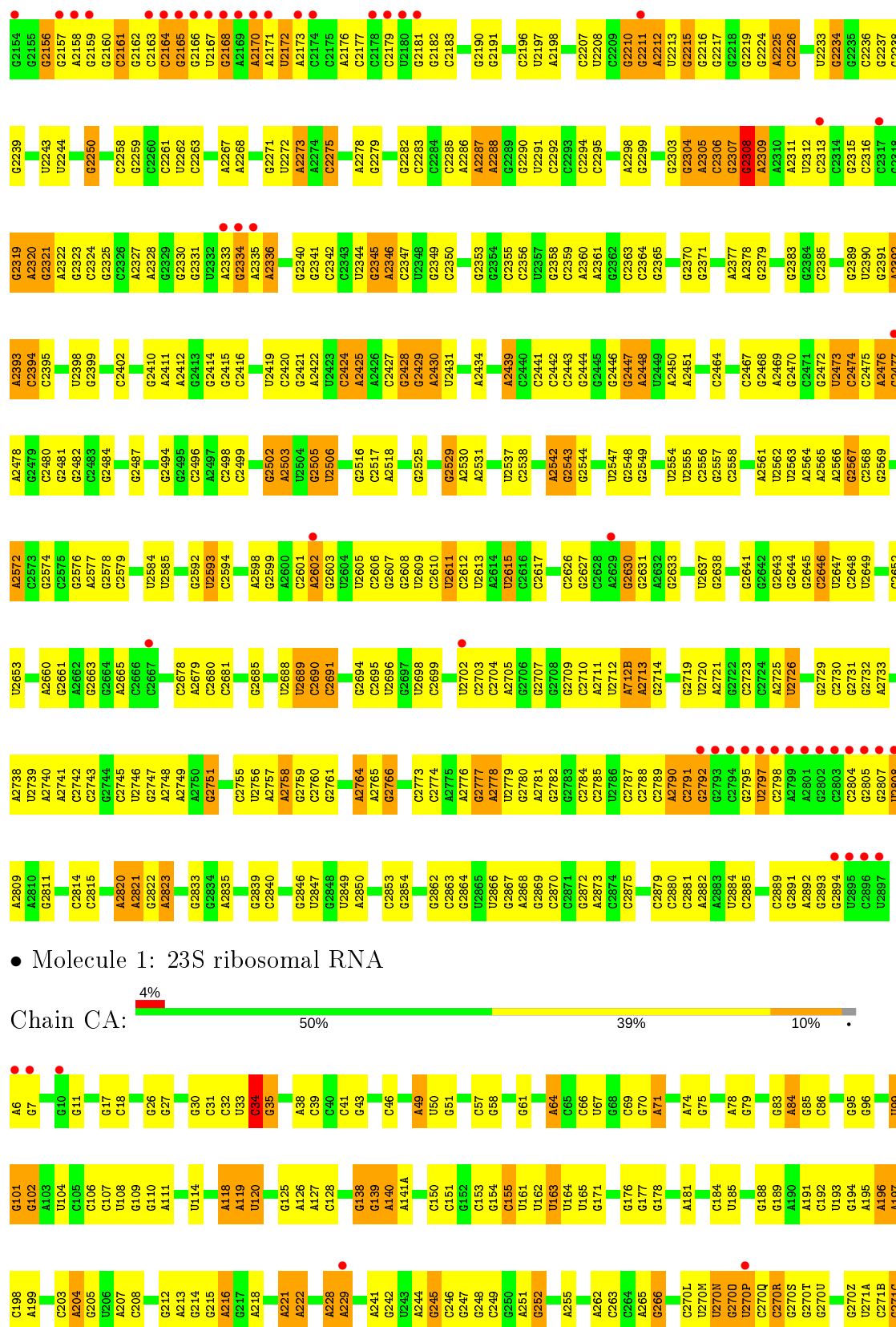
3 Residue-property plots

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

• Molecule 1: 23S ribosomal RNA

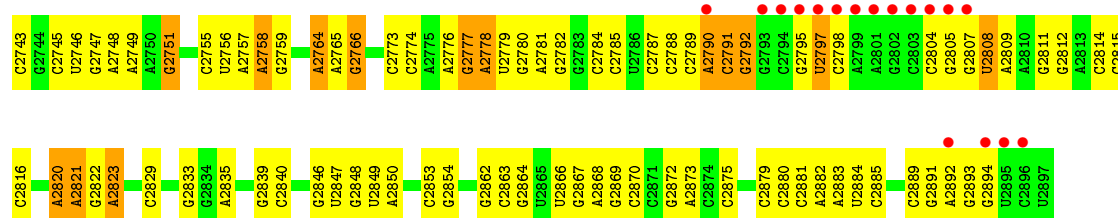


G2069	G1980	G1888	G1678	G1580	G1499	G1414	U1323	U1211	A1128	C991	A910
G2070	A1981	A1889	U1679	G1581	G1500	U1415	U1322	U1217	A1129	C992	A911
U2074	C1982	A1890	G1681	A1582	C1504	C1416	C1327	C1217	U1130	G993	C914
U2075	G1989	A1786	A1786	A1585	C1505	C1417	G1328	C1218	G1135	C994	C915
C2078	A1900	G1788	C1686	A1586	C1506	G1418	U1329	G1219	G1136	G995	G916
U2079	A1901	A1789	U1687	A1587	A1508	A1419	C1330	A1220	G1139	A917	A917
G2080	G1902	C1790	U1688	A1588	A1509	G1421	A1331	C1221A	C1140	A916	A916
U2086	A1791	G1989	G1689	C1589	A1510	G1422	U1332	C1222	U1141	A919	A919
G2087	G1906	U1794	U1693	U1590	A1511	A1427	U1335	G1227	U1142	U999	C924
G2087	G1997	G1795	C1694	C1592	G1512	A1428	A1336	C1230	A1142B	A1000	C925
G2090	G1998	U1796	A1698	C1593	U1514	A1434	G1337	G1231	A1143	C1005	A926
G2093	C1914	C1797	A1698	G1594	C1515			G1232	G1144	C1006	G928
G2094	U1915	U1798	G1703	U1595	U1516	C1437	G1344	G1233	C1145		G929
C2095	G1799	G1594	U1704	C1597	A1517	U1438	C1345	U1234	G1149	A1009	U930
U2096	U1917	C1598	G1705	C1518	C1518	A1439	G1348	G1235	U1150	A1010	G931
C2097	A1918	C1598	U1706	G1521	G1521	G1443	A1349	G1236	C1153	G932	A933
U2109	G1920	A1603	U1709	G1522	G1522	G1444	U1352	A1241	G1154	U1019	G938
G2110	G1921	C1607	C1710	U1523	G1524	A1444B	U1356	A1242	A1155	A1020	A941
A2015	G1922	A1608	U1716	G1525	G1525	C1445	G1357	G1252	G1162	G1021	G942
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G2018	U1926	A1614	G1817	C1532	C1532	U1484	A1359	A1254	G1164	U1023	G944
A2019	G1929	A1615	G1726	C1533	C1533	U1485	A1360	U1255	U1165	G1024	A945
G2115	G1930	A1616	U1727	A1534	G1534	U1485	A1365	G1256	G1166	G1025	G946
G2116	U1931	C1617	G1728	U1535	U1535	A1489	A1366	U1257	U1167	U1026	G947
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G2023	G1932	G1731	G1731	A1537	A1537			G1266	G1169	A1028	
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G2120	U1938	G1742	G1742	G1540	G1540	G1467	A1379	U1273	A1174	U1035	G955
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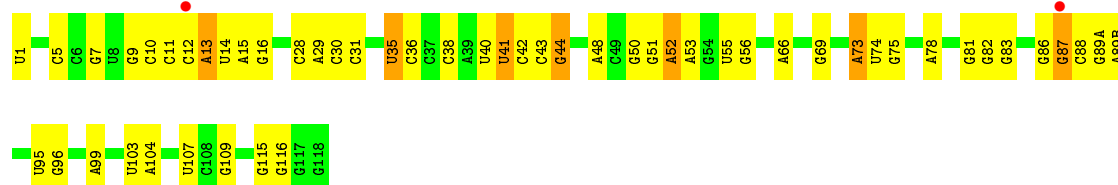




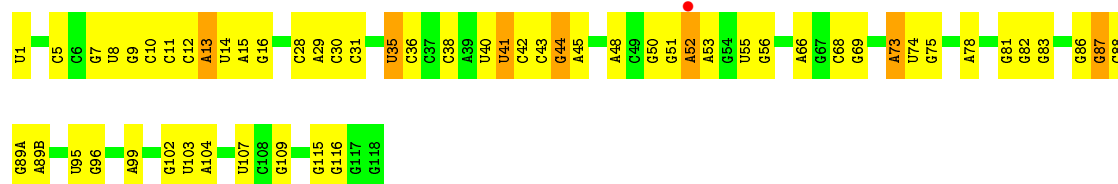




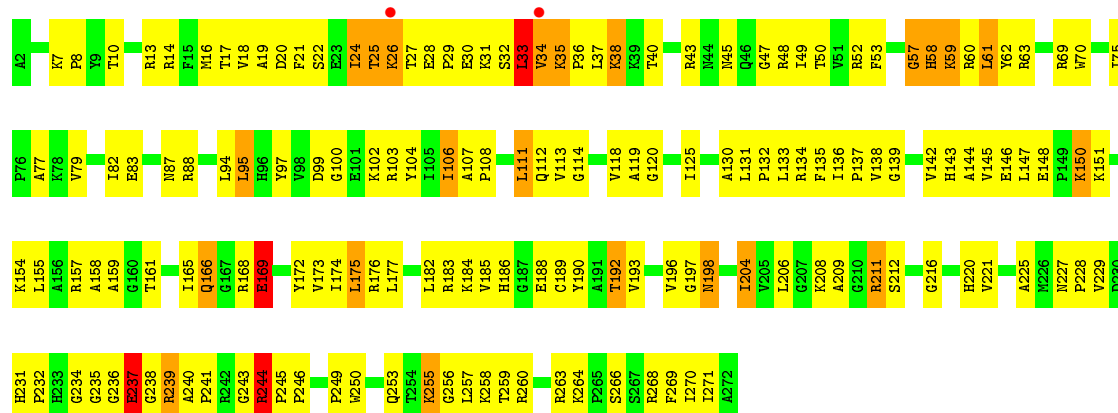
• Molecule 2: 5S ribosomal RNA



• Molecule 2: 5S ribosomal RNA

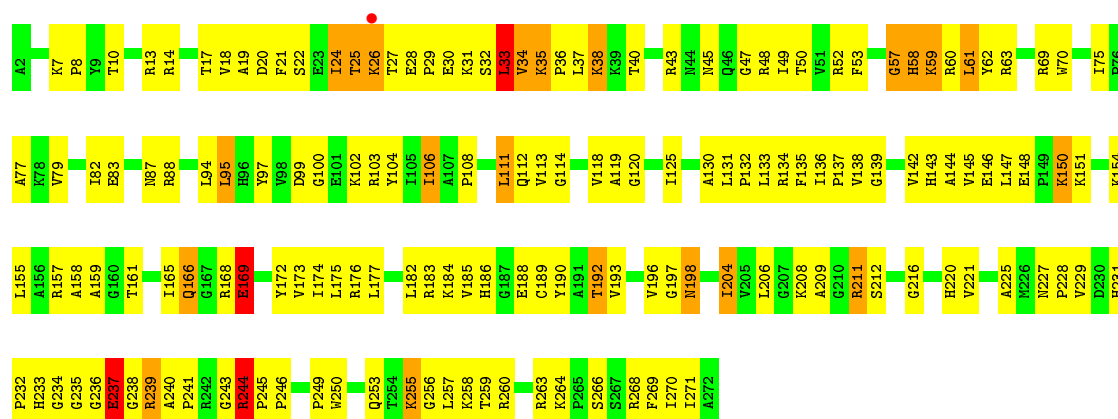


• Molecule 3: 50S ribosomal protein L2

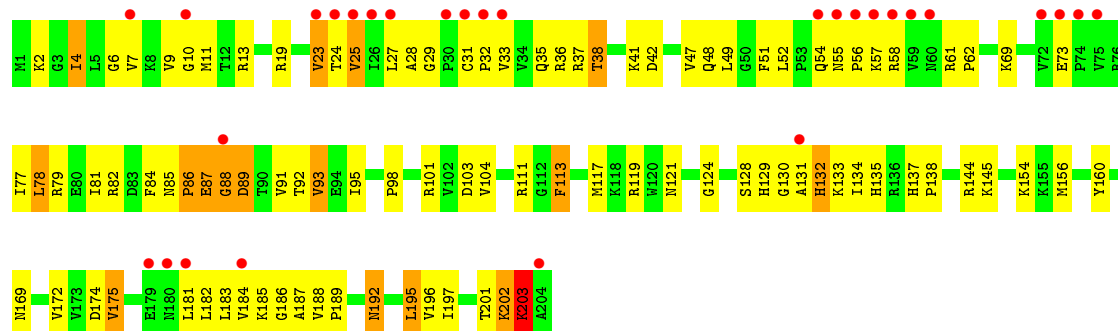


• Molecule 3: 50S ribosomal protein L2

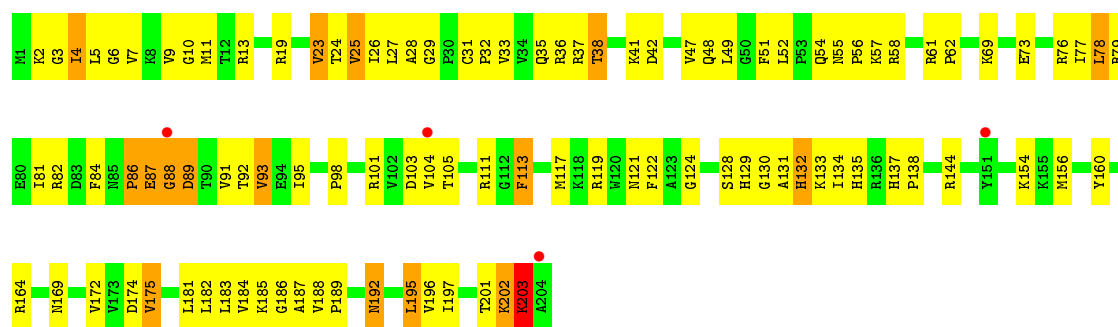




• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3



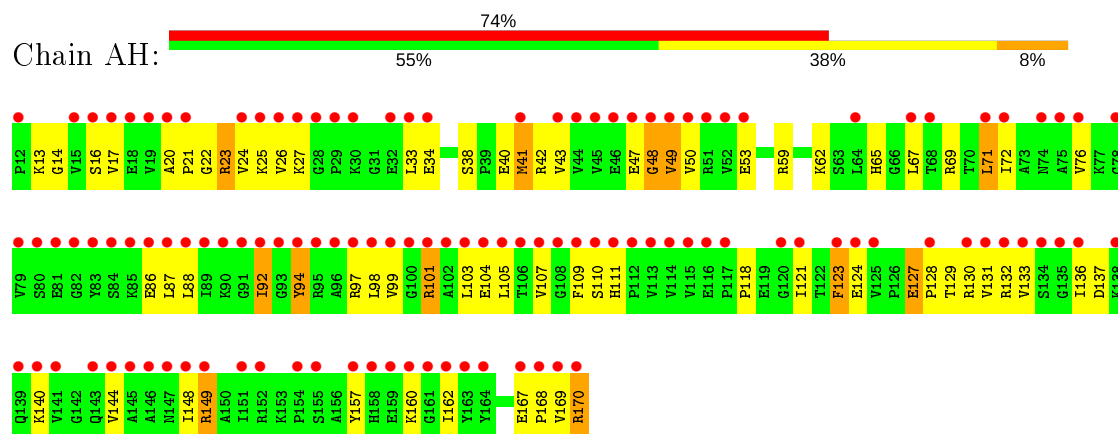
• Molecule 5: 50S ribosomal protein L4





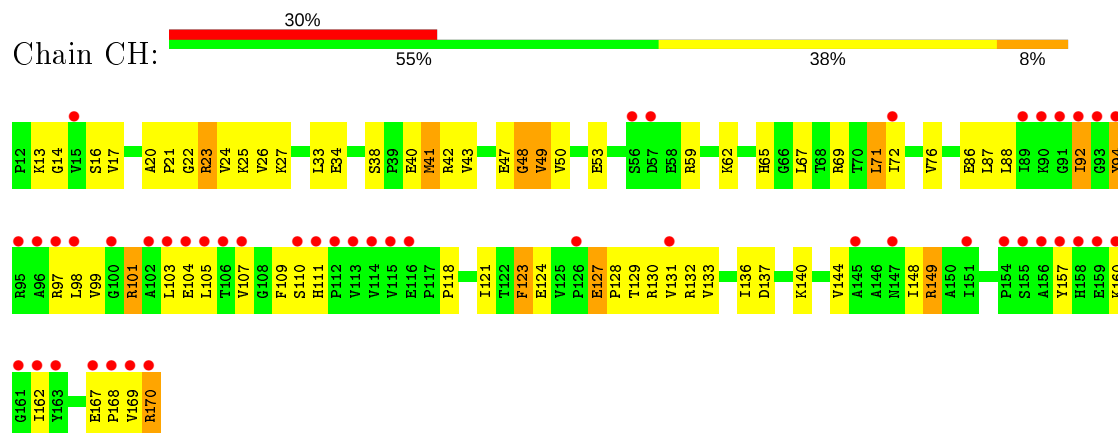
- Molecule 7: 50S ribosomal protein L6

Chain AH:



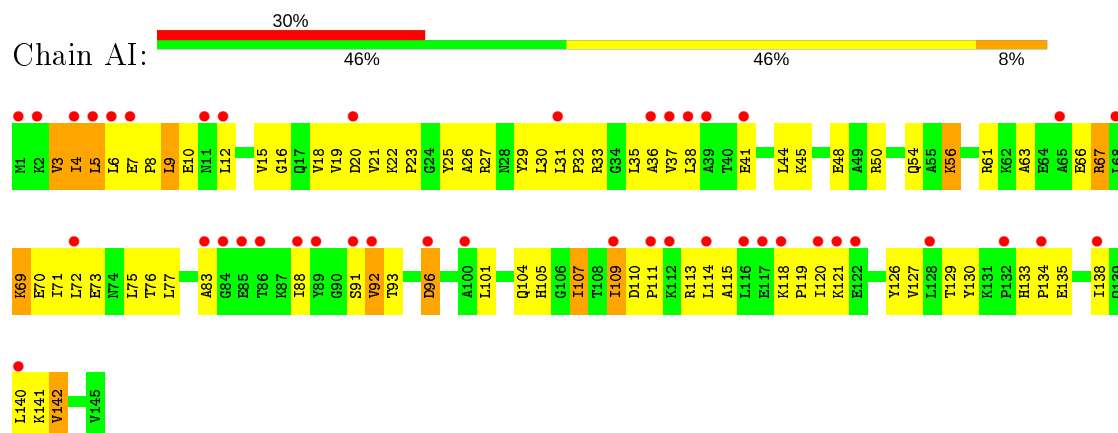
- Molecule 7: 50S ribosomal protein L6

Chain CH:



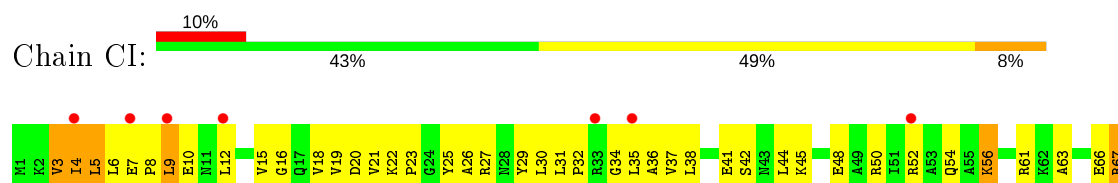
- Molecule 8: 50S ribosomal protein L9

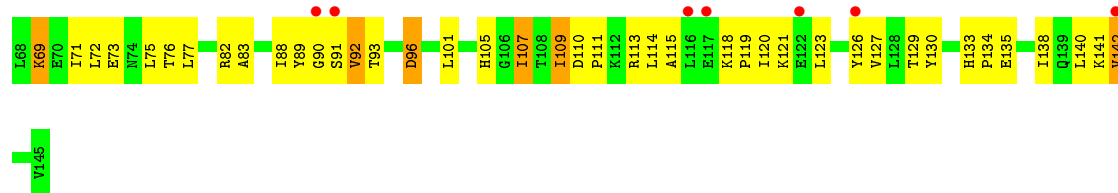
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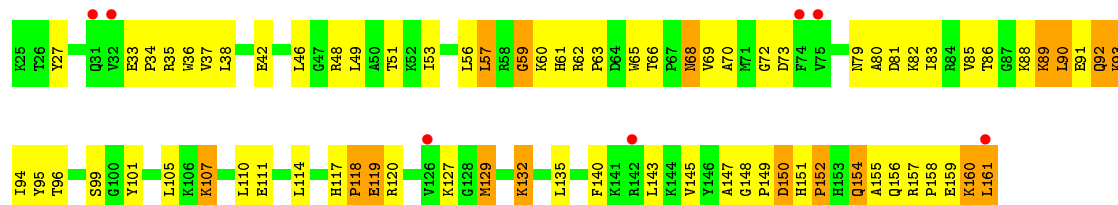
- Molecule 8: 50S ribosomal protein L9

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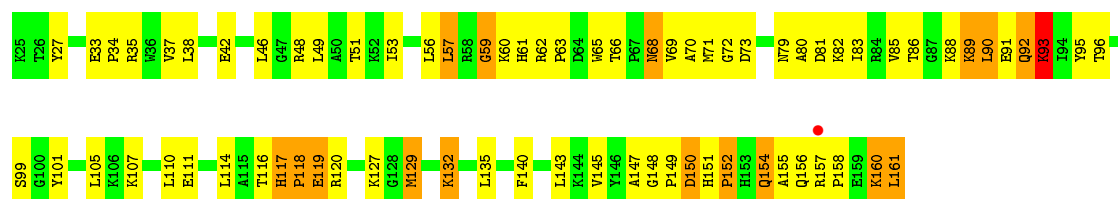




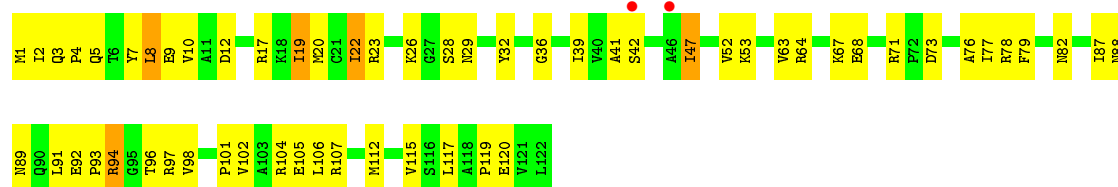
- Molecule 9: 50S ribosomal protein L13



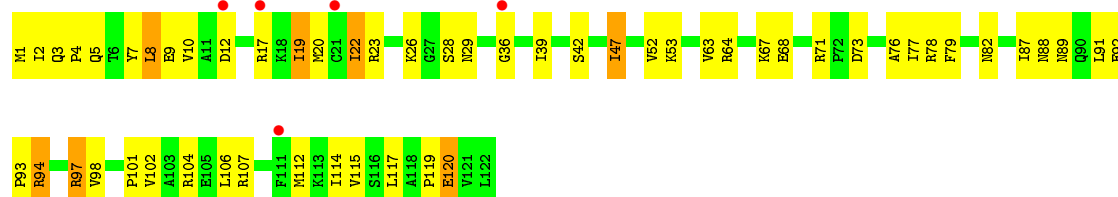
- Molecule 9: 50S ribosomal protein L13

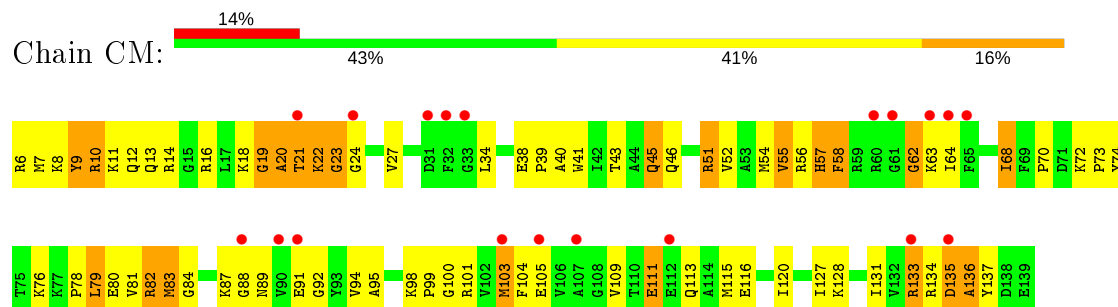


- Molecule 10: 50S ribosomal protein L14

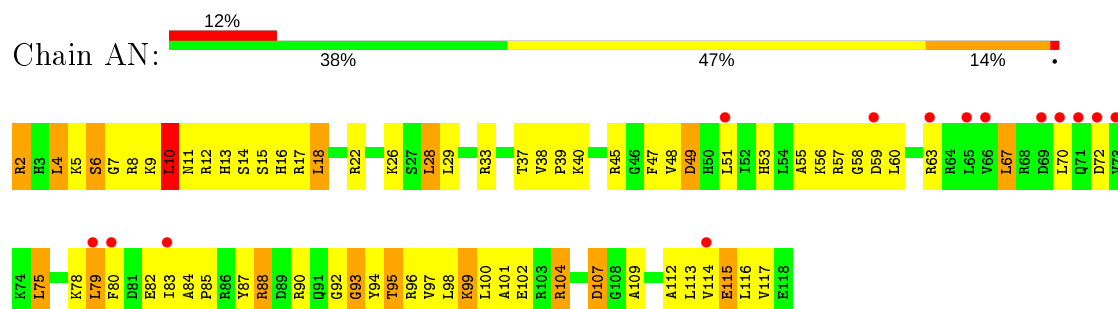


- Molecule 10: 50S ribosomal protein L14

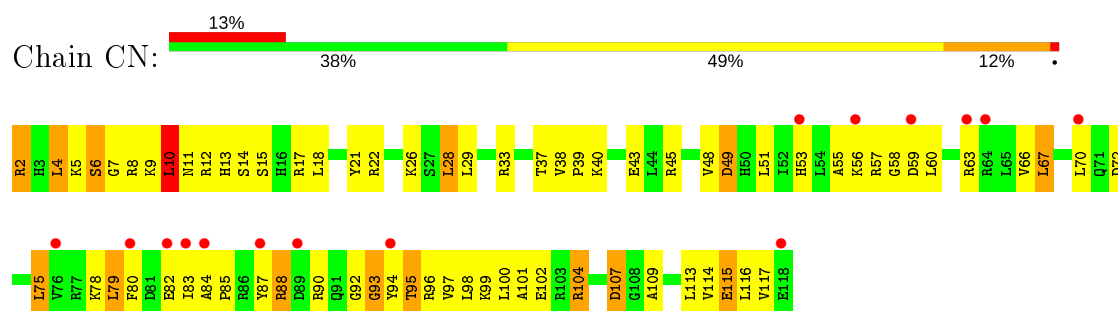




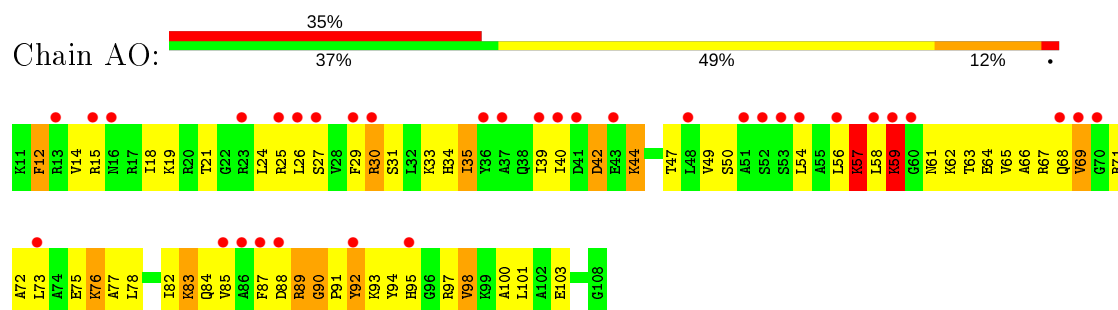
- Molecule 13: 50S ribosomal protein L17



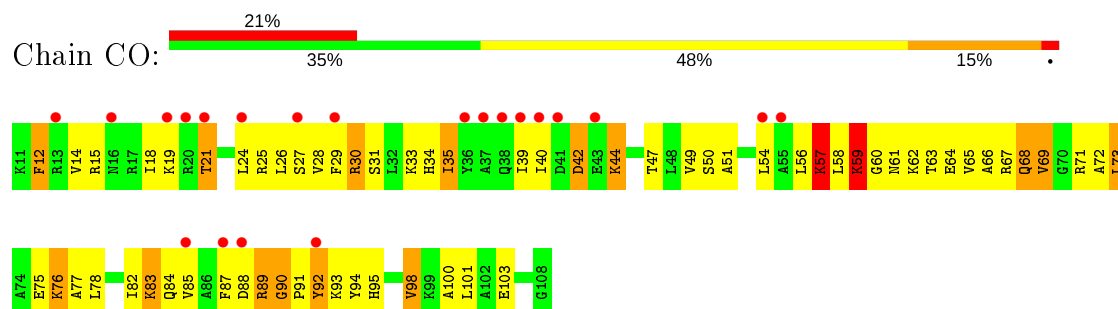
- Molecule 13: 50S ribosomal protein L17



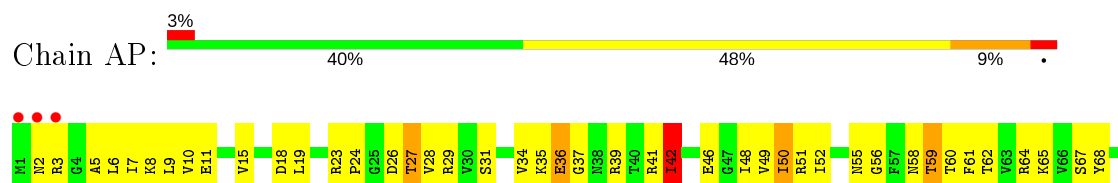
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

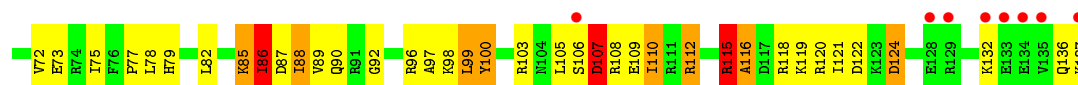
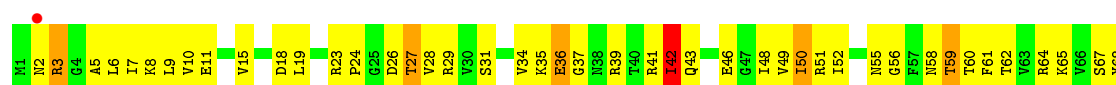


- Molecule 15: 50S ribosomal protein L19

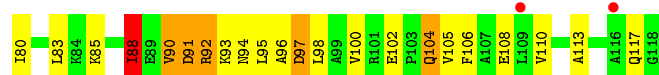




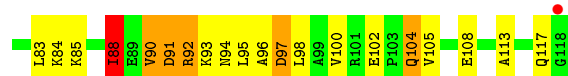
- Molecule 15: 50S ribosomal protein L19



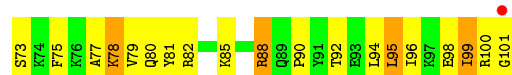
- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20

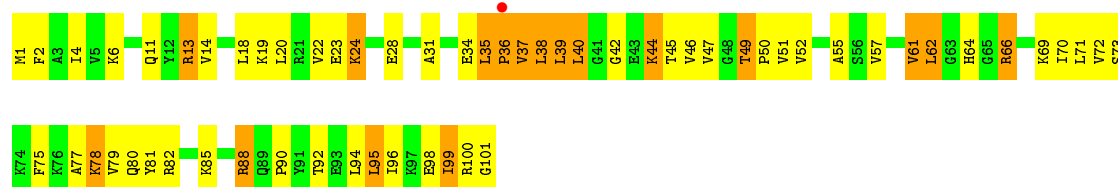


- Molecule 17: 50S ribosomal protein L21

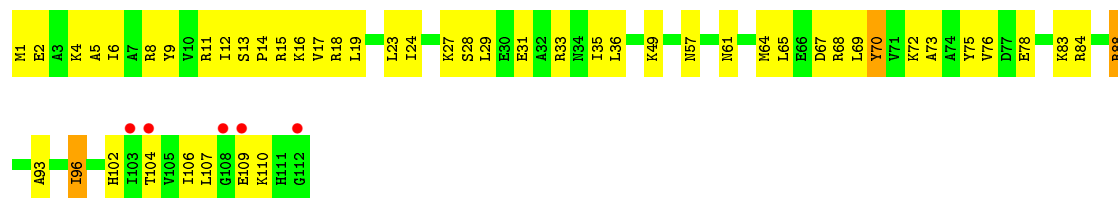


- Molecule 17: 50S ribosomal protein L21





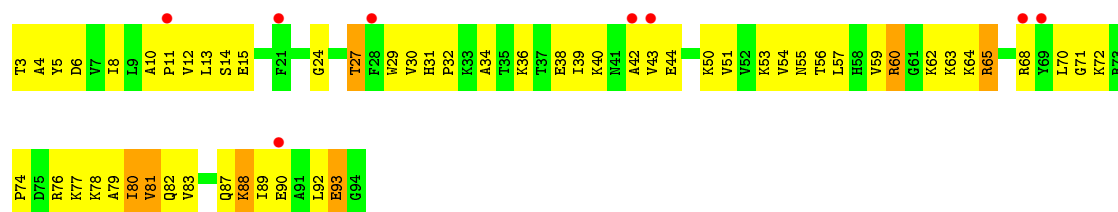
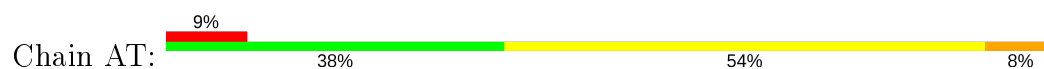
- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



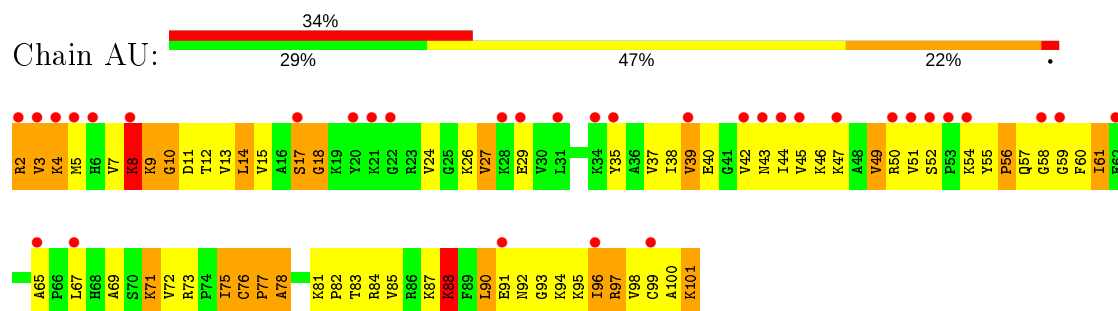
- Molecule 19: 50S ribosomal protein L23



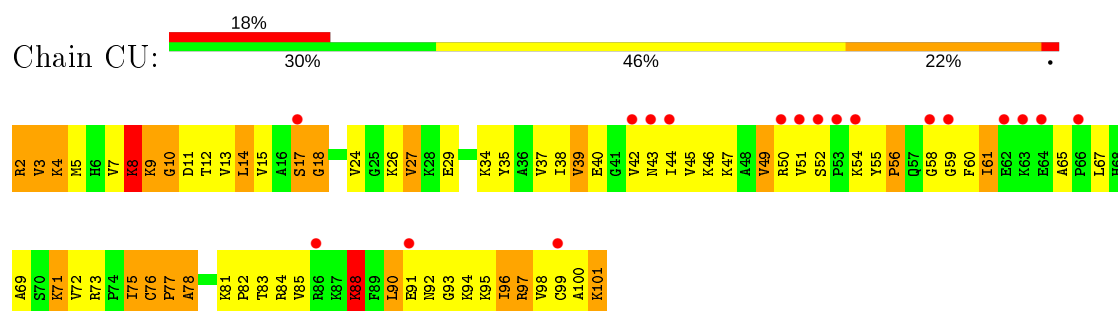
- Molecule 19: 50S ribosomal protein L23



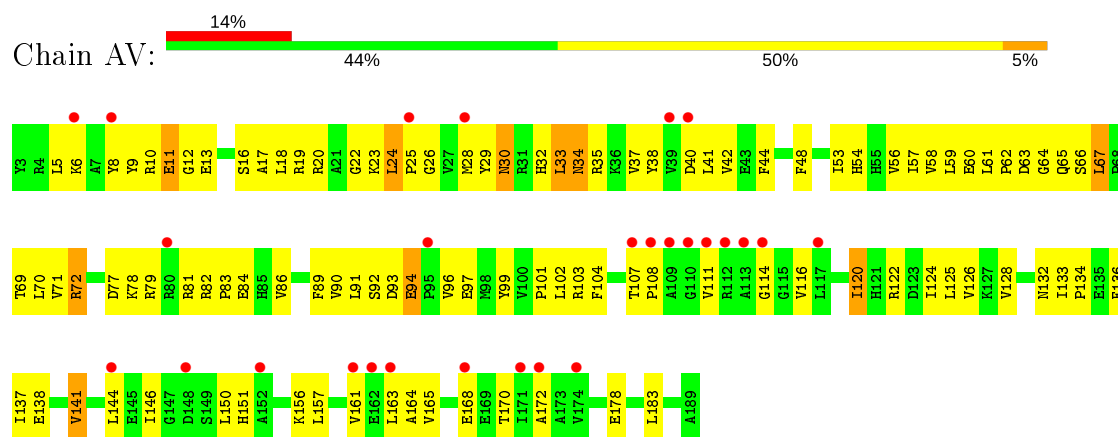
- Molecule 20: 50S ribosomal protein L24



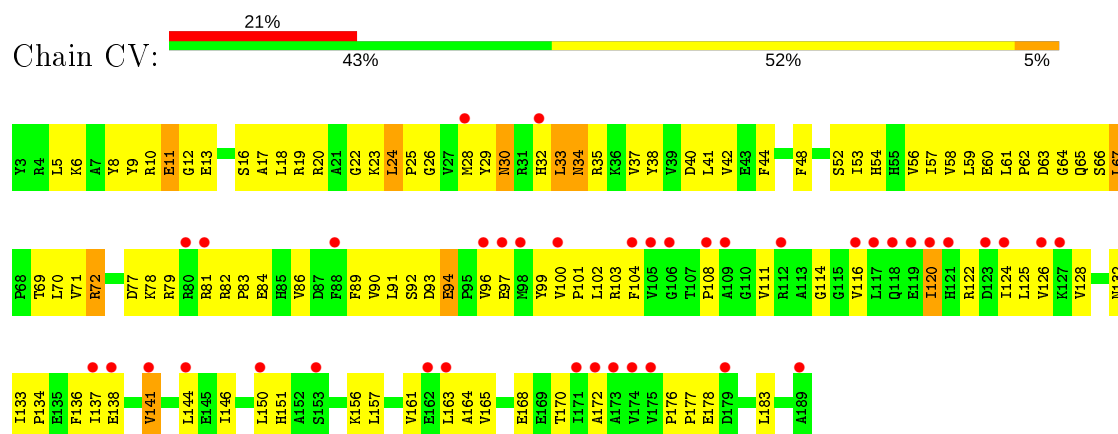
- Molecule 20: 50S ribosomal protein L24



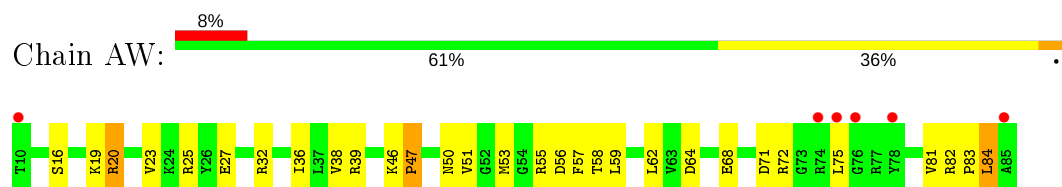
- Molecule 21: 50S ribosomal protein L25



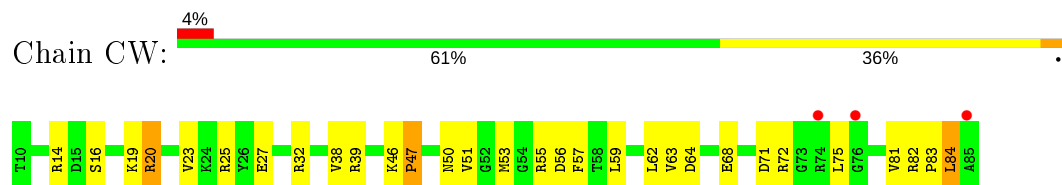
- Molecule 21: 50S ribosomal protein L25



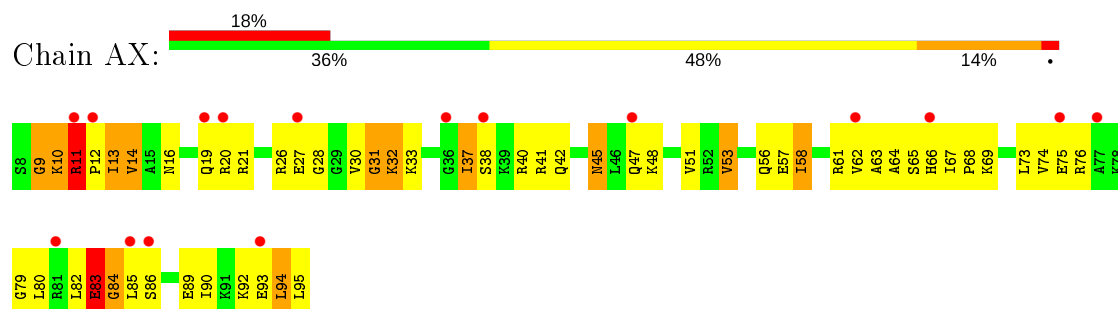
- Molecule 22: 50S ribosomal protein L27



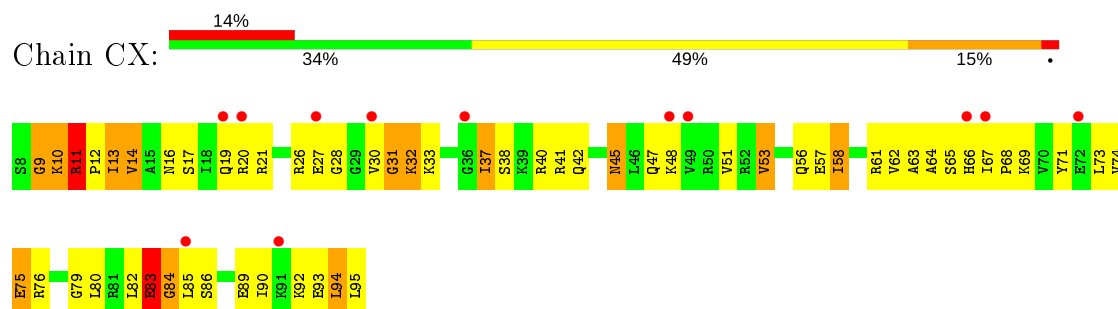
- Molecule 22: 50S ribosomal protein L27



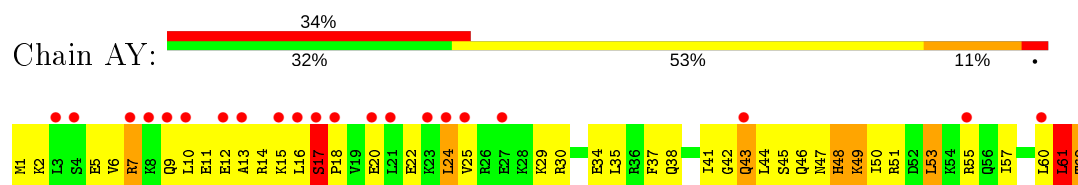
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

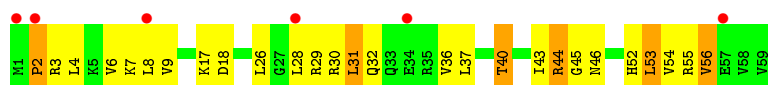


- Molecule 24: 50S ribosomal protein L29

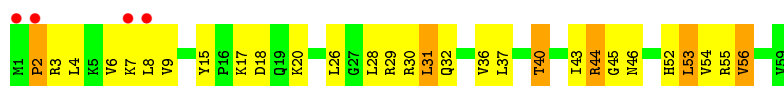




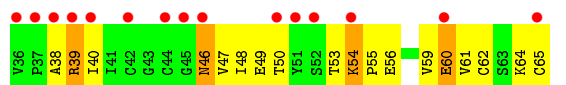
- Molecule 25: 50S ribosomal protein L30



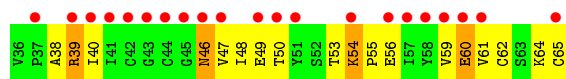
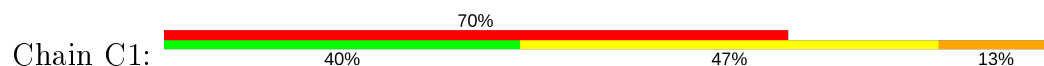
- Molecule 25: 50S ribosomal protein L30



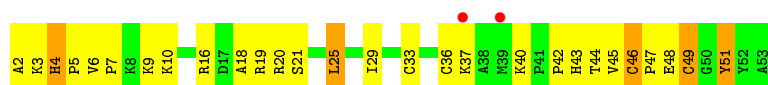
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



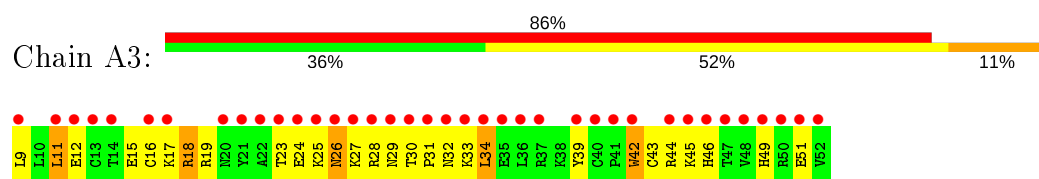
- Molecule 27: 50S ribosomal protein L32



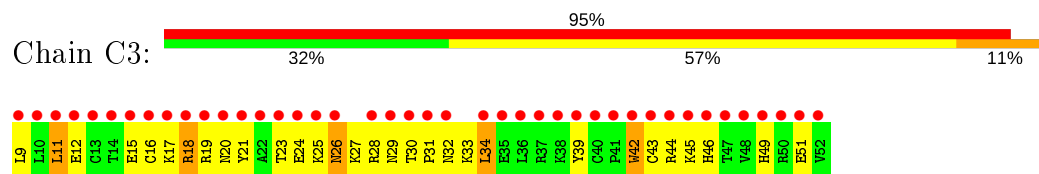
- Molecule 27: 50S ribosomal protein L32



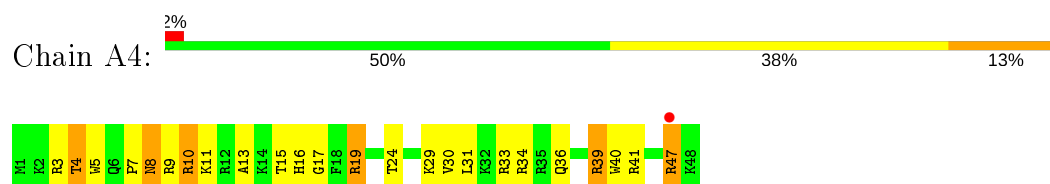
- Molecule 28: 50S ribosomal protein L33



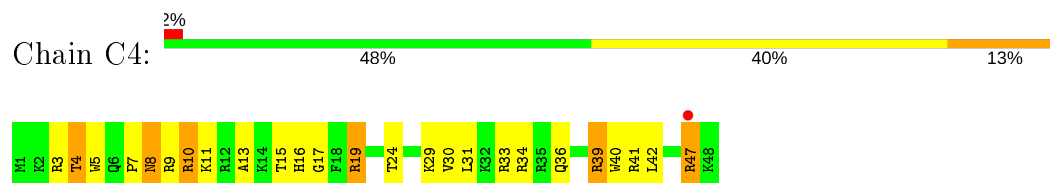
- Molecule 28: 50S ribosomal protein L33



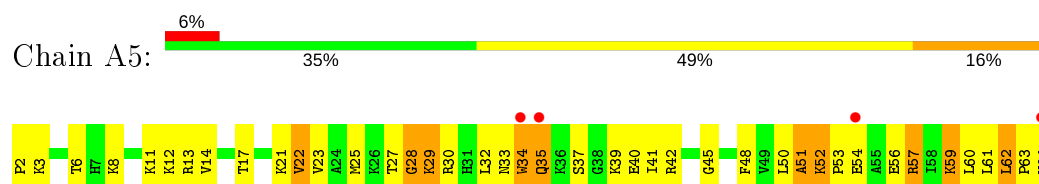
- Molecule 29: 50S ribosomal protein L34



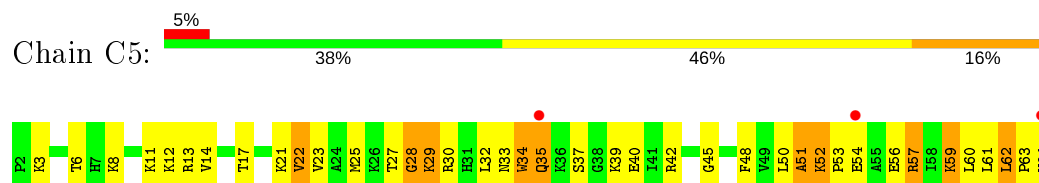
- Molecule 29: 50S ribosomal protein L34



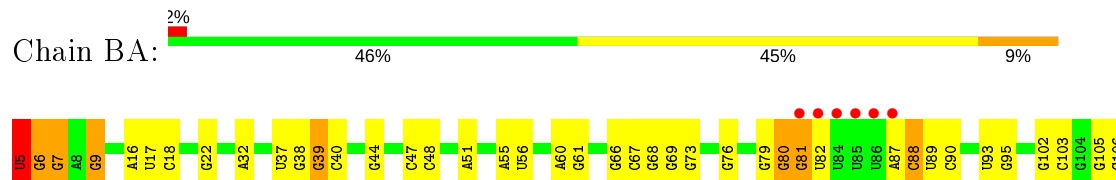
- Molecule 30: 50S ribosomal protein L35



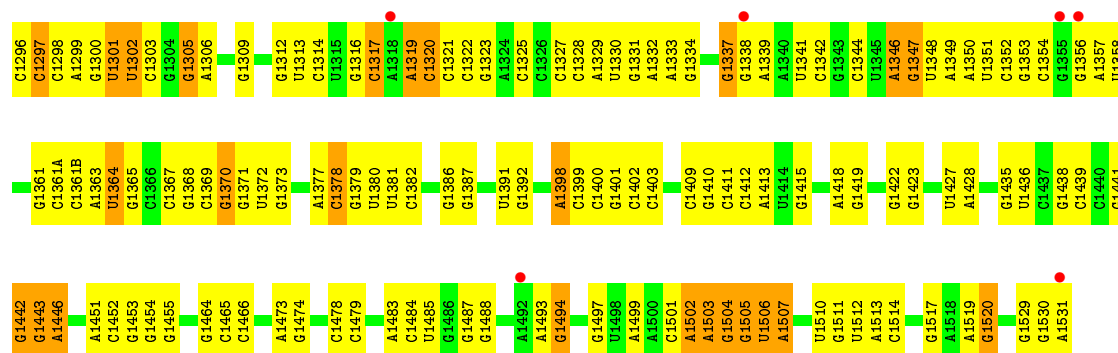
- Molecule 30: 50S ribosomal protein L35



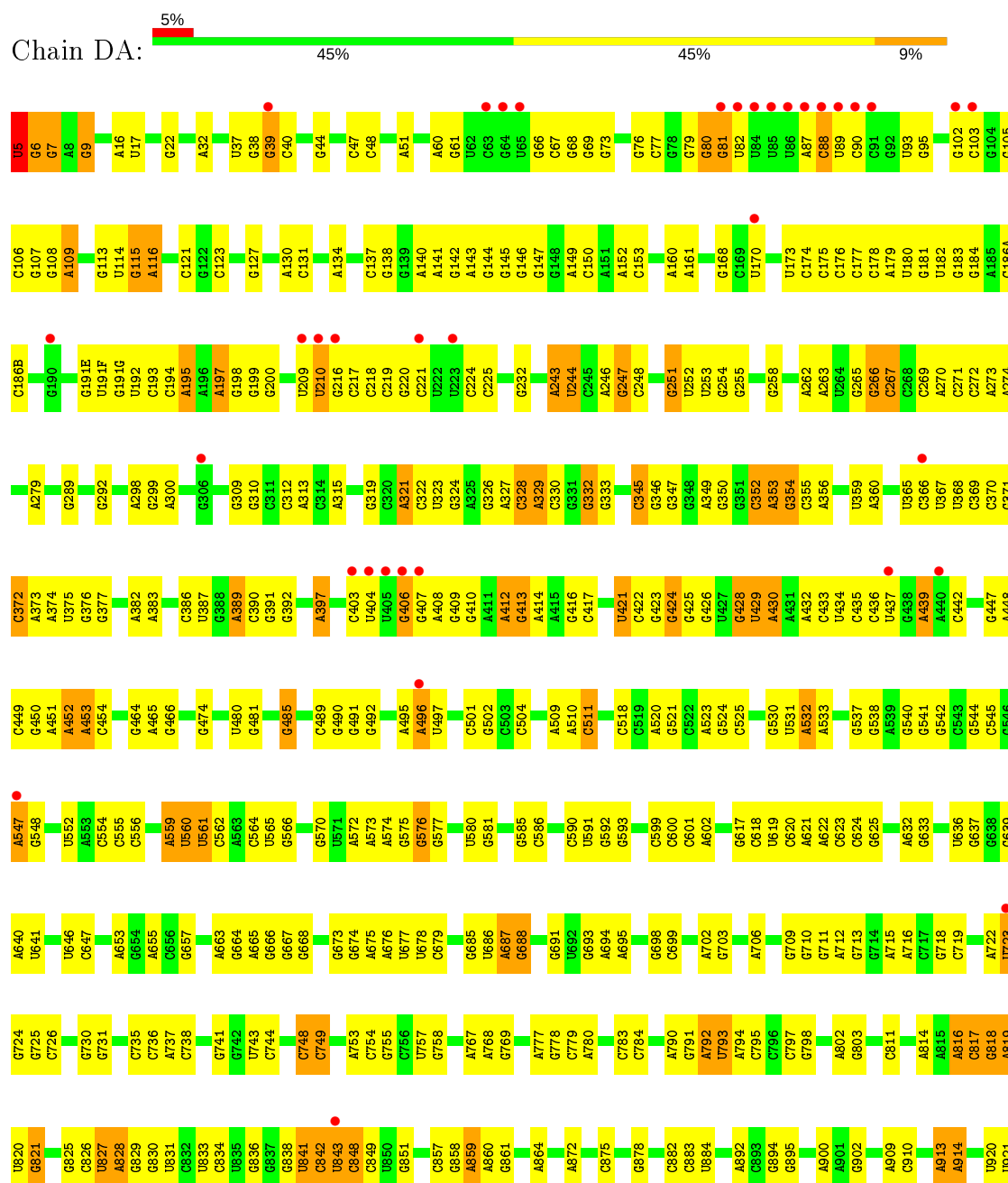
- Molecule 31: 16S ribosomal RNA

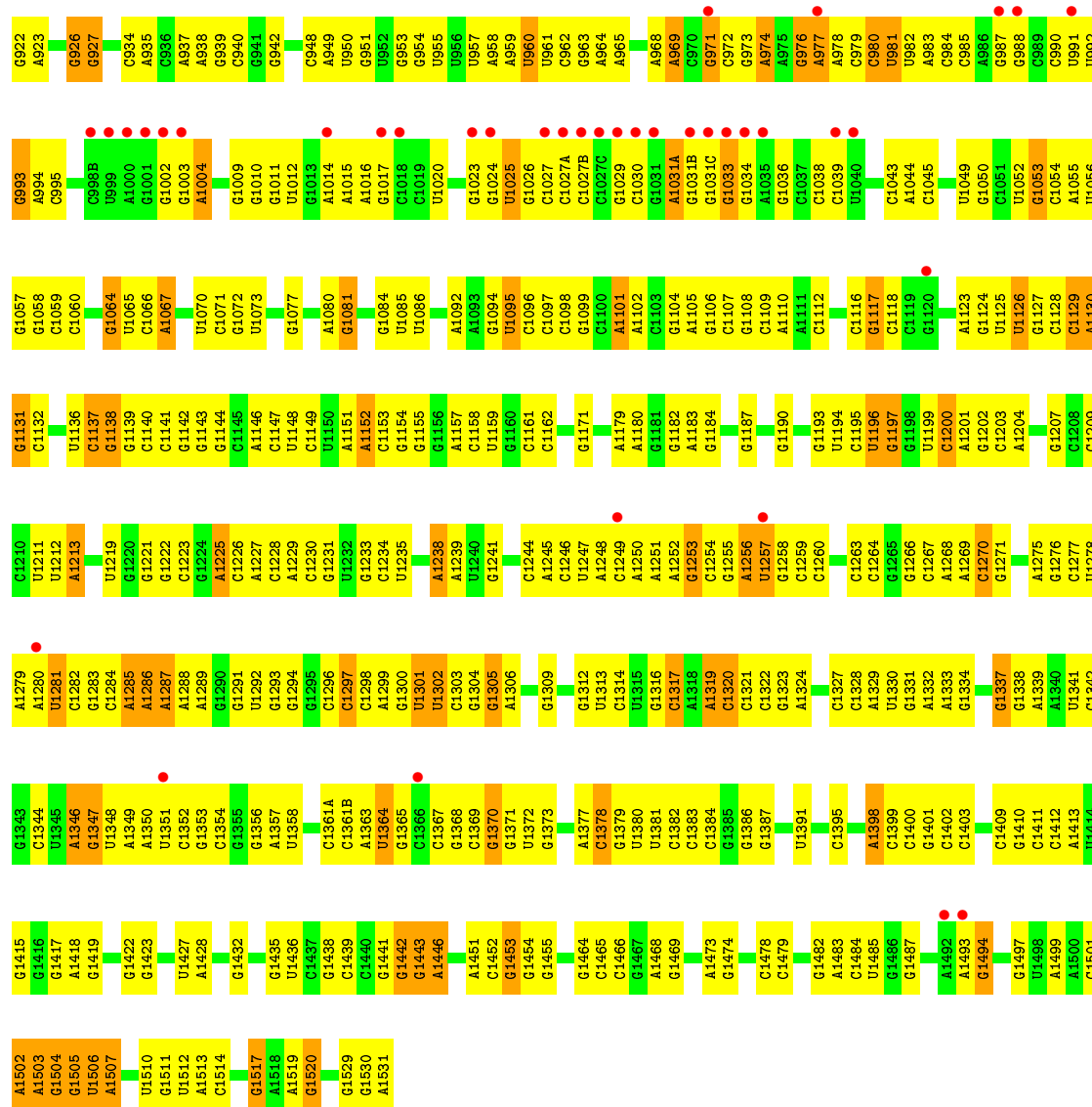


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	C1128	A1055	C990	U920	U820	G710	G620	C525	A431	G350	U253	C163
C1209	A1129	U1056	U991	U921	G713		A621	G529	A432	C353	G255	G168
G1210	A1130	U1057	U992	G922	C826	G718	A622	C530	C433	G354	U256	C169
U1211	G1131	G1058	G993	A923	U827	C719	C623	U531	U434	C355	G257	U170
U1212	C1132	C1059	A994	A926	U827		C624	A533	C436	A356	G258	
A1213	U1136	G1060	C995	G926	C828	A722	G625	G537	U437	U359	A262	C174
C1214	C1137	G1064	G998A	G927	G821	G723	U626	G538	G438	A360	U264	C176
U1215	G1138	U1065	C998B	C934	G821	U724	A632	A539	A439	G365	G265	C177
G1216	C1139	C1066	U999	A935	C826	G718	G633	G540	C442	U366	G266	C178
	A1067	U1067	A1000	C936	U827	C719	G624	G541		C367	C267	A179
U1219	C1141	G1068	G1001	A937	A828		G625	A533		U368	C268	U180
G1220	G1142	C1069	G1002	A938	G829	A722		G537	U437	C369	C269	G181
C1221	G1143	U1070	G1003	G939	G830	G723	A632	G538	G438	A360	U264	C176
G1222	G1144	C1071	C940	U939	U831	U724	G633	A539	A439	G365	G265	C177
C1223	G1145	G1072	G941	G941	C832	G725	G633	G540	C442	C366	G266	A179
A1224	A1146	U1073	G942	G942	U833	G726	G633	G541		U367	C267	U180
A1225	C1147	G1073	G942	G942	C834			G542	G447	U368	C268	G181
C1226	U1148	G1077	U943	U943	U835	C735	U636	G544	A448	C369	C269	U182
G1227	C1149	U1078	G944	G944	G836	C736	G637	C544	C449	C370	G270	G183
C1228	U1150	G1079	G948	C948	U837	C737	G638	G545	G450	G371	C271	G184
A1229	A1151	A1080	A949	A949	G838	C738	A640	G546	A451	C372	C272	A185
G1230	A1152	G1081	U950	U950	U841	C738	A640	A547	A452	A373	A273	C186A
C1231	C1153		C943	C943	C741		U641	G548	A453	A374	A274	C186B

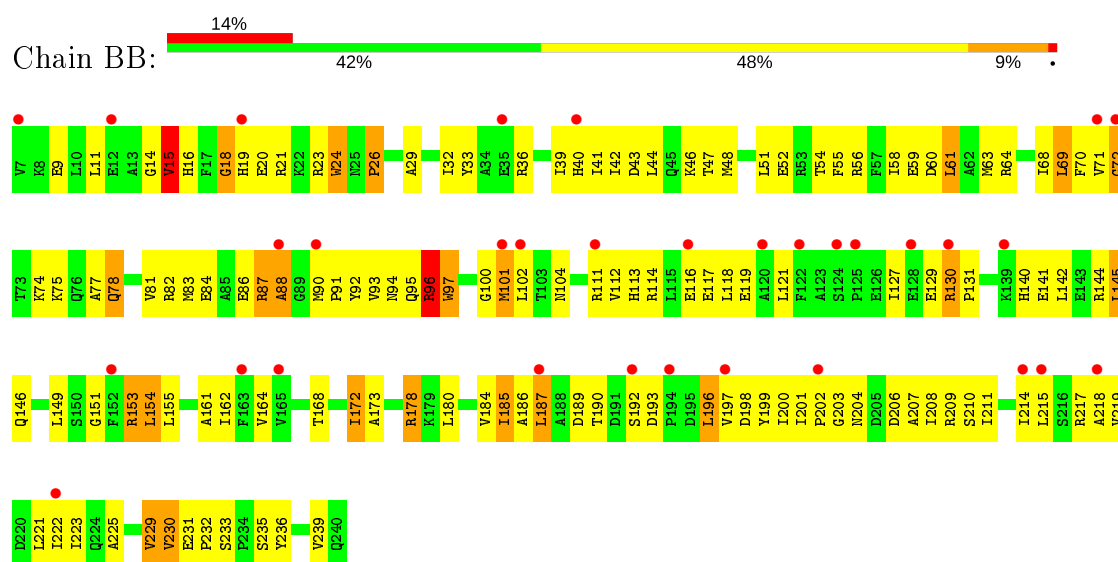


• Molecule 31: 16S ribosomal RNA

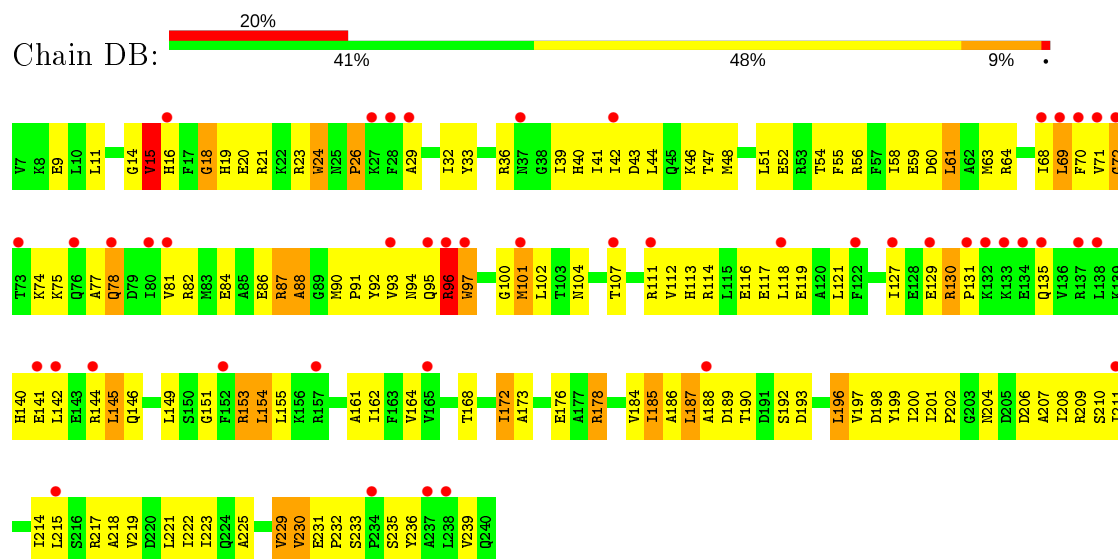




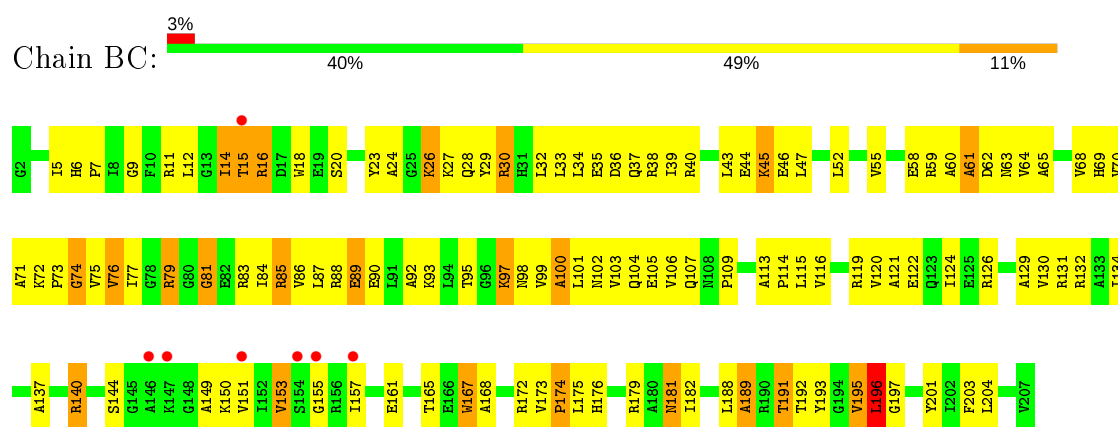
• Molecule 32: 30S ribosomal protein S2



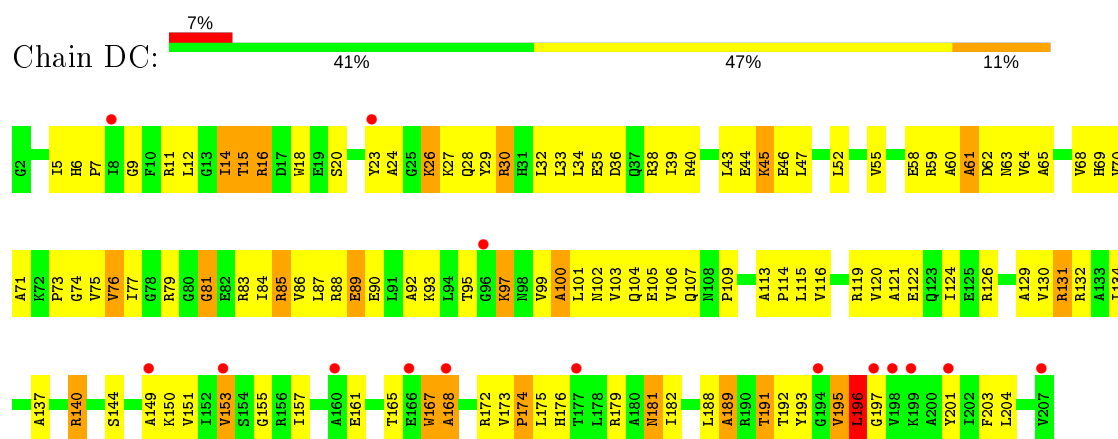
• Molecule 32: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S3

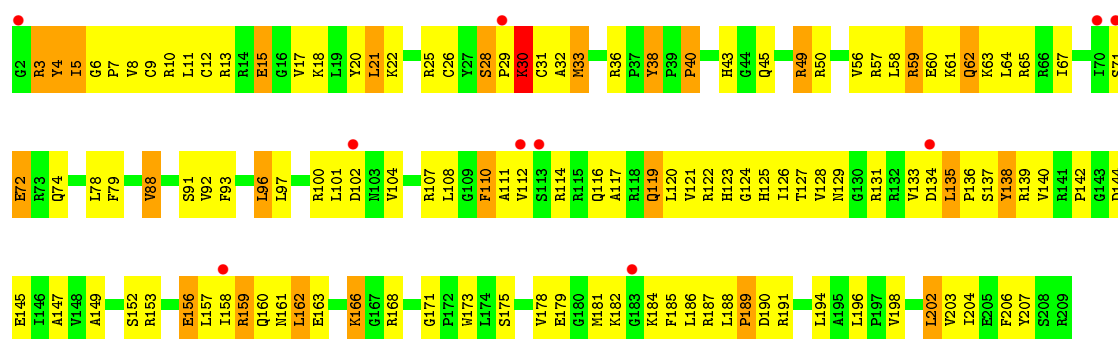


• Molecule 33: 30S ribosomal protein S3

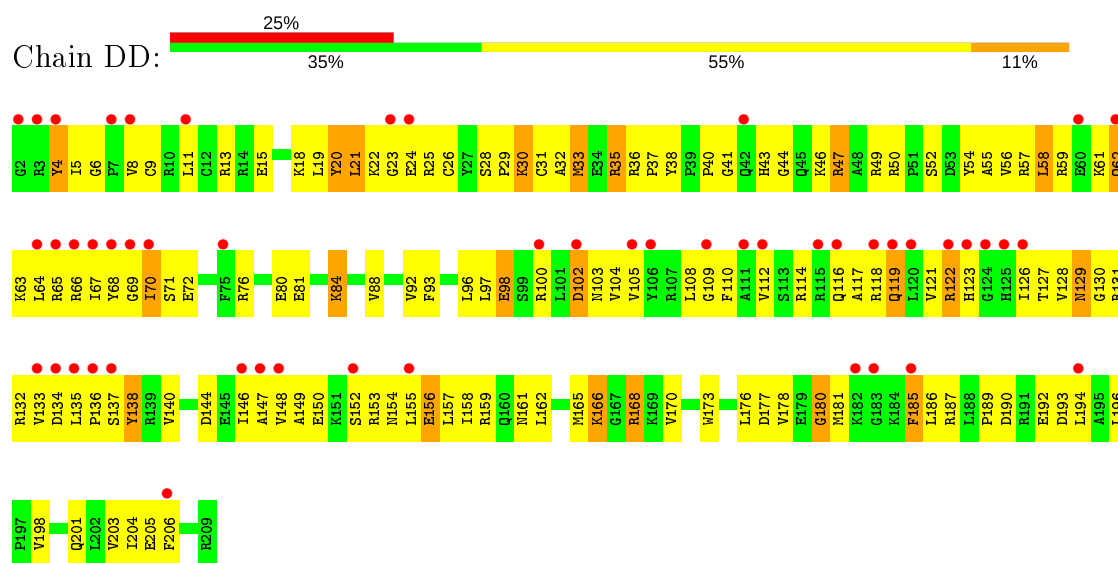


• Molecule 34: 30S ribosomal protein S4

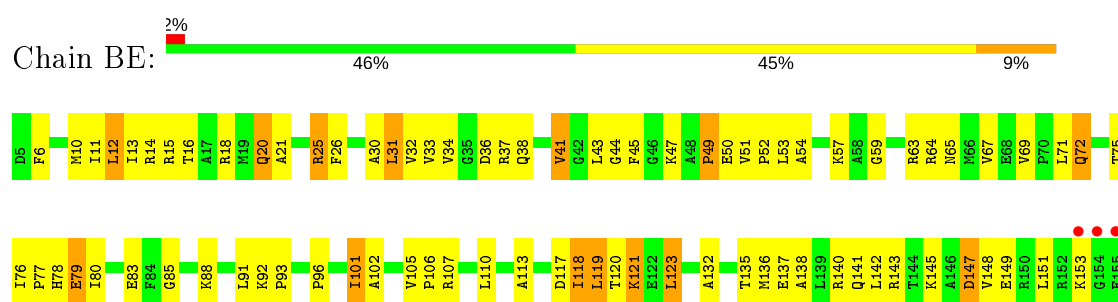




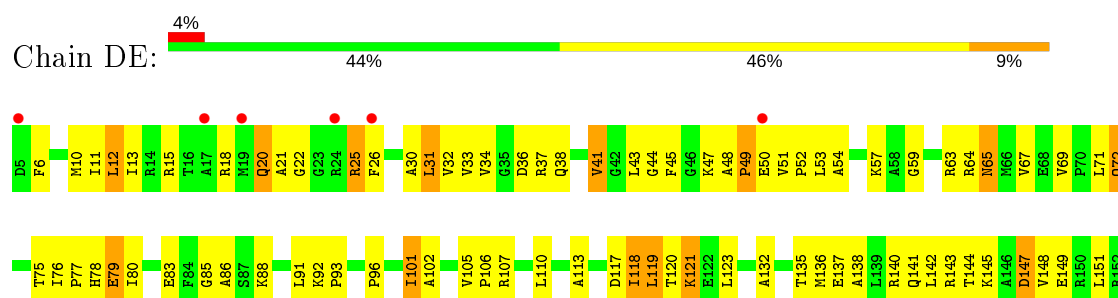
• Molecule 34: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S5



• Molecule 35: 30S ribosomal protein S5

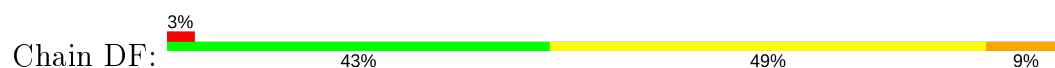




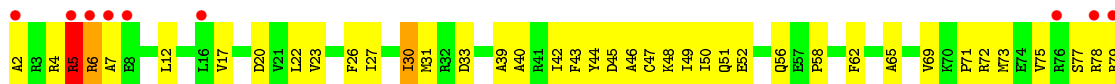
- Molecule 36: 30S ribosomal protein S6



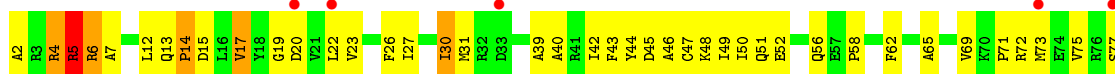
- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

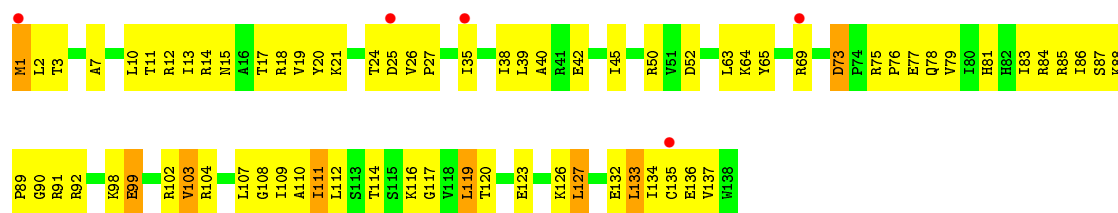


- Molecule 37: 30S ribosomal protein S7

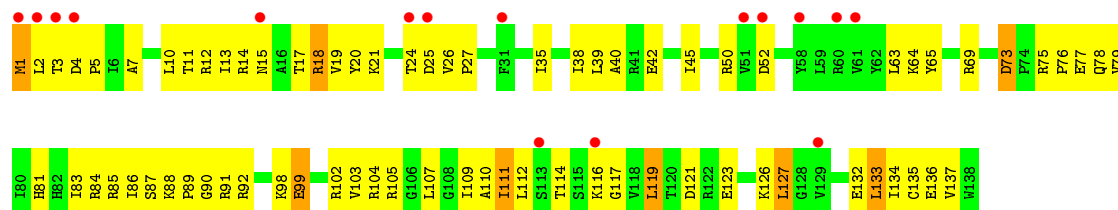


- Molecule 38: 30S ribosomal protein S8

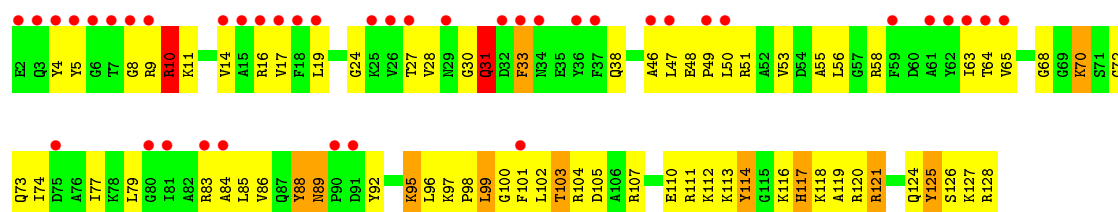
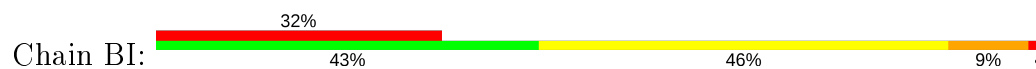




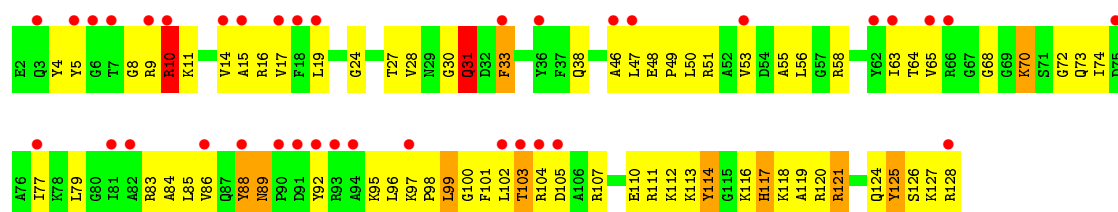
• Molecule 38: 30S ribosomal protein S8



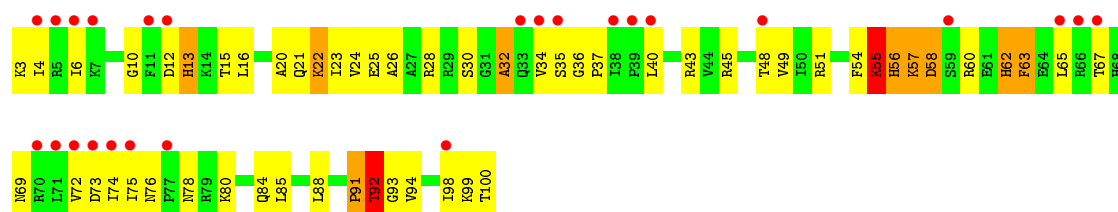
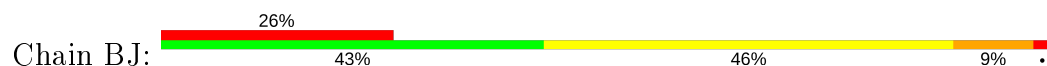
• Molecule 39: 30S ribosomal protein S9



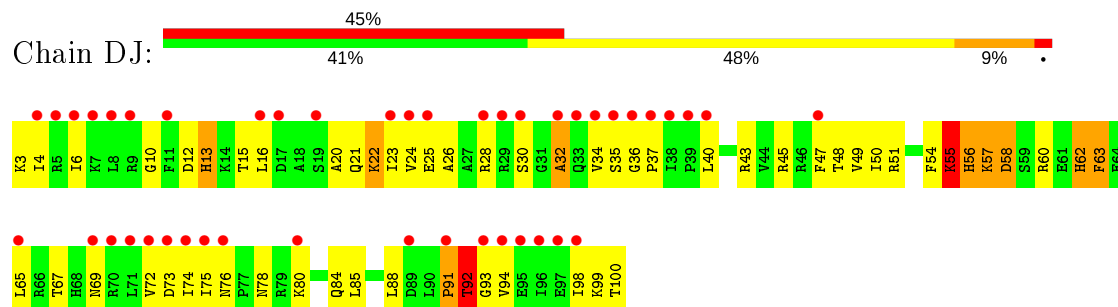
• Molecule 39: 30S ribosomal protein S9



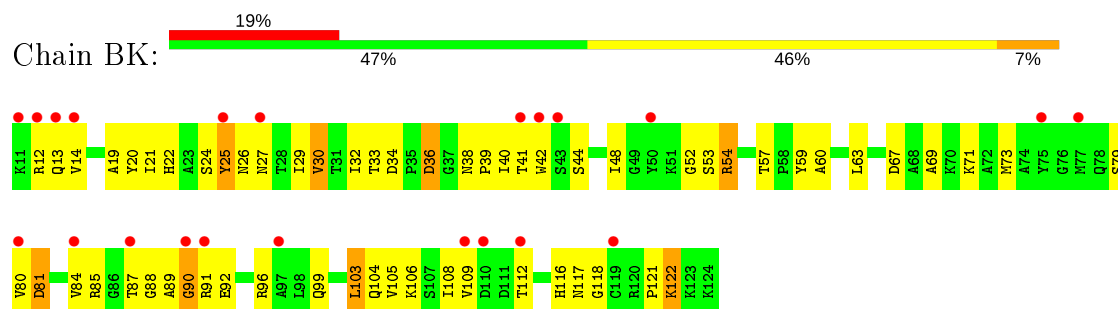
• Molecule 40: 30S ribosomal protein S10



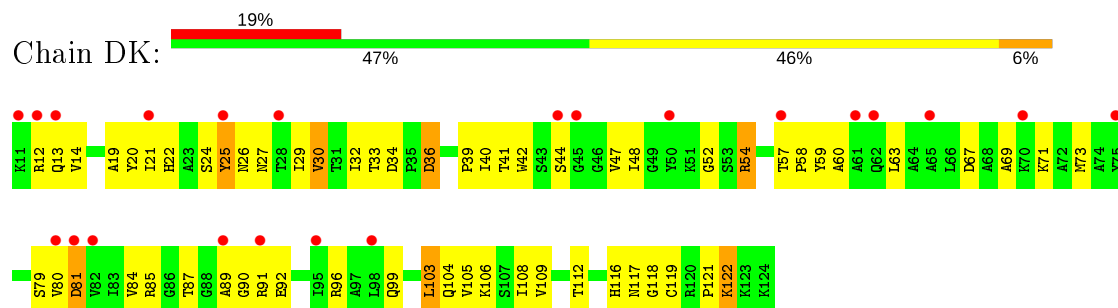
- Molecule 40: 30S ribosomal protein S10



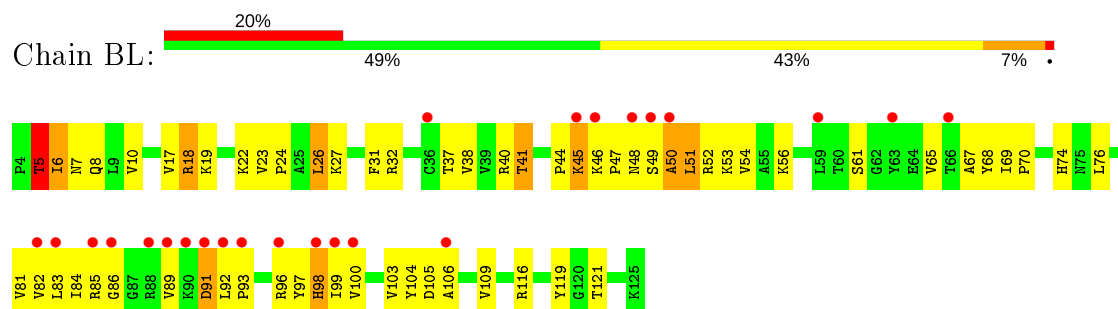
- Molecule 41: 30S ribosomal protein S11



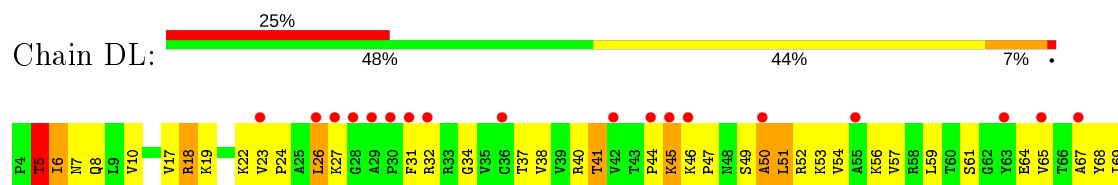
- Molecule 41: 30S ribosomal protein S11

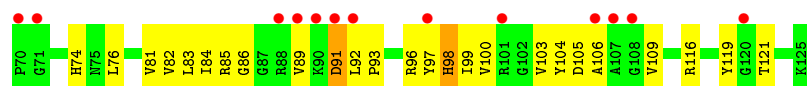


- Molecule 42: 30S ribosomal protein S12

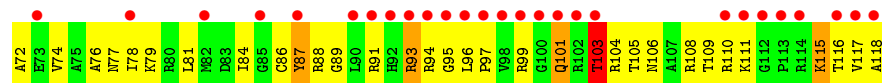
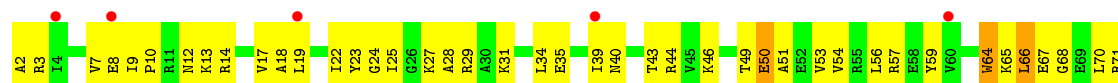


- Molecule 42: 30S ribosomal protein S12

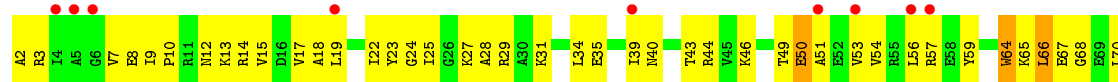
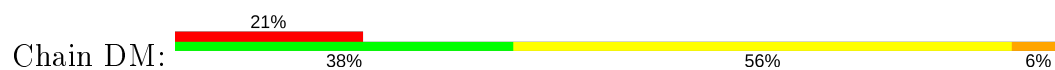




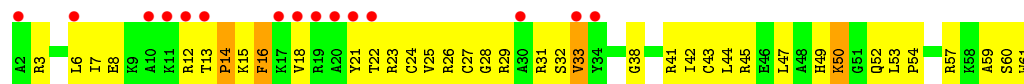
- Molecule 43: 30S ribosomal protein S13



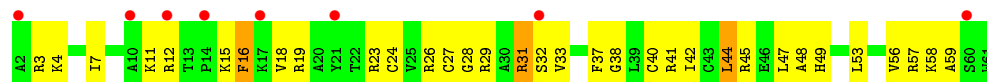
- Molecule 43: 30S ribosomal protein S13



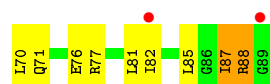
- Molecule 44: 30S ribosomal protein S14



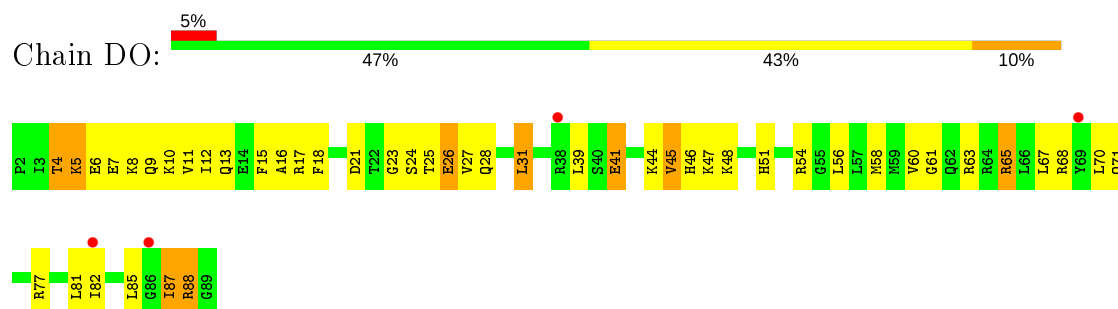
- Molecule 44: 30S ribosomal protein S14



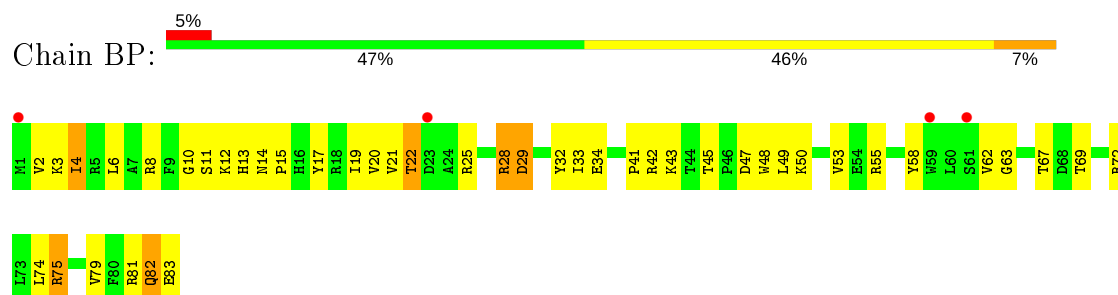
- Molecule 45: 30S ribosomal protein S15



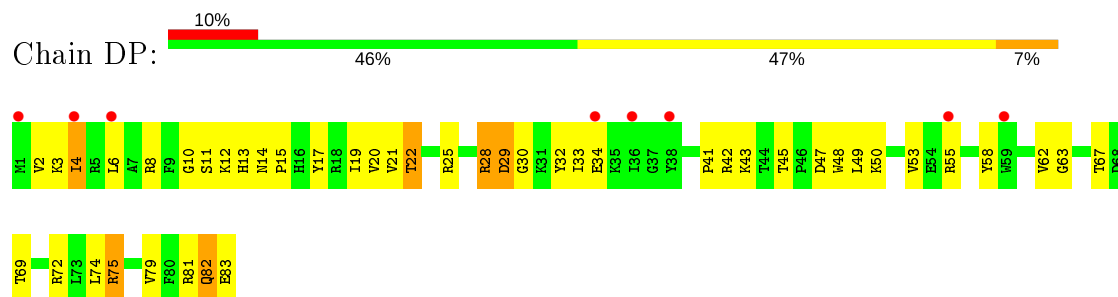
- Molecule 45: 30S ribosomal protein S15



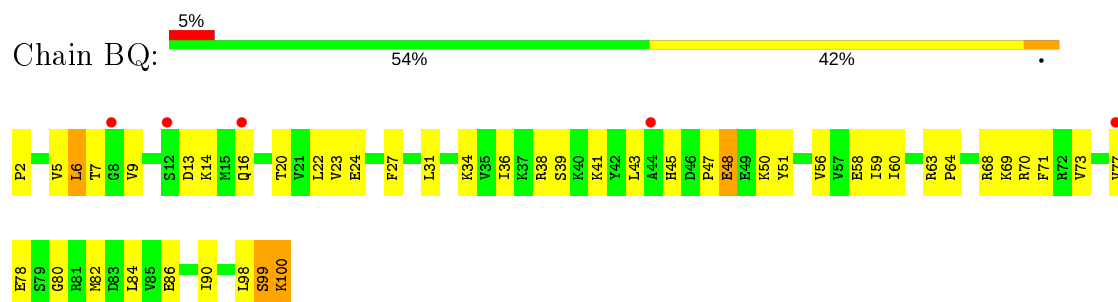
- Molecule 46: 30S ribosomal protein S16



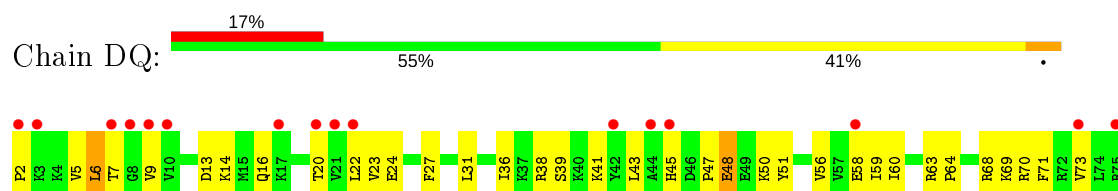
- Molecule 46: 30S ribosomal protein S16

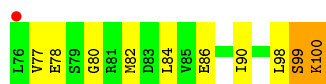


- Molecule 47: 30S ribosomal protein S17



- Molecule 47: 30S ribosomal protein S17

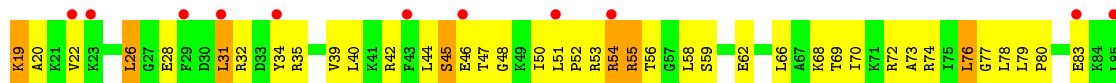




• Molecule 48: 30S ribosomal protein S18



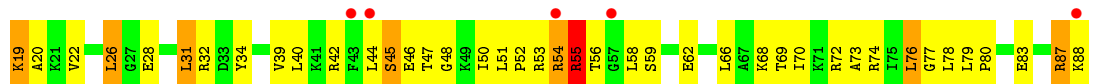
Chain BR:



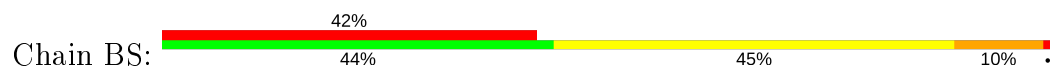
• Molecule 48: 30S ribosomal protein S18



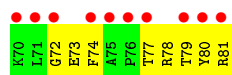
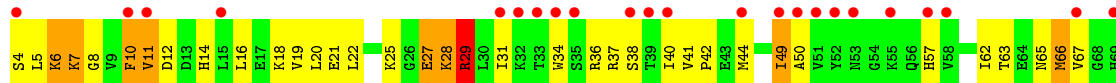
Chain DR:



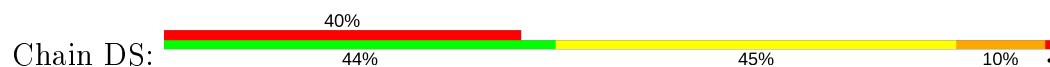
• Molecule 49: 30S ribosomal protein S19



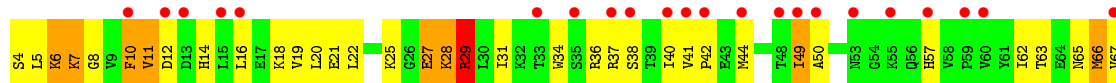
Chain BS:



• Molecule 49: 30S ribosomal protein S19



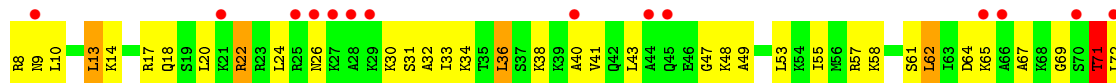
Chain DS:



• Molecule 50: 30S ribosomal protein S20

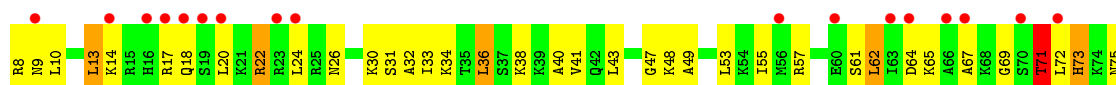
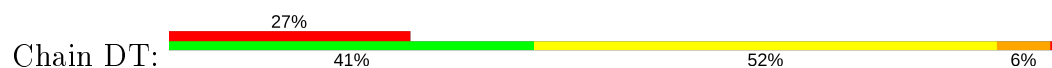


Chain BT:

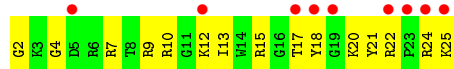
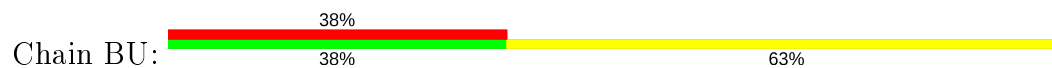




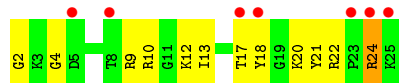
- Molecule 50: 30S ribosomal protein S20



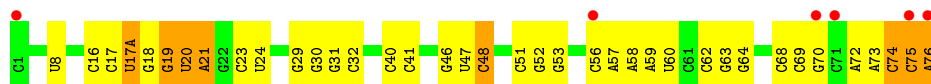
- Molecule 51: 30S ribosomal protein Thx



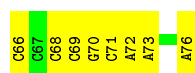
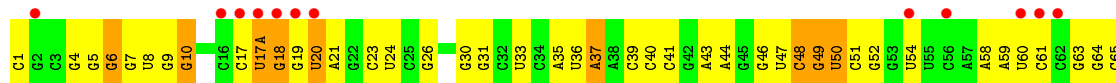
- Molecule 51: 30S ribosomal protein Thx



- Molecule 52: tRNA

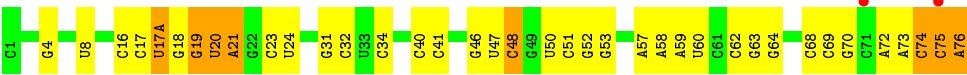


- Molecule 52: tRNA

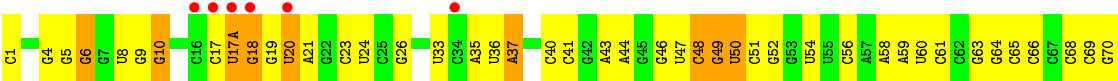


- Molecule 52: tRNA

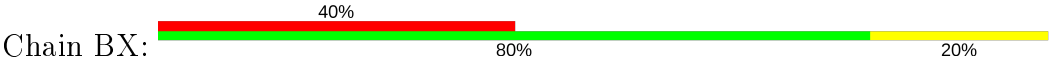




● Molecule 52: tRNA



● Molecule 53: mRNA



● Molecule 53: mRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 454.44Å 620.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.40 69.27 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.98-3.40) 99.6 (69.27-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486), CNS	Depositor
R, R_{free}	0.231 , 0.268 0.230 , 0.267	Depositor DCC
R_{free} test set	16247 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	293113	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, BLS

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	AA	0.34	1/68308 (0.0%)	0.64	11/106635 (0.0%)
1	CA	0.38	1/68308 (0.0%)	0.67	15/106635 (0.0%)
2	AB	0.31	1/2857 (0.0%)	0.52	0/4455
2	CB	0.32	1/2857 (0.0%)	0.53	0/4455
3	AD	0.31	0/2155	0.52	0/2905
3	CD	0.33	0/2155	0.53	0/2905
4	AE	0.27	0/1597	0.49	0/2153
4	CE	0.28	0/1597	0.49	0/2153
5	AF	0.27	0/1622	0.47	0/2194
5	CF	0.28	0/1622	0.47	0/2194
6	AG	0.22	0/1500	0.41	0/2017
6	CG	0.23	0/1500	0.41	0/2017
7	AH	0.22	0/1246	0.43	0/1682
7	CH	0.24	0/1246	0.44	0/1682
8	AI	0.22	0/1148	0.42	0/1552
8	CI	0.24	0/1148	0.43	0/1552
9	AJ	0.26	0/1124	0.49	0/1515
9	CJ	0.29	0/1124	0.50	0/1515
10	AK	0.28	0/942	0.46	0/1268
10	CK	0.28	0/942	0.46	0/1268
11	AL	0.31	0/1131	0.61	0/1504
11	CL	0.33	0/1131	0.62	0/1504
12	AM	0.28	0/1085	0.49	0/1449
12	CM	0.29	0/1085	0.49	0/1449
13	AN	0.28	0/974	0.47	0/1302
13	CN	0.28	0/974	0.48	0/1302
14	AO	0.24	0/779	0.43	0/1036
14	CO	0.25	0/779	0.43	0/1036
15	AP	0.27	0/1158	0.45	0/1544
15	CP	0.27	0/1158	0.45	0/1544
16	AQ	0.28	0/982	0.44	0/1306
16	CQ	0.30	0/982	0.45	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.29	0/790	0.51	0/1057
17	CR	0.31	0/790	0.52	0/1057
18	AS	0.28	0/902	0.46	0/1209
18	CS	0.30	0/902	0.47	0/1209
19	AT	0.29	0/740	0.46	0/993
19	CT	0.32	0/740	0.46	0/993
20	AU	0.30	0/789	0.46	0/1051
20	CU	0.31	0/789	0.47	0/1051
21	AV	0.22	0/1515	0.42	0/2056
21	CV	0.22	0/1515	0.42	0/2056
22	AW	0.28	0/613	0.47	0/816
22	CW	0.27	0/613	0.47	0/816
23	AX	0.32	0/702	0.56	0/932
23	CX	0.34	0/702	0.57	0/932
24	AY	0.27	0/523	0.49	0/690
24	CY	0.30	0/523	0.51	0/690
25	AZ	0.24	0/473	0.46	0/634
25	CZ	0.26	0/473	0.47	0/634
26	A1	0.20	0/229	0.42	0/309
26	C1	0.20	0/229	0.42	0/309
27	A2	0.28	0/419	0.52	0/567
27	C2	0.30	0/419	0.53	0/567
28	A3	0.21	0/388	0.44	0/518
28	C3	0.22	0/388	0.45	0/518
29	A4	0.31	0/427	0.50	0/561
29	C4	0.34	0/427	0.50	0/561
30	A5	0.32	0/516	0.52	0/679
30	C5	0.32	0/516	0.52	0/679
31	BA	0.28	1/36198 (0.0%)	0.55	0/56497
31	DA	0.27	1/36198 (0.0%)	0.55	0/56497
32	BB	0.22	0/1936	0.40	0/2609
32	DB	0.22	0/1936	0.40	0/2609
33	BC	0.22	0/1637	0.40	0/2205
33	DC	0.21	0/1637	0.40	0/2205
34	BD	0.27	0/1733	0.45	0/2318
34	DD	0.25	0/1733	0.42	0/2318
35	BE	0.24	0/1172	0.43	0/1576
35	DE	0.24	0/1172	0.42	0/1576
36	BF	0.24	0/856	0.43	0/1154
36	DF	0.25	0/856	0.44	0/1154
37	BG	0.22	0/1276	0.36	0/1709
37	DG	0.22	0/1276	0.37	0/1709
38	BH	0.23	0/1136	0.44	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DH	0.23	0/1136	0.44	0/1527
39	BI	0.22	0/1029	0.39	0/1378
39	DI	0.22	0/1029	0.39	0/1378
40	BJ	0.21	0/808	0.41	0/1085
40	DJ	0.21	0/808	0.41	0/1085
41	BK	0.23	0/857	0.44	0/1157
41	DK	0.23	0/857	0.44	0/1157
42	BL	0.25	0/973	0.46	0/1301
42	DL	0.25	0/973	0.46	0/1301
43	BM	0.21	0/944	0.41	0/1265
43	DM	0.21	0/944	0.41	0/1265
44	BN	0.24	0/501	0.39	0/664
44	DN	0.23	0/501	0.42	0/664
45	BO	0.25	0/745	0.40	0/992
45	DO	0.25	0/745	0.40	0/992
46	BP	0.26	0/717	0.45	0/963
46	DP	0.23	0/717	0.45	0/963
47	BQ	0.25	0/837	0.42	0/1117
47	DQ	0.25	0/837	0.42	0/1117
48	BR	0.24	0/579	0.44	0/768
48	DR	0.25	0/579	0.44	0/768
49	BS	0.20	0/643	0.40	0/865
49	DS	0.20	0/643	0.40	0/865
50	BT	0.24	0/764	0.42	0/1006
50	DT	0.22	0/764	0.41	0/1006
51	BU	0.20	0/213	0.37	0/277
51	DU	0.20	0/213	0.37	0/277
52	BV	0.21	0/1832	0.48	0/2855
52	BW	0.17	0/1832	0.44	0/2855
52	DV	0.21	0/1832	0.49	0/2855
52	DW	0.17	0/1832	0.44	0/2855
53	BX	0.26	0/122	0.47	0/188
53	DX	0.29	0/122	0.48	0/188
All	All	0.31	6/313948 (0.0%)	0.58	26/469840 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	AN	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	CN	0	1
All	All	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	5	U	OP3-P	-10.80	1.48	1.61
31	DA	5	U	OP3-P	-10.71	1.48	1.61
2	AB	1	U	OP3-P	-10.65	1.48	1.61
2	CB	1	U	OP3-P	-10.63	1.48	1.61
1	CA	6	A	OP3-P	-10.61	1.48	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1420	U	C2-N1-C1'	6.88	125.96	117.70
1	CA	1420	U	C2-N1-C1'	6.84	125.91	117.70
1	CA	1420	U	C6-N1-C1'	-6.61	111.95	121.20
1	AA	1420	U	C6-N1-C1'	-6.57	112.00	121.20
1	CA	2593	U	N3-C4-C5	-6.13	110.92	114.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	AN	10	LEU	Peptide
13	CN	10	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	60991	0	30744	1335	0
1	CA	60991	0	30744	1337	0
2	AB	2555	0	1294	52	0
2	CB	2555	0	1294	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AD	2105	0	2182	184	0
3	CD	2105	0	2182	187	0
4	AE	1564	0	1629	103	0
4	CE	1564	0	1629	115	0
5	AF	1587	0	1632	102	0
5	CF	1587	0	1632	102	0
6	AG	1475	0	1537	127	0
6	CG	1475	0	1537	127	0
7	AH	1223	0	1282	65	0
7	CH	1223	0	1282	65	0
8	AI	1133	0	1220	75	0
8	CI	1133	0	1220	87	0
9	AJ	1097	0	1168	80	0
9	CJ	1097	0	1168	82	0
10	AK	932	0	994	50	0
10	CK	932	0	994	48	0
11	AL	1114	0	1187	196	0
11	CL	1114	0	1187	203	0
12	AM	1065	0	1114	93	0
12	CM	1065	0	1114	97	0
13	AN	960	0	1021	81	0
13	CN	960	0	1021	76	0
14	AO	771	0	832	62	0
14	CO	771	0	832	66	0
15	AP	1144	0	1211	75	0
15	CP	1144	0	1211	91	0
16	AQ	964	0	1022	77	0
16	CQ	964	0	1022	79	0
17	AR	779	0	852	79	0
17	CR	779	0	852	82	0
18	AS	891	0	951	50	0
18	CS	891	0	951	58	0
19	AT	726	0	778	60	0
19	CT	726	0	778	59	0
20	AU	776	0	870	94	0
20	CU	776	0	870	93	0
21	AV	1483	0	1507	88	0
21	CV	1483	0	1507	92	0
22	AW	605	0	628	28	0
22	CW	605	0	628	27	0
23	AX	695	0	764	85	0
23	CX	695	0	764	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	AY	521	0	575	62	0
24	CY	521	0	575	67	0
25	AZ	468	0	523	23	0
25	CZ	468	0	523	25	0
26	A1	226	0	225	22	0
26	C1	226	0	225	22	0
27	A2	405	0	420	43	0
27	C2	405	0	420	44	0
28	A3	381	0	391	33	0
28	C3	381	0	391	34	0
29	A4	419	0	467	29	0
29	C4	419	0	467	29	0
30	A5	508	0	576	64	0
30	C5	508	0	576	64	0
31	BA	32336	0	16317	778	0
31	DA	32336	0	16317	795	0
32	BB	1901	0	1951	125	0
32	DB	1901	0	1951	124	0
33	BC	1613	0	1677	117	0
33	DC	1613	0	1677	112	0
34	BD	1703	0	1764	135	0
34	DD	1703	0	1764	168	0
35	BE	1156	0	1213	73	0
35	DE	1156	0	1213	78	0
36	BF	843	0	857	62	0
36	DF	843	0	857	64	0
37	BG	1257	0	1296	52	0
37	DG	1257	0	1296	53	0
38	BH	1116	0	1177	67	0
38	DH	1116	0	1177	65	0
39	BI	1011	0	1043	95	0
39	DI	1011	0	1043	93	0
40	BJ	795	0	840	62	0
40	DJ	795	0	840	65	0
41	BK	843	0	859	54	0
41	DK	843	0	859	58	0
42	BL	957	0	1046	68	0
42	DL	957	0	1046	67	0
43	BM	934	0	992	76	0
43	DM	934	0	992	79	0
44	BN	492	0	531	46	0
44	DN	492	0	531	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	BO	734	0	771	45	0
45	DO	734	0	771	42	0
46	BP	701	0	720	51	0
46	DP	701	0	720	54	0
47	BQ	824	0	893	42	0
47	DQ	824	0	893	42	0
48	BR	574	0	644	47	0
48	DR	574	0	644	47	0
49	BS	630	0	652	57	0
49	DS	630	0	652	56	0
50	BT	762	0	859	45	0
50	DT	762	0	859	46	0
51	BU	209	0	221	19	0
51	DU	209	0	221	14	0
52	BV	1640	0	837	41	0
52	BW	1640	0	837	52	0
52	DV	1640	0	837	40	0
52	DW	1640	0	837	46	0
53	BX	109	0	55	0	0
53	DX	109	0	55	1	0
54	AA	30	0	24	6	0
54	CA	30	0	24	6	0
55	A3	3	0	0	0	0
55	A4	5	0	0	0	0
55	A5	2	0	0	0	0
55	AA	1296	0	0	0	0
55	AB	50	0	0	0	0
55	AD	4	0	0	0	0
55	AE	4	0	0	0	0
55	AF	6	0	0	0	0
55	AG	2	0	0	0	0
55	AJ	1	0	0	0	0
55	AK	2	0	0	0	0
55	AL	2	0	0	0	0
55	AM	3	0	0	0	0
55	AN	4	0	0	0	0
55	AO	1	0	0	0	0
55	AP	2	0	0	0	0
55	AR	5	0	0	0	0
55	AS	6	0	0	0	0
55	AV	2	0	0	0	0
55	AX	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	AY	1	0	0	0	0
55	BA	570	0	0	0	0
55	BB	2	0	0	0	0
55	BC	3	0	0	0	0
55	BE	5	0	0	0	0
55	BG	2	0	0	0	0
55	BH	1	0	0	0	0
55	BI	2	0	0	0	0
55	BL	2	0	0	0	0
55	BO	1	0	0	0	0
55	BP	1	0	0	0	0
55	BQ	2	0	0	0	0
55	BR	1	0	0	0	0
55	BT	1	0	0	0	0
55	BU	1	0	0	0	0
55	BV	30	0	0	0	0
55	BW	19	0	0	0	0
55	C2	2	0	0	0	0
55	C3	2	0	0	0	0
55	C4	4	0	0	0	0
55	C5	3	0	0	0	0
55	CA	1504	0	0	0	0
55	CB	65	0	0	0	0
55	CD	6	0	0	0	0
55	CE	6	0	0	0	0
55	CF	7	0	0	0	0
55	CG	1	0	0	0	0
55	CI	1	0	0	0	0
55	CJ	2	0	0	0	0
55	CK	2	0	0	0	0
55	CL	7	0	0	0	0
55	CN	3	0	0	0	0
55	CO	1	0	0	0	0
55	CP	1	0	0	0	0
55	CQ	5	0	0	0	0
55	CR	2	0	0	0	0
55	CS	4	0	0	0	0
55	CT	1	0	0	0	0
55	CV	4	0	0	0	0
55	CW	4	0	0	0	0
55	CX	3	0	0	0	0
55	CY	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	DA	604	0	0	0	0
55	DD	2	0	0	0	0
55	DE	2	0	0	0	0
55	DG	1	0	0	0	0
55	DH	3	0	0	0	0
55	DI	1	0	0	0	0
55	DJ	1	0	0	0	0
55	DK	1	0	0	0	0
55	DL	2	0	0	0	0
55	DM	1	0	0	0	0
55	DO	2	0	0	0	0
55	DQ	1	0	0	0	0
55	DR	2	0	0	0	0
55	DT	1	0	0	0	0
55	DV	24	0	0	0	0
55	DW	22	0	0	0	0
55	DX	1	0	0	0	0
56	BD	1	0	0	0	0
56	BN	1	0	0	0	0
56	DD	1	0	0	0	0
56	DN	1	0	0	0	0
All	All	293113	0	195344	10300	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 21.

The worst 5 of 10300 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:AA:1541:U:H3'	1:AA:1542:G:H3'	1.16	1.16
1:CA:2502:G:H5'	1:CA:2503:A:H5''	1.29	1.14
1:AA:2502:G:H5'	1:AA:2503:A:H5''	1.28	1.14
1:CA:1541:U:H3'	1:CA:1542:G:H3'	1.16	1.12
1:CA:2303:G:H2'	1:CA:2304:G:H5''	1.33	1.10

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	AD	269/271 (99%)	220 (82%)	35 (13%)	14 (5%)	2	13
3	CD	269/271 (99%)	220 (82%)	35 (13%)	14 (5%)	2	13
4	AE	202/204 (99%)	164 (81%)	27 (13%)	11 (5%)	2	13
4	CE	202/204 (99%)	164 (81%)	27 (13%)	11 (5%)	2	13
5	AF	200/202 (99%)	168 (84%)	24 (12%)	8 (4%)	3	18
5	CF	200/202 (99%)	167 (84%)	25 (12%)	8 (4%)	3	18
6	AG	179/181 (99%)	128 (72%)	38 (21%)	13 (7%)	1	7
6	CG	179/181 (99%)	129 (72%)	36 (20%)	14 (8%)	1	6
7	AH	157/159 (99%)	122 (78%)	29 (18%)	6 (4%)	3	19
7	CH	157/159 (99%)	122 (78%)	29 (18%)	6 (4%)	3	19
8	AI	143/145 (99%)	120 (84%)	22 (15%)	1 (1%)	22	55
8	CI	143/145 (99%)	121 (85%)	21 (15%)	1 (1%)	22	55
9	AJ	135/137 (98%)	104 (77%)	21 (16%)	10 (7%)	1	7
9	CJ	135/137 (98%)	104 (77%)	21 (16%)	10 (7%)	1	7
10	AK	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	5	26
10	CK	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	4	22
11	AL	144/146 (99%)	89 (62%)	35 (24%)	20 (14%)	0	1
11	CL	144/146 (99%)	89 (62%)	34 (24%)	21 (15%)	0	1
12	AM	132/134 (98%)	96 (73%)	21 (16%)	15 (11%)	0	3
12	CM	132/134 (98%)	96 (73%)	22 (17%)	14 (11%)	0	3
13	AN	115/117 (98%)	92 (80%)	15 (13%)	8 (7%)	1	7
13	CN	115/117 (98%)	92 (80%)	15 (13%)	8 (7%)	1	7
14	AO	96/98 (98%)	65 (68%)	23 (24%)	8 (8%)	1	5
14	CO	96/98 (98%)	65 (68%)	22 (23%)	9 (9%)	0	4
15	AP	135/137 (98%)	105 (78%)	22 (16%)	8 (6%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CP	135/137 (98%)	104 (77%)	23 (17%)	8 (6%)	1	11
16	AQ	115/117 (98%)	102 (89%)	10 (9%)	3 (3%)	5	26
16	CQ	115/117 (98%)	102 (89%)	10 (9%)	3 (3%)	5	26
17	AR	99/101 (98%)	79 (80%)	16 (16%)	4 (4%)	3	18
17	CR	99/101 (98%)	78 (79%)	17 (17%)	4 (4%)	3	18
18	AS	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
18	CS	110/112 (98%)	99 (90%)	11 (10%)	0	100	100
19	AT	90/92 (98%)	76 (84%)	12 (13%)	2 (2%)	6	29
19	CT	90/92 (98%)	75 (83%)	13 (14%)	2 (2%)	6	29
20	AU	98/100 (98%)	63 (64%)	23 (24%)	12 (12%)	0	2
20	CU	98/100 (98%)	65 (66%)	21 (21%)	12 (12%)	0	2
21	AV	185/187 (99%)	159 (86%)	19 (10%)	7 (4%)	3	19
21	CV	185/187 (99%)	159 (86%)	19 (10%)	7 (4%)	3	19
22	AW	74/76 (97%)	59 (80%)	13 (18%)	2 (3%)	5	26
22	CW	74/76 (97%)	59 (80%)	13 (18%)	2 (3%)	5	26
23	AX	86/88 (98%)	56 (65%)	19 (22%)	11 (13%)	0	2
23	CX	86/88 (98%)	56 (65%)	19 (22%)	11 (13%)	0	2
24	AY	60/62 (97%)	47 (78%)	8 (13%)	5 (8%)	1	5
24	CY	60/62 (97%)	47 (78%)	8 (13%)	5 (8%)	1	5
25	AZ	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	8	32
25	CZ	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	8	32
26	A1	28/30 (93%)	13 (46%)	13 (46%)	2 (7%)	1	7
26	C1	28/30 (93%)	13 (46%)	13 (46%)	2 (7%)	1	7
27	A2	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	18
27	C2	50/52 (96%)	45 (90%)	3 (6%)	2 (4%)	3	18
28	A3	42/44 (96%)	26 (62%)	12 (29%)	4 (10%)	0	4
28	C3	42/44 (96%)	26 (62%)	12 (29%)	4 (10%)	0	4
29	A4	46/48 (96%)	44 (96%)	1 (2%)	1 (2%)	6	29
29	C4	46/48 (96%)	44 (96%)	1 (2%)	1 (2%)	6	29
30	A5	61/63 (97%)	46 (75%)	9 (15%)	6 (10%)	0	4
30	C5	61/63 (97%)	46 (75%)	9 (15%)	6 (10%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BB	232/234 (99%)	183 (79%)	36 (16%)	13 (6%)	2	12
32	DB	232/234 (99%)	183 (79%)	36 (16%)	13 (6%)	2	12
33	BC	204/206 (99%)	159 (78%)	28 (14%)	17 (8%)	1	5
33	DC	204/206 (99%)	158 (78%)	28 (14%)	18 (9%)	1	5
34	BD	206/208 (99%)	161 (78%)	34 (16%)	11 (5%)	2	13
34	DD	206/208 (99%)	161 (78%)	34 (16%)	11 (5%)	2	13
35	BE	149/151 (99%)	120 (80%)	26 (17%)	3 (2%)	7	30
35	DE	149/151 (99%)	120 (80%)	25 (17%)	4 (3%)	5	26
36	BF	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15	46
36	DF	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	15	46
37	BG	153/155 (99%)	131 (86%)	17 (11%)	5 (3%)	4	22
37	DG	153/155 (99%)	131 (86%)	15 (10%)	7 (5%)	2	15
38	BH	136/138 (99%)	114 (84%)	20 (15%)	2 (2%)	10	36
38	DH	136/138 (99%)	113 (83%)	21 (15%)	2 (2%)	10	36
39	BI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	1	9
39	DI	125/127 (98%)	92 (74%)	25 (20%)	8 (6%)	1	9
40	BJ	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	2	13
40	DJ	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	2	13
41	BK	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	3	21
41	DK	112/114 (98%)	94 (84%)	14 (12%)	4 (4%)	3	21
42	BL	120/122 (98%)	94 (78%)	22 (18%)	4 (3%)	4	22
42	DL	120/122 (98%)	93 (78%)	23 (19%)	4 (3%)	4	22
43	BM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	26
43	DM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	26
44	BN	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	13
44	DN	58/60 (97%)	43 (74%)	12 (21%)	3 (5%)	2	13
45	BO	86/88 (98%)	75 (87%)	9 (10%)	2 (2%)	6	28
45	DO	86/88 (98%)	74 (86%)	10 (12%)	2 (2%)	6	28
46	BP	81/83 (98%)	65 (80%)	13 (16%)	3 (4%)	3	20
46	DP	81/83 (98%)	66 (82%)	12 (15%)	3 (4%)	3	20
47	BQ	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DQ	97/99 (98%)	80 (82%)	14 (14%)	3 (3%)	4	23
48	BR	68/70 (97%)	55 (81%)	8 (12%)	5 (7%)	1	7
48	DR	68/70 (97%)	55 (81%)	8 (12%)	5 (7%)	1	7
49	BS	76/78 (97%)	57 (75%)	12 (16%)	7 (9%)	1	4
49	DS	76/78 (97%)	58 (76%)	11 (14%)	7 (9%)	1	4
50	BT	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	1	10
50	DT	97/99 (98%)	75 (77%)	16 (16%)	6 (6%)	1	10
51	BU	22/24 (92%)	16 (73%)	5 (23%)	1 (4%)	2	16
51	DU	22/24 (92%)	16 (73%)	5 (23%)	1 (4%)	2	16
All	All	11120/11312 (98%)	8857 (80%)	1670 (15%)	593 (5%)	2	13

5 of 593 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	33	LEU
3	AD	40	THR
3	AD	59	LYS
3	AD	239	ARG
4	AE	86	PRO

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	AD	213/213 (100%)	187 (88%)	26 (12%)	5	18
3	CD	213/213 (100%)	188 (88%)	25 (12%)	5	20
4	AE	165/165 (100%)	147 (89%)	18 (11%)	6	23
4	CE	165/165 (100%)	147 (89%)	18 (11%)	6	23
5	AF	161/161 (100%)	143 (89%)	18 (11%)	6	22
5	CF	161/161 (100%)	143 (89%)	18 (11%)	6	22
6	AG	155/155 (100%)	138 (89%)	17 (11%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CG	155/155 (100%)	137 (88%)	18 (12%)	5	20
7	AH	132/132 (100%)	119 (90%)	13 (10%)	8	28
7	CH	132/132 (100%)	119 (90%)	13 (10%)	8	28
8	AI	122/122 (100%)	107 (88%)	15 (12%)	4	17
8	CI	122/122 (100%)	107 (88%)	15 (12%)	4	17
9	AJ	116/116 (100%)	103 (89%)	13 (11%)	6	22
9	CJ	116/116 (100%)	102 (88%)	14 (12%)	5	18
10	AK	100/100 (100%)	91 (91%)	9 (9%)	9	32
10	CK	100/100 (100%)	91 (91%)	9 (9%)	9	32
11	AL	112/112 (100%)	86 (77%)	26 (23%)	1	2
11	CL	112/112 (100%)	86 (77%)	26 (23%)	1	2
12	AM	105/105 (100%)	92 (88%)	13 (12%)	4	17
12	CM	105/105 (100%)	92 (88%)	13 (12%)	4	17
13	AN	100/100 (100%)	86 (86%)	14 (14%)	3	13
13	CN	100/100 (100%)	86 (86%)	14 (14%)	3	13
14	AO	77/77 (100%)	64 (83%)	13 (17%)	2	8
14	CO	77/77 (100%)	64 (83%)	13 (17%)	2	8
15	AP	121/121 (100%)	102 (84%)	19 (16%)	2	10
15	CP	121/121 (100%)	102 (84%)	19 (16%)	2	10
16	AQ	93/93 (100%)	84 (90%)	9 (10%)	8	28
16	CQ	93/93 (100%)	85 (91%)	8 (9%)	10	35
17	AR	82/82 (100%)	67 (82%)	15 (18%)	1	5
17	CR	82/82 (100%)	66 (80%)	16 (20%)	1	4
18	AS	91/91 (100%)	82 (90%)	9 (10%)	8	27
18	CS	91/91 (100%)	81 (89%)	10 (11%)	6	23
19	AT	74/74 (100%)	66 (89%)	8 (11%)	6	24
19	CT	74/74 (100%)	66 (89%)	8 (11%)	6	24
20	AU	84/84 (100%)	70 (83%)	14 (17%)	2	8
20	CU	84/84 (100%)	70 (83%)	14 (17%)	2	8
21	AV	162/162 (100%)	152 (94%)	10 (6%)	18	48
21	CV	162/162 (100%)	152 (94%)	10 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	AW	61/61 (100%)	55 (90%)	6 (10%)	8	28
22	CW	61/61 (100%)	55 (90%)	6 (10%)	8	28
23	AX	73/73 (100%)	65 (89%)	8 (11%)	6	23
23	CX	73/73 (100%)	64 (88%)	9 (12%)	4	17
24	AY	58/58 (100%)	51 (88%)	7 (12%)	5	18
24	CY	58/58 (100%)	51 (88%)	7 (12%)	5	18
25	AZ	51/51 (100%)	45 (88%)	6 (12%)	5	19
25	CZ	51/51 (100%)	45 (88%)	6 (12%)	5	19
26	A1	27/27 (100%)	24 (89%)	3 (11%)	6	22
26	C1	27/27 (100%)	24 (89%)	3 (11%)	6	22
27	A2	45/45 (100%)	40 (89%)	5 (11%)	6	22
27	C2	45/45 (100%)	40 (89%)	5 (11%)	6	22
28	A3	43/43 (100%)	40 (93%)	3 (7%)	15	44
28	C3	43/43 (100%)	40 (93%)	3 (7%)	15	44
29	A4	41/41 (100%)	33 (80%)	8 (20%)	1	4
29	C4	41/41 (100%)	33 (80%)	8 (20%)	1	4
30	A5	53/53 (100%)	49 (92%)	4 (8%)	13	41
30	C5	53/53 (100%)	49 (92%)	4 (8%)	13	41
32	BB	202/202 (100%)	184 (91%)	18 (9%)	9	33
32	DB	202/202 (100%)	184 (91%)	18 (9%)	9	33
33	BC	160/160 (100%)	144 (90%)	16 (10%)	7	27
33	DC	160/160 (100%)	144 (90%)	16 (10%)	7	27
34	BD	180/180 (100%)	156 (87%)	24 (13%)	4	15
34	DD	180/180 (100%)	159 (88%)	21 (12%)	5	20
35	BE	116/116 (100%)	103 (89%)	13 (11%)	6	22
35	DE	116/116 (100%)	104 (90%)	12 (10%)	7	26
36	BF	90/90 (100%)	78 (87%)	12 (13%)	4	15
36	DF	90/90 (100%)	78 (87%)	12 (13%)	4	15
37	BG	126/126 (100%)	120 (95%)	6 (5%)	25	56
37	DG	126/126 (100%)	120 (95%)	6 (5%)	25	56
38	BH	119/119 (100%)	105 (88%)	14 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DH	119/119 (100%)	105 (88%)	14 (12%)	5	19
39	BI	98/98 (100%)	87 (89%)	11 (11%)	6	22
39	DI	98/98 (100%)	87 (89%)	11 (11%)	6	22
40	BJ	88/88 (100%)	79 (90%)	9 (10%)	7	26
40	DJ	88/88 (100%)	79 (90%)	9 (10%)	7	26
41	BK	86/86 (100%)	77 (90%)	9 (10%)	7	25
41	DK	86/86 (100%)	77 (90%)	9 (10%)	7	25
42	BL	103/103 (100%)	93 (90%)	10 (10%)	8	28
42	DL	103/103 (100%)	93 (90%)	10 (10%)	8	28
43	BM	94/94 (100%)	83 (88%)	11 (12%)	5	20
43	DM	94/94 (100%)	83 (88%)	11 (12%)	5	20
44	BN	49/49 (100%)	46 (94%)	3 (6%)	18	48
44	DN	49/49 (100%)	46 (94%)	3 (6%)	18	48
45	BO	79/79 (100%)	69 (87%)	10 (13%)	4	16
45	DO	79/79 (100%)	69 (87%)	10 (13%)	4	16
46	BP	72/72 (100%)	65 (90%)	7 (10%)	8	28
46	DP	72/72 (100%)	65 (90%)	7 (10%)	8	28
47	BQ	94/94 (100%)	90 (96%)	4 (4%)	29	59
47	DQ	94/94 (100%)	90 (96%)	4 (4%)	29	59
48	BR	61/61 (100%)	56 (92%)	5 (8%)	11	37
48	DR	61/61 (100%)	55 (90%)	6 (10%)	8	28
49	BS	69/69 (100%)	61 (88%)	8 (12%)	5	20
49	DS	69/69 (100%)	61 (88%)	8 (12%)	5	20
50	BT	76/76 (100%)	68 (90%)	8 (10%)	7	25
50	DT	76/76 (100%)	68 (90%)	8 (10%)	7	25
51	BU	19/19 (100%)	19 (100%)	0	100	100
51	DU	19/19 (100%)	19 (100%)	0	100	100
All	All	9396/9396 (100%)	8342 (89%)	1054 (11%)	6	22

5 of 1054 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BM	87	TYR

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Mol	Chain	Res	Type
6	CG	34	LEU
40	DJ	62	HIS
45	BO	41	GLU
3	CD	106	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 216 such sidechains are listed below:

Mol	Chain	Res	Type
43	BM	101	GLN
5	CF	67	GLN
41	DK	117	ASN
45	BO	37	ASN
50	BT	73	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2830/2879 (98%)	442 (15%)	15 (0%)
1	CA	2830/2879 (98%)	441 (15%)	15 (0%)
2	AB	118/119 (99%)	9 (7%)	0
2	CB	118/119 (99%)	9 (7%)	0
31	BA	1504/1504 (100%)	204 (13%)	12 (0%)
31	DA	1504/1504 (100%)	205 (13%)	12 (0%)
52	BV	76/77 (98%)	11 (14%)	0
52	BW	76/77 (98%)	12 (15%)	1 (1%)
52	DV	76/77 (98%)	11 (14%)	0
52	DW	76/77 (98%)	12 (15%)	1 (1%)
53	BX	4/5 (80%)	1 (25%)	0
53	DX	4/5 (80%)	1 (25%)	0
All	All	9216/9322 (98%)	1358 (14%)	56 (0%)

5 of 1358 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	11	G
1	AA	34	C
1	AA	35	G
1	AA	46	C
1	AA	49	A

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	BA	1285	A
1	CA	616	A
31	DA	748	C
31	BA	1504	G
1	CA	34	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4369 ligands modelled in this entry, 4367 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	BLS	CA	4405	-	25,31,31	3.33	9 (36%)	23,43,43	2.65	8 (34%)
54	BLS	AA	4001	-	25,31,31	3.33	9 (36%)	23,43,43	2.56	8 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	BLS	CA	4405	-	-	7/17/38/38	0/2/2/2
54	BLS	AA	4001	-	-	7/17/38/38	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	AA	4001	BLS	C14-N12	8.72	1.54	1.35
54	CA	4405	BLS	C14-N12	8.66	1.54	1.35
54	AA	4001	BLS	C7-N6	7.08	1.49	1.34
54	CA	4405	BLS	C7-N6	7.02	1.49	1.34
54	CA	4405	BLS	O5'-C5'	5.91	1.51	1.44

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	AA	4001	BLS	C1'-C2'-C3'	-8.43	111.48	122.52
54	CA	4405	BLS	C1'-C2'-C3'	-8.05	111.98	122.52
54	CA	4405	BLS	O5'-C1'-C2'	-6.21	109.77	113.13
54	AA	4001	BLS	O5'-C1'-C2'	-4.91	110.48	113.13
54	CA	4405	BLS	C4'-N6-C7	-2.95	119.97	123.13

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	AA	4001	BLS	C10-C11-N12-C13
54	AA	4001	BLS	C10-C11-N12-C14
54	CA	4405	BLS	C10-C11-N12-C13
54	CA	4405	BLS	C10-C11-N12-C14
54	AA	4001	BLS	N6-C7-C8-C9

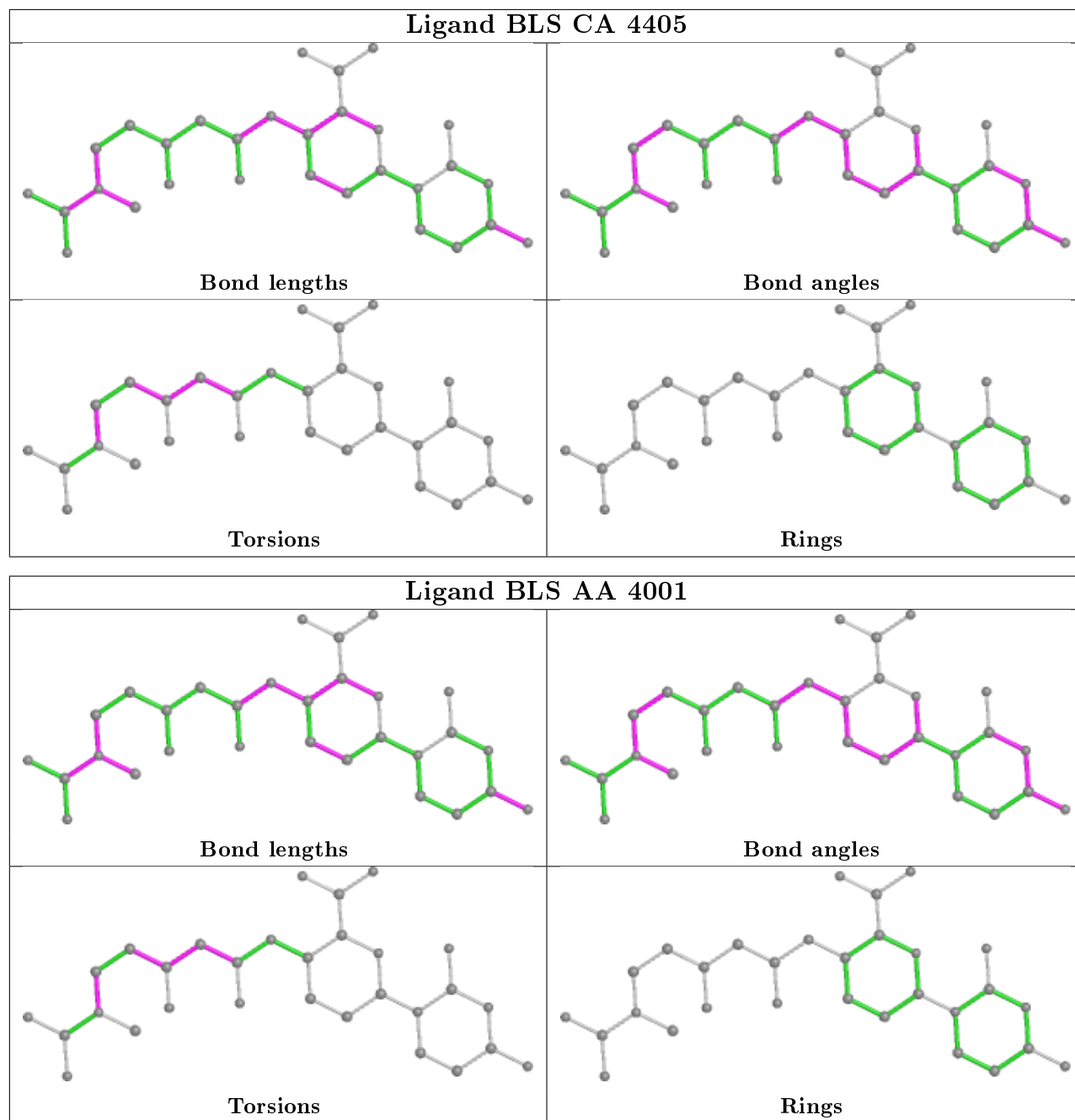
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	CA	4405	BLS	6	0
54	AA	4001	BLS	6	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2832/2879 (98%)	0.44	125 (4%) 34 34	29, 68, 217, 367	0
1	CA	2832/2879 (98%)	0.39	105 (3%) 41 40	22, 55, 182, 409	0
2	AB	119/119 (100%)	0.11	2 (1%) 70 68	68, 117, 172, 246	0
2	CB	119/119 (100%)	0.09	1 (0%) 86 85	54, 97, 141, 234	0
3	AD	271/271 (100%)	0.01	2 (0%) 87 87	23, 61, 104, 243	0
3	CD	271/271 (100%)	0.09	1 (0%) 92 92	7, 46, 92, 203	0
4	AE	204/204 (100%)	0.79	29 (14%) 2 3	20, 77, 134, 263	0
4	CE	204/204 (100%)	0.23	4 (1%) 65 64	13, 60, 116, 249	0
5	AF	202/202 (100%)	0.49	3 (1%) 73 72	27, 67, 131, 220	0
5	CF	202/202 (100%)	0.47	7 (3%) 44 43	9, 58, 130, 240	0
6	AG	181/181 (100%)	1.20	38 (20%) 1 1	75, 134, 205, 230	0
6	CG	181/181 (100%)	1.01	35 (19%) 1 1	53, 117, 201, 226	0
7	AH	159/159 (100%)	3.32	118 (74%) 0 0	88, 157, 258, 279	0
7	CH	159/159 (100%)	1.33	47 (29%) 0 0	39, 83, 142, 266	0
8	AI	145/145 (100%)	1.34	43 (29%) 0 0	46, 131, 204, 288	0
8	CI	145/145 (100%)	0.75	14 (9%) 7 9	37, 103, 167, 210	0
9	AJ	137/137 (100%)	0.53	7 (5%) 28 28	49, 80, 142, 172	0
9	CJ	137/137 (100%)	0.26	1 (0%) 87 87	28, 62, 113, 213	0
10	AK	122/122 (100%)	0.05	2 (1%) 72 70	30, 68, 109, 168	0
10	CK	122/122 (100%)	0.41	5 (4%) 37 36	21, 60, 105, 134	0
11	AL	146/146 (100%)	1.22	28 (19%) 1 1	19, 91, 177, 263	0
11	CL	146/146 (100%)	0.68	8 (5%) 25 25	17, 80, 168, 236	0
12	AM	134/134 (100%)	0.66	7 (5%) 27 27	41, 82, 166, 289	0
12	CM	134/134 (100%)	1.10	19 (14%) 2 3	26, 68, 159, 293	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	AN	117/117 (100%)	0.89	14 (11%)	4	5	19, 72, 139, 184	0
13	CN	117/117 (100%)	0.84	15 (12%)	3	4	16, 60, 111, 207	0
14	AO	98/98 (100%)	1.63	34 (34%)	0	0	63, 120, 186, 243	0
14	CO	98/98 (100%)	1.08	21 (21%)	0	1	63, 97, 157, 178	0
15	AP	137/137 (100%)	0.24	4 (2%)	51	50	41, 82, 160, 246	0
15	CP	137/137 (100%)	0.41	9 (6%)	18	20	30, 74, 184, 271	0
16	AQ	117/117 (100%)	0.57	4 (3%)	45	44	27, 69, 121, 162	0
16	CQ	117/117 (100%)	0.06	1 (0%)	84	83	21, 50, 108, 206	0
17	AR	101/101 (100%)	0.49	5 (4%)	28	29	30, 93, 142, 223	0
17	CR	101/101 (100%)	0.40	1 (0%)	82	81	27, 68, 117, 256	0
18	AS	112/112 (100%)	0.61	5 (4%)	33	33	32, 61, 131, 252	0
18	CS	112/112 (100%)	0.19	2 (1%)	68	67	20, 48, 103, 203	0
19	AT	92/92 (100%)	0.60	8 (8%)	10	12	38, 81, 117, 172	0
19	CT	92/92 (100%)	0.92	4 (4%)	35	35	23, 59, 107, 160	0
20	AU	100/100 (100%)	1.91	34 (34%)	0	0	49, 97, 234, 307	0
20	CU	100/100 (100%)	1.31	18 (18%)	1	1	32, 75, 247, 286	0
21	AV	187/187 (100%)	0.96	27 (14%)	2	3	61, 121, 189, 251	0
21	CV	187/187 (100%)	1.21	40 (21%)	0	1	36, 113, 183, 227	0
22	AW	76/76 (100%)	0.77	6 (7%)	12	14	40, 74, 133, 245	0
22	CW	76/76 (100%)	0.50	3 (3%)	39	38	36, 70, 138, 207	0
23	AX	88/88 (100%)	1.30	16 (18%)	1	1	28, 69, 147, 186	0
23	CX	88/88 (100%)	1.03	12 (13%)	3	3	25, 59, 136, 242	0
24	AY	62/62 (100%)	1.65	21 (33%)	0	0	49, 98, 175, 228	0
24	CY	62/62 (100%)	0.94	7 (11%)	5	6	20, 69, 165, 252	0
25	AZ	59/59 (100%)	0.87	6 (10%)	6	8	46, 80, 146, 204	0
25	CZ	59/59 (100%)	0.37	4 (6%)	17	19	30, 65, 134, 194	0
26	A1	30/30 (100%)	2.26	15 (50%)	0	0	129, 198, 264, 286	0
26	C1	30/30 (100%)	2.72	21 (70%)	0	0	151, 200, 258, 294	0
27	A2	52/52 (100%)	0.28	2 (3%)	40	39	27, 67, 144, 206	0
27	C2	52/52 (100%)	-0.01	1 (1%)	66	65	12, 57, 127, 206	0
28	A3	44/44 (100%)	4.64	38 (86%)	0	0	99, 175, 241, 280	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C3	44/44 (100%)	4.97	42 (95%) 0 0	96, 147, 206, 246	0
29	A4	48/48 (100%)	-0.02	1 (2%) 63 62	26, 53, 102, 159	0
29	C4	48/48 (100%)	-0.07	1 (2%) 63 62	11, 31, 82, 126	0
30	A5	63/63 (100%)	0.56	4 (6%) 20 21	38, 66, 133, 226	0
30	C5	63/63 (100%)	0.39	3 (4%) 30 31	16, 62, 135, 154	0
31	BA	1504/1504 (100%)	0.37	35 (2%) 60 59	44, 89, 187, 268	0
31	DA	1504/1504 (100%)	0.60	74 (4%) 29 29	41, 108, 215, 364	0
32	BB	234/234 (100%)	0.93	32 (13%) 3 3	65, 131, 205, 270	0
32	DB	234/234 (100%)	0.97	46 (19%) 1 1	83, 146, 214, 282	0
33	BC	206/206 (100%)	0.22	7 (3%) 45 44	68, 121, 178, 219	0
33	DC	206/206 (100%)	0.55	15 (7%) 15 17	70, 145, 214, 286	0
34	BD	208/208 (100%)	0.59	10 (4%) 30 31	25, 79, 128, 152	0
34	DD	208/208 (100%)	1.27	51 (24%) 0 0	48, 115, 180, 240	0
35	BE	151/151 (100%)	0.36	3 (1%) 65 64	44, 84, 135, 189	0
35	DE	151/151 (100%)	0.51	6 (3%) 38 37	51, 101, 161, 233	0
36	BF	101/101 (100%)	0.58	5 (4%) 28 29	56, 99, 141, 177	0
36	DF	101/101 (100%)	0.22	3 (2%) 50 49	45, 87, 140, 166	0
37	BG	155/155 (100%)	0.75	23 (14%) 2 3	69, 123, 171, 218	0
37	DG	155/155 (100%)	0.67	20 (12%) 3 4	75, 128, 179, 227	0
38	BH	138/138 (100%)	0.60	5 (3%) 42 42	56, 86, 136, 184	0
38	DH	138/138 (100%)	0.74	16 (11%) 4 5	53, 101, 149, 194	0
39	BI	127/127 (100%)	1.60	41 (32%) 0 0	67, 148, 212, 269	0
39	DI	127/127 (100%)	1.30	37 (29%) 0 0	82, 157, 214, 266	0
40	BJ	98/98 (100%)	1.38	25 (25%) 0 0	77, 145, 238, 266	0
40	DJ	98/98 (100%)	2.52	44 (44%) 0 0	89, 177, 249, 277	0
41	BK	114/114 (100%)	1.21	22 (19%) 1 1	46, 91, 139, 207	0
41	DK	114/114 (100%)	1.19	22 (19%) 1 1	50, 84, 144, 196	0
42	BL	122/122 (100%)	1.08	24 (19%) 1 1	36, 78, 126, 184	0
42	DL	122/122 (100%)	1.25	31 (25%) 0 0	47, 98, 147, 236	0
43	BM	117/117 (100%)	1.26	32 (27%) 0 0	80, 146, 214, 228	0
43	DM	117/117 (100%)	1.22	24 (20%) 1 1	84, 150, 203, 267	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BN	60/60 (100%)	1.21	15 (25%) 0 0	63, 115, 155, 210	0
44	DN	60/60 (100%)	0.93	8 (13%) 3 4	60, 130, 192, 250	0
45	BO	88/88 (100%)	0.75	6 (6%) 17 19	50, 87, 143, 170	0
45	DO	88/88 (100%)	0.49	4 (4%) 33 33	46, 82, 130, 168	0
46	BP	83/83 (100%)	0.67	4 (4%) 30 31	35, 76, 124, 161	0
46	DP	83/83 (100%)	0.90	8 (9%) 8 9	67, 110, 171, 274	0
47	BQ	99/99 (100%)	0.66	5 (5%) 28 28	43, 83, 127, 186	0
47	DQ	99/99 (100%)	1.03	17 (17%) 1 1	57, 93, 134, 200	0
48	BR	70/70 (100%)	1.10	12 (17%) 1 2	45, 95, 159, 191	0
48	DR	70/70 (100%)	0.69	5 (7%) 16 18	49, 92, 161, 188	0
49	BS	78/78 (100%)	1.87	33 (42%) 0 0	103, 145, 213, 241	0
49	DS	78/78 (100%)	1.93	31 (39%) 0 0	93, 158, 216, 254	0
50	BT	99/99 (100%)	1.23	19 (19%) 1 1	42, 95, 175, 218	0
50	DT	99/99 (100%)	1.36	27 (27%) 0 0	66, 122, 199, 230	0
51	BU	24/24 (100%)	1.67	9 (37%) 0 0	107, 163, 225, 270	0
51	DU	24/24 (100%)	1.45	7 (29%) 0 0	73, 151, 199, 257	0
52	BV	77/77 (100%)	0.36	6 (7%) 13 14	80, 135, 208, 244	0
52	BW	77/77 (100%)	0.82	12 (15%) 2 2	71, 190, 252, 308	0
52	DV	77/77 (100%)	0.26	2 (2%) 56 54	77, 122, 191, 213	0
52	DW	77/77 (100%)	0.46	6 (7%) 13 14	62, 173, 228, 302	0
53	BX	5/5 (100%)	1.65	2 (40%) 0 0	72, 73, 112, 168	0
53	DX	5/5 (100%)	1.15	0 100 100	65, 67, 128, 182	0
All	All	20540/20634 (99%)	0.68	1991 (9%) 7 9	7, 85, 195, 409	0

The worst 5 of 1991 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	275	G	20.7
11	AL	150	ALA	15.4
49	BS	81	ARG	14.2
28	A3	26	ASN	14.1
28	A3	14	THR	13.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DW	111	1/1	-0.46	0.14	136,136,136,136	0
55	MG	CA	3903	1/1	-0.38	0.29	135,135,135,135	0
55	MG	BA	2106	1/1	-0.24	0.78	124,124,124,124	0
55	MG	CA	3586	1/1	-0.07	1.27	105,105,105,105	0
55	MG	DA	1638	1/1	-0.01	1.01	126,126,126,126	0
55	MG	BA	1610	1/1	0.01	0.64	93,93,93,93	0
55	MG	DA	1953	1/1	0.04	0.11	140,140,140,140	0
55	MG	BA	1653	1/1	0.06	0.76	76,76,76,76	0
55	MG	CA	2977	1/1	0.07	0.86	88,88,88,88	0
55	MG	AA	4684	1/1	0.09	0.61	73,73,73,73	0
55	MG	DA	1939	1/1	0.10	1.19	214,214,214,214	0
55	MG	AA	5267	1/1	0.13	0.76	96,96,96,96	0
55	MG	AA	5264	1/1	0.15	0.99	87,87,87,87	0
55	MG	DA	2172	1/1	0.16	0.55	96,96,96,96	0
55	MG	CA	3013	1/1	0.17	0.89	128,128,128,128	0
55	MG	CA	4358	1/1	0.19	1.49	78,78,78,78	0
55	MG	DA	1949	1/1	0.19	0.46	88,88,88,88	0
55	MG	CA	3949	1/1	0.19	0.82	110,110,110,110	0
55	MG	DA	1913	1/1	0.19	0.45	93,93,93,93	0
55	MG	AA	4979	1/1	0.20	0.67	83,83,83,83	0
55	MG	DA	1898	1/1	0.20	0.66	96,96,96,96	0
55	MG	CA	4403	1/1	0.20	0.34	175,175,175,175	0
55	MG	DA	2122	1/1	0.22	0.32	150,150,150,150	0
55	MG	DA	1917	1/1	0.22	0.09	143,143,143,143	0
55	MG	DA	1650	1/1	0.23	0.93	116,116,116,116	0
55	MG	CA	3804	1/1	0.24	0.41	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4539	1/1	0.24	0.52	90,90,90,90	0
55	MG	DA	1916	1/1	0.24	0.78	87,87,87,87	0
55	MG	BA	2097	1/1	0.24	0.68	95,95,95,95	0
55	MG	AA	4807	1/1	0.26	0.91	88,88,88,88	0
55	MG	AA	4972	1/1	0.26	0.92	171,171,171,171	0
55	MG	CA	4248	1/1	0.27	0.61	88,88,88,88	0
55	MG	DA	1602	1/1	0.28	1.32	94,94,94,94	0
55	MG	AA	4120	1/1	0.28	0.74	92,92,92,92	0
55	MG	CA	3088	1/1	0.28	0.37	76,76,76,76	0
55	MG	DA	1811	1/1	0.29	0.65	73,73,73,73	0
55	MG	AX	101	1/1	0.30	0.29	99,99,99,99	0
55	MG	DA	1676	1/1	0.31	0.41	71,71,71,71	0
55	MG	BA	2152	1/1	0.31	0.71	83,83,83,83	0
55	MG	CA	3776	1/1	0.31	0.26	95,95,95,95	0
55	MG	BA	1867	1/1	0.31	1.12	100,100,100,100	0
55	MG	BA	2125	1/1	0.32	0.80	84,84,84,84	0
55	MG	BA	1879	1/1	0.32	0.84	94,94,94,94	0
55	MG	AA	4007	1/1	0.33	0.20	88,88,88,88	0
55	MG	AA	5023	1/1	0.33	0.97	57,57,57,57	0
55	MG	AA	4822	1/1	0.33	0.85	87,87,87,87	0
55	MG	BA	1792	1/1	0.34	1.75	76,76,76,76	0
55	MG	BA	1615	1/1	0.34	0.56	134,134,134,134	0
55	MG	BV	104	1/1	0.35	0.15	84,84,84,84	0
55	MG	CA	4213	1/1	0.35	0.64	70,70,70,70	0
55	MG	DA	1630	1/1	0.35	1.60	133,133,133,133	0
55	MG	CA	2944	1/1	0.36	0.67	94,94,94,94	0
55	MG	DA	2052	1/1	0.36	0.32	66,66,66,66	0
55	MG	CA	3065	1/1	0.36	0.52	88,88,88,88	0
55	MG	AA	4602	1/1	0.37	0.19	134,134,134,134	0
55	MG	CA	4373	1/1	0.38	0.59	92,92,92,92	0
55	MG	BA	1882	1/1	0.38	0.30	92,92,92,92	0
55	MG	AA	4688	1/1	0.38	0.58	65,65,65,65	0
55	MG	AA	5202	1/1	0.38	0.43	72,72,72,72	0
55	MG	AA	5099	1/1	0.38	0.25	111,111,111,111	0
55	MG	AA	4510	1/1	0.38	0.92	167,167,167,167	0
55	MG	CA	3920	1/1	0.38	0.69	85,85,85,85	0
55	MG	BA	2100	1/1	0.38	0.30	112,112,112,112	0
55	MG	BA	1949	1/1	0.38	0.64	102,102,102,102	0
55	MG	CA	4157	1/1	0.38	0.82	63,63,63,63	0
55	MG	DA	1643	1/1	0.39	0.32	91,91,91,91	0
55	MG	AA	4953	1/1	0.40	0.13	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3916	1/1	0.40	0.25	73,73,73,73	0
55	MG	AA	5297	1/1	0.41	1.42	71,71,71,71	0
55	MG	AA	5292	1/1	0.41	0.54	76,76,76,76	0
55	MG	DA	2106	1/1	0.41	0.32	94,94,94,94	0
55	MG	CA	3499	1/1	0.41	0.54	71,71,71,71	0
55	MG	DA	1845	1/1	0.42	1.20	117,117,117,117	0
55	MG	AA	4999	1/1	0.42	0.19	100,100,100,100	0
55	MG	DA	2153	1/1	0.42	0.72	87,87,87,87	0
55	MG	DA	1626	1/1	0.42	1.23	123,123,123,123	0
55	MG	CA	4369	1/1	0.42	0.50	111,111,111,111	0
55	MG	AB	224	1/1	0.43	0.17	94,94,94,94	0
55	MG	CA	3529	1/1	0.43	0.18	78,78,78,78	0
55	MG	BA	1975	1/1	0.43	0.44	75,75,75,75	0
55	MG	CA	4257	1/1	0.44	0.40	74,74,74,74	0
55	MG	BA	1904	1/1	0.45	0.72	79,79,79,79	0
55	MG	CA	2941	1/1	0.45	0.80	71,71,71,71	0
55	MG	AA	5296	1/1	0.45	0.27	74,74,74,74	0
55	MG	CA	3455	1/1	0.45	0.70	60,60,60,60	0
55	MG	AA	4718	1/1	0.45	0.20	89,89,89,89	0
55	MG	AB	243	1/1	0.45	0.73	164,164,164,164	0
55	MG	AA	4874	1/1	0.45	0.46	41,41,41,41	0
55	MG	DA	2180	1/1	0.46	0.47	123,123,123,123	0
55	MG	BA	2060	1/1	0.46	0.80	73,73,73,73	0
55	MG	BA	1840	1/1	0.46	0.43	96,96,96,96	0
55	MG	CA	2920	1/1	0.46	0.57	63,63,63,63	0
55	MG	AA	4697	1/1	0.46	0.79	82,82,82,82	0
55	MG	AA	4135	1/1	0.47	0.68	127,127,127,127	0
55	MG	AA	4536	1/1	0.47	0.32	126,126,126,126	0
55	MG	BA	1801	1/1	0.47	0.68	88,88,88,88	0
55	MG	DA	1929	1/1	0.47	0.19	93,93,93,93	0
55	MG	DA	1831	1/1	0.47	0.29	99,99,99,99	0
55	MG	AA	5214	1/1	0.47	0.33	54,54,54,54	0
55	MG	BA	1661	1/1	0.47	0.20	90,90,90,90	0
55	MG	CA	4278	1/1	0.47	0.70	58,58,58,58	0
55	MG	CA	3885	1/1	0.47	0.45	77,77,77,77	0
55	MG	CA	3082	1/1	0.48	0.76	113,113,113,113	0
55	MG	BA	1964	1/1	0.48	0.16	70,70,70,70	0
55	MG	CA	3915	1/1	0.48	0.74	80,80,80,80	0
55	MG	CQ	205	1/1	0.48	0.56	81,81,81,81	0
55	MG	AA	4169	1/1	0.49	0.72	67,67,67,67	0
55	MG	DA	2146	1/1	0.49	0.36	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AB	223	1/1	0.49	0.25	95,95,95,95	0
55	MG	DA	1677	1/1	0.49	0.46	124,124,124,124	0
55	MG	AA	5039	1/1	0.49	0.63	51,51,51,51	0
55	MG	AA	4665	1/1	0.49	0.31	78,78,78,78	0
55	MG	DA	1908	1/1	0.49	0.27	88,88,88,88	0
55	MG	AA	4788	1/1	0.49	0.66	55,55,55,55	0
55	MG	DA	2068	1/1	0.50	0.20	105,105,105,105	0
55	MG	CA	3799	1/1	0.50	0.56	111,111,111,111	0
55	MG	DA	2191	1/1	0.50	0.67	92,92,92,92	0
55	MG	BV	122	1/1	0.50	0.39	97,97,97,97	0
55	MG	CA	3997	1/1	0.51	0.27	51,51,51,51	0
55	MG	CA	3795	1/1	0.51	0.54	51,51,51,51	0
55	MG	BA	2010	1/1	0.51	0.52	78,78,78,78	0
55	MG	CA	3935	1/1	0.51	0.72	61,61,61,61	0
55	MG	AA	5002	1/1	0.51	0.83	90,90,90,90	0
55	MG	DA	2067	1/1	0.51	0.54	55,55,55,55	0
55	MG	AA	5037	1/1	0.52	1.00	95,95,95,95	0
55	MG	AB	237	1/1	0.52	0.62	72,72,72,72	0
55	MG	AA	5205	1/1	0.52	0.22	83,83,83,83	0
55	MG	BA	2102	1/1	0.52	0.56	80,80,80,80	0
55	MG	CA	3054	1/1	0.52	1.35	68,68,68,68	0
55	MG	BA	1925	1/1	0.52	1.12	75,75,75,75	0
55	MG	CA	3684	1/1	0.52	0.32	90,90,90,90	0
55	MG	BA	1624	1/1	0.53	1.04	79,79,79,79	0
55	MG	AA	4295	1/1	0.53	0.27	61,61,61,61	0
55	MG	AA	4123	1/1	0.53	0.54	74,74,74,74	0
55	MG	CV	203	1/1	0.53	0.21	85,85,85,85	0
55	MG	AA	4397	1/1	0.53	3.28	82,82,82,82	0
55	MG	BA	1852	1/1	0.53	0.76	121,121,121,121	0
55	MG	DA	2109	1/1	0.53	0.17	93,93,93,93	0
55	MG	CA	4326	1/1	0.53	0.56	57,57,57,57	0
55	MG	AA	4803	1/1	0.53	0.55	85,85,85,85	0
55	MG	AA	5146	1/1	0.53	0.36	110,110,110,110	0
55	MG	CA	3079	1/1	0.53	0.34	103,103,103,103	0
55	MG	DA	2125	1/1	0.54	0.66	63,63,63,63	0
55	MG	BA	2033	1/1	0.54	0.53	56,56,56,56	0
55	MG	BA	2057	1/1	0.54	0.54	46,46,46,46	0
55	MG	AA	4779	1/1	0.54	0.48	71,71,71,71	0
55	MG	DA	1999	1/1	0.54	0.53	108,108,108,108	0
55	MG	AA	4338	1/1	0.54	0.22	58,58,58,58	0
55	MG	AA	4741	1/1	0.54	0.45	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	2925	1/1	0.54	0.18	128,128,128,128	0
55	MG	DA	2202	1/1	0.54	0.25	80,80,80,80	0
55	MG	AA	4502	1/1	0.54	0.47	53,53,53,53	0
55	MG	DA	1952	1/1	0.54	0.50	66,66,66,66	0
55	MG	CA	4035	1/1	0.54	0.46	50,50,50,50	0
55	MG	AA	4770	1/1	0.55	0.47	83,83,83,83	0
55	MG	BA	1781	1/1	0.55	0.62	64,64,64,64	0
55	MG	BA	1647	1/1	0.55	0.60	93,93,93,93	0
55	MG	DA	1649	1/1	0.55	0.75	118,118,118,118	0
55	MG	AA	4723	1/1	0.55	0.45	83,83,83,83	0
55	MG	DA	1806	1/1	0.55	0.21	69,69,69,69	0
55	MG	CV	201	1/1	0.55	0.45	78,78,78,78	0
55	MG	CD	306	1/1	0.55	0.46	65,65,65,65	0
55	MG	AA	5228	1/1	0.55	0.84	73,73,73,73	0
55	MG	BA	2145	1/1	0.55	0.21	97,97,97,97	0
55	MG	BA	1634	1/1	0.55	0.90	104,104,104,104	0
55	MG	AA	4069	1/1	0.55	0.59	68,68,68,68	0
55	MG	DV	123	1/1	0.55	0.25	104,104,104,104	0
55	MG	AA	4828	1/1	0.55	0.28	53,53,53,53	0
55	MG	AA	4497	1/1	0.55	0.32	66,66,66,66	0
55	MG	AA	4436	1/1	0.56	0.28	76,76,76,76	0
55	MG	AA	4616	1/1	0.56	0.42	140,140,140,140	0
55	MG	A3	102	1/1	0.56	0.39	77,77,77,77	0
55	MG	BA	2019	1/1	0.56	0.28	83,83,83,83	0
55	MG	CA	4207	1/1	0.56	0.29	62,62,62,62	0
55	MG	BV	115	1/1	0.56	0.33	107,107,107,107	0
55	MG	AA	5045	1/1	0.56	0.27	80,80,80,80	0
55	MG	DA	1682	1/1	0.56	0.63	68,68,68,68	0
55	MG	BA	1604	1/1	0.56	0.52	96,96,96,96	0
55	MG	AA	4593	1/1	0.56	0.44	82,82,82,82	0
55	MG	AB	210	1/1	0.56	0.38	68,68,68,68	0
55	MG	AA	4097	1/1	0.56	0.57	78,78,78,78	0
55	MG	CA	4181	1/1	0.56	0.25	57,57,57,57	0
55	MG	DA	1991	1/1	0.57	0.56	56,56,56,56	0
55	MG	BA	1682	1/1	0.57	0.10	105,105,105,105	0
55	MG	DA	1841	1/1	0.57	1.07	75,75,75,75	0
55	MG	BA	1943	1/1	0.57	0.82	79,79,79,79	0
55	MG	AA	4923	1/1	0.57	0.71	64,64,64,64	0
55	MG	DA	1912	1/1	0.57	0.18	88,88,88,88	0
55	MG	AA	4363	1/1	0.57	0.44	57,57,57,57	0
55	MG	CA	4136	1/1	0.57	0.71	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1903	1/1	0.57	0.40	62,62,62,62	0
55	MG	CA	3941	1/1	0.57	0.53	58,58,58,58	0
55	MG	BA	1995	1/1	0.57	0.29	61,61,61,61	0
55	MG	BA	2141	1/1	0.57	0.36	85,85,85,85	0
55	MG	DA	2140	1/1	0.58	0.19	107,107,107,107	0
55	MG	CA	4195	1/1	0.58	0.86	64,64,64,64	0
55	MG	AA	4632	1/1	0.58	0.38	81,81,81,81	0
55	MG	CA	4335	1/1	0.58	0.14	110,110,110,110	0
55	MG	AA	4769	1/1	0.58	0.68	69,69,69,69	0
55	MG	CB	242	1/1	0.58	0.33	77,77,77,77	0
55	MG	BA	1818	1/1	0.58	0.94	75,75,75,75	0
55	MG	CA	3936	1/1	0.58	0.54	82,82,82,82	0
55	MG	BA	1913	1/1	0.58	0.72	84,84,84,84	0
55	MG	BA	2121	1/1	0.58	0.29	81,81,81,81	0
55	MG	AA	4767	1/1	0.58	0.50	89,89,89,89	0
55	MG	AA	5032	1/1	0.58	0.50	65,65,65,65	0
55	MG	CA	3764	1/1	0.58	0.59	75,75,75,75	0
55	MG	CA	2935	1/1	0.58	0.22	65,65,65,65	0
55	MG	CB	259	1/1	0.58	0.25	78,78,78,78	0
55	MG	DA	1690	1/1	0.58	0.72	79,79,79,79	0
55	MG	AA	4717	1/1	0.58	0.14	68,68,68,68	0
55	MG	AA	4047	1/1	0.59	0.46	65,65,65,65	0
55	MG	DA	1833	1/1	0.59	0.22	103,103,103,103	0
55	MG	AA	4970	1/1	0.59	0.23	60,60,60,60	0
55	MG	CA	4179	1/1	0.59	0.40	105,105,105,105	0
55	MG	DA	2121	1/1	0.59	1.00	96,96,96,96	0
55	MG	DA	2037	1/1	0.59	0.67	95,95,95,95	0
55	MG	AA	4453	1/1	0.59	0.51	48,48,48,48	0
55	MG	AA	5164	1/1	0.59	0.08	125,125,125,125	0
55	MG	AA	5100	1/1	0.59	0.46	91,91,91,91	0
55	MG	BA	1999	1/1	0.59	0.21	85,85,85,85	0
55	MG	DA	2117	1/1	0.59	0.49	68,68,68,68	0
55	MG	CA	3090	1/1	0.59	0.41	82,82,82,82	0
55	MG	AA	4096	1/1	0.59	0.43	70,70,70,70	0
55	MG	AA	5086	1/1	0.59	0.40	65,65,65,65	0
55	MG	AA	5078	1/1	0.59	0.63	64,64,64,64	0
55	MG	CA	3888	1/1	0.59	0.43	73,73,73,73	0
55	MG	DA	1951	1/1	0.60	0.58	68,68,68,68	0
55	MG	BA	1626	1/1	0.60	0.50	81,81,81,81	0
55	MG	AA	4584	1/1	0.60	0.53	67,67,67,67	0
55	MG	CA	3072	1/1	0.60	0.62	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1816	1/1	0.60	0.14	86,86,86,86	0
55	MG	AA	4703	1/1	0.60	0.30	92,92,92,92	0
55	MG	DA	1937	1/1	0.60	0.52	85,85,85,85	0
55	MG	CA	4339	1/1	0.60	0.62	67,67,67,67	0
55	MG	DA	1850	1/1	0.60	0.23	101,101,101,101	0
55	MG	CA	3692	1/1	0.60	0.80	65,65,65,65	0
55	MG	DA	1932	1/1	0.60	1.48	66,66,66,66	0
55	MG	CA	3805	1/1	0.60	0.23	72,72,72,72	0
55	MG	AA	5250	1/1	0.60	1.06	70,70,70,70	0
55	MG	DA	1799	1/1	0.60	0.17	80,80,80,80	0
55	MG	DA	1611	1/1	0.60	0.61	99,99,99,99	0
55	MG	BA	1823	1/1	0.60	0.39	103,103,103,103	0
55	MG	DA	1995	1/1	0.60	0.48	71,71,71,71	0
55	MG	AA	4751	1/1	0.60	0.30	96,96,96,96	0
55	MG	CB	231	1/1	0.60	0.26	76,76,76,76	0
55	MG	BA	2093	1/1	0.60	0.61	75,75,75,75	0
55	MG	DA	1681	1/1	0.60	0.42	83,83,83,83	0
55	MG	CA	4183	1/1	0.60	0.83	71,71,71,71	0
55	MG	BA	1737	1/1	0.60	0.23	46,46,46,46	0
55	MG	DA	2101	1/1	0.60	0.27	155,155,155,155	0
55	MG	DA	2032	1/1	0.60	0.22	60,60,60,60	0
55	MG	DW	113	1/1	0.61	0.24	68,68,68,68	0
55	MG	CA	3786	1/1	0.61	0.67	64,64,64,64	0
55	MG	CA	3424	1/1	0.61	0.30	48,48,48,48	0
55	MG	AA	5137	1/1	0.61	0.57	64,64,64,64	0
55	MG	CA	3059	1/1	0.61	0.83	92,92,92,92	0
55	MG	AA	4061	1/1	0.61	0.33	52,52,52,52	0
55	MG	CA	2972	1/1	0.61	0.93	64,64,64,64	0
55	MG	BA	1914	1/1	0.61	0.27	82,82,82,82	0
55	MG	CA	3873	1/1	0.61	0.16	77,77,77,77	0
55	MG	AA	4144	1/1	0.61	0.34	63,63,63,63	0
55	MG	CA	3858	1/1	0.61	0.42	53,53,53,53	0
55	MG	AA	5201	1/1	0.61	0.44	49,49,49,49	0
55	MG	AA	5265	1/1	0.61	0.53	68,68,68,68	0
55	MG	CA	2994	1/1	0.61	0.54	49,49,49,49	0
55	MG	DA	2162	1/1	0.61	0.34	72,72,72,72	0
55	MG	CA	3388	1/1	0.61	0.50	61,61,61,61	0
55	MG	BA	2170	1/1	0.61	0.16	105,105,105,105	0
55	MG	DA	1673	1/1	0.61	0.58	90,90,90,90	0
55	MG	AA	5013	1/1	0.61	0.16	79,79,79,79	0
55	MG	CA	4332	1/1	0.61	0.38	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	2069	1/1	0.61	0.56	76,76,76,76	0
55	MG	AA	4032	1/1	0.61	0.80	82,82,82,82	0
55	MG	AA	4755	1/1	0.61	0.75	68,68,68,68	0
55	MG	CA	2952	1/1	0.61	0.19	130,130,130,130	0
55	MG	AA	4798	1/1	0.61	0.80	76,76,76,76	0
55	MG	AA	5121	1/1	0.61	0.14	78,78,78,78	0
55	MG	AB	204	1/1	0.61	0.46	56,56,56,56	0
55	MG	CJ	201	1/1	0.61	0.38	71,71,71,71	0
55	MG	CA	2903	1/1	0.61	0.44	80,80,80,80	0
55	MG	AA	5279	1/1	0.61	1.09	59,59,59,59	0
55	MG	BA	2129	1/1	0.61	0.77	36,36,36,36	0
55	MG	AA	5143	1/1	0.61	0.42	71,71,71,71	0
55	MG	CA	2902	1/1	0.62	0.46	65,65,65,65	0
55	MG	DW	120	1/1	0.62	0.17	73,73,73,73	0
55	MG	CA	3326	1/1	0.62	0.47	61,61,61,61	0
55	MG	DA	1866	1/1	0.62	0.37	74,74,74,74	0
55	MG	AA	4138	1/1	0.62	0.33	69,69,69,69	0
55	MG	BV	111	1/1	0.62	0.23	65,65,65,65	0
55	MG	AA	4546	1/1	0.62	0.56	76,76,76,76	0
55	MG	CA	3972	1/1	0.62	0.40	46,46,46,46	0
55	MG	BA	1878	1/1	0.62	0.26	77,77,77,77	0
55	MG	AA	5200	1/1	0.62	0.56	64,64,64,64	0
55	MG	BA	1974	1/1	0.62	0.33	66,66,66,66	0
55	MG	CA	3844	1/1	0.62	0.45	54,54,54,54	0
55	MG	AA	4057	1/1	0.62	0.78	71,71,71,71	0
55	MG	AA	4556	1/1	0.62	0.27	80,80,80,80	0
55	MG	AA	5147	1/1	0.62	0.42	61,61,61,61	0
55	MG	DA	2123	1/1	0.62	0.55	94,94,94,94	0
55	MG	DA	1607	1/1	0.62	0.93	74,74,74,74	0
55	MG	CA	3824	1/1	0.62	0.96	78,78,78,78	0
55	MG	CA	3722	1/1	0.62	0.24	82,82,82,82	0
55	MG	AA	4837	1/1	0.62	0.30	107,107,107,107	0
55	MG	BV	102	1/1	0.62	0.44	56,56,56,56	0
55	MG	AA	4978	1/1	0.62	0.14	99,99,99,99	0
55	MG	CA	3517	1/1	0.62	0.59	71,71,71,71	0
55	MG	DW	103	1/1	0.62	0.10	93,93,93,93	0
55	MG	AA	4780	1/1	0.62	0.81	68,68,68,68	0
55	MG	BA	2028	1/1	0.62	0.28	64,64,64,64	0
55	MG	BA	2127	1/1	0.62	0.73	69,69,69,69	0
55	MG	CF	303	1/1	0.62	1.15	53,53,53,53	0
55	MG	AA	4025	1/1	0.62	0.54	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	2003	1/1	0.62	0.33	49,49,49,49	0
55	MG	CA	3892	1/1	0.63	0.70	63,63,63,63	0
55	MG	CA	2954	1/1	0.63	0.34	76,76,76,76	0
55	MG	BA	1902	1/1	0.63	0.47	63,63,63,63	0
55	MG	CA	4147	1/1	0.63	0.57	64,64,64,64	0
55	MG	CA	3944	1/1	0.63	0.30	39,39,39,39	0
55	MG	BW	105	1/1	0.63	0.12	69,69,69,69	0
55	MG	CA	4294	1/1	0.63	0.48	94,94,94,94	0
55	MG	CA	4151	1/1	0.63	0.47	57,57,57,57	0
55	MG	DA	1671	1/1	0.63	0.75	78,78,78,78	0
55	MG	AA	4473	1/1	0.63	0.50	91,91,91,91	0
55	MG	DA	2192	1/1	0.63	0.55	58,58,58,58	0
55	MG	AA	4110	1/1	0.63	0.59	89,89,89,89	0
55	MG	AS	206	1/1	0.63	0.23	77,77,77,77	0
55	MG	AA	4375	1/1	0.63	0.46	61,61,61,61	0
55	MG	BA	1659	1/1	0.63	0.47	85,85,85,85	0
55	MG	AA	4121	1/1	0.63	0.81	82,82,82,82	0
55	MG	AA	4024	1/1	0.63	0.29	82,82,82,82	0
55	MG	DA	2119	1/1	0.63	0.31	75,75,75,75	0
55	MG	AA	4592	1/1	0.63	0.40	61,61,61,61	0
55	MG	AA	4514	1/1	0.63	0.54	81,81,81,81	0
55	MG	AA	4716	1/1	0.63	0.47	76,76,76,76	0
55	MG	BA	1859	1/1	0.64	0.47	53,53,53,53	0
55	MG	AA	5110	1/1	0.64	0.44	60,60,60,60	0
55	MG	CA	4190	1/1	0.64	0.38	51,51,51,51	0
55	MG	CA	3493	1/1	0.64	0.58	57,57,57,57	0
55	MG	AA	4924	1/1	0.64	0.28	78,78,78,78	0
55	MG	AA	4396	1/1	0.64	0.30	66,66,66,66	0
55	MG	BA	1628	1/1	0.64	0.94	99,99,99,99	0
55	MG	AA	5178	1/1	0.64	0.44	74,74,74,74	0
55	MG	AA	4112	1/1	0.64	0.27	92,92,92,92	0
55	MG	BA	2134	1/1	0.64	0.58	63,63,63,63	0
55	MG	CK	202	1/1	0.64	0.36	57,57,57,57	0
55	MG	AA	4162	1/1	0.64	0.48	67,67,67,67	0
55	MG	BA	1652	1/1	0.64	0.63	84,84,84,84	0
55	MG	AA	4829	1/1	0.64	0.29	82,82,82,82	0
55	MG	CA	3755	1/1	0.64	0.33	52,52,52,52	0
55	MG	CA	4174	1/1	0.64	0.38	53,53,53,53	0
55	MG	CA	3841	1/1	0.64	0.18	71,71,71,71	0
55	MG	AA	4825	1/1	0.64	0.26	84,84,84,84	0
55	MG	BA	1930	1/1	0.64	0.19	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4430	1/1	0.64	0.32	59,59,59,59	0
55	MG	AB	216	1/1	0.64	0.59	63,63,63,63	0
55	MG	CA	3089	1/1	0.64	0.13	81,81,81,81	0
55	MG	CA	3881	1/1	0.64	0.59	84,84,84,84	0
55	MG	CA	4402	1/1	0.64	0.24	94,94,94,94	0
55	MG	DQ	201	1/1	0.64	0.34	57,57,57,57	0
55	MG	BA	2052	1/1	0.64	0.35	81,81,81,81	0
55	MG	AA	4750	1/1	0.65	0.94	62,62,62,62	0
55	MG	AA	4842	1/1	0.65	0.49	111,111,111,111	0
55	MG	AF	306	1/1	0.65	0.27	53,53,53,53	0
55	MG	CA	3856	1/1	0.65	0.30	67,67,67,67	0
55	MG	DA	2129	1/1	0.65	0.21	72,72,72,72	0
55	MG	CA	4228	1/1	0.65	1.43	74,74,74,74	0
55	MG	CA	4289	1/1	0.65	0.33	65,65,65,65	0
55	MG	CA	3797	1/1	0.65	0.51	83,83,83,83	0
55	MG	CA	3677	1/1	0.65	0.45	67,67,67,67	0
55	MG	BA	2112	1/1	0.65	0.29	84,84,84,84	0
55	MG	AA	4844	1/1	0.65	1.15	59,59,59,59	0
55	MG	CA	4304	1/1	0.65	0.23	81,81,81,81	0
55	MG	AA	4737	1/1	0.65	0.51	71,71,71,71	0
55	MG	DA	1924	1/1	0.65	0.51	90,90,90,90	0
55	MG	BA	1765	1/1	0.65	0.18	93,93,93,93	0
55	MG	AB	233	1/1	0.65	0.17	64,64,64,64	0
55	MG	DA	2041	1/1	0.65	0.37	112,112,112,112	0
55	MG	AA	4594	1/1	0.65	1.30	75,75,75,75	0
55	MG	CA	4141	1/1	0.65	0.49	54,54,54,54	0
55	MG	CA	2914	1/1	0.65	0.72	66,66,66,66	0
55	MG	BA	1673	1/1	0.65	0.41	66,66,66,66	0
55	MG	CA	4026	1/1	0.65	0.35	66,66,66,66	0
55	MG	AA	4529	1/1	0.65	0.49	88,88,88,88	0
55	MG	DA	1922	1/1	0.65	0.32	94,94,94,94	0
55	MG	DA	1752	1/1	0.65	0.45	89,89,89,89	0
55	MG	BA	1819	1/1	0.65	0.23	67,67,67,67	0
55	MG	AA	4305	1/1	0.66	0.76	55,55,55,55	0
55	MG	CA	3945	1/1	0.66	0.82	65,65,65,65	0
55	MG	CA	3412	1/1	0.66	0.17	57,57,57,57	0
55	MG	CA	4061	1/1	0.66	0.29	73,73,73,73	0
55	MG	AA	4067	1/1	0.66	0.74	82,82,82,82	0
55	MG	DV	114	1/1	0.66	0.25	68,68,68,68	0
55	MG	AA	4142	1/1	0.66	0.35	65,65,65,65	0
55	MG	DA	1763	1/1	0.66	0.90	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	2950	1/1	0.66	0.66	84,84,84,84	0
55	MG	DA	1612	1/1	0.66	0.42	141,141,141,141	0
55	MG	AA	5239	1/1	0.66	0.76	69,69,69,69	0
55	MG	DA	1680	1/1	0.66	0.37	83,83,83,83	0
55	MG	CB	212	1/1	0.66	0.52	104,104,104,104	0
55	MG	DA	1992	1/1	0.66	0.39	53,53,53,53	0
55	MG	BA	2139	1/1	0.66	0.96	96,96,96,96	0
55	MG	CW	103	1/1	0.66	0.54	47,47,47,47	0
55	MG	CA	4105	1/1	0.66	0.17	60,60,60,60	0
55	MG	CA	3554	1/1	0.66	0.40	62,62,62,62	0
55	MG	BA	1911	1/1	0.66	0.43	73,73,73,73	0
55	MG	CA	3800	1/1	0.66	0.51	92,92,92,92	0
55	MG	BA	2098	1/1	0.66	0.62	82,82,82,82	0
55	MG	AA	5295	1/1	0.66	0.36	103,103,103,103	0
55	MG	DI	201	1/1	0.66	0.54	72,72,72,72	0
55	MG	DA	1927	1/1	0.66	0.40	92,92,92,92	0
55	MG	CA	3623	1/1	0.66	0.50	69,69,69,69	0
55	MG	DV	117	1/1	0.66	0.19	81,81,81,81	0
55	MG	CA	3641	1/1	0.66	0.34	57,57,57,57	0
55	MG	DA	2151	1/1	0.66	0.14	124,124,124,124	0
55	MG	AB	228	1/1	0.66	0.18	75,75,75,75	0
55	MG	CA	4144	1/1	0.66	0.47	55,55,55,55	0
55	MG	CA	3024	1/1	0.67	0.56	75,75,75,75	0
55	MG	CA	4389	1/1	0.67	0.19	93,93,93,93	0
55	MG	DA	2054	1/1	0.67	0.15	77,77,77,77	0
55	MG	BA	1803	1/1	0.67	0.41	61,61,61,61	0
55	MG	CA	3917	1/1	0.67	0.48	70,70,70,70	0
55	MG	AA	4918	1/1	0.67	0.58	54,54,54,54	0
55	MG	CA	3039	1/1	0.67	0.24	81,81,81,81	0
55	MG	CA	3578	1/1	0.67	0.29	58,58,58,58	0
55	MG	AA	4760	1/1	0.67	0.37	89,89,89,89	0
55	MG	AA	4885	1/1	0.67	0.23	88,88,88,88	0
55	MG	CA	3721	1/1	0.67	0.37	56,56,56,56	0
55	MG	CA	4349	1/1	0.67	0.43	84,84,84,84	0
55	MG	CA	3085	1/1	0.67	0.48	81,81,81,81	0
55	MG	CA	4070	1/1	0.67	0.56	46,46,46,46	0
55	MG	DA	1622	1/1	0.67	0.55	77,77,77,77	0
55	MG	DA	1773	1/1	0.67	0.27	83,83,83,83	0
55	MG	AA	5033	1/1	0.67	0.30	88,88,88,88	0
55	MG	AA	5041	1/1	0.67	0.39	84,84,84,84	0
55	MG	CA	4050	1/1	0.67	0.51	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DV	116	1/1	0.67	0.13	77,77,77,77	0
55	MG	CA	4347	1/1	0.67	0.80	81,81,81,81	0
55	MG	AA	4350	1/1	0.67	0.27	43,43,43,43	0
55	MG	AA	5089	1/1	0.67	0.34	57,57,57,57	0
55	MG	CA	4233	1/1	0.67	1.35	76,76,76,76	0
55	MG	CA	4308	1/1	0.67	0.15	83,83,83,83	0
55	MG	CA	3165	1/1	0.67	0.59	26,26,26,26	0
55	MG	BA	1970	1/1	0.67	0.27	61,61,61,61	0
55	MG	CA	3252	1/1	0.67	0.19	61,61,61,61	0
55	MG	AA	5243	1/1	0.67	0.23	107,107,107,107	0
55	MG	AA	4113	1/1	0.67	0.52	84,84,84,84	0
55	MG	CA	4395	1/1	0.67	0.86	85,85,85,85	0
55	MG	BA	2099	1/1	0.67	0.60	54,54,54,54	0
55	MG	DA	2075	1/1	0.67	0.24	72,72,72,72	0
55	MG	AA	4078	1/1	0.67	0.35	60,60,60,60	0
55	MG	AA	4986	1/1	0.68	0.50	65,65,65,65	0
55	MG	AA	5092	1/1	0.68	0.19	55,55,55,55	0
55	MG	BA	2160	1/1	0.68	0.37	91,91,91,91	0
55	MG	AA	4990	1/1	0.68	0.39	60,60,60,60	0
55	MG	DA	2058	1/1	0.68	0.15	86,86,86,86	0
55	MG	AA	4313	1/1	0.68	0.37	39,39,39,39	0
55	MG	AA	4159	1/1	0.68	0.98	77,77,77,77	0
55	MG	BA	2076	1/1	0.68	0.37	66,66,66,66	0
55	MG	CB	262	1/1	0.68	0.41	67,67,67,67	0
55	MG	CA	3825	1/1	0.68	0.27	83,83,83,83	0
55	MG	DA	1766	1/1	0.68	0.15	91,91,91,91	0
55	MG	BA	2077	1/1	0.68	0.37	72,72,72,72	0
55	MG	BA	1645	1/1	0.68	0.42	86,86,86,86	0
55	MG	AA	5162	1/1	0.68	0.17	47,47,47,47	0
55	MG	CA	3651	1/1	0.68	0.16	70,70,70,70	0
55	MG	CA	4352	1/1	0.68	0.67	80,80,80,80	0
55	MG	CA	3583	1/1	0.68	0.45	111,111,111,111	0
55	MG	CA	4199	1/1	0.68	0.17	70,70,70,70	0
55	MG	AA	4945	1/1	0.68	0.45	58,58,58,58	0
55	MG	AA	4447	1/1	0.68	0.49	63,63,63,63	0
55	MG	BA	2142	1/1	0.68	0.30	78,78,78,78	0
55	MG	CA	4218	1/1	0.68	0.23	75,75,75,75	0
55	MG	AA	4576	1/1	0.68	0.26	60,60,60,60	0
55	MG	BA	2046	1/1	0.68	0.79	82,82,82,82	0
55	MG	AA	4994	1/1	0.68	0.53	63,63,63,63	0
55	MG	CA	3466	1/1	0.68	0.27	56,56,56,56	0
55	MG	CA	4046	1/1	0.68	0.57	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4763	1/1	0.68	0.60	137,137,137,137	0
55	MG	CB	228	1/1	0.68	0.23	67,67,67,67	0
55	MG	BA	2133	1/1	0.68	0.52	77,77,77,77	0
55	MG	DA	1859	1/1	0.68	0.22	91,91,91,91	0
55	MG	CA	3540	1/1	0.68	0.72	49,49,49,49	0
55	MG	AB	221	1/1	0.68	0.16	74,74,74,74	0
55	MG	CA	3541	1/1	0.68	0.37	63,63,63,63	0
55	MG	AA	5059	1/1	0.68	0.48	48,48,48,48	0
55	MG	CA	3522	1/1	0.68	0.43	56,56,56,56	0
55	MG	CA	4273	1/1	0.68	0.41	82,82,82,82	0
55	MG	AA	5177	1/1	0.68	0.45	63,63,63,63	0
55	MG	AA	4653	1/1	0.69	0.47	90,90,90,90	0
55	MG	BA	1979	1/1	0.69	0.11	64,64,64,64	0
55	MG	AA	4130	1/1	0.69	0.44	78,78,78,78	0
55	MG	BA	2109	1/1	0.69	0.76	63,63,63,63	0
55	MG	AA	4429	1/1	0.69	0.20	36,36,36,36	0
55	MG	AA	4696	1/1	0.69	0.56	50,50,50,50	0
55	MG	CA	3454	1/1	0.69	0.26	55,55,55,55	0
55	MG	AA	4759	1/1	0.69	0.53	55,55,55,55	0
55	MG	AA	4342	1/1	0.69	0.47	40,40,40,40	0
55	MG	AA	5131	1/1	0.69	0.17	86,86,86,86	0
55	MG	CA	4300	1/1	0.69	0.40	46,46,46,46	0
55	MG	DA	2099	1/1	0.69	0.42	55,55,55,55	0
55	MG	BA	1992	1/1	0.69	0.80	67,67,67,67	0
55	MG	BA	2068	1/1	0.69	0.32	69,69,69,69	0
55	MG	CA	3883	1/1	0.69	0.91	77,77,77,77	0
55	MG	AA	4992	1/1	0.69	0.36	48,48,48,48	0
55	MG	AA	4508	1/1	0.69	0.19	89,89,89,89	0
55	MG	CA	4175	1/1	0.69	0.40	64,64,64,64	0
55	MG	CA	4109	1/1	0.69	0.51	45,45,45,45	0
55	MG	CA	4192	1/1	0.69	0.34	43,43,43,43	0
55	MG	AA	5028	1/1	0.69	0.26	68,68,68,68	0
55	MG	DV	111	1/1	0.69	0.28	75,75,75,75	0
55	MG	AA	5063	1/1	0.69	0.51	59,59,59,59	0
55	MG	AA	4106	1/1	0.69	0.25	54,54,54,54	0
55	MG	AA	4093	1/1	0.69	0.31	104,104,104,104	0
55	MG	AA	4958	1/1	0.69	0.41	78,78,78,78	0
55	MG	CA	4243	1/1	0.69	0.29	68,68,68,68	0
55	MG	CA	4362	1/1	0.69	0.42	58,58,58,58	0
55	MG	DA	1849	1/1	0.69	0.28	65,65,65,65	0
55	MG	CA	4058	1/1	0.69	0.45	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	2113	1/1	0.69	0.27	58,58,58,58	0
55	MG	AA	4855	1/1	0.69	0.25	36,36,36,36	0
55	MG	DA	1933	1/1	0.69	0.55	61,61,61,61	0
55	MG	DA	2126	1/1	0.69	0.40	59,59,59,59	0
55	MG	CA	3626	1/1	0.69	0.51	103,103,103,103	0
55	MG	DA	2038	1/1	0.69	0.19	114,114,114,114	0
55	MG	AA	4114	1/1	0.69	0.51	64,64,64,64	0
55	MG	CA	4106	1/1	0.69	0.16	49,49,49,49	0
55	MG	BA	1640	1/1	0.69	0.35	75,75,75,75	0
55	MG	BA	2044	1/1	0.69	0.30	56,56,56,56	0
55	MG	BA	2002	1/1	0.69	0.63	71,71,71,71	0
55	MG	BA	1967	1/1	0.69	0.86	56,56,56,56	0
55	MG	AA	5271	1/1	0.69	0.24	82,82,82,82	0
55	MG	BA	2138	1/1	0.69	0.27	51,51,51,51	0
55	MG	AA	4115	1/1	0.69	0.24	86,86,86,86	0
55	MG	CA	3339	1/1	0.69	0.14	50,50,50,50	0
55	MG	BA	1752	1/1	0.69	0.57	69,69,69,69	0
55	MG	BA	1836	1/1	0.69	0.32	79,79,79,79	0
55	MG	BA	1954	1/1	0.69	0.29	56,56,56,56	0
55	MG	AA	4023	1/1	0.70	0.45	71,71,71,71	0
55	MG	AA	4378	1/1	0.70	0.21	54,54,54,54	0
55	MG	AA	4906	1/1	0.70	0.74	63,63,63,63	0
55	MG	CA	4404	1/1	0.70	0.76	66,66,66,66	0
55	MG	AA	4471	1/1	0.70	0.38	53,53,53,53	0
55	MG	CA	3438	1/1	0.70	0.21	54,54,54,54	0
55	MG	DA	1893	1/1	0.70	0.37	65,65,65,65	0
55	MG	AA	5020	1/1	0.70	0.44	57,57,57,57	0
55	MG	DA	1684	1/1	0.70	0.42	72,72,72,72	0
55	MG	CA	2926	1/1	0.70	0.71	56,56,56,56	0
55	MG	CA	3729	1/1	0.70	0.31	101,101,101,101	0
55	MG	AA	4314	1/1	0.70	0.37	36,36,36,36	0
55	MG	CA	4276	1/1	0.70	0.34	61,61,61,61	0
55	MG	BA	1931	1/1	0.70	0.76	61,61,61,61	0
55	MG	AA	4916	1/1	0.70	0.38	58,58,58,58	0
55	MG	BA	1833	1/1	0.70	0.57	55,55,55,55	0
55	MG	CB	255	1/1	0.70	0.23	62,62,62,62	0
55	MG	BA	2086	1/1	0.70	0.54	71,71,71,71	0
55	MG	DA	1619	1/1	0.70	0.54	77,77,77,77	0
55	MG	AA	4721	1/1	0.70	0.30	76,76,76,76	0
55	MG	AA	5248	1/1	0.70	0.45	59,59,59,59	0
55	MG	CA	3891	1/1	0.70	0.44	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	5190	1/1	0.70	0.73	73,73,73,73	0
55	MG	AA	4549	1/1	0.70	0.41	39,39,39,39	0
55	MG	BA	2049	1/1	0.70	0.26	59,59,59,59	0
55	MG	DA	1921	1/1	0.70	0.41	53,53,53,53	0
55	MG	AA	4748	1/1	0.70	0.39	104,104,104,104	0
55	MG	DA	2152	1/1	0.70	0.15	69,69,69,69	0
55	MG	BA	1841	1/1	0.70	0.33	60,60,60,60	0
55	MG	BA	1827	1/1	0.70	0.52	73,73,73,73	0
55	MG	DA	1646	1/1	0.70	0.36	72,72,72,72	0
55	MG	CA	3462	1/1	0.70	0.48	64,64,64,64	0
55	MG	BA	1808	1/1	0.70	0.46	67,67,67,67	0
55	MG	CA	3566	1/1	0.70	0.28	63,63,63,63	0
55	MG	AA	4573	1/1	0.70	0.24	59,59,59,59	0
55	MG	DA	1973	1/1	0.70	0.71	49,49,49,49	0
55	MG	AB	205	1/1	0.70	0.55	88,88,88,88	0
55	MG	CA	3050	1/1	0.70	0.39	80,80,80,80	0
55	MG	AA	4973	1/1	0.70	0.47	65,65,65,65	0
55	MG	AA	4809	1/1	0.71	0.52	65,65,65,65	0
55	MG	CA	3269	1/1	0.71	0.34	40,40,40,40	0
55	MG	CA	3417	1/1	0.71	0.14	45,45,45,45	0
55	MG	CA	2981	1/1	0.71	0.45	48,48,48,48	0
55	MG	CA	4112	1/1	0.71	0.16	49,49,49,49	0
55	MG	CB	244	1/1	0.71	0.30	76,76,76,76	0
55	MG	BA	1900	1/1	0.71	0.40	98,98,98,98	0
55	MG	CG	201	1/1	0.71	0.30	86,86,86,86	0
55	MG	CA	3956	1/1	0.71	0.39	64,64,64,64	0
55	MG	CA	3898	1/1	0.71	0.45	65,65,65,65	0
55	MG	CA	4008	1/1	0.71	0.32	61,61,61,61	0
55	MG	AA	4810	1/1	0.71	0.41	74,74,74,74	0
55	MG	DA	1787	1/1	0.71	0.27	81,81,81,81	0
55	MG	BV	121	1/1	0.71	0.36	65,65,65,65	0
55	MG	DA	1935	1/1	0.71	0.48	69,69,69,69	0
55	MG	AA	4477	1/1	0.71	0.39	59,59,59,59	0
55	MG	BA	1745	1/1	0.71	0.30	70,70,70,70	0
55	MG	AA	4757	1/1	0.71	0.39	78,78,78,78	0
55	MG	CA	3716	1/1	0.71	0.52	105,105,105,105	0
55	MG	BA	1785	1/1	0.71	0.18	73,73,73,73	0
55	MG	CA	3849	1/1	0.71	0.47	119,119,119,119	0
55	MG	DA	2195	1/1	0.71	0.86	78,78,78,78	0
55	MG	CA	3938	1/1	0.71	0.42	64,64,64,64	0
55	MG	CA	3996	1/1	0.71	0.28	49,49,49,49	0
55	MG	CV	204	1/1	0.71	0.14	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	2179	1/1	0.71	0.35	73,73,73,73	0
55	MG	DA	1725	1/1	0.71	0.29	59,59,59,59	0
55	MG	AA	5154	1/1	0.71	0.64	45,45,45,45	0
55	MG	AA	4944	1/1	0.71	0.31	53,53,53,53	0
55	MG	AA	4524	1/1	0.71	0.47	87,87,87,87	0
55	MG	CA	3995	1/1	0.71	0.84	36,36,36,36	0
55	MG	AB	227	1/1	0.71	0.28	95,95,95,95	0
55	MG	AA	4746	1/1	0.71	0.25	71,71,71,71	0
55	MG	BW	106	1/1	0.71	0.18	91,91,91,91	0
55	MG	DA	1717	1/1	0.71	0.65	91,91,91,91	0
55	MG	DA	1761	1/1	0.71	0.73	76,76,76,76	0
55	MG	AA	4125	1/1	0.71	0.39	66,66,66,66	0
55	MG	BA	2101	1/1	0.71	0.33	59,59,59,59	0
55	MG	AA	4756	1/1	0.71	1.22	69,69,69,69	0
55	MG	DA	1731	1/1	0.71	0.30	47,47,47,47	0
55	MG	DA	1826	1/1	0.71	0.53	73,73,73,73	0
55	MG	CA	3352	1/1	0.71	0.21	61,61,61,61	0
55	MG	CA	4221	1/1	0.71	0.44	69,69,69,69	0
55	MG	CA	4334	1/1	0.71	0.35	102,102,102,102	0
55	MG	CA	3720	1/1	0.71	0.73	60,60,60,60	0
55	MG	CA	4116	1/1	0.71	0.34	56,56,56,56	0
55	MG	DA	1904	1/1	0.71	0.29	57,57,57,57	0
55	MG	DA	2199	1/1	0.71	0.30	59,59,59,59	0
55	MG	BA	2115	1/1	0.71	0.29	56,56,56,56	0
55	MG	CA	4263	1/1	0.71	0.42	61,61,61,61	0
55	MG	CA	3871	1/1	0.71	0.57	64,64,64,64	0
55	MG	CA	3532	1/1	0.71	0.56	64,64,64,64	0
55	MG	AA	5294	1/1	0.71	0.26	61,61,61,61	0
55	MG	AB	202	1/1	0.71	0.45	95,95,95,95	0
55	MG	CA	4194	1/1	0.71	0.41	78,78,78,78	0
55	MG	DA	1818	1/1	0.71	0.42	68,68,68,68	0
55	MG	BV	129	1/1	0.71	0.16	92,92,92,92	0
55	MG	BA	1846	1/1	0.72	0.33	87,87,87,87	0
55	MG	BA	1724	1/1	0.72	0.45	55,55,55,55	0
55	MG	AA	4794	1/1	0.72	0.28	106,106,106,106	0
55	MG	BV	116	1/1	0.72	0.44	74,74,74,74	0
55	MG	AA	5268	1/1	0.72	0.55	62,62,62,62	0
55	MG	BA	1847	1/1	0.72	0.12	52,52,52,52	0
55	MG	BA	1720	1/1	0.72	0.32	54,54,54,54	0
55	MG	BA	1790	1/1	0.72	0.16	109,109,109,109	0
55	MG	AA	4982	1/1	0.72	0.57	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1857	1/1	0.72	0.17	72,72,72,72	0
55	MG	CA	3835	1/1	0.72	0.27	69,69,69,69	0
55	MG	CA	3862	1/1	0.72	0.43	44,44,44,44	0
55	MG	BR	101	1/1	0.72	0.56	77,77,77,77	0
55	MG	CA	4348	1/1	0.72	0.76	89,89,89,89	0
55	MG	AA	4361	1/1	0.72	0.35	47,47,47,47	0
55	MG	DA	1721	1/1	0.72	0.23	79,79,79,79	0
55	MG	AA	5212	1/1	0.72	0.30	74,74,74,74	0
55	MG	CA	3070	1/1	0.72	0.39	39,39,39,39	0
55	MG	AA	5000	1/1	0.72	0.38	50,50,50,50	0
55	MG	AA	4680	1/1	0.72	0.43	68,68,68,68	0
55	MG	AA	4354	1/1	0.72	0.42	55,55,55,55	0
55	MG	AA	4954	1/1	0.72	0.21	42,42,42,42	0
55	MG	BA	1761	1/1	0.72	0.44	61,61,61,61	0
55	MG	BA	2132	1/1	0.72	0.46	82,82,82,82	0
55	MG	CA	4237	1/1	0.72	0.36	55,55,55,55	0
55	MG	CA	4182	1/1	0.72	0.25	47,47,47,47	0
55	MG	CA	4025	1/1	0.72	0.38	76,76,76,76	0
55	MG	CA	3782	1/1	0.72	0.69	76,76,76,76	0
55	MG	CA	3500	1/1	0.72	0.69	69,69,69,69	0
55	MG	BA	1824	1/1	0.72	0.39	76,76,76,76	0
55	MG	CA	3209	1/1	0.72	0.39	38,38,38,38	0
55	MG	DA	1648	1/1	0.72	0.47	68,68,68,68	0
55	MG	DA	2194	1/1	0.72	0.29	79,79,79,79	0
55	MG	AA	4567	1/1	0.72	0.69	83,83,83,83	0
55	MG	BA	1915	1/1	0.72	0.18	58,58,58,58	0
55	MG	AA	4702	1/1	0.72	0.48	89,89,89,89	0
55	MG	CA	3058	1/1	0.72	0.59	66,66,66,66	0
55	MG	AA	4089	1/1	0.72	0.43	96,96,96,96	0
55	MG	DA	2003	1/1	0.72	0.22	53,53,53,53	0
55	MG	AA	5159	1/1	0.72	1.00	69,69,69,69	0
55	MG	DA	2083	1/1	0.72	0.68	53,53,53,53	0
55	MG	AA	4499	1/1	0.72	0.42	74,74,74,74	0
55	MG	CA	3713	1/1	0.72	0.41	54,54,54,54	0
55	MG	AA	4732	1/1	0.72	1.04	112,112,112,112	0
55	MG	AA	4152	1/1	0.72	0.34	68,68,68,68	0
55	MG	CA	3100	1/1	0.72	0.29	86,86,86,86	0
55	MG	AA	5140	1/1	0.72	0.37	84,84,84,84	0
55	MG	CA	3882	1/1	0.72	0.12	60,60,60,60	0
55	MG	AA	4833	1/1	0.72	0.47	69,69,69,69	0
55	MG	CA	4367	1/1	0.73	0.60	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3322	1/1	0.73	1.37	66,66,66,66	0
55	MG	AA	4074	1/1	0.73	0.42	54,54,54,54	0
55	MG	CA	3324	1/1	0.73	0.35	53,53,53,53	0
55	MG	CA	4346	1/1	0.73	0.18	60,60,60,60	0
55	MG	DA	2157	1/1	0.73	0.33	31,31,31,31	0
55	MG	BA	1939	1/1	0.73	0.31	69,69,69,69	0
55	MG	CA	4261	1/1	0.73	0.37	48,48,48,48	0
55	MG	BC	301	1/1	0.73	0.72	64,64,64,64	0
55	MG	AA	5108	1/1	0.73	0.28	66,66,66,66	0
55	MG	DA	2010	1/1	0.73	0.09	61,61,61,61	0
55	MG	CA	4222	1/1	0.73	1.05	62,62,62,62	0
55	MG	CA	4242	1/1	0.73	0.39	47,47,47,47	0
55	MG	CA	3535	1/1	0.73	0.43	53,53,53,53	0
55	MG	CA	3356	1/1	0.73	0.60	34,34,34,34	0
55	MG	BA	1901	1/1	0.73	1.03	48,48,48,48	0
55	MG	DA	1896	1/1	0.73	0.45	74,74,74,74	0
55	MG	CA	4039	1/1	0.73	0.23	60,60,60,60	0
55	MG	DA	1651	1/1	0.73	0.49	69,69,69,69	0
55	MG	CA	4235	1/1	0.73	0.51	51,51,51,51	0
55	MG	AA	4310	1/1	0.73	0.46	37,37,37,37	0
55	MG	CA	3877	1/1	0.73	0.48	65,65,65,65	0
55	MG	AA	4448	1/1	0.73	0.14	59,59,59,59	0
55	MG	CA	4283	1/1	0.73	0.25	55,55,55,55	0
55	MG	AA	4749	1/1	0.73	0.52	51,51,51,51	0
55	MG	BA	1875	1/1	0.73	0.69	78,78,78,78	0
55	MG	CA	3727	1/1	0.73	0.41	89,89,89,89	0
55	MG	AA	5185	1/1	0.73	0.37	102,102,102,102	0
55	MG	BA	1947	1/1	0.73	0.62	69,69,69,69	0
55	MG	DA	1800	1/1	0.73	0.34	63,63,63,63	0
55	MG	DA	1901	1/1	0.73	0.60	68,68,68,68	0
55	MG	CA	4117	1/1	0.73	1.26	76,76,76,76	0
55	MG	AA	5169	1/1	0.73	0.89	71,71,71,71	0
55	MG	BA	1923	1/1	0.73	0.45	54,54,54,54	0
55	MG	DA	1789	1/1	0.73	0.14	90,90,90,90	0
55	MG	DA	2198	1/1	0.73	0.49	87,87,87,87	0
55	MG	AA	5226	1/1	0.73	0.40	78,78,78,78	0
55	MG	BA	1739	1/1	0.73	0.52	73,73,73,73	0
55	MG	AA	4708	1/1	0.73	0.44	72,72,72,72	0
55	MG	CA	3789	1/1	0.73	0.47	94,94,94,94	0
55	MG	AA	4628	1/1	0.73	0.68	68,68,68,68	0
55	MG	AA	5229	1/1	0.73	0.44	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4004	1/1	0.73	0.72	48,48,48,48	0
55	MG	DW	105	1/1	0.73	0.11	92,92,92,92	0
55	MG	CA	3023	1/1	0.73	0.29	64,64,64,64	0
55	MG	AA	4629	1/1	0.73	0.24	112,112,112,112	0
55	MG	AA	4606	1/1	0.73	0.56	109,109,109,109	0
55	MG	CA	3551	1/1	0.73	0.52	87,87,87,87	0
55	MG	CA	3439	1/1	0.73	0.37	36,36,36,36	0
55	MG	DA	2104	1/1	0.73	0.18	124,124,124,124	0
55	MG	BA	1608	1/1	0.73	0.48	69,69,69,69	0
55	MG	BA	1897	1/1	0.73	0.12	53,53,53,53	0
55	MG	AB	218	1/1	0.73	0.84	93,93,93,93	0
55	MG	CA	3561	1/1	0.73	0.51	68,68,68,68	0
55	MG	CA	2989	1/1	0.73	0.32	83,83,83,83	0
55	MG	DA	2183	1/1	0.73	0.35	96,96,96,96	0
55	MG	AA	4817	1/1	0.73	0.08	98,98,98,98	0
55	MG	AA	4009	1/1	0.73	0.15	56,56,56,56	0
55	MG	DA	2184	1/1	0.73	0.66	79,79,79,79	0
55	MG	CA	3932	1/1	0.73	0.42	54,54,54,54	0
55	MG	BA	1731	1/1	0.73	0.82	37,37,37,37	0
55	MG	AA	4084	1/1	0.73	0.46	61,61,61,61	0
55	MG	AA	4055	1/1	0.73	0.37	92,92,92,92	0
55	MG	AA	4965	1/1	0.73	0.50	51,51,51,51	0
55	MG	CA	3081	1/1	0.73	0.20	80,80,80,80	0
55	MG	CA	3730	1/1	0.73	0.20	74,74,74,74	0
55	MG	CA	3473	1/1	0.74	0.20	80,80,80,80	0
55	MG	CA	3593	1/1	0.74	0.50	62,62,62,62	0
55	MG	BA	1966	1/1	0.74	0.32	69,69,69,69	0
55	MG	CA	3433	1/1	0.74	0.35	67,67,67,67	0
55	MG	CA	3620	1/1	0.74	0.30	89,89,89,89	0
55	MG	DA	1957	1/1	0.74	0.18	43,43,43,43	0
55	MG	CA	3041	1/1	0.74	0.37	72,72,72,72	0
55	MG	CA	4193	1/1	0.74	0.26	58,58,58,58	0
55	MG	AA	5072	1/1	0.74	0.27	78,78,78,78	0
55	MG	AA	4731	1/1	0.74	0.29	119,119,119,119	0
55	MG	DA	1662	1/1	0.74	0.21	64,64,64,64	0
55	MG	AF	303	1/1	0.74	0.38	62,62,62,62	0
55	MG	CA	3766	1/1	0.74	0.34	89,89,89,89	0
55	MG	CA	4280	1/1	0.74	0.49	84,84,84,84	0
55	MG	AA	4861	1/1	0.74	0.10	79,79,79,79	0
55	MG	CA	3321	1/1	0.74	0.53	45,45,45,45	0
55	MG	DA	2072	1/1	0.74	0.30	49,49,49,49	0
55	MG	CA	3837	1/1	0.74	0.38	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1787	1/1	0.74	0.22	98,98,98,98	0
55	MG	BW	118	1/1	0.74	0.44	61,61,61,61	0
55	MG	AA	4521	1/1	0.74	0.15	64,64,64,64	0
55	MG	CA	3080	1/1	0.74	0.43	65,65,65,65	0
55	MG	AA	4664	1/1	0.74	0.43	74,74,74,74	0
55	MG	DA	1678	1/1	0.74	0.57	74,74,74,74	0
55	MG	BA	1810	1/1	0.74	0.48	75,75,75,75	0
55	MG	AA	5235	1/1	0.74	0.51	67,67,67,67	0
55	MG	DA	2177	1/1	0.74	0.27	105,105,105,105	0
55	MG	BA	2118	1/1	0.74	0.39	64,64,64,64	0
55	MG	DA	1872	1/1	0.74	0.87	96,96,96,96	0
55	MG	DA	2028	1/1	0.74	0.67	82,82,82,82	0
55	MG	DA	2150	1/1	0.74	0.47	57,57,57,57	0
55	MG	CB	227	1/1	0.74	0.25	76,76,76,76	0
55	MG	BA	2038	1/1	0.74	0.27	51,51,51,51	0
55	MG	BA	1991	1/1	0.74	0.28	62,62,62,62	0
55	MG	CA	3453	1/1	0.74	0.45	49,49,49,49	0
55	MG	CA	3803	1/1	0.74	0.89	121,121,121,121	0
55	MG	CA	2984	1/1	0.74	0.47	103,103,103,103	0
55	MG	AA	4948	1/1	0.74	0.33	56,56,56,56	0
55	MG	AA	5050	1/1	0.74	0.30	63,63,63,63	0
55	MG	BA	1972	1/1	0.74	0.75	55,55,55,55	0
55	MG	AA	5142	1/1	0.74	0.58	69,69,69,69	0
55	MG	AA	4150	1/1	0.74	0.40	86,86,86,86	0
55	MG	BA	1993	1/1	0.74	0.24	28,28,28,28	0
55	MG	AA	5173	1/1	0.74	0.27	68,68,68,68	0
55	MG	CA	3958	1/1	0.74	0.46	51,51,51,51	0
55	MG	AA	4462	1/1	0.74	0.39	48,48,48,48	0
55	MG	CA	3008	1/1	0.74	0.46	57,57,57,57	0
55	MG	DA	2055	1/1	0.74	0.53	59,59,59,59	0
55	MG	CL	201	1/1	0.74	0.40	76,76,76,76	0
55	MG	DA	2169	1/1	0.74	0.44	54,54,54,54	0
55	MG	AA	4017	1/1	0.74	1.20	155,155,155,155	0
55	MG	AA	4951	1/1	0.74	0.34	64,64,64,64	0
55	MG	AA	5160	1/1	0.74	0.43	55,55,55,55	0
55	MG	CA	3399	1/1	0.74	0.43	37,37,37,37	0
55	MG	DA	1942	1/1	0.74	0.38	58,58,58,58	0
55	MG	DA	2144	1/1	0.74	0.96	63,63,63,63	0
55	MG	BA	2008	1/1	0.74	0.65	45,45,45,45	0
55	MG	DA	1834	1/1	0.74	0.33	123,123,123,123	0
55	MG	CA	3833	1/1	0.74	0.22	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AM	201	1/1	0.74	0.38	62,62,62,62	0
55	MG	DA	1753	1/1	0.74	0.33	52,52,52,52	0
55	MG	BA	1641	1/1	0.74	0.42	63,63,63,63	0
55	MG	DA	1928	1/1	0.74	0.73	68,68,68,68	0
55	MG	DA	2155	1/1	0.74	0.14	83,83,83,83	0
55	MG	AA	4987	1/1	0.74	0.15	78,78,78,78	0
55	MG	BA	2151	1/1	0.74	0.40	76,76,76,76	0
55	MG	DA	2051	1/1	0.74	0.54	65,65,65,65	0
55	MG	AA	4773	1/1	0.74	0.54	69,69,69,69	0
55	MG	AA	4515	1/1	0.74	0.28	62,62,62,62	0
55	MG	BH	201	1/1	0.74	0.27	64,64,64,64	0
55	MG	DA	1883	1/1	0.74	0.37	75,75,75,75	0
55	MG	DA	2087	1/1	0.74	0.59	64,64,64,64	0
55	MG	AA	5253	1/1	0.74	0.13	90,90,90,90	0
55	MG	DW	119	1/1	0.75	0.36	49,49,49,49	0
55	MG	DA	1654	1/1	0.75	0.35	131,131,131,131	0
55	MG	DA	2138	1/1	0.75	0.18	58,58,58,58	0
55	MG	DA	1660	1/1	0.75	0.29	126,126,126,126	0
55	MG	DA	1686	1/1	0.75	0.11	97,97,97,97	0
55	MG	CA	3382	1/1	0.75	0.65	38,38,38,38	0
55	MG	CA	3528	1/1	0.75	0.43	43,43,43,43	0
55	MG	DA	1871	1/1	0.75	0.10	69,69,69,69	0
55	MG	CA	4161	1/1	0.75	0.29	65,65,65,65	0
55	MG	CA	2938	1/1	0.75	0.75	107,107,107,107	0
55	MG	AA	4694	1/1	0.75	0.34	92,92,92,92	0
55	MG	CA	3948	1/1	0.75	0.62	66,66,66,66	0
55	MG	BA	1680	1/1	0.75	0.44	72,72,72,72	0
55	MG	BA	2082	1/1	0.75	0.47	54,54,54,54	0
55	MG	CA	4036	1/1	0.75	0.13	83,83,83,83	0
55	MG	AF	301	1/1	0.75	0.67	59,59,59,59	0
55	MG	CA	4239	1/1	0.75	0.55	56,56,56,56	0
55	MG	AA	5275	1/1	0.75	0.31	59,59,59,59	0
55	MG	AG	202	1/1	0.75	0.41	76,76,76,76	0
55	MG	CA	3003	1/1	0.75	0.10	69,69,69,69	0
55	MG	AA	5240	1/1	0.75	0.53	93,93,93,93	0
55	MG	AA	5184	1/1	0.75	0.39	73,73,73,73	0
55	MG	CB	257	1/1	0.75	0.73	81,81,81,81	0
55	MG	AA	5232	1/1	0.75	0.33	76,76,76,76	0
55	MG	BA	1896	1/1	0.75	0.16	66,66,66,66	0
55	MG	BA	2007	1/1	0.75	0.23	82,82,82,82	0
55	MG	CA	3986	1/1	0.75	0.65	38,38,38,38	0
55	MG	BA	1639	1/1	0.75	0.44	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4989	1/1	0.75	0.12	72,72,72,72	0
55	MG	AA	4065	1/1	0.75	0.40	100,100,100,100	0
55	MG	DA	2089	1/1	0.75	0.35	58,58,58,58	0
55	MG	AA	4806	1/1	0.75	0.37	48,48,48,48	0
55	MG	CA	3649	1/1	0.75	0.40	54,54,54,54	0
55	MG	BA	1929	1/1	0.75	0.47	72,72,72,72	0
55	MG	AA	4838	1/1	0.75	0.21	73,73,73,73	0
55	MG	CA	4359	1/1	0.75	0.45	56,56,56,56	0
55	MG	CA	4284	1/1	0.75	0.37	63,63,63,63	0
55	MG	CA	3459	1/1	0.75	0.34	45,45,45,45	0
55	MG	BA	2047	1/1	0.75	0.27	58,58,58,58	0
55	MG	AA	4347	1/1	0.75	0.34	54,54,54,54	0
55	MG	CB	220	1/1	0.75	0.17	31,31,31,31	0
55	MG	BA	1898	1/1	0.75	0.44	54,54,54,54	0
55	MG	BA	1744	1/1	0.75	0.39	51,51,51,51	0
55	MG	AA	4678	1/1	0.75	0.40	62,62,62,62	0
55	MG	AA	4783	1/1	0.75	0.14	70,70,70,70	0
55	MG	AA	4797	1/1	0.75	0.55	50,50,50,50	0
55	MG	BA	1793	1/1	0.75	0.18	73,73,73,73	0
55	MG	BA	1863	1/1	0.75	0.44	56,56,56,56	0
55	MG	CA	3226	1/1	0.75	0.16	25,25,25,25	0
55	MG	CA	3864	1/1	0.75	0.48	55,55,55,55	0
55	MG	DA	2127	1/1	0.75	0.45	68,68,68,68	0
55	MG	CB	245	1/1	0.75	0.27	51,51,51,51	0
55	MG	CA	3062	1/1	0.75	0.65	68,68,68,68	0
55	MG	AA	5244	1/1	0.75	0.38	68,68,68,68	0
55	MG	CA	4220	1/1	0.75	0.14	95,95,95,95	0
55	MG	AA	4435	1/1	0.75	0.25	38,38,38,38	0
55	MG	BW	117	1/1	0.75	0.44	77,77,77,77	0
55	MG	AA	4481	1/1	0.75	0.49	58,58,58,58	0
55	MG	DA	1838	1/1	0.75	0.24	73,73,73,73	0
55	MG	CA	3460	1/1	0.75	0.43	45,45,45,45	0
55	MG	BA	1775	1/1	0.75	0.52	64,64,64,64	0
55	MG	CA	4142	1/1	0.75	0.14	103,103,103,103	0
55	MG	CA	3653	1/1	0.75	0.91	82,82,82,82	0
55	MG	AA	4643	1/1	0.75	0.20	65,65,65,65	0
55	MG	AA	5223	1/1	0.75	0.43	70,70,70,70	0
55	MG	BA	2123	1/1	0.75	0.86	82,82,82,82	0
55	MG	BA	1675	1/1	0.76	0.37	60,60,60,60	0
55	MG	AA	4821	1/1	0.76	0.31	70,70,70,70	0
55	MG	AA	4942	1/1	0.76	0.18	56,56,56,56	0
55	MG	CA	3002	1/1	0.76	0.46	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BV	107	1/1	0.76	0.16	68,68,68,68	0
55	MG	CA	4122	1/1	0.76	0.74	49,49,49,49	0
55	MG	AA	4676	1/1	0.76	0.23	74,74,74,74	0
55	MG	CA	4180	1/1	0.76	0.18	63,63,63,63	0
55	MG	CA	4048	1/1	0.76	0.24	65,65,65,65	0
55	MG	AA	4656	1/1	0.76	0.92	69,69,69,69	0
55	MG	CA	3809	1/1	0.76	0.36	62,62,62,62	0
55	MG	BA	1909	1/1	0.76	0.26	67,67,67,67	0
55	MG	AA	5188	1/1	0.76	0.29	77,77,77,77	0
55	MG	AA	4913	1/1	0.76	0.26	36,36,36,36	0
55	MG	CA	3770	1/1	0.76	0.28	62,62,62,62	0
55	MG	AA	4912	1/1	0.76	0.37	49,49,49,49	0
55	MG	CA	3544	1/1	0.76	0.35	53,53,53,53	0
55	MG	AA	5249	1/1	0.76	0.45	69,69,69,69	0
55	MG	AA	4804	1/1	0.76	0.60	57,57,57,57	0
55	MG	AA	5109	1/1	0.76	0.35	88,88,88,88	0
55	MG	BA	1866	1/1	0.76	0.33	57,57,57,57	0
55	MG	BA	1660	1/1	0.76	0.25	73,73,73,73	0
55	MG	DA	1911	1/1	0.76	0.25	58,58,58,58	0
55	MG	CA	4272	1/1	0.76	0.40	65,65,65,65	0
55	MG	AA	4147	1/1	0.76	0.36	75,75,75,75	0
55	MG	AA	4947	1/1	0.76	0.46	61,61,61,61	0
55	MG	BA	1980	1/1	0.76	0.37	53,53,53,53	0
55	MG	CA	3857	1/1	0.76	0.45	44,44,44,44	0
55	MG	AA	5281	1/1	0.76	0.29	56,56,56,56	0
55	MG	DA	1878	1/1	0.76	0.38	111,111,111,111	0
55	MG	CA	3495	1/1	0.76	0.32	58,58,58,58	0
55	MG	CA	3291	1/1	0.76	0.21	31,31,31,31	0
55	MG	AA	4587	1/1	0.76	0.11	107,107,107,107	0
55	MG	CA	3718	1/1	0.76	0.41	71,71,71,71	0
55	MG	AS	205	1/1	0.76	0.47	70,70,70,70	0
55	MG	CY	102	1/1	0.76	0.28	100,100,100,100	0
55	MG	CA	4223	1/1	0.76	0.37	30,30,30,30	0
55	MG	DA	1679	1/1	0.76	0.38	41,41,41,41	0
55	MG	CA	2996	1/1	0.76	0.71	55,55,55,55	0
55	MG	BA	2126	1/1	0.76	0.60	106,106,106,106	0
55	MG	AA	4374	1/1	0.76	0.27	46,46,46,46	0
55	MG	AA	4667	1/1	0.76	0.83	120,120,120,120	0
55	MG	CR	202	1/1	0.76	0.52	66,66,66,66	0
55	MG	AA	4835	1/1	0.76	0.41	131,131,131,131	0
55	MG	AA	5117	1/1	0.76	1.11	77,77,77,77	0
55	MG	CA	4270	1/1	0.76	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3942	1/1	0.76	0.41	60,60,60,60	0
55	MG	BA	2055	1/1	0.76	0.31	95,95,95,95	0
55	MG	CA	4119	1/1	0.76	0.57	51,51,51,51	0
55	MG	BA	1862	1/1	0.76	0.39	65,65,65,65	0
55	MG	BA	2140	1/1	0.76	0.42	88,88,88,88	0
55	MG	AA	5080	1/1	0.76	0.29	56,56,56,56	0
55	MG	CA	3004	1/1	0.76	1.07	89,89,89,89	0
55	MG	AA	4904	1/1	0.76	0.36	49,49,49,49	0
55	MG	AA	5251	1/1	0.76	0.47	55,55,55,55	0
55	MG	AA	5051	1/1	0.76	0.31	69,69,69,69	0
55	MG	CA	3447	1/1	0.76	0.20	57,57,57,57	0
55	MG	CA	2919	1/1	0.76	0.81	62,62,62,62	0
55	MG	AA	4099	1/1	0.76	0.46	88,88,88,88	0
55	MG	AA	4267	1/1	0.76	0.40	50,50,50,50	0
55	MG	DW	107	1/1	0.76	0.21	155,155,155,155	0
55	MG	CA	3066	1/1	0.76	0.38	92,92,92,92	0
55	MG	CA	4177	1/1	0.76	0.36	54,54,54,54	0
55	MG	CA	3489	1/1	0.76	0.65	69,69,69,69	0
55	MG	DA	1683	1/1	0.76	0.35	98,98,98,98	0
55	MG	AA	5075	1/1	0.76	0.49	49,49,49,49	0
55	MG	AA	4054	1/1	0.76	0.47	79,79,79,79	0
55	MG	AA	4805	1/1	0.76	0.38	61,61,61,61	0
55	MG	BA	1780	1/1	0.76	0.28	72,72,72,72	0
55	MG	BO	101	1/1	0.76	0.42	91,91,91,91	0
55	MG	AA	4006	1/1	0.76	0.37	59,59,59,59	0
55	MG	CA	3040	1/1	0.76	0.27	60,60,60,60	0
55	MG	CA	3037	1/1	0.76	0.18	66,66,66,66	0
55	MG	AA	4870	1/1	0.76	0.85	63,63,63,63	0
55	MG	BA	2016	1/1	0.76	0.28	47,47,47,47	0
55	MG	AA	4377	1/1	0.76	0.63	52,52,52,52	0
55	MG	CA	3686	1/1	0.76	0.62	83,83,83,83	0
55	MG	BA	1649	1/1	0.76	0.67	96,96,96,96	0
55	MG	DA	2200	1/1	0.76	0.45	61,61,61,61	0
55	MG	CA	3950	1/1	0.76	0.31	75,75,75,75	0
55	MG	DA	1632	1/1	0.76	0.36	81,81,81,81	0
55	MG	BA	1843	1/1	0.77	0.71	87,87,87,87	0
55	MG	CB	250	1/1	0.77	0.31	74,74,74,74	0
55	MG	BA	2105	1/1	0.77	0.28	96,96,96,96	0
55	MG	CA	3905	1/1	0.77	0.11	64,64,64,64	0
55	MG	CA	4325	1/1	0.77	0.41	72,72,72,72	0
55	MG	CA	3075	1/1	0.77	1.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1795	1/1	0.77	0.68	70,70,70,70	0
55	MG	DA	1900	1/1	0.77	0.11	87,87,87,87	0
55	MG	C3	102	1/1	0.77	0.13	46,46,46,46	0
55	MG	DD	302	1/1	0.77	0.25	48,48,48,48	0
55	MG	BA	2024	1/1	0.77	0.09	68,68,68,68	0
55	MG	AA	4933	1/1	0.77	0.22	62,62,62,62	0
55	MG	AA	4151	1/1	0.77	0.41	83,83,83,83	0
55	MG	CA	3310	1/1	0.77	0.50	48,48,48,48	0
55	MG	BA	1621	1/1	0.77	0.40	67,67,67,67	0
55	MG	CA	4323	1/1	0.77	0.40	49,49,49,49	0
55	MG	DA	1910	1/1	0.77	0.44	104,104,104,104	0
55	MG	CA	4252	1/1	0.77	0.18	66,66,66,66	0
55	MG	AA	4421	1/1	0.77	0.42	47,47,47,47	0
55	MG	DL	202	1/1	0.77	0.48	60,60,60,60	0
55	MG	CA	3060	1/1	0.77	0.32	100,100,100,100	0
55	MG	AA	4512	1/1	0.77	0.17	55,55,55,55	0
55	MG	DA	1672	1/1	0.77	0.42	62,62,62,62	0
55	MG	CF	305	1/1	0.77	0.31	89,89,89,89	0
55	MG	AA	5247	1/1	0.77	1.42	91,91,91,91	0
55	MG	CA	4224	1/1	0.77	0.20	58,58,58,58	0
55	MG	BA	2165	1/1	0.77	0.30	66,66,66,66	0
55	MG	DA	2118	1/1	0.77	0.26	54,54,54,54	0
55	MG	CA	4388	1/1	0.77	0.45	59,59,59,59	0
55	MG	DA	1918	1/1	0.77	0.12	88,88,88,88	0
55	MG	CA	4396	1/1	0.77	0.18	90,90,90,90	0
55	MG	BA	1722	1/1	0.77	0.28	43,43,43,43	0
55	MG	CA	3830	1/1	0.77	0.41	66,66,66,66	0
55	MG	BA	1835	1/1	0.77	0.32	106,106,106,106	0
55	MG	DA	1687	1/1	0.77	0.34	86,86,86,86	0
55	MG	CA	3706	1/1	0.77	0.41	48,48,48,48	0
55	MG	CA	4216	1/1	0.77	0.36	60,60,60,60	0
55	MG	AA	5044	1/1	0.77	0.45	72,72,72,72	0
55	MG	CA	3815	1/1	0.77	0.30	66,66,66,66	0
55	MG	BA	1656	1/1	0.77	0.45	70,70,70,70	0
55	MG	CA	3760	1/1	0.77	0.94	74,74,74,74	0
55	MG	CA	3709	1/1	0.77	1.14	82,82,82,82	0
55	MG	AA	5219	1/1	0.77	0.43	79,79,79,79	0
55	MG	AA	4819	1/1	0.77	0.33	77,77,77,77	0
55	MG	DA	1613	1/1	0.77	0.34	60,60,60,60	0
55	MG	AA	5010	1/1	0.77	0.59	81,81,81,81	0
55	MG	CA	2918	1/1	0.77	0.34	89,89,89,89	0
55	MG	BA	1784	1/1	0.77	0.39	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4865	1/1	0.77	0.77	52,52,52,52	0
55	MG	CA	3814	1/1	0.77	0.37	76,76,76,76	0
55	MG	CA	3732	1/1	0.77	0.39	74,74,74,74	0
55	MG	AA	5145	1/1	0.77	0.32	58,58,58,58	0
55	MG	AA	5206	1/1	0.77	0.38	78,78,78,78	0
55	MG	AA	5174	1/1	0.77	0.38	63,63,63,63	0
55	MG	CA	3851	1/1	0.77	0.40	74,74,74,74	0
55	MG	BA	1905	1/1	0.77	0.37	64,64,64,64	0
55	MG	CX	101	1/1	0.77	1.00	71,71,71,71	0
55	MG	CA	3895	1/1	0.77	0.35	58,58,58,58	0
55	MG	CA	4128	1/1	0.77	0.29	64,64,64,64	0
55	MG	CA	3343	1/1	0.77	0.15	54,54,54,54	0
55	MG	CA	3009	1/1	0.77	0.38	56,56,56,56	0
55	MG	AA	4469	1/1	0.77	0.16	66,66,66,66	0
55	MG	CA	3449	1/1	0.77	0.15	49,49,49,49	0
55	MG	BA	2114	1/1	0.77	0.44	60,60,60,60	0
55	MG	AA	4824	1/1	0.78	0.32	51,51,51,51	0
55	MG	AA	4570	1/1	0.78	0.30	76,76,76,76	0
55	MG	CA	3546	1/1	0.78	0.43	55,55,55,55	0
55	MG	AA	5245	1/1	0.78	0.48	76,76,76,76	0
55	MG	CA	3374	1/1	0.78	0.20	56,56,56,56	0
55	MG	CB	237	1/1	0.78	0.46	72,72,72,72	0
55	MG	DA	2088	1/1	0.78	0.28	94,94,94,94	0
55	MG	BA	1717	1/1	0.78	0.51	75,75,75,75	0
55	MG	CA	3954	1/1	0.78	0.18	92,92,92,92	0
55	MG	CA	3606	1/1	0.78	0.34	55,55,55,55	0
55	MG	CA	2915	1/1	0.78	0.27	64,64,64,64	0
55	MG	AA	4442	1/1	0.78	0.56	55,55,55,55	0
55	MG	DA	2203	1/1	0.78	0.33	53,53,53,53	0
55	MG	CA	3984	1/1	0.78	0.21	65,65,65,65	0
55	MG	DA	2011	1/1	0.78	0.27	79,79,79,79	0
55	MG	DA	2137	1/1	0.78	0.23	98,98,98,98	0
55	MG	AA	4590	1/1	0.78	0.47	66,66,66,66	0
55	MG	CA	4266	1/1	0.78	0.60	63,63,63,63	0
55	MG	CA	4333	1/1	0.78	0.25	76,76,76,76	0
55	MG	CA	3754	1/1	0.78	0.30	67,67,67,67	0
55	MG	DA	2181	1/1	0.78	0.47	68,68,68,68	0
55	MG	CA	2998	1/1	0.78	0.38	62,62,62,62	0
55	MG	AA	5087	1/1	0.78	0.37	43,43,43,43	0
55	MG	AA	4525	1/1	0.78	0.33	43,43,43,43	0
55	MG	CA	4121	1/1	0.78	0.30	39,39,39,39	0
55	MG	BA	2051	1/1	0.78	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1872	1/1	0.78	0.34	64,64,64,64	0
55	MG	AA	4575	1/1	0.78	0.11	87,87,87,87	0
55	MG	CA	4307	1/1	0.78	0.37	58,58,58,58	0
55	MG	AA	5141	1/1	0.78	0.21	58,58,58,58	0
55	MG	DA	1816	1/1	0.78	0.30	79,79,79,79	0
55	MG	AA	4841	1/1	0.78	0.45	67,67,67,67	0
55	MG	DA	1754	1/1	0.78	0.18	69,69,69,69	0
55	MG	AA	4081	1/1	0.78	0.26	78,78,78,78	0
55	MG	CA	3558	1/1	0.78	0.27	50,50,50,50	0
55	MG	CA	3401	1/1	0.78	0.41	55,55,55,55	0
55	MG	BA	1719	1/1	0.78	0.12	50,50,50,50	0
55	MG	DA	1685	1/1	0.78	0.24	59,59,59,59	0
55	MG	CA	4340	1/1	0.78	0.32	40,40,40,40	0
55	MG	CA	3704	1/1	0.78	0.28	61,61,61,61	0
55	MG	CA	3788	1/1	0.78	0.49	57,57,57,57	0
55	MG	AA	4650	1/1	0.78	0.62	70,70,70,70	0
55	MG	CA	3807	1/1	0.78	0.68	66,66,66,66	0
55	MG	BA	1861	1/1	0.78	0.38	67,67,67,67	0
55	MG	BA	1655	1/1	0.78	0.35	77,77,77,77	0
55	MG	AO	201	1/1	0.78	0.17	67,67,67,67	0
55	MG	CA	2960	1/1	0.78	0.41	77,77,77,77	0
55	MG	DA	2158	1/1	0.78	0.12	76,76,76,76	0
55	MG	AA	4328	1/1	0.78	1.05	40,40,40,40	0
55	MG	CA	3647	1/1	0.78	0.41	69,69,69,69	0
55	MG	AA	4635	1/1	0.78	0.60	79,79,79,79	0
55	MG	AA	4963	1/1	0.78	0.37	62,62,62,62	0
55	MG	AA	4426	1/1	0.78	0.22	64,64,64,64	0
55	MG	AA	5282	1/1	0.78	0.19	87,87,87,87	0
55	MG	CA	4062	1/1	0.78	0.27	50,50,50,50	0
55	MG	CA	3423	1/1	0.78	0.14	56,56,56,56	0
55	MG	BA	1671	1/1	0.78	0.28	112,112,112,112	0
55	MG	BA	1648	1/1	0.78	0.41	61,61,61,61	0
55	MG	AA	4511	1/1	0.78	1.17	71,71,71,71	0
55	MG	CA	3145	1/1	0.78	0.16	22,22,22,22	0
55	MG	CA	2907	1/1	0.78	0.75	70,70,70,70	0
55	MG	CB	263	1/1	0.78	0.11	73,73,73,73	0
55	MG	CA	4191	1/1	0.78	0.11	55,55,55,55	0
55	MG	BA	1942	1/1	0.78	0.27	77,77,77,77	0
55	MG	AA	4818	1/1	0.78	0.41	79,79,79,79	0
55	MG	CA	3010	1/1	0.78	0.69	65,65,65,65	0
55	MG	CA	3450	1/1	0.78	0.50	49,49,49,49	0
55	MG	CA	4350	1/1	0.78	0.40	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4531	1/1	0.78	0.23	57,57,57,57	0
55	MG	CA	4102	1/1	0.78	0.66	69,69,69,69	0
55	MG	AA	4355	1/1	0.78	1.33	69,69,69,69	0
55	MG	CA	3735	1/1	0.78	0.18	64,64,64,64	0
55	MG	CA	3813	1/1	0.78	0.27	58,58,58,58	0
55	MG	AA	4670	1/1	0.78	0.31	66,66,66,66	0
55	MG	AA	5094	1/1	0.78	0.17	55,55,55,55	0
55	MG	CA	3842	1/1	0.78	0.32	71,71,71,71	0
55	MG	AA	4129	1/1	0.78	0.40	66,66,66,66	0
55	MG	AA	4630	1/1	0.78	0.33	72,72,72,72	0
55	MG	CA	3756	1/1	0.79	0.26	90,90,90,90	0
55	MG	CA	4379	1/1	0.79	0.34	59,59,59,59	0
55	MG	CA	3084	1/1	0.79	0.19	95,95,95,95	0
55	MG	AA	5090	1/1	0.79	0.79	73,73,73,73	0
55	MG	CA	3515	1/1	0.79	0.30	42,42,42,42	0
55	MG	CA	4133	1/1	0.79	0.39	51,51,51,51	0
55	MG	AA	5236	1/1	0.79	0.53	66,66,66,66	0
55	MG	CA	3930	1/1	0.79	0.36	74,74,74,74	0
55	MG	AA	5115	1/1	0.79	0.26	65,65,65,65	0
55	MG	CA	4205	1/1	0.79	0.60	82,82,82,82	0
55	MG	BA	1625	1/1	0.79	0.46	91,91,91,91	0
55	MG	CA	4100	1/1	0.79	0.41	65,65,65,65	0
55	MG	CA	4337	1/1	0.79	0.52	69,69,69,69	0
55	MG	AA	4293	1/1	0.79	0.65	43,43,43,43	0
55	MG	CA	2986	1/1	0.79	0.29	51,51,51,51	0
55	MG	CA	3435	1/1	0.79	0.64	45,45,45,45	0
55	MG	AA	4843	1/1	0.79	0.40	51,51,51,51	0
55	MG	AA	5005	1/1	0.79	0.29	61,61,61,61	0
55	MG	CA	3347	1/1	0.79	0.35	60,60,60,60	0
55	MG	AA	4905	1/1	0.79	0.07	71,71,71,71	0
55	MG	AA	4568	1/1	0.79	0.33	41,41,41,41	0
55	MG	CA	3570	1/1	0.79	0.29	57,57,57,57	0
55	MG	DA	1814	1/1	0.79	0.32	59,59,59,59	0
55	MG	CA	3625	1/1	0.79	0.30	59,59,59,59	0
55	MG	AB	231	1/1	0.79	0.20	78,78,78,78	0
55	MG	BA	1920	1/1	0.79	0.17	92,92,92,92	0
55	MG	CA	4030	1/1	0.79	0.27	37,37,37,37	0
55	MG	BW	116	1/1	0.79	0.15	82,82,82,82	0
55	MG	CA	4366	1/1	0.79	0.34	70,70,70,70	0
55	MG	DA	1783	1/1	0.79	0.15	72,72,72,72	0
55	MG	DH	202	1/1	0.79	1.14	87,87,87,87	0
55	MG	DA	1863	1/1	0.79	0.63	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BV	114	1/1	0.79	0.20	70,70,70,70	0
55	MG	AA	4677	1/1	0.79	0.36	95,95,95,95	0
55	MG	BB	301	1/1	0.79	0.24	54,54,54,54	0
55	MG	CA	3022	1/1	0.79	0.68	56,56,56,56	0
55	MG	CA	3436	1/1	0.79	0.42	46,46,46,46	0
55	MG	BA	1828	1/1	0.79	0.30	68,68,68,68	0
55	MG	CA	3472	1/1	0.79	0.34	50,50,50,50	0
55	MG	DA	1907	1/1	0.79	0.68	71,71,71,71	0
55	MG	DA	1786	1/1	0.79	0.14	93,93,93,93	0
55	MG	CA	4163	1/1	0.79	0.44	64,64,64,64	0
55	MG	DA	1895	1/1	0.79	0.26	80,80,80,80	0
55	MG	DA	1794	1/1	0.79	0.62	64,64,64,64	0
55	MG	AA	5284	1/1	0.79	0.28	52,52,52,52	0
55	MG	BA	1802	1/1	0.79	0.33	66,66,66,66	0
55	MG	CA	4131	1/1	0.79	0.27	70,70,70,70	0
55	MG	DA	2080	1/1	0.79	0.32	71,71,71,71	0
55	MG	AA	4952	1/1	0.79	0.19	89,89,89,89	0
55	MG	CA	2922	1/1	0.79	0.28	56,56,56,56	0
55	MG	BA	1788	1/1	0.79	0.68	58,58,58,58	0
55	MG	CA	3052	1/1	0.79	0.38	86,86,86,86	0
55	MG	BA	2062	1/1	0.79	0.38	79,79,79,79	0
55	MG	AA	4901	1/1	0.79	0.18	42,42,42,42	0
55	MG	CA	4209	1/1	0.79	0.53	55,55,55,55	0
55	MG	DV	119	1/1	0.79	0.19	72,72,72,72	0
55	MG	CA	3301	1/1	0.79	0.34	35,35,35,35	0
55	MG	CA	3866	1/1	0.79	0.29	65,65,65,65	0
55	MG	CA	4265	1/1	0.79	0.30	64,64,64,64	0
55	MG	AA	4282	1/1	0.79	0.26	23,23,23,23	0
55	MG	AA	4035	1/1	0.79	0.45	65,65,65,65	0
55	MG	BA	1988	1/1	0.79	0.19	66,66,66,66	0
55	MG	DA	1735	1/1	0.79	0.21	57,57,57,57	0
55	MG	AX	104	1/1	0.79	0.38	65,65,65,65	0
55	MG	CA	4041	1/1	0.79	0.64	61,61,61,61	0
55	MG	AA	4997	1/1	0.79	0.56	68,68,68,68	0
55	MG	CB	253	1/1	0.79	0.10	76,76,76,76	0
55	MG	CA	3521	1/1	0.79	0.29	42,42,42,42	0
55	MG	CA	3351	1/1	0.79	0.27	39,39,39,39	0
55	MG	CA	4082	1/1	0.79	0.32	43,43,43,43	0
55	MG	CA	3539	1/1	0.79	0.12	78,78,78,78	0
55	MG	BA	1945	1/1	0.79	0.60	82,82,82,82	0
55	MG	BA	2001	1/1	0.79	0.36	68,68,68,68	0
55	MG	DA	2095	1/1	0.79	0.22	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4445	1/1	0.79	0.15	61,61,61,61	0
55	MG	AR	204	1/1	0.79	0.28	40,40,40,40	0
55	MG	DA	1748	1/1	0.79	0.43	73,73,73,73	0
55	MG	CA	3283	1/1	0.79	0.28	47,47,47,47	0
55	MG	AA	4040	1/1	0.79	0.38	60,60,60,60	0
55	MG	AA	4011	1/1	0.79	0.63	59,59,59,59	0
55	MG	CA	3525	1/1	0.79	0.82	61,61,61,61	0
55	MG	BA	2089	1/1	0.79	0.38	66,66,66,66	0
55	MG	AA	5119	1/1	0.79	0.47	80,80,80,80	0
55	MG	CA	3355	1/1	0.79	0.27	54,54,54,54	0
55	MG	CA	3775	1/1	0.79	0.20	66,66,66,66	0
55	MG	AN	204	1/1	0.79	0.47	48,48,48,48	0
55	MG	BA	1854	1/1	0.79	0.23	71,71,71,71	0
55	MG	CA	3178	1/1	0.79	0.16	25,25,25,25	0
55	MG	BA	1973	1/1	0.79	0.16	58,58,58,58	0
55	MG	AA	4715	1/1	0.79	0.97	80,80,80,80	0
55	MG	CA	3501	1/1	0.79	0.33	65,65,65,65	0
55	MG	CA	3744	1/1	0.79	0.15	90,90,90,90	0
55	MG	AA	5216	1/1	0.79	0.30	58,58,58,58	0
55	MG	DA	2076	1/1	0.79	0.34	62,62,62,62	0
55	MG	BA	1921	1/1	0.79	0.23	42,42,42,42	0
55	MG	DA	1857	1/1	0.79	0.32	79,79,79,79	0
55	MG	CA	4063	1/1	0.79	0.82	58,58,58,58	0
55	MG	AA	4409	1/1	0.79	0.12	83,83,83,83	0
55	MG	DH	201	1/1	0.79	0.20	100,100,100,100	0
55	MG	BA	2137	1/1	0.79	0.59	75,75,75,75	0
55	MG	AA	4086	1/1	0.79	0.86	57,57,57,57	0
55	MG	BA	2009	1/1	0.79	0.45	94,94,94,94	0
55	MG	DA	2066	1/1	0.79	0.52	55,55,55,55	0
55	MG	DA	1728	1/1	0.79	0.30	32,32,32,32	0
55	MG	CA	4238	1/1	0.79	0.14	91,91,91,91	0
55	MG	DA	2113	1/1	0.79	0.22	46,46,46,46	0
55	MG	BA	1607	1/1	0.80	0.29	90,90,90,90	0
55	MG	CA	3752	1/1	0.80	0.25	68,68,68,68	0
55	MG	CA	3834	1/1	0.80	0.23	69,69,69,69	0
55	MG	DA	2139	1/1	0.80	0.28	83,83,83,83	0
55	MG	C4	103	1/1	0.80	0.41	74,74,74,74	0
55	MG	DA	1812	1/1	0.80	0.64	116,116,116,116	0
55	MG	CA	2943	1/1	0.80	0.31	69,69,69,69	0
55	MG	CA	4291	1/1	0.80	0.20	46,46,46,46	0
55	MG	BA	2103	1/1	0.80	0.41	38,38,38,38	0
55	MG	AA	5149	1/1	0.80	0.25	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4005	1/1	0.80	0.24	49,49,49,49	0
55	MG	BA	1637	1/1	0.80	0.38	70,70,70,70	0
55	MG	DA	1705	1/1	0.80	0.79	34,34,34,34	0
55	MG	CA	3913	1/1	0.80	0.26	77,77,77,77	0
55	MG	CA	4344	1/1	0.80	0.23	41,41,41,41	0
55	MG	CA	2964	1/1	0.80	0.30	56,56,56,56	0
55	MG	DA	1967	1/1	0.80	0.41	36,36,36,36	0
55	MG	CA	4137	1/1	0.80	0.62	64,64,64,64	0
55	MG	AA	4304	1/1	0.80	0.40	38,38,38,38	0
55	MG	BW	111	1/1	0.80	0.23	53,53,53,53	0
55	MG	AA	4882	1/1	0.80	0.31	42,42,42,42	0
55	MG	DA	2027	1/1	0.80	0.52	57,57,57,57	0
55	MG	BA	1917	1/1	0.80	0.40	73,73,73,73	0
55	MG	AA	5047	1/1	0.80	0.44	60,60,60,60	0
55	MG	CA	3497	1/1	0.80	0.67	107,107,107,107	0
55	MG	AA	5273	1/1	0.80	0.33	75,75,75,75	0
55	MG	CA	4049	1/1	0.80	0.26	62,62,62,62	0
55	MG	AA	4535	1/1	0.80	0.58	70,70,70,70	0
55	MG	DW	104	1/1	0.80	0.29	95,95,95,95	0
55	MG	CA	3440	1/1	0.80	0.27	52,52,52,52	0
55	MG	AA	4581	1/1	0.80	0.13	59,59,59,59	0
55	MG	BA	2013	1/1	0.80	1.20	88,88,88,88	0
55	MG	CB	207	1/1	0.80	0.38	75,75,75,75	0
55	MG	BA	1969	1/1	0.80	0.32	60,60,60,60	0
55	MG	AA	5287	1/1	0.80	0.38	58,58,58,58	0
55	MG	CA	3042	1/1	0.80	0.33	67,67,67,67	0
55	MG	CA	4380	1/1	0.80	0.38	63,63,63,63	0
55	MG	CA	3879	1/1	0.80	0.33	43,43,43,43	0
55	MG	CA	3166	1/1	0.80	0.73	44,44,44,44	0
55	MG	AA	5179	1/1	0.80	0.62	61,61,61,61	0
55	MG	BA	1642	1/1	0.80	0.68	67,67,67,67	0
55	MG	CA	4211	1/1	0.80	0.29	67,67,67,67	0
55	MG	AA	4853	1/1	0.80	0.13	52,52,52,52	0
55	MG	BA	2130	1/1	0.80	0.65	33,33,33,33	0
55	MG	DA	1784	1/1	0.80	0.11	133,133,133,133	0
55	MG	CA	4146	1/1	0.80	0.41	47,47,47,47	0
55	MG	AA	4550	1/1	0.80	0.24	62,62,62,62	0
55	MG	BA	1766	1/1	0.80	0.41	50,50,50,50	0
55	MG	BA	2094	1/1	0.80	0.41	41,41,41,41	0
55	MG	AA	4454	1/1	0.80	0.29	49,49,49,49	0
55	MG	AA	4309	1/1	0.80	0.29	57,57,57,57	0
55	MG	CA	3661	1/1	0.80	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3034	1/1	0.80	0.52	43,43,43,43	0
55	MG	AB	203	1/1	0.80	0.33	65,65,65,65	0
55	MG	DA	1955	1/1	0.80	0.20	24,24,24,24	0
55	MG	AA	4391	1/1	0.80	0.61	63,63,63,63	0
55	MG	AE	303	1/1	0.80	0.57	53,53,53,53	0
55	MG	CA	3434	1/1	0.80	0.51	56,56,56,56	0
55	MG	AB	219	1/1	0.80	0.14	107,107,107,107	0
55	MG	AA	4552	1/1	0.80	0.23	71,71,71,71	0
55	MG	BA	1742	1/1	0.80	0.23	60,60,60,60	0
55	MG	BA	1708	1/1	0.80	0.19	36,36,36,36	0
55	MG	CA	3965	1/1	0.80	0.20	42,42,42,42	0
55	MG	CA	2973	1/1	0.80	0.52	99,99,99,99	0
55	MG	CA	3376	1/1	0.80	0.23	44,44,44,44	0
55	MG	CA	4210	1/1	0.80	0.31	63,63,63,63	0
55	MG	AA	5130	1/1	0.80	0.22	83,83,83,83	0
55	MG	CA	3556	1/1	0.80	0.11	55,55,55,55	0
55	MG	AA	4292	1/1	0.80	0.17	65,65,65,65	0
55	MG	AA	4425	1/1	0.80	0.38	66,66,66,66	0
55	MG	BA	2071	1/1	0.80	0.16	71,71,71,71	0
55	MG	AA	4796	1/1	0.80	0.34	64,64,64,64	0
55	MG	DA	2023	1/1	0.80	0.19	65,65,65,65	0
55	MG	CA	3859	1/1	0.80	0.48	96,96,96,96	0
55	MG	CA	3656	1/1	0.80	0.55	44,44,44,44	0
55	MG	DA	2112	1/1	0.80	0.33	55,55,55,55	0
55	MG	BA	1733	1/1	0.80	0.68	54,54,54,54	0
55	MG	CA	4214	1/1	0.80	0.29	63,63,63,63	0
55	MG	CA	4068	1/1	0.80	0.49	66,66,66,66	0
55	MG	AA	5286	1/1	0.80	0.36	65,65,65,65	0
55	MG	CA	3061	1/1	0.80	0.28	82,82,82,82	0
55	MG	DA	2156	1/1	0.80	1.24	97,97,97,97	0
55	MG	BA	1876	1/1	0.80	0.24	91,91,91,91	0
55	MG	DV	118	1/1	0.80	0.21	78,78,78,78	0
55	MG	DA	1979	1/1	0.80	0.17	48,48,48,48	0
55	MG	AA	4625	1/1	0.80	0.64	68,68,68,68	0
55	MG	BA	1779	1/1	0.80	0.40	54,54,54,54	0
55	MG	CA	3650	1/1	0.80	0.41	122,122,122,122	0
55	MG	CA	3884	1/1	0.80	0.81	86,86,86,86	0
55	MG	CA	2953	1/1	0.80	0.32	71,71,71,71	0
55	MG	DA	1865	1/1	0.80	1.16	75,75,75,75	0
55	MG	CA	3929	1/1	0.80	0.24	53,53,53,53	0
55	MG	CA	3964	1/1	0.80	0.57	48,48,48,48	0
55	MG	AA	5136	1/1	0.80	0.38	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4355	1/1	0.80	0.23	47,47,47,47	0
55	MG	CA	4394	1/1	0.80	0.68	81,81,81,81	0
55	MG	DA	1724	1/1	0.80	0.36	41,41,41,41	0
55	MG	AA	5018	1/1	0.80	0.16	44,44,44,44	0
55	MG	AA	4476	1/1	0.80	0.30	61,61,61,61	0
55	MG	BA	2053	1/1	0.80	0.46	64,64,64,64	0
55	MG	CA	3921	1/1	0.80	0.30	59,59,59,59	0
55	MG	CA	3731	1/1	0.80	0.32	53,53,53,53	0
55	MG	DO	102	1/1	0.80	1.15	113,113,113,113	0
55	MG	AA	4858	1/1	0.80	0.36	50,50,50,50	0
55	MG	AA	4826	1/1	0.80	0.42	73,73,73,73	0
55	MG	AA	5118	1/1	0.80	0.65	54,54,54,54	0
55	MG	CA	3749	1/1	0.80	0.40	105,105,105,105	0
55	MG	BA	1874	1/1	0.80	0.32	82,82,82,82	0
55	MG	CA	3846	1/1	0.80	0.17	126,126,126,126	0
55	MG	AA	4290	1/1	0.80	0.80	38,38,38,38	0
55	MG	CA	4017	1/1	0.80	0.31	48,48,48,48	0
55	MG	CA	3309	1/1	0.80	0.63	61,61,61,61	0
55	MG	CA	3258	1/1	0.80	0.16	41,41,41,41	0
55	MG	CA	3608	1/1	0.80	0.48	82,82,82,82	0
55	MG	CA	2958	1/1	0.80	0.25	71,71,71,71	0
55	MG	AA	4108	1/1	0.80	0.30	61,61,61,61	0
55	MG	DA	1605	1/1	0.80	0.34	80,80,80,80	0
55	MG	DA	1909	1/1	0.80	0.33	73,73,73,73	0
55	MG	AA	5038	1/1	0.80	0.92	52,52,52,52	0
55	MG	CA	3422	1/1	0.81	0.74	44,44,44,44	0
55	MG	AA	5168	1/1	0.81	0.30	71,71,71,71	0
55	MG	AA	4618	1/1	0.81	0.25	64,64,64,64	0
55	MG	CA	3596	1/1	0.81	0.18	79,79,79,79	0
55	MG	CA	3599	1/1	0.81	0.36	46,46,46,46	0
55	MG	DA	2077	1/1	0.81	0.31	109,109,109,109	0
55	MG	AM	202	1/1	0.81	0.37	52,52,52,52	0
55	MG	AB	246	1/1	0.81	0.22	94,94,94,94	0
55	MG	BA	1815	1/1	0.81	0.42	47,47,47,47	0
55	MG	DA	2056	1/1	0.81	0.69	105,105,105,105	0
55	MG	DA	2061	1/1	0.81	0.21	57,57,57,57	0
55	MG	AA	5161	1/1	0.81	0.25	48,48,48,48	0
55	MG	CA	4318	1/1	0.81	0.27	71,71,71,71	0
55	MG	DA	2120	1/1	0.81	0.43	95,95,95,95	0
55	MG	AA	4863	1/1	0.81	0.68	51,51,51,51	0
55	MG	AA	4037	1/1	0.81	0.35	62,62,62,62	0
55	MG	DV	113	1/1	0.81	0.19	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4517	1/1	0.81	0.45	48,48,48,48	0
55	MG	DA	2166	1/1	0.81	0.39	69,69,69,69	0
55	MG	AA	4730	1/1	0.81	0.24	73,73,73,73	0
55	MG	CA	4052	1/1	0.81	0.67	60,60,60,60	0
55	MG	CA	3432	1/1	0.81	0.32	32,32,32,32	0
55	MG	AA	4003	1/1	0.81	0.31	57,57,57,57	0
55	MG	CA	3259	1/1	0.81	0.42	39,39,39,39	0
55	MG	CF	304	1/1	0.81	0.54	55,55,55,55	0
55	MG	AA	5256	1/1	0.81	0.37	55,55,55,55	0
55	MG	DA	1604	1/1	0.81	0.41	101,101,101,101	0
55	MG	CA	3714	1/1	0.81	0.51	80,80,80,80	0
55	MG	DA	2141	1/1	0.81	0.23	85,85,85,85	0
55	MG	DA	1746	1/1	0.81	0.24	67,67,67,67	0
55	MG	AA	4261	1/1	0.81	0.42	34,34,34,34	0
55	MG	CB	211	1/1	0.81	0.09	90,90,90,90	0
55	MG	BA	1881	1/1	0.81	0.29	68,68,68,68	0
55	MG	CA	2934	1/1	0.81	0.32	59,59,59,59	0
55	MG	AA	4686	1/1	0.81	0.42	81,81,81,81	0
55	MG	BA	1934	1/1	0.81	0.31	87,87,87,87	0
55	MG	AA	4895	1/1	0.81	0.21	70,70,70,70	0
55	MG	AA	5112	1/1	0.81	0.57	47,47,47,47	0
55	MG	CA	4356	1/1	0.81	0.67	60,60,60,60	0
55	MG	BA	2148	1/1	0.81	0.15	88,88,88,88	0
55	MG	AA	4766	1/1	0.81	0.32	63,63,63,63	0
55	MG	CA	3605	1/1	0.81	0.28	66,66,66,66	0
55	MG	AA	5289	1/1	0.81	0.13	73,73,73,73	0
55	MG	AA	4754	1/1	0.81	0.69	42,42,42,42	0
55	MG	DA	2063	1/1	0.81	0.14	77,77,77,77	0
55	MG	AA	4085	1/1	0.81	0.29	89,89,89,89	0
55	MG	AA	4695	1/1	0.81	0.13	65,65,65,65	0
55	MG	DA	1854	1/1	0.81	0.45	47,47,47,47	0
55	MG	AA	5060	1/1	0.81	0.34	54,54,54,54	0
55	MG	CA	4400	1/1	0.81	0.27	45,45,45,45	0
55	MG	AA	5111	1/1	0.81	0.52	53,53,53,53	0
55	MG	DA	2014	1/1	0.81	0.14	78,78,78,78	0
55	MG	CB	203	1/1	0.81	0.33	100,100,100,100	0
55	MG	AA	4243	1/1	0.81	0.37	45,45,45,45	0
55	MG	AX	105	1/1	0.81	0.32	58,58,58,58	0
55	MG	BV	101	1/1	0.81	0.11	105,105,105,105	0
55	MG	DA	2134	1/1	0.81	0.23	74,74,74,74	0
55	MG	BA	1922	1/1	0.81	0.34	54,54,54,54	0
55	MG	AA	5071	1/1	0.81	0.58	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	2090	1/1	0.81	0.79	55,55,55,55	0
55	MG	CA	2955	1/1	0.81	0.53	52,52,52,52	0
55	MG	BA	1994	1/1	0.81	0.34	52,52,52,52	0
55	MG	CA	3053	1/1	0.81	0.94	81,81,81,81	0
55	MG	CA	3197	1/1	0.81	0.44	28,28,28,28	0
55	MG	CA	3479	1/1	0.81	0.13	45,45,45,45	0
55	MG	AA	4259	1/1	0.81	0.64	42,42,42,42	0
55	MG	CA	3425	1/1	0.81	0.10	57,57,57,57	0
55	MG	CA	3753	1/1	0.81	0.34	69,69,69,69	0
55	MG	AA	4109	1/1	0.81	0.77	59,59,59,59	0
55	MG	CA	4285	1/1	0.81	0.17	46,46,46,46	0
55	MG	CA	3635	1/1	0.81	0.48	63,63,63,63	0
55	MG	CA	3387	1/1	0.81	0.19	29,29,29,29	0
55	MG	DW	109	1/1	0.81	0.27	85,85,85,85	0
55	MG	AA	5233	1/1	0.81	0.17	74,74,74,74	0
55	MG	AA	4087	1/1	0.81	0.38	86,86,86,86	0
55	MG	CA	3981	1/1	0.81	0.24	35,35,35,35	0
55	MG	CA	4398	1/1	0.81	0.47	68,68,68,68	0
55	MG	BA	1743	1/1	0.81	0.13	76,76,76,76	0
55	MG	CA	3821	1/1	0.81	0.07	94,94,94,94	0
55	MG	CA	3740	1/1	0.81	0.69	77,77,77,77	0
55	MG	AA	5198	1/1	0.81	0.16	62,62,62,62	0
55	MG	AA	4561	1/1	0.81	0.72	67,67,67,67	0
55	MG	CV	202	1/1	0.81	0.11	78,78,78,78	0
55	MG	CA	4293	1/1	0.81	0.32	60,60,60,60	0
55	MG	AA	4160	1/1	0.81	0.26	94,94,94,94	0
55	MG	AA	4577	1/1	0.81	0.56	110,110,110,110	0
55	MG	CA	2974	1/1	0.81	0.13	59,59,59,59	0
55	MG	AA	4034	1/1	0.81	0.44	84,84,84,84	0
55	MG	BA	2150	1/1	0.81	0.28	82,82,82,82	0
55	MG	DA	2090	1/1	0.81	0.27	86,86,86,86	0
55	MG	DA	2020	1/1	0.81	0.21	66,66,66,66	0
55	MG	CA	4345	1/1	0.81	0.51	86,86,86,86	0
55	MG	AA	5046	1/1	0.81	0.37	37,37,37,37	0
55	MG	BA	2149	1/1	0.81	0.19	70,70,70,70	0
55	MG	DR	102	1/1	0.81	0.38	70,70,70,70	0
55	MG	CA	3350	1/1	0.81	0.39	47,47,47,47	0
55	MG	AA	4041	1/1	0.81	0.16	57,57,57,57	0
55	MG	AA	4329	1/1	0.81	0.45	76,76,76,76	0
55	MG	DA	2046	1/1	0.81	0.23	47,47,47,47	0
55	MG	DG	201	1/1	0.81	0.39	73,73,73,73	0
55	MG	CA	4079	1/1	0.81	0.36	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4031	1/1	0.81	0.21	109,109,109,109	0
55	MG	CA	3248	1/1	0.81	0.66	40,40,40,40	0
55	MG	AA	5290	1/1	0.81	0.38	69,69,69,69	0
55	MG	BA	2128	1/1	0.81	0.42	83,83,83,83	0
55	MG	CA	4377	1/1	0.81	0.14	84,84,84,84	0
55	MG	AA	4662	1/1	0.81	0.38	77,77,77,77	0
55	MG	AA	4742	1/1	0.81	0.27	69,69,69,69	0
55	MG	CA	3177	1/1	0.81	0.92	42,42,42,42	0
55	MG	CA	3577	1/1	0.81	0.63	69,69,69,69	0
55	MG	CA	4158	1/1	0.81	0.32	83,83,83,83	0
55	MG	CA	3999	1/1	0.81	0.39	37,37,37,37	0
55	MG	DE	202	1/1	0.81	0.29	73,73,73,73	0
55	MG	CA	3827	1/1	0.81	0.33	70,70,70,70	0
55	MG	AA	4622	1/1	0.81	0.28	79,79,79,79	0
55	MG	AA	5148	1/1	0.81	0.14	59,59,59,59	0
55	MG	AA	4265	1/1	0.81	0.64	51,51,51,51	0
55	MG	DM	201	1/1	0.81	0.26	69,69,69,69	0
55	MG	AB	245	1/1	0.81	0.40	63,63,63,63	0
55	MG	DA	2161	1/1	0.81	0.35	61,61,61,61	0
55	MG	DA	1998	1/1	0.81	0.38	59,59,59,59	0
55	MG	BA	1611	1/1	0.81	0.30	67,67,67,67	0
55	MG	AA	4505	1/1	0.81	0.87	126,126,126,126	0
55	MG	BA	1941	1/1	0.81	0.15	81,81,81,81	0
55	MG	AA	4488	1/1	0.81	0.34	50,50,50,50	0
55	MG	BA	2030	1/1	0.81	0.65	55,55,55,55	0
55	MG	DA	1695	1/1	0.81	0.26	55,55,55,55	0
55	MG	AA	4758	1/1	0.81	0.31	71,71,71,71	0
55	MG	DA	1994	1/1	0.81	0.26	63,63,63,63	0
55	MG	CA	4299	1/1	0.81	0.58	73,73,73,73	0
55	MG	CA	4074	1/1	0.81	0.37	59,59,59,59	0
55	MG	BU	101	1/1	0.81	0.34	109,109,109,109	0
55	MG	CA	3378	1/1	0.81	0.13	44,44,44,44	0
55	MG	CA	3951	1/1	0.82	0.34	94,94,94,94	0
55	MG	AA	5255	1/1	0.82	0.37	61,61,61,61	0
55	MG	DA	2042	1/1	0.82	0.38	87,87,87,87	0
55	MG	CA	4187	1/1	0.82	0.26	69,69,69,69	0
55	MG	AA	4604	1/1	0.82	0.31	54,54,54,54	0
55	MG	CW	104	1/1	0.82	1.42	64,64,64,64	0
55	MG	CA	3750	1/1	0.82	0.58	140,140,140,140	0
55	MG	CA	4269	1/1	0.82	0.58	49,49,49,49	0
55	MG	AA	4640	1/1	0.82	0.33	73,73,73,73	0
55	MG	AA	4166	1/1	0.82	0.23	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	2105	1/1	0.82	0.27	52,52,52,52	0
55	MG	AA	4700	1/1	0.82	0.58	107,107,107,107	0
55	MG	DA	2085	1/1	0.82	0.37	68,68,68,68	0
55	MG	AA	4896	1/1	0.82	0.28	42,42,42,42	0
55	MG	AA	4157	1/1	0.82	0.41	64,64,64,64	0
55	MG	AA	4229	1/1	0.82	0.44	34,34,34,34	0
55	MG	BA	1870	1/1	0.82	0.10	92,92,92,92	0
55	MG	CA	4226	1/1	0.82	0.22	50,50,50,50	0
55	MG	CB	241	1/1	0.82	0.19	82,82,82,82	0
55	MG	DA	2135	1/1	0.82	0.17	93,93,93,93	0
55	MG	DA	1943	1/1	0.82	0.37	64,64,64,64	0
55	MG	AA	4168	1/1	0.82	0.52	65,65,65,65	0
55	MG	AA	4470	1/1	0.82	0.31	62,62,62,62	0
55	MG	CA	4129	1/1	0.82	0.37	79,79,79,79	0
55	MG	DA	1629	1/1	0.82	0.45	89,89,89,89	0
55	MG	CA	3861	1/1	0.82	0.23	56,56,56,56	0
55	MG	CA	3886	1/1	0.82	0.09	58,58,58,58	0
55	MG	DA	1970	1/1	0.82	0.33	30,30,30,30	0
55	MG	CA	4225	1/1	0.82	0.46	48,48,48,48	0
55	MG	AA	5231	1/1	0.82	0.39	78,78,78,78	0
55	MG	CA	4148	1/1	0.82	0.55	43,43,43,43	0
55	MG	BA	1940	1/1	0.82	0.11	65,65,65,65	0
55	MG	CA	2982	1/1	0.82	0.48	69,69,69,69	0
55	MG	AA	4026	1/1	0.82	0.40	55,55,55,55	0
55	MG	AA	5101	1/1	0.82	0.55	77,77,77,77	0
55	MG	AS	201	1/1	0.82	0.40	62,62,62,62	0
55	MG	AA	4279	1/1	0.82	0.28	37,37,37,37	0
55	MG	CA	3923	1/1	0.82	0.34	63,63,63,63	0
55	MG	CA	4384	1/1	0.82	0.54	65,65,65,65	0
55	MG	BA	2025	1/1	0.82	0.30	62,62,62,62	0
55	MG	AA	4468	1/1	0.82	0.42	66,66,66,66	0
55	MG	CA	3071	1/1	0.82	0.64	66,66,66,66	0
55	MG	AA	5082	1/1	0.82	0.29	72,72,72,72	0
55	MG	CA	2908	1/1	0.82	0.62	74,74,74,74	0
55	MG	AA	5009	1/1	0.82	0.50	65,65,65,65	0
55	MG	BV	103	1/1	0.82	1.10	66,66,66,66	0
55	MG	BA	1977	1/1	0.82	0.23	65,65,65,65	0
55	MG	AA	4393	1/1	0.82	0.11	57,57,57,57	0
55	MG	CI	201	1/1	0.82	0.70	62,62,62,62	0
55	MG	AA	4002	1/1	0.82	0.68	130,130,130,130	0
55	MG	DA	1920	1/1	0.82	0.41	72,72,72,72	0
55	MG	AA	4412	1/1	0.82	0.77	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1903	1/1	0.82	0.23	79,79,79,79	0
55	MG	CA	3168	1/1	0.82	0.41	27,27,27,27	0
55	MG	AA	4137	1/1	0.82	0.93	85,85,85,85	0
55	MG	AA	4890	1/1	0.82	0.42	37,37,37,37	0
55	MG	CA	3922	1/1	0.82	0.38	72,72,72,72	0
55	MG	CA	3904	1/1	0.82	0.24	98,98,98,98	0
55	MG	AA	4634	1/1	0.82	0.48	86,86,86,86	0
55	MG	DO	101	1/1	0.82	0.35	98,98,98,98	0
55	MG	DA	2096	1/1	0.82	0.18	38,38,38,38	0
55	MG	AA	4967	1/1	0.82	0.14	60,60,60,60	0
55	MG	AA	4713	1/1	0.82	0.22	87,87,87,87	0
55	MG	CA	4282	1/1	0.82	0.45	56,56,56,56	0
55	MG	AA	5048	1/1	0.82	0.38	69,69,69,69	0
55	MG	DA	2165	1/1	0.82	0.57	61,61,61,61	0
55	MG	AB	211	1/1	0.82	0.65	62,62,62,62	0
55	MG	AK	202	1/1	0.82	0.20	72,72,72,72	0
55	MG	AA	4595	1/1	0.82	0.44	62,62,62,62	0
55	MG	CA	3415	1/1	0.82	0.20	44,44,44,44	0
55	MG	DA	2029	1/1	0.82	0.21	53,53,53,53	0
55	MG	AA	4596	1/1	0.82	0.39	103,103,103,103	0
55	MG	DA	1919	1/1	0.82	0.27	66,66,66,66	0
55	MG	CA	3125	1/1	0.82	0.52	13,13,13,13	0
55	MG	CA	3667	1/1	0.82	0.34	64,64,64,64	0
55	MG	CA	4254	1/1	0.82	0.38	61,61,61,61	0
55	MG	AA	4461	1/1	0.82	0.41	53,53,53,53	0
55	MG	CA	4186	1/1	0.82	0.36	47,47,47,47	0
55	MG	CA	4290	1/1	0.82	0.24	68,68,68,68	0
55	MG	AA	4620	1/1	0.82	0.20	70,70,70,70	0
55	MG	CA	3655	1/1	0.82	0.60	63,63,63,63	0
55	MG	AA	4939	1/1	0.82	0.55	56,56,56,56	0
55	MG	CA	3018	1/1	0.82	0.46	70,70,70,70	0
55	MG	AA	5083	1/1	0.82	0.23	56,56,56,56	0
55	MG	AA	4551	1/1	0.82	0.22	72,72,72,72	0
55	MG	CA	3076	1/1	0.82	0.36	101,101,101,101	0
55	MG	CA	3584	1/1	0.82	0.17	55,55,55,55	0
55	MG	AA	5254	1/1	0.82	0.43	54,54,54,54	0
55	MG	DA	2102	1/1	0.82	1.13	87,87,87,87	0
55	MG	BA	1916	1/1	0.82	0.73	65,65,65,65	0
55	MG	CA	3398	1/1	0.82	0.16	53,53,53,53	0
55	MG	AA	4868	1/1	0.82	0.79	62,62,62,62	0
55	MG	CA	3247	1/1	0.82	0.26	23,23,23,23	0
55	MG	CA	3705	1/1	0.82	0.41	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4404	1/1	0.82	0.60	41,41,41,41	0
55	MG	AA	4039	1/1	0.82	0.18	85,85,85,85	0
55	MG	CA	2927	1/1	0.82	0.36	57,57,57,57	0
55	MG	CE	306	1/1	0.82	0.29	64,64,64,64	0
55	MG	A5	101	1/1	0.82	0.31	30,30,30,30	0
55	MG	CA	3389	1/1	0.82	0.14	46,46,46,46	0
55	MG	AB	238	1/1	0.82	0.11	55,55,55,55	0
55	MG	CA	3078	1/1	0.82	0.20	72,72,72,72	0
55	MG	AA	4626	1/1	0.82	0.28	55,55,55,55	0
55	MG	CA	4154	1/1	0.82	0.88	61,61,61,61	0
55	MG	AA	5106	1/1	0.82	0.31	56,56,56,56	0
55	MG	CA	3498	1/1	0.82	0.30	44,44,44,44	0
55	MG	BA	1723	1/1	0.82	0.27	38,38,38,38	0
55	MG	DA	2012	1/1	0.82	0.32	65,65,65,65	0
55	MG	BA	1657	1/1	0.82	0.16	52,52,52,52	0
55	MG	DA	1793	1/1	0.82	0.13	84,84,84,84	0
55	MG	AA	5192	1/1	0.82	0.35	46,46,46,46	0
55	MG	CA	3275	1/1	0.82	0.94	40,40,40,40	0
55	MG	CA	3512	1/1	0.82	0.11	60,60,60,60	0
55	MG	AA	4907	1/1	0.82	0.29	42,42,42,42	0
55	MG	DJ	201	1/1	0.82	0.30	83,83,83,83	0
55	MG	AA	5246	1/1	0.82	0.29	46,46,46,46	0
55	MG	DA	1714	1/1	0.82	0.19	46,46,46,46	0
55	MG	CA	4096	1/1	0.82	0.32	72,72,72,72	0
55	MG	CA	3240	1/1	0.82	0.59	33,33,33,33	0
55	MG	CA	3229	1/1	0.83	0.18	45,45,45,45	0
55	MG	DA	2145	1/1	0.83	0.20	84,84,84,84	0
55	MG	CA	2993	1/1	0.83	0.52	64,64,64,64	0
55	MG	DA	1779	1/1	0.83	0.08	87,87,87,87	0
55	MG	CA	4298	1/1	0.83	0.35	62,62,62,62	0
55	MG	CA	3675	1/1	0.83	0.17	72,72,72,72	0
55	MG	BA	1962	1/1	0.83	0.54	49,49,49,49	0
55	MG	CL	204	1/1	0.83	0.44	41,41,41,41	0
55	MG	AA	4158	1/1	0.83	0.30	100,100,100,100	0
55	MG	AA	5040	1/1	0.83	0.48	64,64,64,64	0
55	MG	CB	235	1/1	0.83	0.15	58,58,58,58	0
55	MG	AA	5064	1/1	0.83	0.18	46,46,46,46	0
55	MG	CA	3043	1/1	0.83	0.11	95,95,95,95	0
55	MG	BA	1845	1/1	0.83	0.14	103,103,103,103	0
55	MG	CA	3494	1/1	0.83	0.28	40,40,40,40	0
55	MG	AA	5097	1/1	0.83	0.36	37,37,37,37	0
55	MG	AA	4315	1/1	0.83	0.93	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3914	1/1	0.83	1.60	73,73,73,73	0
55	MG	CA	3306	1/1	0.83	0.32	25,25,25,25	0
55	MG	A4	105	1/1	0.83	0.74	94,94,94,94	0
55	MG	CA	2976	1/1	0.83	0.53	61,61,61,61	0
55	MG	BA	2119	1/1	0.83	0.28	88,88,88,88	0
55	MG	BA	1899	1/1	0.83	0.48	79,79,79,79	0
55	MG	CA	3359	1/1	0.83	0.38	43,43,43,43	0
55	MG	CE	304	1/1	0.83	0.67	59,59,59,59	0
55	MG	AA	5227	1/1	0.83	0.24	75,75,75,75	0
55	MG	CA	3015	1/1	0.83	0.20	71,71,71,71	0
55	MG	AA	5269	1/1	0.83	0.73	109,109,109,109	0
55	MG	AA	4633	1/1	0.83	0.54	59,59,59,59	0
55	MG	CA	3426	1/1	0.83	0.43	39,39,39,39	0
55	MG	DA	1986	1/1	0.83	0.65	60,60,60,60	0
55	MG	DA	2108	1/1	0.83	0.25	92,92,92,92	0
55	MG	BA	2116	1/1	0.83	0.42	93,93,93,93	0
55	MG	AA	4943	1/1	0.83	0.35	45,45,45,45	0
55	MG	AB	250	1/1	0.83	0.23	68,68,68,68	0
55	MG	BW	108	1/1	0.83	0.15	93,93,93,93	0
55	MG	CA	3739	1/1	0.83	0.43	45,45,45,45	0
55	MG	CA	3416	1/1	0.83	0.36	54,54,54,54	0
55	MG	CA	3697	1/1	0.83	0.51	71,71,71,71	0
55	MG	CA	3271	1/1	0.83	0.59	52,52,52,52	0
55	MG	CA	3628	1/1	0.83	0.84	69,69,69,69	0
55	MG	CA	3358	1/1	0.83	0.70	41,41,41,41	0
55	MG	BV	125	1/1	0.83	0.31	81,81,81,81	0
55	MG	BA	1885	1/1	0.83	0.15	60,60,60,60	0
55	MG	AA	4597	1/1	0.83	0.39	54,54,54,54	0
55	MG	CA	4060	1/1	0.83	0.24	49,49,49,49	0
55	MG	CA	3161	1/1	0.83	0.61	30,30,30,30	0
55	MG	DA	2086	1/1	0.83	0.15	57,57,57,57	0
55	MG	AA	4887	1/1	0.83	0.27	40,40,40,40	0
55	MG	AA	4935	1/1	0.83	0.58	46,46,46,46	0
55	MG	CA	4343	1/1	0.83	0.41	73,73,73,73	0
55	MG	AA	4218	1/1	0.83	0.18	34,34,34,34	0
55	MG	BA	1795	1/1	0.83	0.33	75,75,75,75	0
55	MG	BA	1848	1/1	0.83	0.24	79,79,79,79	0
55	MG	CA	2937	1/1	0.83	0.29	86,86,86,86	0
55	MG	CA	3429	1/1	0.83	0.37	44,44,44,44	0
55	MG	BA	1782	1/1	0.83	0.43	69,69,69,69	0
55	MG	AA	4392	1/1	0.83	0.21	39,39,39,39	0
55	MG	AA	4832	1/1	0.83	0.30	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BV	123	1/1	0.83	0.47	56,56,56,56	0
55	MG	CA	4327	1/1	0.83	0.23	58,58,58,58	0
55	MG	DV	108	1/1	0.83	0.36	111,111,111,111	0
55	MG	DA	1781	1/1	0.83	0.09	107,107,107,107	0
55	MG	CA	3603	1/1	0.83	0.14	57,57,57,57	0
55	MG	CS	204	1/1	0.83	0.31	76,76,76,76	0
55	MG	CA	4371	1/1	0.83	0.31	76,76,76,76	0
55	MG	AA	4458	1/1	0.83	0.56	65,65,65,65	0
55	MG	BA	1669	1/1	0.83	0.22	60,60,60,60	0
55	MG	CA	3952	1/1	0.83	0.40	70,70,70,70	0
55	MG	AB	215	1/1	0.83	0.31	99,99,99,99	0
55	MG	DA	1755	1/1	0.83	0.60	93,93,93,93	0
55	MG	BC	302	1/1	0.83	0.32	60,60,60,60	0
55	MG	C5	101	1/1	0.83	0.45	63,63,63,63	0
55	MG	AA	4266	1/1	0.83	0.57	43,43,43,43	0
55	MG	DW	115	1/1	0.83	0.14	127,127,127,127	0
55	MG	AA	5053	1/1	0.83	0.30	75,75,75,75	0
55	MG	AA	4714	1/1	0.83	0.22	73,73,73,73	0
55	MG	CA	3798	1/1	0.83	0.37	98,98,98,98	0
55	MG	CB	226	1/1	0.83	0.19	40,40,40,40	0
55	MG	DW	117	1/1	0.83	0.19	74,74,74,74	0
55	MG	CA	4360	1/1	0.83	0.28	52,52,52,52	0
55	MG	CA	3569	1/1	0.83	0.37	74,74,74,74	0
55	MG	CA	3063	1/1	0.83	0.22	82,82,82,82	0
55	MG	CA	4173	1/1	0.83	0.41	49,49,49,49	0
55	MG	AA	4424	1/1	0.83	0.51	48,48,48,48	0
55	MG	DA	1899	1/1	0.83	0.17	71,71,71,71	0
55	MG	BA	1789	1/1	0.83	1.15	79,79,79,79	0
55	MG	CB	206	1/1	0.83	0.14	61,61,61,61	0
55	MG	AA	5027	1/1	0.83	0.09	68,68,68,68	0
55	MG	CA	3607	1/1	0.83	0.35	47,47,47,47	0
55	MG	AA	4098	1/1	0.83	0.56	87,87,87,87	0
55	MG	CA	2990	1/1	0.83	0.09	68,68,68,68	0
55	MG	BA	1630	1/1	0.83	0.53	47,47,47,47	0
55	MG	AA	5008	1/1	0.83	0.41	71,71,71,71	0
55	MG	AA	5151	1/1	0.83	0.32	58,58,58,58	0
55	MG	AA	4957	1/1	0.83	0.25	47,47,47,47	0
55	MG	AA	4627	1/1	0.83	0.37	42,42,42,42	0
55	MG	AA	4774	1/1	0.83	0.37	63,63,63,63	0
55	MG	DA	1807	1/1	0.83	0.19	53,53,53,53	0
55	MG	CA	4015	1/1	0.83	0.17	53,53,53,53	0
55	MG	AA	5120	1/1	0.83	0.38	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1799	1/1	0.83	0.36	64,64,64,64	0
55	MG	CA	3955	1/1	0.83	0.36	51,51,51,51	0
55	MG	CA	3346	1/1	0.83	0.36	39,39,39,39	0
55	MG	CA	4321	1/1	0.83	0.60	63,63,63,63	0
55	MG	CA	4381	1/1	0.83	0.57	74,74,74,74	0
55	MG	BQ	202	1/1	0.83	0.36	78,78,78,78	0
55	MG	DA	1822	1/1	0.83	0.49	111,111,111,111	0
55	MG	CA	4204	1/1	0.83	0.46	49,49,49,49	0
55	MG	BA	1946	1/1	0.83	0.19	69,69,69,69	0
55	MG	CA	4176	1/1	0.83	0.28	68,68,68,68	0
55	MG	DA	1616	1/1	0.83	0.19	113,113,113,113	0
55	MG	AA	4483	1/1	0.83	0.21	51,51,51,51	0
55	MG	AA	5096	1/1	0.83	1.09	63,63,63,63	0
55	MG	DA	1926	1/1	0.83	0.10	54,54,54,54	0
55	MG	DA	2189	1/1	0.83	0.29	58,58,58,58	0
55	MG	CA	3654	1/1	0.83	0.12	56,56,56,56	0
55	MG	AA	5230	1/1	0.83	0.16	102,102,102,102	0
55	MG	BA	1736	1/1	0.83	0.30	36,36,36,36	0
55	MG	CA	3906	1/1	0.83	0.29	47,47,47,47	0
55	MG	CA	3513	1/1	0.83	0.15	52,52,52,52	0
55	MG	CA	3926	1/1	0.83	0.58	45,45,45,45	0
55	MG	AA	4153	1/1	0.83	0.48	62,62,62,62	0
55	MG	DK	201	1/1	0.83	0.26	49,49,49,49	0
55	MG	BA	2135	1/1	0.83	0.27	76,76,76,76	0
55	MG	AA	4532	1/1	0.83	0.62	46,46,46,46	0
55	MG	CA	3021	1/1	0.83	0.41	68,68,68,68	0
55	MG	CA	3669	1/1	0.83	0.64	44,44,44,44	0
55	MG	AA	4013	1/1	0.83	0.27	55,55,55,55	0
55	MG	CA	3353	1/1	0.83	0.71	50,50,50,50	0
55	MG	CA	3927	1/1	0.83	0.40	64,64,64,64	0
55	MG	CA	4075	1/1	0.83	0.38	69,69,69,69	0
55	MG	AA	4376	1/1	0.83	0.14	53,53,53,53	0
55	MG	CA	3218	1/1	0.83	0.46	23,23,23,23	0
55	MG	BA	1666	1/1	0.83	0.64	45,45,45,45	0
55	MG	AA	4959	1/1	0.83	0.30	37,37,37,37	0
55	MG	AA	4929	1/1	0.83	0.41	35,35,35,35	0
55	MG	BA	2043	1/1	0.83	0.37	62,62,62,62	0
55	MG	BA	1989	1/1	0.83	0.30	74,74,74,74	0
55	MG	DA	1813	1/1	0.84	0.38	79,79,79,79	0
55	MG	CA	4045	1/1	0.84	0.21	49,49,49,49	0
55	MG	DA	2204	1/1	0.84	0.20	66,66,66,66	0
55	MG	CA	2923	1/1	0.84	0.26	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	5081	1/1	0.84	0.12	92,92,92,92	0
55	MG	CB	240	1/1	0.84	0.49	54,54,54,54	0
55	MG	DA	2065	1/1	0.84	0.21	59,59,59,59	0
55	MG	A4	103	1/1	0.84	0.50	76,76,76,76	0
55	MG	DA	1823	1/1	0.84	0.14	88,88,88,88	0
55	MG	CA	3442	1/1	0.84	0.11	45,45,45,45	0
55	MG	DE	201	1/1	0.84	0.39	137,137,137,137	0
55	MG	BA	2169	1/1	0.84	0.33	72,72,72,72	0
55	MG	CA	4188	1/1	0.84	0.35	45,45,45,45	0
55	MG	AA	4850	1/1	0.84	0.30	50,50,50,50	0
55	MG	BA	1990	1/1	0.84	0.45	59,59,59,59	0
55	MG	CA	3287	1/1	0.84	0.34	36,36,36,36	0
55	MG	BA	1612	1/1	0.84	0.27	98,98,98,98	0
55	MG	CB	254	1/1	0.84	0.19	71,71,71,71	0
55	MG	DA	2168	1/1	0.84	0.27	54,54,54,54	0
55	MG	AA	4572	1/1	0.84	0.47	61,61,61,61	0
55	MG	AA	4014	1/1	0.84	0.25	80,80,80,80	0
55	MG	BA	2032	1/1	0.84	0.52	59,59,59,59	0
55	MG	CA	3235	1/1	0.84	0.42	35,35,35,35	0
55	MG	DA	1764	1/1	0.84	0.55	71,71,71,71	0
55	MG	DV	103	1/1	0.84	0.21	79,79,79,79	0
55	MG	CA	4316	1/1	0.84	0.30	60,60,60,60	0
55	MG	CA	3542	1/1	0.84	0.28	63,63,63,63	0
55	MG	AA	5220	1/1	0.84	0.30	51,51,51,51	0
55	MG	AA	5194	1/1	0.84	0.82	70,70,70,70	0
55	MG	CA	4150	1/1	0.84	0.55	75,75,75,75	0
55	MG	AA	4214	1/1	0.84	0.37	33,33,33,33	0
55	MG	DX	101	1/1	0.84	0.32	62,62,62,62	0
55	MG	BA	1968	1/1	0.84	0.20	49,49,49,49	0
55	MG	AA	4927	1/1	0.84	0.27	50,50,50,50	0
55	MG	DA	1914	1/1	0.84	0.18	77,77,77,77	0
55	MG	AA	4985	1/1	0.84	0.36	61,61,61,61	0
55	MG	AA	5211	1/1	0.84	1.13	74,74,74,74	0
55	MG	CA	3580	1/1	0.84	0.34	59,59,59,59	0
55	MG	AA	4554	1/1	0.84	0.38	73,73,73,73	0
55	MG	AA	4133	1/1	0.84	0.76	82,82,82,82	0
55	MG	DA	1837	1/1	0.84	0.48	88,88,88,88	0
55	MG	AA	5029	1/1	0.84	0.09	111,111,111,111	0
55	MG	CA	3557	1/1	0.84	0.22	59,59,59,59	0
55	MG	BW	115	1/1	0.84	0.18	70,70,70,70	0
55	MG	AA	4358	1/1	0.84	0.29	46,46,46,46	0
55	MG	AA	4297	1/1	0.84	0.73	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4588	1/1	0.84	0.49	80,80,80,80	0
55	MG	CA	4241	1/1	0.84	0.28	86,86,86,86	0
55	MG	CA	3652	1/1	0.84	0.29	51,51,51,51	0
55	MG	AB	249	1/1	0.84	0.15	73,73,73,73	0
55	MG	DW	106	1/1	0.84	0.30	113,113,113,113	0
55	MG	BA	1679	1/1	0.84	0.33	46,46,46,46	0
55	MG	AA	4646	1/1	0.84	0.20	91,91,91,91	0
55	MG	BA	2156	1/1	0.84	0.23	95,95,95,95	0
55	MG	DA	2159	1/1	0.84	0.28	63,63,63,63	0
55	MG	CA	4208	1/1	0.84	0.18	68,68,68,68	0
55	MG	AA	4278	1/1	0.84	0.49	44,44,44,44	0
55	MG	BA	2058	1/1	0.84	0.18	63,63,63,63	0
55	MG	AA	4389	1/1	0.84	0.21	61,61,61,61	0
55	MG	CA	3437	1/1	0.84	0.57	62,62,62,62	0
55	MG	AA	4998	1/1	0.84	0.13	86,86,86,86	0
55	MG	AA	4064	1/1	0.84	0.53	66,66,66,66	0
55	MG	CA	3027	1/1	0.84	0.30	48,48,48,48	0
55	MG	AA	4909	1/1	0.84	0.29	57,57,57,57	0
55	MG	AA	5207	1/1	0.84	0.28	65,65,65,65	0
55	MG	CA	3889	1/1	0.84	0.13	59,59,59,59	0
55	MG	AA	4523	1/1	0.84	0.42	66,66,66,66	0
55	MG	AA	4416	1/1	0.84	0.86	56,56,56,56	0
55	MG	CA	2959	1/1	0.84	0.25	60,60,60,60	0
55	MG	DA	2092	1/1	0.84	0.13	70,70,70,70	0
55	MG	AA	4165	1/1	0.84	0.61	104,104,104,104	0
55	MG	DA	2017	1/1	0.84	0.26	76,76,76,76	0
55	MG	AA	4083	1/1	0.84	0.24	78,78,78,78	0
55	MG	BA	2069	1/1	0.84	0.53	52,52,52,52	0
55	MG	DA	1734	1/1	0.84	0.80	61,61,61,61	0
55	MG	CA	3748	1/1	0.84	0.09	56,56,56,56	0
55	MG	CA	3372	1/1	0.84	0.18	38,38,38,38	0
55	MG	DA	1639	1/1	0.84	0.32	138,138,138,138	0
55	MG	CA	4042	1/1	0.84	0.24	46,46,46,46	0
55	MG	DA	1843	1/1	0.84	0.57	60,60,60,60	0
55	MG	BA	1716	1/1	0.84	0.51	56,56,56,56	0
55	MG	BE	204	1/1	0.84	0.19	46,46,46,46	0
55	MG	A3	103	1/1	0.84	0.64	77,77,77,77	0
55	MG	BA	1676	1/1	0.84	0.60	90,90,90,90	0
55	MG	CA	4341	1/1	0.84	0.34	51,51,51,51	0
55	MG	CA	3594	1/1	0.84	0.26	55,55,55,55	0
55	MG	CA	4077	1/1	0.84	0.37	47,47,47,47	0
55	MG	DA	1693	1/1	0.84	0.56	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3947	1/1	0.84	0.11	41,41,41,41	0
55	MG	CA	3368	1/1	0.84	0.31	41,41,41,41	0
55	MG	BA	1830	1/1	0.84	0.23	61,61,61,61	0
55	MG	DA	1804	1/1	0.84	0.45	69,69,69,69	0
55	MG	DV	101	1/1	0.84	0.21	103,103,103,103	0
55	MG	BA	1948	1/1	0.84	0.86	85,85,85,85	0
55	MG	BA	2063	1/1	0.84	0.46	37,37,37,37	0
55	MG	DA	1623	1/1	0.84	0.22	85,85,85,85	0
55	MG	CA	4055	1/1	0.84	0.24	49,49,49,49	0
55	MG	AA	4975	1/1	0.84	0.15	57,57,57,57	0
55	MG	CA	3946	1/1	0.84	0.32	51,51,51,51	0
55	MG	CN	202	1/1	0.84	0.38	57,57,57,57	0
55	MG	BA	1932	1/1	0.84	0.78	99,99,99,99	0
55	MG	BA	2048	1/1	0.84	0.32	47,47,47,47	0
55	MG	DA	1706	1/1	0.84	0.27	54,54,54,54	0
55	MG	DA	1747	1/1	0.84	0.59	56,56,56,56	0
55	MG	CA	4162	1/1	0.84	0.26	62,62,62,62	0
55	MG	CA	3293	1/1	0.84	0.36	45,45,45,45	0
55	MG	CA	3771	1/1	0.84	0.61	111,111,111,111	0
55	MG	BW	109	1/1	0.84	0.29	57,57,57,57	0
55	MG	AA	5238	1/1	0.84	0.42	59,59,59,59	0
55	MG	CA	4401	1/1	0.84	0.21	77,77,77,77	0
55	MG	AA	4903	1/1	0.84	0.26	48,48,48,48	0
55	MG	AA	4353	1/1	0.84	0.14	36,36,36,36	0
55	MG	AA	4528	1/1	0.84	0.34	63,63,63,63	0
55	MG	AA	4956	1/1	0.84	0.24	55,55,55,55	0
55	MG	DV	124	1/1	0.84	0.62	61,61,61,61	0
55	MG	CA	3064	1/1	0.84	1.08	75,75,75,75	0
55	MG	CB	209	1/1	0.84	0.84	66,66,66,66	0
55	MG	BA	1924	1/1	0.84	0.33	53,53,53,53	0
55	MG	AA	4362	1/1	0.84	0.51	49,49,49,49	0
55	MG	AA	5204	1/1	0.84	0.41	71,71,71,71	0
55	MG	AA	4601	1/1	0.84	0.17	68,68,68,68	0
55	MG	BA	2075	1/1	0.84	0.20	60,60,60,60	0
55	MG	CA	4306	1/1	0.84	0.35	53,53,53,53	0
55	MG	AA	4745	1/1	0.84	0.47	64,64,64,64	0
55	MG	BA	2110	1/1	0.84	0.40	88,88,88,88	0
55	MG	CA	3627	1/1	0.84	0.12	88,88,88,88	0
55	MG	AA	5007	1/1	0.84	0.27	60,60,60,60	0
55	MG	CA	3901	1/1	0.84	0.38	58,58,58,58	0
55	MG	AA	5138	1/1	0.84	0.25	72,72,72,72	0
55	MG	AA	4197	1/1	0.84	0.65	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4080	1/1	0.84	0.43	59,59,59,59	0
55	MG	AA	5025	1/1	0.84	0.39	92,92,92,92	0
55	MG	CA	3933	1/1	0.84	0.31	52,52,52,52	0
55	MG	CA	3678	1/1	0.84	0.29	77,77,77,77	0
55	MG	BA	1936	1/1	0.84	0.14	74,74,74,74	0
55	MG	AD	304	1/1	0.84	0.33	84,84,84,84	0
55	MG	AA	4012	1/1	0.84	0.44	65,65,65,65	0
55	MG	CA	2970	1/1	0.84	0.28	78,78,78,78	0
55	MG	DA	2009	1/1	0.84	0.26	55,55,55,55	0
55	MG	AA	5257	1/1	0.84	0.32	69,69,69,69	0
55	MG	BW	113	1/1	0.84	0.18	56,56,56,56	0
55	MG	DA	1688	1/1	0.84	0.33	58,58,58,58	0
55	MG	CA	3340	1/1	0.84	0.48	33,33,33,33	0
55	MG	CA	3793	1/1	0.84	0.16	77,77,77,77	0
55	MG	AA	5152	1/1	0.84	0.82	71,71,71,71	0
55	MG	CA	3482	1/1	0.85	0.23	47,47,47,47	0
55	MG	CA	4115	1/1	0.85	0.23	46,46,46,46	0
55	MG	BA	1807	1/1	0.85	0.90	77,77,77,77	0
55	MG	AA	4073	1/1	0.85	0.78	43,43,43,43	0
55	MG	CA	3504	1/1	0.85	0.29	43,43,43,43	0
55	MG	BA	1928	1/1	0.85	0.20	53,53,53,53	0
55	MG	CA	2916	1/1	0.85	0.37	66,66,66,66	0
55	MG	CA	3743	1/1	0.85	0.36	58,58,58,58	0
55	MG	CA	3242	1/1	0.85	0.25	33,33,33,33	0
55	MG	CA	4172	1/1	0.85	0.31	43,43,43,43	0
55	MG	BA	2155	1/1	0.85	0.19	40,40,40,40	0
55	MG	CA	3467	1/1	0.85	0.37	41,41,41,41	0
55	MG	DA	2045	1/1	0.85	0.17	98,98,98,98	0
55	MG	CA	3164	1/1	0.85	0.20	9,9,9,9	0
55	MG	DA	2124	1/1	0.85	0.84	88,88,88,88	0
55	MG	CA	4234	1/1	0.85	0.27	46,46,46,46	0
55	MG	DA	1631	1/1	0.85	0.49	71,71,71,71	0
55	MG	CA	3555	1/1	0.85	0.61	73,73,73,73	0
55	MG	CA	4140	1/1	0.85	0.30	57,57,57,57	0
55	MG	DT	201	1/1	0.85	0.24	57,57,57,57	0
55	MG	AA	4607	1/1	0.85	0.63	91,91,91,91	0
55	MG	DA	1659	1/1	0.85	0.26	83,83,83,83	0
55	MG	DA	2187	1/1	0.85	0.39	55,55,55,55	0
55	MG	BA	2005	1/1	0.85	0.20	63,63,63,63	0
55	MG	AA	4541	1/1	0.85	0.35	78,78,78,78	0
55	MG	CA	3637	1/1	0.85	0.16	47,47,47,47	0
55	MG	CA	3288	1/1	0.85	0.94	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4480	1/1	0.85	0.34	48,48,48,48	0
55	MG	CA	3375	1/1	0.85	0.08	59,59,59,59	0
55	MG	CA	3719	1/1	0.85	0.13	46,46,46,46	0
55	MG	DA	1989	1/1	0.85	0.11	85,85,85,85	0
55	MG	DA	1809	1/1	0.85	0.24	86,86,86,86	0
55	MG	AA	4876	1/1	0.85	0.40	57,57,57,57	0
55	MG	DA	1938	1/1	0.85	0.09	128,128,128,128	0
55	MG	DA	1948	1/1	0.85	0.28	58,58,58,58	0
55	MG	BA	1762	1/1	0.85	0.60	71,71,71,71	0
55	MG	CA	3445	1/1	0.85	0.48	44,44,44,44	0
55	MG	AA	4814	1/1	0.85	0.32	75,75,75,75	0
55	MG	DA	1947	1/1	0.85	0.25	84,84,84,84	0
55	MG	CA	3890	1/1	0.85	0.38	56,56,56,56	0
55	MG	AA	4500	1/1	0.85	0.55	63,63,63,63	0
55	MG	AA	4852	1/1	0.85	0.39	28,28,28,28	0
55	MG	BA	1681	1/1	0.85	0.62	162,162,162,162	0
55	MG	CA	3277	1/1	0.85	0.31	49,49,49,49	0
55	MG	BA	1644	1/1	0.85	0.29	91,91,91,91	0
55	MG	DA	2059	1/1	0.85	0.43	52,52,52,52	0
55	MG	AA	4609	1/1	0.85	0.37	76,76,76,76	0
55	MG	CA	3286	1/1	0.85	0.35	27,27,27,27	0
55	MG	AA	4615	1/1	0.85	0.36	79,79,79,79	0
55	MG	DA	1829	1/1	0.85	0.32	123,123,123,123	0
55	MG	AA	4335	1/1	0.85	0.46	52,52,52,52	0
55	MG	BA	1667	1/1	0.85	0.58	50,50,50,50	0
55	MG	AA	4795	1/1	0.85	0.36	105,105,105,105	0
55	MG	AA	4777	1/1	0.85	0.43	48,48,48,48	0
55	MG	CB	230	1/1	0.85	0.54	77,77,77,77	0
55	MG	AA	4516	1/1	0.85	0.40	69,69,69,69	0
55	MG	BV	112	1/1	0.85	0.14	89,89,89,89	0
55	MG	AA	4238	1/1	0.85	0.30	42,42,42,42	0
55	MG	CA	3030	1/1	0.85	0.26	61,61,61,61	0
55	MG	AS	202	1/1	0.85	0.28	56,56,56,56	0
55	MG	BA	1877	1/1	0.85	0.21	84,84,84,84	0
55	MG	AA	5061	1/1	0.85	0.49	49,49,49,49	0
55	MG	CA	3491	1/1	0.85	0.32	59,59,59,59	0
55	MG	BA	2070	1/1	0.85	0.63	66,66,66,66	0
55	MG	AA	4926	1/1	0.85	0.29	53,53,53,53	0
55	MG	BA	1687	1/1	0.85	0.37	25,25,25,25	0
55	MG	DA	1771	1/1	0.85	0.24	77,77,77,77	0
55	MG	CA	4361	1/1	0.85	0.50	65,65,65,65	0
55	MG	AA	4289	1/1	0.85	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3334	1/1	0.85	0.50	32,32,32,32	0
55	MG	CA	4156	1/1	0.85	0.56	68,68,68,68	0
55	MG	CA	3939	1/1	0.85	0.51	65,65,65,65	0
55	MG	BA	1774	1/1	0.85	0.17	57,57,57,57	0
55	MG	AA	4127	1/1	0.85	0.56	72,72,72,72	0
55	MG	BA	1696	1/1	0.85	0.41	50,50,50,50	0
55	MG	CA	4168	1/1	0.85	0.24	64,64,64,64	0
55	MG	AA	5288	1/1	0.85	0.43	68,68,68,68	0
55	MG	DA	1858	1/1	0.85	0.61	68,68,68,68	0
55	MG	CA	4330	1/1	0.85	0.53	61,61,61,61	0
55	MG	CA	4375	1/1	0.85	0.87	85,85,85,85	0
55	MG	CA	3689	1/1	0.85	0.19	47,47,47,47	0
55	MG	AA	5165	1/1	0.85	0.56	62,62,62,62	0
55	MG	AA	5221	1/1	0.85	0.48	55,55,55,55	0
55	MG	AA	4681	1/1	0.85	0.60	69,69,69,69	0
55	MG	CA	3777	1/1	0.85	0.58	59,59,59,59	0
55	MG	CA	4073	1/1	0.85	0.43	45,45,45,45	0
55	MG	AA	4827	1/1	0.85	0.31	64,64,64,64	0
55	MG	AA	4119	1/1	0.85	0.78	67,67,67,67	0
55	MG	DA	1902	1/1	0.85	0.53	70,70,70,70	0
55	MG	DA	1993	1/1	0.85	0.59	55,55,55,55	0
55	MG	BV	118	1/1	0.85	0.26	94,94,94,94	0
55	MG	AA	5195	1/1	0.85	0.32	80,80,80,80	0
55	MG	CA	3878	1/1	0.85	0.40	67,67,67,67	0
55	MG	CA	3876	1/1	0.85	0.30	76,76,76,76	0
55	MG	AA	4080	1/1	0.85	0.67	71,71,71,71	0
55	MG	CB	236	1/1	0.85	0.35	93,93,93,93	0
55	MG	CA	3410	1/1	0.85	0.17	44,44,44,44	0
55	MG	CA	3017	1/1	0.85	0.39	68,68,68,68	0
55	MG	DW	114	1/1	0.85	0.27	97,97,97,97	0
55	MG	CA	4259	1/1	0.85	0.48	35,35,35,35	0
55	MG	CA	4312	1/1	0.85	0.26	57,57,57,57	0
55	MG	CA	4123	1/1	0.85	0.39	43,43,43,43	0
55	MG	BA	2157	1/1	0.85	0.38	49,49,49,49	0
55	MG	CA	2966	1/1	0.85	0.29	75,75,75,75	0
55	MG	CA	3159	1/1	0.85	0.32	24,24,24,24	0
55	MG	DA	1931	1/1	0.85	0.52	50,50,50,50	0
55	MG	CA	3622	1/1	0.85	0.47	53,53,53,53	0
55	MG	BA	2083	1/1	0.85	0.21	92,92,92,92	0
55	MG	AA	4878	1/1	0.85	0.45	29,29,29,29	0
55	MG	CL	207	1/1	0.85	0.52	41,41,41,41	0
55	MG	BA	2078	1/1	0.85	0.08	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4884	1/1	0.85	0.19	47,47,47,47	0
55	MG	DA	1819	1/1	0.85	0.29	101,101,101,101	0
55	MG	CA	3699	1/1	0.85	0.24	75,75,75,75	0
55	MG	AA	4270	1/1	0.85	0.46	45,45,45,45	0
55	MG	BA	1728	1/1	0.85	0.28	69,69,69,69	0
55	MG	AA	4365	1/1	0.85	0.24	39,39,39,39	0
55	MG	AA	4018	1/1	0.85	0.31	125,125,125,125	0
55	MG	AA	5062	1/1	0.85	0.34	56,56,56,56	0
55	MG	AA	4239	1/1	0.85	1.29	47,47,47,47	0
55	MG	BA	1837	1/1	0.85	0.34	61,61,61,61	0
55	MG	DA	2060	1/1	0.85	0.57	72,72,72,72	0
55	MG	BA	1664	1/1	0.85	0.36	86,86,86,86	0
55	MG	CA	3391	1/1	0.85	0.40	72,72,72,72	0
55	MG	CA	4212	1/1	0.85	0.21	44,44,44,44	0
55	MG	AA	4565	1/1	0.85	0.27	61,61,61,61	0
55	MG	AA	5181	1/1	0.85	0.19	67,67,67,67	0
55	MG	AA	5011	1/1	0.85	0.24	87,87,87,87	0
55	MG	CA	2968	1/1	0.85	0.54	74,74,74,74	0
55	MG	BW	104	1/1	0.85	0.24	96,96,96,96	0
55	MG	CA	3550	1/1	0.85	0.45	41,41,41,41	0
55	MG	DA	1703	1/1	0.85	0.26	34,34,34,34	0
55	MG	BA	2029	1/1	0.85	0.15	64,64,64,64	0
55	MG	BA	1826	1/1	0.85	0.21	48,48,48,48	0
55	MG	BA	1883	1/1	0.85	0.23	77,77,77,77	0
55	MG	CA	2928	1/1	0.85	0.49	55,55,55,55	0
55	MG	CA	3048	1/1	0.85	0.33	88,88,88,88	0
55	MG	AA	5139	1/1	0.85	0.37	66,66,66,66	0
55	MG	DA	1745	1/1	0.85	0.29	54,54,54,54	0
55	MG	AB	220	1/1	0.85	0.31	84,84,84,84	0
55	MG	AA	4326	1/1	0.85	0.59	29,29,29,29	0
55	MG	AA	5182	1/1	0.85	0.48	52,52,52,52	0
55	MG	CA	3056	1/1	0.85	0.48	47,47,47,47	0
55	MG	DA	1855	1/1	0.85	0.28	69,69,69,69	0
55	MG	DA	2019	1/1	0.85	0.56	62,62,62,62	0
55	MG	BA	2059	1/1	0.85	0.42	48,48,48,48	0
55	MG	DV	106	1/1	0.85	0.13	93,93,93,93	0
55	MG	CA	3394	1/1	0.85	0.28	54,54,54,54	0
55	MG	AA	4062	1/1	0.85	0.52	126,126,126,126	0
55	MG	AA	4928	1/1	0.85	0.55	54,54,54,54	0
55	MG	BA	2034	1/1	0.85	0.17	47,47,47,47	0
55	MG	AA	4689	1/1	0.85	0.27	64,64,64,64	0
55	MG	DA	2016	1/1	0.85	0.45	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3560	1/1	0.85	0.11	69,69,69,69	0
55	MG	BA	2080	1/1	0.85	0.26	56,56,56,56	0
55	MG	AA	4451	1/1	0.85	0.42	60,60,60,60	0
55	MG	AA	4761	1/1	0.85	0.19	64,64,64,64	0
55	MG	BA	1956	1/1	0.85	0.25	50,50,50,50	0
55	MG	CA	3200	1/1	0.85	0.26	27,27,27,27	0
55	MG	DA	2073	1/1	0.86	0.18	60,60,60,60	0
55	MG	CA	4393	1/1	0.86	0.25	69,69,69,69	0
55	MG	DW	102	1/1	0.86	0.32	76,76,76,76	0
55	MG	AA	4540	1/1	0.86	0.28	87,87,87,87	0
55	MG	AA	5215	1/1	0.86	0.29	68,68,68,68	0
55	MG	CA	3634	1/1	0.86	0.61	118,118,118,118	0
55	MG	BA	1770	1/1	0.86	0.14	58,58,58,58	0
55	MG	DA	1620	1/1	0.86	0.20	101,101,101,101	0
55	MG	CA	2978	1/1	0.86	0.73	56,56,56,56	0
55	MG	DA	1875	1/1	0.86	0.20	77,77,77,77	0
55	MG	AA	4212	1/1	0.86	0.60	39,39,39,39	0
55	MG	DA	1749	1/1	0.86	0.24	39,39,39,39	0
55	MG	AA	4272	1/1	0.86	0.80	46,46,46,46	0
55	MG	CA	3970	1/1	0.86	0.45	29,29,29,29	0
55	MG	AA	4322	1/1	0.86	0.10	43,43,43,43	0
55	MG	CB	229	1/1	0.86	0.18	84,84,84,84	0
55	MG	AA	4537	1/1	0.86	0.36	58,58,58,58	0
55	MG	CA	3745	1/1	0.86	0.31	60,60,60,60	0
55	MG	BE	202	1/1	0.86	0.96	65,65,65,65	0
55	MG	DA	2074	1/1	0.86	0.64	72,72,72,72	0
55	MG	CA	4378	1/1	0.86	0.29	42,42,42,42	0
55	MG	AA	4743	1/1	0.86	0.33	59,59,59,59	0
55	MG	AA	5091	1/1	0.86	0.17	52,52,52,52	0
55	MG	CA	3910	1/1	0.86	0.27	77,77,77,77	0
55	MG	CA	3802	1/1	0.86	0.55	70,70,70,70	0
55	MG	CA	4385	1/1	0.86	0.12	61,61,61,61	0
55	MG	CA	2983	1/1	0.86	0.22	64,64,64,64	0
55	MG	CA	4336	1/1	0.86	0.36	62,62,62,62	0
55	MG	AN	203	1/1	0.86	0.17	64,64,64,64	0
55	MG	AA	4443	1/1	0.86	0.29	43,43,43,43	0
55	MG	AA	4802	1/1	0.86	0.28	82,82,82,82	0
55	MG	BA	1886	1/1	0.86	0.16	63,63,63,63	0
55	MG	DA	2064	1/1	0.86	0.37	52,52,52,52	0
55	MG	DA	1977	1/1	0.86	0.16	61,61,61,61	0
55	MG	BA	1842	1/1	0.86	0.59	63,63,63,63	0
55	MG	BA	1730	1/1	0.86	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4786	1/1	0.86	0.24	55,55,55,55	0
55	MG	DA	1873	1/1	0.86	0.30	90,90,90,90	0
55	MG	AA	4492	1/1	0.86	0.36	41,41,41,41	0
55	MG	CA	4153	1/1	0.86	0.23	57,57,57,57	0
55	MG	AA	4090	1/1	0.86	0.47	87,87,87,87	0
55	MG	CA	3067	1/1	0.86	0.25	73,73,73,73	0
55	MG	BA	1605	1/1	0.86	0.52	75,75,75,75	0
55	MG	CA	2905	1/1	0.86	0.72	89,89,89,89	0
55	MG	CA	3937	1/1	0.86	0.20	52,52,52,52	0
55	MG	A5	102	1/1	0.86	0.60	62,62,62,62	0
55	MG	DA	1744	1/1	0.86	0.42	69,69,69,69	0
55	MG	DA	1990	1/1	0.86	0.25	68,68,68,68	0
55	MG	CA	3614	1/1	0.86	0.53	84,84,84,84	0
55	MG	AB	207	1/1	0.86	0.19	59,59,59,59	0
55	MG	DA	1738	1/1	0.86	0.56	40,40,40,40	0
55	MG	CA	4353	1/1	0.86	0.68	53,53,53,53	0
55	MG	BA	1890	1/1	0.86	0.18	64,64,64,64	0
55	MG	BV	126	1/1	0.86	0.40	75,75,75,75	0
55	MG	CA	3552	1/1	0.86	0.92	56,56,56,56	0
55	MG	AA	5276	1/1	0.86	0.21	41,41,41,41	0
55	MG	CA	4003	1/1	0.86	0.34	56,56,56,56	0
55	MG	AA	5189	1/1	0.86	0.59	65,65,65,65	0
55	MG	AA	4659	1/1	0.86	0.43	69,69,69,69	0
55	MG	DA	2170	1/1	0.86	0.54	107,107,107,107	0
55	MG	CA	3211	1/1	0.86	0.28	28,28,28,28	0
55	MG	DA	2131	1/1	0.86	0.30	56,56,56,56	0
55	MG	CA	4155	1/1	0.86	0.41	54,54,54,54	0
55	MG	CA	3217	1/1	0.86	0.25	24,24,24,24	0
55	MG	DA	1750	1/1	0.86	0.16	27,27,27,27	0
55	MG	CA	4088	1/1	0.86	0.26	66,66,66,66	0
55	MG	DA	1889	1/1	0.86	0.54	107,107,107,107	0
55	MG	CA	3968	1/1	0.86	0.30	33,33,33,33	0
55	MG	BA	1609	1/1	0.86	0.55	88,88,88,88	0
55	MG	CL	203	1/1	0.86	0.40	49,49,49,49	0
55	MG	AA	4974	1/1	0.86	0.51	73,73,73,73	0
55	MG	AA	4094	1/1	0.86	0.42	62,62,62,62	0
55	MG	DD	301	1/1	0.86	0.28	73,73,73,73	0
55	MG	CA	3591	1/1	0.86	0.51	58,58,58,58	0
55	MG	DA	1775	1/1	0.86	0.20	68,68,68,68	0
55	MG	BA	2056	1/1	0.86	0.17	72,72,72,72	0
55	MG	BA	1663	1/1	0.86	0.43	95,95,95,95	0
55	MG	AA	4384	1/1	0.86	0.34	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3967	1/1	0.86	0.18	39,39,39,39	0
55	MG	AA	4100	1/1	0.86	0.50	58,58,58,58	0
55	MG	AA	4487	1/1	0.86	0.38	43,43,43,43	0
55	MG	CA	3990	1/1	0.86	0.49	39,39,39,39	0
55	MG	CA	3481	1/1	0.86	0.36	38,38,38,38	0
55	MG	AA	4648	1/1	0.86	0.26	70,70,70,70	0
55	MG	CA	3839	1/1	0.86	0.22	27,27,27,27	0
55	MG	DA	1827	1/1	0.86	0.28	98,98,98,98	0
55	MG	CA	3899	1/1	0.86	0.31	71,71,71,71	0
55	MG	AA	4614	1/1	0.86	0.11	79,79,79,79	0
55	MG	AA	4762	1/1	0.86	0.63	113,113,113,113	0
55	MG	BV	113	1/1	0.86	0.18	82,82,82,82	0
55	MG	DA	1888	1/1	0.86	0.15	98,98,98,98	0
55	MG	BA	1665	1/1	0.86	0.50	83,83,83,83	0
55	MG	DA	1712	1/1	0.86	0.33	48,48,48,48	0
55	MG	AA	4753	1/1	0.86	0.19	51,51,51,51	0
55	MG	CA	4043	1/1	0.86	0.24	47,47,47,47	0
55	MG	AV	201	1/1	0.86	0.17	62,62,62,62	0
55	MG	CA	3520	1/1	0.86	0.63	57,57,57,57	0
55	MG	CA	3865	1/1	0.86	0.32	55,55,55,55	0
55	MG	AA	5049	1/1	0.86	0.20	69,69,69,69	0
55	MG	CA	3855	1/1	0.86	0.34	42,42,42,42	0
55	MG	DA	1696	1/1	0.86	0.30	25,25,25,25	0
55	MG	CA	4262	1/1	0.86	0.55	55,55,55,55	0
55	MG	CA	3507	1/1	0.86	0.57	55,55,55,55	0
55	MG	CA	4139	1/1	0.86	0.15	51,51,51,51	0
55	MG	AA	4077	1/1	0.86	0.29	62,62,62,62	0
55	MG	CA	4245	1/1	0.86	0.31	43,43,43,43	0
55	MG	CA	3683	1/1	0.86	0.12	62,62,62,62	0
55	MG	CA	4382	1/1	0.86	0.26	65,65,65,65	0
55	MG	CA	4255	1/1	0.86	0.13	89,89,89,89	0
55	MG	CA	4185	1/1	0.86	0.54	53,53,53,53	0
55	MG	BA	1805	1/1	0.86	0.14	64,64,64,64	0
55	MG	CA	3854	1/1	0.86	0.42	66,66,66,66	0
55	MG	CA	4253	1/1	0.86	0.22	53,53,53,53	0
55	MG	AA	4390	1/1	0.86	0.36	59,59,59,59	0
55	MG	CA	3869	1/1	0.86	0.22	43,43,43,43	0
55	MG	DA	1860	1/1	0.86	0.29	74,74,74,74	0
55	MG	AA	5095	1/1	0.86	0.68	57,57,57,57	0
55	MG	AA	4494	1/1	0.86	0.20	50,50,50,50	0
55	MG	AA	5133	1/1	0.86	0.42	74,74,74,74	0
55	MG	CA	4087	1/1	0.86	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4044	1/1	0.86	0.42	66,66,66,66	0
55	MG	AA	4045	1/1	0.86	0.28	72,72,72,72	0
55	MG	CA	4229	1/1	0.86	0.61	42,42,42,42	0
55	MG	AA	4417	1/1	0.86	0.29	55,55,55,55	0
55	MG	BW	114	1/1	0.86	0.19	58,58,58,58	0
55	MG	CA	4028	1/1	0.86	0.24	47,47,47,47	0
55	MG	BV	124	1/1	0.86	0.21	62,62,62,62	0
55	MG	DW	122	1/1	0.86	0.18	72,72,72,72	0
55	MG	AA	5065	1/1	0.86	0.30	44,44,44,44	0
55	MG	DA	1830	1/1	0.86	0.20	56,56,56,56	0
55	MG	AA	4772	1/1	0.86	0.31	51,51,51,51	0
55	MG	CA	3796	1/1	0.86	0.43	54,54,54,54	0
55	MG	AA	4145	1/1	0.86	0.37	63,63,63,63	0
55	MG	AA	4432	1/1	0.86	0.25	56,56,56,56	0
55	MG	DA	2176	1/1	0.86	0.32	57,57,57,57	0
55	MG	AA	4095	1/1	0.86	0.26	57,57,57,57	0
55	MG	CA	3978	1/1	0.86	0.16	32,32,32,32	0
55	MG	DA	1774	1/1	0.86	0.23	71,71,71,71	0
55	MG	CA	2939	1/1	0.86	0.41	47,47,47,47	0
55	MG	AA	4765	1/1	0.86	0.98	59,59,59,59	0
55	MG	CA	3338	1/1	0.86	0.69	43,43,43,43	0
55	MG	BA	1773	1/1	0.86	0.14	74,74,74,74	0
55	MG	AA	4449	1/1	0.86	0.26	58,58,58,58	0
55	MG	DA	1768	1/1	0.86	0.56	138,138,138,138	0
55	MG	DA	1628	1/1	0.86	0.20	135,135,135,135	0
55	MG	CA	4331	1/1	0.86	0.22	51,51,51,51	0
55	MG	CA	3989	1/1	0.86	0.23	14,14,14,14	0
55	MG	CA	3943	1/1	0.86	0.29	114,114,114,114	0
55	MG	CA	3192	1/1	0.86	0.26	24,24,24,24	0
55	MG	BA	1619	1/1	0.86	0.18	81,81,81,81	0
55	MG	AA	4854	1/1	0.86	0.45	43,43,43,43	0
55	MG	CA	4203	1/1	0.86	0.55	32,32,32,32	0
55	MG	DA	1862	1/1	0.86	0.51	75,75,75,75	0
55	MG	CA	3702	1/1	0.86	0.98	90,90,90,90	0
55	MG	CA	3405	1/1	0.86	0.38	32,32,32,32	0
55	MG	BA	2066	1/1	0.86	0.15	58,58,58,58	0
55	MG	AA	4993	1/1	0.86	1.03	59,59,59,59	0
55	MG	BA	1986	1/1	0.86	0.19	56,56,56,56	0
55	MG	CA	3911	1/1	0.86	0.22	63,63,63,63	0
55	MG	CA	3458	1/1	0.86	0.41	68,68,68,68	0
55	MG	CA	4114	1/1	0.86	0.34	50,50,50,50	0
55	MG	AA	4185	1/1	0.86	0.34	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	2124	1/1	0.86	0.64	64,64,64,64	0
55	MG	CA	4365	1/1	0.86	0.29	84,84,84,84	0
55	MG	BI	202	1/1	0.87	0.78	94,94,94,94	0
55	MG	AA	5054	1/1	0.87	0.18	48,48,48,48	0
55	MG	DA	2103	1/1	0.87	0.23	80,80,80,80	0
55	MG	AA	4506	1/1	0.87	0.22	65,65,65,65	0
55	MG	AA	5166	1/1	0.87	0.15	93,93,93,93	0
55	MG	CA	3979	1/1	0.87	0.17	29,29,29,29	0
55	MG	CA	3421	1/1	0.87	0.49	55,55,55,55	0
55	MG	BA	1721	1/1	0.87	0.09	46,46,46,46	0
55	MG	AA	4258	1/1	0.87	0.41	42,42,42,42	0
55	MG	CA	3033	1/1	0.87	0.27	61,61,61,61	0
55	MG	CA	2999	1/1	0.87	0.14	85,85,85,85	0
55	MG	CA	3563	1/1	0.87	0.28	62,62,62,62	0
55	MG	CB	247	1/1	0.87	0.14	55,55,55,55	0
55	MG	BA	2158	1/1	0.87	0.22	59,59,59,59	0
55	MG	AA	5132	1/1	0.87	0.67	62,62,62,62	0
55	MG	BA	2073	1/1	0.87	0.10	68,68,68,68	0
55	MG	CA	3187	1/1	0.87	0.25	36,36,36,36	0
55	MG	CA	3420	1/1	0.87	0.29	43,43,43,43	0
55	MG	BA	2042	1/1	0.87	0.41	73,73,73,73	0
55	MG	BV	105	1/1	0.87	0.14	56,56,56,56	0
55	MG	BA	2061	1/1	0.87	0.39	65,65,65,65	0
55	MG	CA	3672	1/1	0.87	0.45	72,72,72,72	0
55	MG	AE	304	1/1	0.87	0.26	29,29,29,29	0
55	MG	DV	120	1/1	0.87	0.13	54,54,54,54	0
55	MG	CA	3411	1/1	0.87	0.50	53,53,53,53	0
55	MG	CB	261	1/1	0.87	0.22	61,61,61,61	0
55	MG	AA	4337	1/1	0.87	0.37	24,24,24,24	0
55	MG	DA	1751	1/1	0.87	0.69	58,58,58,58	0
55	MG	DA	2154	1/1	0.87	0.32	68,68,68,68	0
55	MG	CA	3441	1/1	0.87	0.28	63,63,63,63	0
55	MG	CA	3595	1/1	0.87	0.39	54,54,54,54	0
55	MG	AA	4816	1/1	0.87	0.27	82,82,82,82	0
55	MG	BB	302	1/1	0.87	0.16	61,61,61,61	0
55	MG	AA	5225	1/1	0.87	0.11	56,56,56,56	0
55	MG	CA	2987	1/1	0.87	0.41	67,67,67,67	0
55	MG	CA	3349	1/1	0.87	0.14	48,48,48,48	0
55	MG	AA	4513	1/1	0.87	0.25	42,42,42,42	0
55	MG	DA	2034	1/1	0.87	0.12	43,43,43,43	0
55	MG	DA	1964	1/1	0.87	0.42	38,38,38,38	0
55	MG	AA	4823	1/1	0.87	0.28	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	2088	1/1	0.87	0.36	55,55,55,55	0
55	MG	DA	1987	1/1	0.87	0.32	42,42,42,42	0
55	MG	CA	3496	1/1	0.87	0.13	45,45,45,45	0
55	MG	CA	3163	1/1	0.87	0.49	16,16,16,16	0
55	MG	AA	4332	1/1	0.87	0.32	53,53,53,53	0
55	MG	AA	5167	1/1	0.87	0.35	58,58,58,58	0
55	MG	AA	4189	1/1	0.87	0.38	27,27,27,27	0
55	MG	AA	4543	1/1	0.87	0.27	77,77,77,77	0
55	MG	AA	4311	1/1	0.87	0.53	60,60,60,60	0
55	MG	AA	4864	1/1	0.87	0.24	30,30,30,30	0
55	MG	CA	3860	1/1	0.87	0.33	46,46,46,46	0
55	MG	AA	4790	1/1	0.87	0.26	43,43,43,43	0
55	MG	CA	4027	1/1	0.87	0.23	67,67,67,67	0
55	MG	AA	4931	1/1	0.87	0.26	41,41,41,41	0
55	MG	CA	3734	1/1	0.87	0.59	43,43,43,43	0
55	MG	AA	4747	1/1	0.87	0.34	37,37,37,37	0
55	MG	AA	4071	1/1	0.87	0.25	54,54,54,54	0
55	MG	BA	1813	1/1	0.87	0.67	60,60,60,60	0
55	MG	BA	2131	1/1	0.87	0.41	70,70,70,70	0
55	MG	BA	2081	1/1	0.87	0.17	92,92,92,92	0
55	MG	AA	5016	1/1	0.87	0.51	68,68,68,68	0
55	MG	AA	4791	1/1	0.87	0.42	57,57,57,57	0
55	MG	DA	1668	1/1	0.87	0.88	93,93,93,93	0
55	MG	CA	3648	1/1	0.87	0.28	41,41,41,41	0
55	MG	CA	4037	1/1	0.87	0.15	45,45,45,45	0
55	MG	CA	3446	1/1	0.87	0.46	53,53,53,53	0
55	MG	DA	2004	1/1	0.87	0.41	40,40,40,40	0
55	MG	CB	265	1/1	0.87	0.30	55,55,55,55	0
55	MG	CA	4351	1/1	0.87	0.19	59,59,59,59	0
55	MG	AA	4799	1/1	0.87	0.34	37,37,37,37	0
55	MG	AA	4063	1/1	0.87	0.67	80,80,80,80	0
55	MG	CA	4126	1/1	0.87	0.16	48,48,48,48	0
55	MG	CA	3998	1/1	0.87	0.23	35,35,35,35	0
55	MG	CB	204	1/1	0.87	0.21	92,92,92,92	0
55	MG	CA	4069	1/1	0.87	0.31	41,41,41,41	0
55	MG	CA	2921	1/1	0.87	0.15	63,63,63,63	0
55	MG	AA	5293	1/1	0.87	0.34	49,49,49,49	0
55	MG	CA	3817	1/1	0.87	0.95	59,59,59,59	0
55	MG	CA	3893	1/1	0.87	0.36	54,54,54,54	0
55	MG	AA	5266	1/1	0.87	0.32	64,64,64,64	0
55	MG	AA	4254	1/1	0.87	0.52	33,33,33,33	0
55	MG	DA	1603	1/1	0.87	0.66	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CT	101	1/1	0.87	0.31	51,51,51,51	0
55	MG	CA	4010	1/1	0.87	0.51	42,42,42,42	0
55	MG	CA	3783	1/1	0.87	1.20	96,96,96,96	0
55	MG	AA	4495	1/1	0.87	0.31	53,53,53,53	0
55	MG	CA	3516	1/1	0.87	0.16	46,46,46,46	0
55	MG	DA	2070	1/1	0.87	0.19	90,90,90,90	0
55	MG	C3	101	1/1	0.87	0.35	57,57,57,57	0
55	MG	AA	4603	1/1	0.87	0.20	68,68,68,68	0
55	MG	DA	1805	1/1	0.87	0.30	85,85,85,85	0
55	MG	AA	4503	1/1	0.87	0.20	48,48,48,48	0
55	MG	BA	2014	1/1	0.87	0.26	58,58,58,58	0
55	MG	AA	4316	1/1	0.87	0.31	31,31,31,31	0
55	MG	BA	2039	1/1	0.87	0.29	62,62,62,62	0
55	MG	DA	2050	1/1	0.87	0.39	77,77,77,77	0
55	MG	BA	1794	1/1	0.87	0.11	53,53,53,53	0
55	MG	CA	4189	1/1	0.87	0.48	49,49,49,49	0
55	MG	CA	4287	1/1	0.87	0.41	77,77,77,77	0
55	MG	CA	3853	1/1	0.87	0.24	21,21,21,21	0
55	MG	A4	102	1/1	0.87	0.63	101,101,101,101	0
55	MG	CA	3470	1/1	0.87	0.41	49,49,49,49	0
55	MG	CA	3480	1/1	0.87	0.67	49,49,49,49	0
55	MG	BA	1750	1/1	0.87	0.48	55,55,55,55	0
55	MG	DA	1723	1/1	0.87	0.38	65,65,65,65	0
55	MG	AA	4124	1/1	0.87	0.40	75,75,75,75	0
55	MG	AA	4660	1/1	0.87	1.25	140,140,140,140	0
55	MG	AA	4246	1/1	0.87	0.47	43,43,43,43	0
55	MG	CB	223	1/1	0.87	0.56	36,36,36,36	0
55	MG	AA	4219	1/1	0.87	0.17	16,16,16,16	0
55	MG	DA	1700	1/1	0.87	0.10	48,48,48,48	0
55	MG	DA	2188	1/1	0.87	0.51	91,91,91,91	0
55	MG	AB	214	1/1	0.87	0.24	84,84,84,84	0
55	MG	CB	217	1/1	0.87	0.28	35,35,35,35	0
55	MG	CA	3335	1/1	0.87	0.20	34,34,34,34	0
55	MG	CA	3327	1/1	0.87	0.28	36,36,36,36	0
55	MG	CA	3400	1/1	0.87	0.45	32,32,32,32	0
55	MG	BA	1767	1/1	0.87	0.32	39,39,39,39	0
55	MG	CA	3616	1/1	0.87	0.17	53,53,53,53	0
55	MG	AB	226	1/1	0.87	0.20	59,59,59,59	0
55	MG	BA	1834	1/1	0.87	1.08	67,67,67,67	0
55	MG	CA	3126	1/1	0.87	0.37	14,14,14,14	0
55	MG	AA	4411	1/1	0.87	0.17	63,63,63,63	0
55	MG	AA	4372	1/1	0.87	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DR	101	1/1	0.87	0.83	62,62,62,62	0
55	MG	AA	5258	1/1	0.87	0.07	76,76,76,76	0
55	MG	DA	1941	1/1	0.87	0.30	38,38,38,38	0
55	MG	DH	203	1/1	0.87	0.92	102,102,102,102	0
55	MG	AA	5203	1/1	0.87	0.25	80,80,80,80	0
55	MG	BA	2011	1/1	0.87	0.12	73,73,73,73	0
55	MG	AA	4644	1/1	0.87	0.53	75,75,75,75	0
55	MG	CA	4099	1/1	0.87	0.31	47,47,47,47	0
55	MG	CA	3912	1/1	0.87	0.30	56,56,56,56	0
55	MG	CA	3243	1/1	0.87	0.52	54,54,54,54	0
55	MG	CA	4364	1/1	0.87	0.13	74,74,74,74	0
55	MG	BA	1963	1/1	0.87	0.17	51,51,51,51	0
55	MG	CA	3099	1/1	0.87	0.27	41,41,41,41	0
55	MG	DA	2164	1/1	0.87	0.25	54,54,54,54	0
55	MG	AA	4866	1/1	0.87	0.43	24,24,24,24	0
55	MG	BA	1757	1/1	0.87	0.46	66,66,66,66	0
55	MG	BA	1971	1/1	0.87	0.27	34,34,34,34	0
55	MG	CA	2917	1/1	0.87	0.35	41,41,41,41	0
55	MG	AA	4257	1/1	0.87	0.79	41,41,41,41	0
55	MG	AA	5055	1/1	0.87	0.27	48,48,48,48	0
55	MG	AA	4068	1/1	0.87	0.22	66,66,66,66	0
55	MG	CA	3524	1/1	0.87	0.12	39,39,39,39	0
55	MG	CA	3562	1/1	0.87	0.32	48,48,48,48	0
55	MG	CA	3549	1/1	0.87	0.27	36,36,36,36	0
55	MG	DA	2160	1/1	0.87	0.78	63,63,63,63	0
55	MG	CA	4000	1/1	0.87	0.23	47,47,47,47	0
55	MG	AA	4107	1/1	0.87	0.32	61,61,61,61	0
55	MG	CA	3597	1/1	0.87	0.28	89,89,89,89	0
55	MG	AA	4318	1/1	0.87	1.05	56,56,56,56	0
55	MG	CA	3005	1/1	0.87	0.53	91,91,91,91	0
55	MG	CA	3210	1/1	0.87	0.38	35,35,35,35	0
55	MG	BA	2117	1/1	0.87	0.19	56,56,56,56	0
55	MG	CA	3592	1/1	0.87	0.18	49,49,49,49	0
55	MG	DA	1657	1/1	0.87	0.73	68,68,68,68	0
55	MG	AA	5116	1/1	0.87	0.19	50,50,50,50	0
55	MG	AA	4848	1/1	0.87	0.16	30,30,30,30	0
55	MG	CA	4275	1/1	0.87	0.31	74,74,74,74	0
55	MG	BA	1658	1/1	0.87	0.20	73,73,73,73	0
55	MG	AA	5123	1/1	0.87	0.13	60,60,60,60	0
55	MG	BA	1933	1/1	0.87	0.15	64,64,64,64	0
55	MG	AA	5014	1/1	0.87	0.21	45,45,45,45	0
55	MG	CA	3468	1/1	0.87	0.57	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1838	1/1	0.87	0.26	90,90,90,90	0
55	MG	AA	4720	1/1	0.87	0.32	92,92,92,92	0
55	MG	DA	2116	1/1	0.87	0.39	89,89,89,89	0
55	MG	CB	238	1/1	0.88	0.25	52,52,52,52	0
55	MG	AP	202	1/1	0.88	0.33	79,79,79,79	0
55	MG	BA	1627	1/1	0.88	0.29	61,61,61,61	0
55	MG	CA	3186	1/1	0.88	0.25	29,29,29,29	0
55	MG	AA	4325	1/1	0.88	0.26	44,44,44,44	0
55	MG	CA	4021	1/1	0.88	0.10	56,56,56,56	0
55	MG	CA	3519	1/1	0.88	0.26	68,68,68,68	0
55	MG	AA	4922	1/1	0.88	0.12	67,67,67,67	0
55	MG	AA	4446	1/1	0.88	0.32	51,51,51,51	0
55	MG	AA	4564	1/1	0.88	0.12	66,66,66,66	0
55	MG	CA	2991	1/1	0.88	0.33	51,51,51,51	0
55	MG	AA	4420	1/1	0.88	0.17	52,52,52,52	0
55	MG	CA	2979	1/1	0.88	0.60	74,74,74,74	0
55	MG	DA	2007	1/1	0.88	0.11	75,75,75,75	0
55	MG	AA	4941	1/1	0.88	0.21	48,48,48,48	0
55	MG	AA	4117	1/1	0.88	0.96	71,71,71,71	0
55	MG	CA	3181	1/1	0.88	0.34	39,39,39,39	0
55	MG	DA	1971	1/1	0.88	0.19	45,45,45,45	0
55	MG	AA	4645	1/1	0.88	0.18	57,57,57,57	0
55	MG	CA	3318	1/1	0.88	0.31	29,29,29,29	0
55	MG	BA	1703	1/1	0.88	0.14	32,32,32,32	0
55	MG	BA	1614	1/1	0.88	0.54	83,83,83,83	0
55	MG	DA	2167	1/1	0.88	0.28	41,41,41,41	0
55	MG	CA	4236	1/1	0.88	0.50	45,45,45,45	0
55	MG	AA	4051	1/1	0.88	0.16	54,54,54,54	0
55	MG	CA	4363	1/1	0.88	0.13	58,58,58,58	0
55	MG	CB	213	1/1	0.88	0.25	65,65,65,65	0
55	MG	CA	4165	1/1	0.88	0.13	37,37,37,37	0
55	MG	BA	1602	1/1	0.88	0.26	101,101,101,101	0
55	MG	AA	4155	1/1	0.88	0.54	75,75,75,75	0
55	MG	AA	4128	1/1	0.88	0.17	69,69,69,69	0
55	MG	CA	3276	1/1	0.88	0.55	58,58,58,58	0
55	MG	BA	1918	1/1	0.88	0.15	65,65,65,65	0
55	MG	DA	1963	1/1	0.88	0.14	46,46,46,46	0
55	MG	AA	4740	1/1	0.88	1.33	103,103,103,103	0
55	MG	AA	4136	1/1	0.88	0.19	91,91,91,91	0
55	MG	BA	1631	1/1	0.88	0.17	94,94,94,94	0
55	MG	AA	4919	1/1	0.88	0.66	64,64,64,64	0
55	MG	AA	5124	1/1	0.88	0.27	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	2104	1/1	0.88	0.25	62,62,62,62	0
55	MG	DA	2098	1/1	0.88	0.36	57,57,57,57	0
55	MG	CA	3902	1/1	0.88	0.19	68,68,68,68	0
55	MG	DA	2033	1/1	0.88	0.35	45,45,45,45	0
55	MG	CA	3205	1/1	0.88	0.32	34,34,34,34	0
55	MG	CA	3994	1/1	0.88	0.15	66,66,66,66	0
55	MG	AA	4657	1/1	0.88	0.77	69,69,69,69	0
55	MG	CA	3366	1/1	0.88	0.26	42,42,42,42	0
55	MG	AA	4995	1/1	0.88	0.12	71,71,71,71	0
55	MG	AA	4654	1/1	0.88	0.19	42,42,42,42	0
55	MG	DA	2081	1/1	0.88	0.48	68,68,68,68	0
55	MG	CA	2936	1/1	0.88	0.29	61,61,61,61	0
55	MG	BA	1983	1/1	0.88	0.28	58,58,58,58	0
55	MG	BA	1706	1/1	0.88	0.14	35,35,35,35	0
55	MG	DA	1726	1/1	0.88	0.14	28,28,28,28	0
55	MG	AA	5043	1/1	0.88	0.30	79,79,79,79	0
55	MG	CX	103	1/1	0.88	0.20	31,31,31,31	0
55	MG	BA	1817	1/1	0.88	0.06	77,77,77,77	0
55	MG	DA	2111	1/1	0.88	0.23	52,52,52,52	0
55	MG	BA	2012	1/1	0.88	0.75	64,64,64,64	0
55	MG	CA	4006	1/1	0.88	0.17	33,33,33,33	0
55	MG	BA	1906	1/1	0.88	1.40	90,90,90,90	0
55	MG	CA	3255	1/1	0.88	0.13	33,33,33,33	0
55	MG	CA	3477	1/1	0.88	0.16	45,45,45,45	0
55	MG	BW	103	1/1	0.88	0.34	60,60,60,60	0
55	MG	CA	3514	1/1	0.88	0.60	74,74,74,74	0
55	MG	AA	5012	1/1	0.88	0.51	59,59,59,59	0
55	MG	DA	1658	1/1	0.88	0.30	87,87,87,87	0
55	MG	CA	2924	1/1	0.88	0.63	91,91,91,91	0
55	MG	AA	4932	1/1	0.88	0.25	45,45,45,45	0
55	MG	DA	1732	1/1	0.88	0.43	64,64,64,64	0
55	MG	AA	5172	1/1	0.88	0.17	65,65,65,65	0
55	MG	DA	1718	1/1	0.88	0.57	43,43,43,43	0
55	MG	BA	2015	1/1	0.88	0.40	53,53,53,53	0
55	MG	CA	3537	1/1	0.88	0.22	60,60,60,60	0
55	MG	CA	3503	1/1	0.88	0.32	53,53,53,53	0
55	MG	CA	3228	1/1	0.88	0.32	34,34,34,34	0
55	MG	BA	1798	1/1	0.88	0.23	60,60,60,60	0
55	MG	CA	3097	1/1	0.88	0.27	60,60,60,60	0
55	MG	CA	3264	1/1	0.88	0.25	34,34,34,34	0
55	MG	BI	201	1/1	0.88	0.34	96,96,96,96	0
55	MG	AA	4860	1/1	0.88	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3957	1/1	0.88	0.71	55,55,55,55	0
55	MG	CQ	204	1/1	0.88	0.52	75,75,75,75	0
55	MG	CA	3418	1/1	0.88	0.39	49,49,49,49	0
55	MG	CA	3759	1/1	0.88	0.47	57,57,57,57	0
55	MG	DA	2100	1/1	0.88	0.16	48,48,48,48	0
55	MG	AB	232	1/1	0.88	0.13	93,93,93,93	0
55	MG	CA	4019	1/1	0.88	0.42	43,43,43,43	0
55	MG	DA	1982	1/1	0.88	0.22	61,61,61,61	0
55	MG	AA	4976	1/1	0.88	0.34	78,78,78,78	0
55	MG	AA	4889	1/1	0.88	0.26	41,41,41,41	0
55	MG	AA	4955	1/1	0.88	0.42	54,54,54,54	0
55	MG	AA	4431	1/1	0.88	0.32	59,59,59,59	0
55	MG	BA	2146	1/1	0.88	0.30	53,53,53,53	0
55	MG	DA	1870	1/1	0.88	0.11	76,76,76,76	0
55	MG	CA	2985	1/1	0.88	0.28	43,43,43,43	0
55	MG	CA	3452	1/1	0.88	0.20	50,50,50,50	0
55	MG	AA	4548	1/1	0.88	0.18	78,78,78,78	0
55	MG	BA	1820	1/1	0.88	0.38	66,66,66,66	0
55	MG	AA	5155	1/1	0.88	0.85	69,69,69,69	0
55	MG	BA	1646	1/1	0.88	0.20	59,59,59,59	0
55	MG	CA	3300	1/1	0.88	0.36	60,60,60,60	0
55	MG	CA	3518	1/1	0.88	0.11	75,75,75,75	0
55	MG	BA	1889	1/1	0.88	0.27	98,98,98,98	0
55	MG	CA	3688	1/1	0.88	0.39	70,70,70,70	0
55	MG	CA	3640	1/1	0.88	0.26	73,73,73,73	0
55	MG	DA	1944	1/1	0.88	0.27	64,64,64,64	0
55	MG	CA	4160	1/1	0.88	0.25	67,67,67,67	0
55	MG	CA	3658	1/1	0.88	0.21	51,51,51,51	0
55	MG	DA	2047	1/1	0.88	0.58	52,52,52,52	0
55	MG	AA	4857	1/1	0.88	0.35	28,28,28,28	0
55	MG	AA	4666	1/1	0.88	0.72	48,48,48,48	0
55	MG	AA	4574	1/1	0.88	0.80	71,71,71,71	0
55	MG	DA	2186	1/1	0.88	0.19	71,71,71,71	0
55	MG	CA	4231	1/1	0.88	0.42	48,48,48,48	0
55	MG	AA	4004	1/1	0.88	0.37	52,52,52,52	0
55	MG	BA	1672	1/1	0.88	0.23	60,60,60,60	0
55	MG	DA	1689	1/1	0.88	0.66	118,118,118,118	0
55	MG	BA	1714	1/1	0.88	0.51	56,56,56,56	0
55	MG	AA	4856	1/1	0.88	0.20	42,42,42,42	0
55	MG	AA	4319	1/1	0.88	0.20	50,50,50,50	0
55	MG	CA	3698	1/1	0.88	0.19	65,65,65,65	0
55	MG	DA	1874	1/1	0.88	0.58	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	2000	1/1	0.88	0.47	87,87,87,87	0
55	MG	AA	4131	1/1	0.88	0.19	48,48,48,48	0
55	MG	AA	5088	1/1	0.88	0.50	78,78,78,78	0
55	MG	AA	5042	1/1	0.88	0.37	57,57,57,57	0
55	MG	AA	5098	1/1	0.88	0.37	80,80,80,80	0
55	MG	AA	4052	1/1	0.88	0.33	72,72,72,72	0
55	MG	CB	218	1/1	0.88	0.53	46,46,46,46	0
55	MG	CA	3244	1/1	0.88	1.14	47,47,47,47	0
55	MG	DA	2062	1/1	0.88	0.34	65,65,65,65	0
55	MG	AA	4244	1/1	0.88	0.19	31,31,31,31	0
55	MG	AB	201	1/1	0.88	1.19	87,87,87,87	0
55	MG	AA	4784	1/1	0.88	0.34	43,43,43,43	0
55	MG	AA	4441	1/1	0.88	0.30	43,43,43,43	0
55	MG	CA	3870	1/1	0.88	0.34	51,51,51,51	0
55	MG	DA	1742	1/1	0.88	0.28	53,53,53,53	0
55	MG	DA	1945	1/1	0.88	0.21	78,78,78,78	0
55	MG	BA	2000	1/1	0.88	0.21	76,76,76,76	0
55	MG	CA	3331	1/1	0.88	0.14	27,27,27,27	0
55	MG	AA	4038	1/1	0.88	0.26	117,117,117,117	0
55	MG	CA	3919	1/1	0.88	0.24	51,51,51,51	0
55	MG	CA	2948	1/1	0.88	0.43	85,85,85,85	0
55	MG	CA	3428	1/1	0.88	0.16	35,35,35,35	0
55	MG	AA	4479	1/1	0.88	0.33	80,80,80,80	0
55	MG	CA	3055	1/1	0.88	0.19	59,59,59,59	0
55	MG	BA	1952	1/1	0.88	0.31	22,22,22,22	0
55	MG	AA	4284	1/1	0.88	0.38	28,28,28,28	0
55	MG	DA	1815	1/1	0.88	0.31	75,75,75,75	0
55	MG	CA	4198	1/1	0.88	0.64	93,93,93,93	0
55	MG	CA	4271	1/1	0.88	0.32	29,29,29,29	0
55	MG	DA	1790	1/1	0.88	0.37	91,91,91,91	0
55	MG	CA	3642	1/1	0.88	0.32	46,46,46,46	0
55	MG	AA	4873	1/1	0.88	0.40	34,34,34,34	0
55	MG	AB	206	1/1	0.88	0.25	112,112,112,112	0
55	MG	DA	1934	1/1	0.88	0.13	75,75,75,75	0
55	MG	CA	3488	1/1	0.88	0.25	55,55,55,55	0
55	MG	BA	1950	1/1	0.88	0.28	84,84,84,84	0
55	MG	CA	4322	1/1	0.88	0.29	66,66,66,66	0
55	MG	DA	1663	1/1	0.88	0.22	64,64,64,64	0
55	MG	CA	3256	1/1	0.88	0.15	31,31,31,31	0
55	MG	CA	4390	1/1	0.88	0.15	54,54,54,54	0
55	MG	AA	4283	1/1	0.88	0.18	39,39,39,39	0
55	MG	CA	3977	1/1	0.88	0.16	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4562	1/1	0.88	0.13	73,73,73,73	0
55	MG	AA	4915	1/1	0.88	0.31	64,64,64,64	0
55	MG	CA	3396	1/1	0.88	0.33	39,39,39,39	0
55	MG	AA	4019	1/1	0.88	0.12	85,85,85,85	0
55	MG	AA	4519	1/1	0.88	0.32	50,50,50,50	0
55	MG	AA	4217	1/1	0.88	0.82	43,43,43,43	0
55	MG	CA	4328	1/1	0.88	0.68	76,76,76,76	0
55	MG	AA	4373	1/1	0.88	0.49	40,40,40,40	0
55	MG	CA	3816	1/1	0.88	0.10	68,68,68,68	0
55	MG	AA	4423	1/1	0.88	0.24	45,45,45,45	0
55	MG	AA	4553	1/1	0.88	0.31	39,39,39,39	0
55	MG	AA	4059	1/1	0.88	0.36	73,73,73,73	0
55	MG	AA	4072	1/1	0.88	0.33	57,57,57,57	0
55	MG	CA	3548	1/1	0.88	0.34	55,55,55,55	0
55	MG	AA	4752	1/1	0.88	0.34	78,78,78,78	0
55	MG	AA	4623	1/1	0.88	0.43	69,69,69,69	0
55	MG	CA	3474	1/1	0.88	0.39	55,55,55,55	0
55	MG	CA	4067	1/1	0.88	0.30	50,50,50,50	0
55	MG	BA	1821	1/1	0.88	0.64	81,81,81,81	0
55	MG	CP	201	1/1	0.88	0.20	57,57,57,57	0
55	MG	BA	1772	1/1	0.88	0.14	43,43,43,43	0
55	MG	AA	4734	1/1	0.88	0.30	21,21,21,21	0
55	MG	BA	1705	1/1	0.88	0.12	55,55,55,55	0
55	MG	AA	4518	1/1	0.88	0.55	98,98,98,98	0
55	MG	AA	4352	1/1	0.88	0.32	66,66,66,66	0
55	MG	BA	2168	1/1	0.88	0.34	59,59,59,59	0
55	MG	AA	4401	1/1	0.88	0.41	42,42,42,42	0
55	MG	BW	119	1/1	0.88	0.17	73,73,73,73	0
55	MG	CA	4258	1/1	0.88	0.47	48,48,48,48	0
55	MG	CA	3887	1/1	0.88	0.41	48,48,48,48	0
55	MG	DA	2171	1/1	0.88	0.21	96,96,96,96	0
55	MG	BV	130	1/1	0.88	0.13	43,43,43,43	0
55	MG	CA	3670	1/1	0.88	0.90	78,78,78,78	0
55	MG	AB	247	1/1	0.88	0.12	49,49,49,49	0
55	MG	BA	1960	1/1	0.88	0.35	35,35,35,35	0
55	MG	AA	4381	1/1	0.88	0.34	79,79,79,79	0
55	MG	BA	1984	1/1	0.88	0.08	69,69,69,69	0
55	MG	CA	3456	1/1	0.88	0.25	51,51,51,51	0
55	MG	C4	104	1/1	0.88	0.28	56,56,56,56	0
55	MG	AA	5001	1/1	0.88	0.67	53,53,53,53	0
55	MG	CA	4372	1/1	0.88	0.35	55,55,55,55	0
55	MG	CA	4196	1/1	0.88	0.24	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	5058	1/1	0.88	0.26	49,49,49,49	0
55	MG	DA	2174	1/1	0.88	0.23	65,65,65,65	0
55	MG	AA	4983	1/1	0.88	0.21	51,51,51,51	0
55	MG	AA	4545	1/1	0.88	0.57	65,65,65,65	0
55	MG	AA	4691	1/1	0.88	0.15	76,76,76,76	0
55	MG	CA	4297	1/1	0.88	0.35	49,49,49,49	0
55	MG	CA	3000	1/1	0.88	0.57	37,37,37,37	0
55	MG	AA	4877	1/1	0.88	0.24	48,48,48,48	0
55	MG	CA	3035	1/1	0.88	0.20	70,70,70,70	0
55	MG	CA	2962	1/1	0.89	0.30	71,71,71,71	0
55	MG	DA	1950	1/1	0.89	0.21	155,155,155,155	0
55	MG	CA	4264	1/1	0.89	0.10	68,68,68,68	0
55	MG	CB	248	1/1	0.89	0.55	63,63,63,63	0
55	MG	CB	252	1/1	0.89	0.22	64,64,64,64	0
55	MG	AA	4555	1/1	0.89	0.47	66,66,66,66	0
55	MG	CB	260	1/1	0.89	0.20	54,54,54,54	0
55	MG	DA	1656	1/1	0.89	0.13	96,96,96,96	0
55	MG	BA	1638	1/1	0.89	0.22	65,65,65,65	0
55	MG	AA	4701	1/1	0.89	0.43	71,71,71,71	0
55	MG	BA	1616	1/1	0.89	0.38	65,65,65,65	0
55	MG	AA	4719	1/1	0.89	0.26	74,74,74,74	0
55	MG	AA	4403	1/1	0.89	0.18	55,55,55,55	0
55	MG	CA	4103	1/1	0.89	0.33	43,43,43,43	0
55	MG	CA	3273	1/1	0.89	0.35	43,43,43,43	0
55	MG	AA	4642	1/1	0.89	0.67	73,73,73,73	0
55	MG	AA	4262	1/1	0.89	0.19	34,34,34,34	0
55	MG	DA	1767	1/1	0.89	0.20	118,118,118,118	0
55	MG	BA	2096	1/1	0.89	0.39	76,76,76,76	0
55	MG	CA	4240	1/1	0.89	0.28	44,44,44,44	0
55	MG	CA	3179	1/1	0.89	0.12	41,41,41,41	0
55	MG	AA	4438	1/1	0.89	0.20	76,76,76,76	0
55	MG	CA	3510	1/1	0.89	0.24	58,58,58,58	0
55	MG	AA	4980	1/1	0.89	0.16	55,55,55,55	0
55	MG	BA	2079	1/1	0.89	0.17	57,57,57,57	0
55	MG	CA	3138	1/1	0.89	0.55	19,19,19,19	0
55	MG	CA	3266	1/1	0.89	0.49	25,25,25,25	0
55	MG	DA	1915	1/1	0.89	0.11	113,113,113,113	0
55	MG	AA	4408	1/1	0.89	0.24	50,50,50,50	0
55	MG	BA	1937	1/1	0.89	0.26	48,48,48,48	0
55	MG	AA	4460	1/1	0.89	0.26	62,62,62,62	0
55	MG	CA	4120	1/1	0.89	0.32	42,42,42,42	0
55	MG	BA	1777	1/1	0.89	0.29	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3791	1/1	0.89	0.37	61,61,61,61	0
55	MG	AA	4775	1/1	0.89	0.14	66,66,66,66	0
55	MG	AB	212	1/1	0.89	0.10	45,45,45,45	0
55	MG	AB	241	1/1	0.89	0.41	98,98,98,98	0
55	MG	BA	1753	1/1	0.89	0.42	39,39,39,39	0
55	MG	CA	3383	1/1	0.89	0.19	38,38,38,38	0
55	MG	CA	4064	1/1	0.89	0.24	49,49,49,49	0
55	MG	CA	4132	1/1	0.89	0.40	57,57,57,57	0
55	MG	AA	4268	1/1	0.89	0.28	25,25,25,25	0
55	MG	CA	3527	1/1	0.89	0.34	27,27,27,27	0
55	MG	CA	3169	1/1	0.89	0.53	21,21,21,21	0
55	MG	CA	3245	1/1	0.89	0.23	31,31,31,31	0
55	MG	AA	4126	1/1	0.89	0.47	95,95,95,95	0
55	MG	AA	5186	1/1	0.89	0.63	69,69,69,69	0
55	MG	CA	4397	1/1	0.89	0.21	69,69,69,69	0
55	MG	CA	3370	1/1	0.89	0.25	52,52,52,52	0
55	MG	AA	5024	1/1	0.89	0.14	52,52,52,52	0
55	MG	CA	4022	1/1	0.89	0.28	55,55,55,55	0
55	MG	DA	1835	1/1	0.89	0.20	85,85,85,85	0
55	MG	CA	2980	1/1	0.89	0.17	67,67,67,67	0
55	MG	DA	2044	1/1	0.89	0.25	65,65,65,65	0
55	MG	DA	2082	1/1	0.89	0.13	81,81,81,81	0
55	MG	AA	5134	1/1	0.89	0.73	77,77,77,77	0
55	MG	BA	2065	1/1	0.89	0.14	39,39,39,39	0
55	MG	CA	3918	1/1	0.89	0.20	58,58,58,58	0
55	MG	AA	4343	1/1	0.89	0.27	43,43,43,43	0
55	MG	AA	5180	1/1	0.89	0.45	82,82,82,82	0
55	MG	CA	4020	1/1	0.89	0.50	21,21,21,21	0
55	MG	CA	3601	1/1	0.89	0.29	58,58,58,58	0
55	MG	DA	1848	1/1	0.89	0.26	67,67,67,67	0
55	MG	DA	2091	1/1	0.89	0.42	50,50,50,50	0
55	MG	CA	4044	1/1	0.89	0.34	25,25,25,25	0
55	MG	CA	3894	1/1	0.89	0.21	55,55,55,55	0
55	MG	CA	4202	1/1	0.89	0.24	61,61,61,61	0
55	MG	CA	3031	1/1	0.89	0.56	62,62,62,62	0
55	MG	BA	2161	1/1	0.89	0.27	69,69,69,69	0
55	MG	CA	3547	1/1	0.89	0.28	32,32,32,32	0
55	MG	DA	1828	1/1	0.89	0.41	100,100,100,100	0
55	MG	CA	3657	1/1	0.89	0.36	53,53,53,53	0
55	MG	CA	3046	1/1	0.89	0.88	80,80,80,80	0
55	MG	CA	3613	1/1	0.89	0.23	72,72,72,72	0
55	MG	CA	3348	1/1	0.89	0.47	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4167	1/1	0.89	0.17	45,45,45,45	0
55	MG	CB	239	1/1	0.89	0.22	43,43,43,43	0
55	MG	CA	3207	1/1	0.89	0.20	14,14,14,14	0
55	MG	DA	1978	1/1	0.89	0.41	51,51,51,51	0
55	MG	AA	4563	1/1	0.89	0.26	54,54,54,54	0
55	MG	AA	4273	1/1	0.89	0.43	43,43,43,43	0
55	MG	CA	3925	1/1	0.89	0.28	69,69,69,69	0
55	MG	AA	4465	1/1	0.89	0.40	57,57,57,57	0
55	MG	AB	244	1/1	0.89	0.28	100,100,100,100	0
55	MG	AA	4395	1/1	0.89	0.10	53,53,53,53	0
55	MG	DA	2035	1/1	0.89	0.72	59,59,59,59	0
55	MG	AA	4398	1/1	0.89	0.48	52,52,52,52	0
55	MG	DA	1876	1/1	0.89	0.34	56,56,56,56	0
55	MG	DA	1891	1/1	0.89	0.62	116,116,116,116	0
55	MG	AA	4663	1/1	0.89	0.31	49,49,49,49	0
55	MG	AA	4968	1/1	0.89	0.22	65,65,65,65	0
55	MG	BA	1683	1/1	0.89	0.34	29,29,29,29	0
55	MG	DA	1625	1/1	0.89	0.41	81,81,81,81	0
55	MG	CA	4013	1/1	0.89	0.22	46,46,46,46	0
55	MG	DA	1864	1/1	0.89	0.90	97,97,97,97	0
55	MG	CA	3402	1/1	0.89	0.19	63,63,63,63	0
55	MG	CB	232	1/1	0.89	0.15	54,54,54,54	0
55	MG	DA	1946	1/1	0.89	0.20	86,86,86,86	0
55	MG	CA	4031	1/1	0.89	0.10	40,40,40,40	0
55	MG	DA	1877	1/1	0.89	0.39	88,88,88,88	0
55	MG	DA	1777	1/1	0.89	0.28	124,124,124,124	0
55	MG	CE	302	1/1	0.89	0.62	31,31,31,31	0
55	MG	DA	1697	1/1	0.89	0.45	57,57,57,57	0
55	MG	CA	3406	1/1	0.89	0.30	49,49,49,49	0
55	MG	CA	4093	1/1	0.89	0.24	56,56,56,56	0
55	MG	CA	3298	1/1	0.89	0.45	56,56,56,56	0
55	MG	BA	1849	1/1	0.89	0.40	135,135,135,135	0
55	MG	AA	4917	1/1	0.89	0.19	41,41,41,41	0
55	MG	AA	4027	1/1	0.89	0.28	48,48,48,48	0
55	MG	CA	3223	1/1	0.89	0.42	51,51,51,51	0
55	MG	CA	3598	1/1	0.89	0.29	81,81,81,81	0
55	MG	CA	3492	1/1	0.89	0.57	124,124,124,124	0
55	MG	AA	4589	1/1	0.89	0.34	70,70,70,70	0
55	MG	CA	3633	1/1	0.89	0.54	63,63,63,63	0
55	MG	CA	4249	1/1	0.89	0.77	84,84,84,84	0
55	MG	AA	4076	1/1	0.89	0.56	90,90,90,90	0
55	MG	CA	3342	1/1	0.89	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1798	1/1	0.89	0.20	117,117,117,117	0
55	MG	AA	4707	1/1	0.89	0.41	73,73,73,73	0
55	MG	CA	4085	1/1	0.89	0.25	54,54,54,54	0
55	MG	CA	3014	1/1	0.89	0.37	68,68,68,68	0
55	MG	AA	4111	1/1	0.89	0.90	81,81,81,81	0
55	MG	CA	3850	1/1	0.89	0.25	89,89,89,89	0
55	MG	CO	201	1/1	0.89	0.18	43,43,43,43	0
55	MG	CA	4310	1/1	0.89	0.33	44,44,44,44	0
55	MG	CA	3431	1/1	0.89	0.19	40,40,40,40	0
55	MG	AA	4675	1/1	0.89	0.28	52,52,52,52	0
55	MG	CA	3036	1/1	0.89	0.66	77,77,77,77	0
55	MG	AA	4482	1/1	0.89	0.28	67,67,67,67	0
55	MG	CA	4107	1/1	0.89	0.19	52,52,52,52	0
55	MG	CB	264	1/1	0.89	0.18	62,62,62,62	0
55	MG	AA	4102	1/1	0.89	0.73	58,58,58,58	0
55	MG	DA	1608	1/1	0.89	0.19	71,71,71,71	0
55	MG	AF	305	1/1	0.89	0.27	45,45,45,45	0
55	MG	BA	2163	1/1	0.89	0.25	38,38,38,38	0
55	MG	CA	4084	1/1	0.89	0.22	67,67,67,67	0
55	MG	CA	3016	1/1	0.89	0.72	48,48,48,48	0
55	MG	DA	2114	1/1	0.89	0.29	74,74,74,74	0
55	MG	AA	5019	1/1	0.89	0.33	67,67,67,67	0
55	MG	BA	1629	1/1	0.89	0.09	55,55,55,55	0
55	MG	AA	4808	1/1	0.89	1.03	73,73,73,73	0
55	MG	AB	225	1/1	0.89	0.19	89,89,89,89	0
55	MG	BA	2023	1/1	0.89	0.23	45,45,45,45	0
55	MG	AA	4134	1/1	0.89	0.31	52,52,52,52	0
55	MG	AA	4709	1/1	0.89	0.22	67,67,67,67	0
55	MG	AA	4739	1/1	0.89	0.34	65,65,65,65	0
55	MG	BA	1855	1/1	0.89	0.21	75,75,75,75	0
55	MG	AA	4638	1/1	0.89	0.42	139,139,139,139	0
55	MG	AA	5187	1/1	0.89	0.17	69,69,69,69	0
55	MG	DA	1730	1/1	0.89	0.33	44,44,44,44	0
55	MG	CA	3057	1/1	0.89	0.23	51,51,51,51	0
55	MG	C5	102	1/1	0.89	0.35	55,55,55,55	0
55	MG	BA	2026	1/1	0.89	0.34	59,59,59,59	0
55	MG	CA	3095	1/1	0.89	0.12	82,82,82,82	0
55	MG	CA	3836	1/1	0.89	0.31	77,77,77,77	0
55	MG	AA	5085	1/1	0.89	0.30	77,77,77,77	0
55	MG	CA	4089	1/1	0.89	0.07	53,53,53,53	0
55	MG	DV	112	1/1	0.89	0.18	35,35,35,35	0
55	MG	DV	122	1/1	0.89	0.45	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	5157	1/1	0.89	0.30	58,58,58,58	0
55	MG	AA	4962	1/1	0.89	0.31	49,49,49,49	0
55	MG	CA	3638	1/1	0.89	0.49	44,44,44,44	0
55	MG	DA	1923	1/1	0.89	0.10	69,69,69,69	0
55	MG	DA	2078	1/1	0.89	0.29	63,63,63,63	0
55	MG	AA	5105	1/1	0.89	0.28	47,47,47,47	0
55	MG	CA	3409	1/1	0.89	0.15	38,38,38,38	0
55	MG	DA	1720	1/1	0.89	0.59	66,66,66,66	0
55	MG	BA	1712	1/1	0.89	0.16	41,41,41,41	0
55	MG	AA	4776	1/1	0.89	0.70	105,105,105,105	0
55	MG	BA	1701	1/1	0.89	0.28	36,36,36,36	0
55	MG	AA	4248	1/1	0.89	0.41	39,39,39,39	0
55	MG	AA	5158	1/1	0.89	0.30	50,50,50,50	0
55	MG	AA	5129	1/1	0.89	0.32	66,66,66,66	0
55	MG	BA	1654	1/1	0.89	0.09	89,89,89,89	0
55	MG	AA	5004	1/1	0.89	0.15	49,49,49,49	0
55	MG	CA	3567	1/1	0.89	0.45	71,71,71,71	0
55	MG	CA	4072	1/1	0.89	0.32	61,61,61,61	0
55	MG	CA	4098	1/1	0.89	0.43	76,76,76,76	0
55	MG	BG	202	1/1	0.89	0.19	61,61,61,61	0
55	MG	CA	3476	1/1	0.89	0.73	74,74,74,74	0
55	MG	AA	5127	1/1	0.89	0.08	83,83,83,83	0
55	MG	BA	1763	1/1	0.89	0.27	54,54,54,54	0
55	MG	CA	4302	1/1	0.89	0.40	26,26,26,26	0
55	MG	BA	1618	1/1	0.89	0.28	62,62,62,62	0
55	MG	CA	3553	1/1	0.89	0.62	48,48,48,48	0
55	MG	DA	1966	1/1	0.89	0.79	50,50,50,50	0
55	MG	DL	201	1/1	0.89	0.46	58,58,58,58	0
55	MG	BA	1783	1/1	0.89	0.52	82,82,82,82	0
55	MG	DA	1890	1/1	0.89	0.14	97,97,97,97	0
55	MG	DA	1906	1/1	0.89	0.10	79,79,79,79	0
55	MG	BT	201	1/1	0.89	0.92	67,67,67,67	0
55	MG	CA	3285	1/1	0.89	0.34	45,45,45,45	0
55	MG	DA	2079	1/1	0.89	0.28	57,57,57,57	0
55	MG	CA	3609	1/1	0.90	0.30	77,77,77,77	0
55	MG	CA	3367	1/1	0.90	0.78	50,50,50,50	0
55	MG	AA	5069	1/1	0.90	0.76	80,80,80,80	0
55	MG	CA	3430	1/1	0.90	0.35	52,52,52,52	0
55	MG	BA	1985	1/1	0.90	0.33	44,44,44,44	0
55	MG	CB	251	1/1	0.90	0.24	61,61,61,61	0
55	MG	AA	4463	1/1	0.90	0.31	35,35,35,35	0
55	MG	DA	1760	1/1	0.90	0.34	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4167	1/1	0.90	0.29	68,68,68,68	0
55	MG	CA	3464	1/1	0.90	0.20	64,64,64,64	0
55	MG	BA	1702	1/1	0.90	0.27	52,52,52,52	0
55	MG	CA	3696	1/1	0.90	0.19	47,47,47,47	0
55	MG	CA	3457	1/1	0.90	0.41	42,42,42,42	0
55	MG	DA	1655	1/1	0.90	0.77	85,85,85,85	0
55	MG	CA	3747	1/1	0.90	0.42	46,46,46,46	0
55	MG	CA	3153	1/1	0.90	0.55	27,27,27,27	0
55	MG	AM	203	1/1	0.90	0.19	55,55,55,55	0
55	MG	CA	3362	1/1	0.90	0.40	64,64,64,64	0
55	MG	CA	3296	1/1	0.90	0.20	41,41,41,41	0
55	MG	CA	3227	1/1	0.90	0.26	29,29,29,29	0
55	MG	AA	4433	1/1	0.90	0.09	63,63,63,63	0
55	MG	CA	3665	1/1	0.90	0.19	50,50,50,50	0
55	MG	BA	2092	1/1	0.90	0.54	52,52,52,52	0
55	MG	CA	4314	1/1	0.90	0.18	62,62,62,62	0
55	MG	DA	2128	1/1	0.90	0.19	40,40,40,40	0
55	MG	AA	4046	1/1	0.90	0.28	108,108,108,108	0
55	MG	AA	4571	1/1	0.90	0.35	48,48,48,48	0
55	MG	AA	4930	1/1	0.90	0.26	39,39,39,39	0
55	MG	CA	3781	1/1	0.90	0.53	53,53,53,53	0
55	MG	AA	4379	1/1	0.90	0.24	60,60,60,60	0
55	MG	BA	1907	1/1	0.90	0.41	58,58,58,58	0
55	MG	AA	5017	1/1	0.90	0.29	72,72,72,72	0
55	MG	DA	1727	1/1	0.90	0.26	33,33,33,33	0
55	MG	CA	4217	1/1	0.90	0.26	41,41,41,41	0
55	MG	AA	4830	1/1	0.90	0.23	65,65,65,65	0
55	MG	DA	2163	1/1	0.90	0.27	66,66,66,66	0
55	MG	DA	2008	1/1	0.90	0.36	70,70,70,70	0
55	MG	AA	5259	1/1	0.90	0.41	55,55,55,55	0
55	MG	DA	2071	1/1	0.90	0.26	58,58,58,58	0
55	MG	AA	4897	1/1	0.90	0.10	51,51,51,51	0
55	MG	CA	3703	1/1	0.90	0.20	57,57,57,57	0
55	MG	AA	5006	1/1	0.90	0.46	47,47,47,47	0
55	MG	AA	4991	1/1	0.90	0.26	52,52,52,52	0
55	MG	DA	2021	1/1	0.90	0.42	49,49,49,49	0
55	MG	DA	1740	1/1	0.90	0.40	46,46,46,46	0
55	MG	CA	3012	1/1	0.90	0.26	75,75,75,75	0
55	MG	AA	4655	1/1	0.90	0.71	60,60,60,60	0
55	MG	CA	3769	1/1	0.90	0.34	50,50,50,50	0
55	MG	AA	4184	1/1	0.90	0.50	19,19,19,19	0
55	MG	AA	4275	1/1	0.90	0.22	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1955	1/1	0.90	0.22	24,24,24,24	0
55	MG	AA	4668	1/1	0.90	0.31	74,74,74,74	0
55	MG	AA	4317	1/1	0.90	0.19	47,47,47,47	0
55	MG	AA	4364	1/1	0.90	0.65	77,77,77,77	0
55	MG	BA	1868	1/1	0.90	0.23	55,55,55,55	0
55	MG	AA	4728	1/1	0.90	0.33	60,60,60,60	0
55	MG	DA	1642	1/1	0.90	0.27	87,87,87,87	0
55	MG	AA	5093	1/1	0.90	0.23	48,48,48,48	0
55	MG	AA	4612	1/1	0.90	0.32	59,59,59,59	0
55	MG	DA	2093	1/1	0.90	0.19	89,89,89,89	0
55	MG	CF	306	1/1	0.90	0.29	26,26,26,26	0
55	MG	CA	3868	1/1	0.90	0.37	46,46,46,46	0
55	MG	AA	4198	1/1	0.90	0.28	46,46,46,46	0
55	MG	DA	1669	1/1	0.90	0.31	98,98,98,98	0
55	MG	CA	3832	1/1	0.90	0.88	52,52,52,52	0
55	MG	CA	3826	1/1	0.90	0.23	61,61,61,61	0
55	MG	CA	4051	1/1	0.90	0.19	54,54,54,54	0
55	MG	DA	2036	1/1	0.90	0.31	54,54,54,54	0
55	MG	CA	3736	1/1	0.90	1.00	99,99,99,99	0
55	MG	CA	3983	1/1	0.90	0.27	18,18,18,18	0
55	MG	DA	2002	1/1	0.90	0.13	59,59,59,59	0
55	MG	CA	4296	1/1	0.90	0.24	78,78,78,78	0
55	MG	AA	4914	1/1	0.90	0.32	43,43,43,43	0
55	MG	CA	3115	1/1	0.90	0.48	16,16,16,16	0
55	MG	AA	5144	1/1	0.90	0.40	59,59,59,59	0
55	MG	CA	3230	1/1	0.90	0.12	21,21,21,21	0
55	MG	BA	1764	1/1	0.90	0.25	51,51,51,51	0
55	MG	DA	1644	1/1	0.90	0.12	92,92,92,92	0
55	MG	AA	4834	1/1	0.90	0.22	50,50,50,50	0
55	MG	BA	1987	1/1	0.90	0.26	47,47,47,47	0
55	MG	BA	2084	1/1	0.90	0.41	71,71,71,71	0
55	MG	AA	4181	1/1	0.90	0.55	25,25,25,25	0
55	MG	CA	2951	1/1	0.90	0.36	125,125,125,125	0
55	MG	CA	3664	1/1	0.90	0.14	48,48,48,48	0
55	MG	CA	3191	1/1	0.90	0.10	36,36,36,36	0
55	MG	DA	1965	1/1	0.90	0.26	39,39,39,39	0
55	MG	AR	202	1/1	0.90	0.70	78,78,78,78	0
55	MG	BA	2154	1/1	0.90	0.32	39,39,39,39	0
55	MG	AA	4566	1/1	0.90	0.35	72,72,72,72	0
55	MG	CA	4092	1/1	0.90	0.37	53,53,53,53	0
55	MG	CA	4376	1/1	0.90	0.73	33,33,33,33	0
55	MG	BA	1749	1/1	0.90	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3646	1/1	0.90	0.24	73,73,73,73	0
55	MG	DA	1981	1/1	0.90	0.27	68,68,68,68	0
55	MG	AA	4428	1/1	0.90	0.16	36,36,36,36	0
55	MG	CA	3250	1/1	0.90	0.31	32,32,32,32	0
55	MG	CA	3254	1/1	0.90	0.39	46,46,46,46	0
55	MG	AA	4831	1/1	0.90	0.82	78,78,78,78	0
55	MG	CA	3812	1/1	0.90	0.27	78,78,78,78	0
55	MG	AA	4030	1/1	0.90	0.73	62,62,62,62	0
55	MG	A3	101	1/1	0.90	0.33	100,100,100,100	0
55	MG	AA	4839	1/1	0.90	0.21	98,98,98,98	0
55	MG	AA	5056	1/1	0.90	0.44	63,63,63,63	0
55	MG	AA	5066	1/1	0.90	0.21	37,37,37,37	0
55	MG	DA	1715	1/1	0.90	0.16	30,30,30,30	0
55	MG	BA	1809	1/1	0.90	0.24	62,62,62,62	0
55	MG	CE	305	1/1	0.90	1.18	44,44,44,44	0
55	MG	CA	4145	1/1	0.90	0.40	147,147,147,147	0
55	MG	DA	1698	1/1	0.90	0.46	35,35,35,35	0
55	MG	CA	4292	1/1	0.90	0.27	64,64,64,64	0
55	MG	DA	2001	1/1	0.90	0.17	70,70,70,70	0
55	MG	AA	4299	1/1	0.90	0.67	45,45,45,45	0
55	MG	CA	3582	1/1	0.90	0.29	49,49,49,49	0
55	MG	CB	249	1/1	0.90	0.26	50,50,50,50	0
55	MG	AA	5067	1/1	0.90	0.34	53,53,53,53	0
55	MG	BA	2036	1/1	0.90	0.19	74,74,74,74	0
55	MG	AA	4879	1/1	0.90	0.40	56,56,56,56	0
55	MG	BA	1865	1/1	0.90	0.21	86,86,86,86	0
55	MG	DA	1886	1/1	0.90	0.26	83,83,83,83	0
55	MG	BA	1697	1/1	0.90	0.29	40,40,40,40	0
55	MG	DA	1996	1/1	0.90	0.63	51,51,51,51	0
55	MG	AA	5222	1/1	0.90	0.12	84,84,84,84	0
55	MG	AA	4208	1/1	0.90	0.50	34,34,34,34	0
55	MG	DA	2107	1/1	0.90	0.23	49,49,49,49	0
55	MG	BA	1919	1/1	0.90	0.31	59,59,59,59	0
55	MG	BA	2159	1/1	0.90	0.20	63,63,63,63	0
55	MG	CA	3644	1/1	0.90	0.16	83,83,83,83	0
55	MG	AA	4351	1/1	0.90	0.46	63,63,63,63	0
55	MG	AA	4706	1/1	0.90	0.46	58,58,58,58	0
55	MG	CA	3251	1/1	0.90	0.26	27,27,27,27	0
55	MG	AB	213	1/1	0.90	0.44	76,76,76,76	0
55	MG	AA	4459	1/1	0.90	0.23	58,58,58,58	0
55	MG	CA	3908	1/1	0.90	0.32	55,55,55,55	0
55	MG	CA	4130	1/1	0.90	0.29	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3710	1/1	0.90	0.54	89,89,89,89	0
55	MG	CA	4184	1/1	0.90	0.24	56,56,56,56	0
55	MG	CA	3975	1/1	0.90	0.45	34,34,34,34	0
55	MG	AA	4291	1/1	0.90	0.55	46,46,46,46	0
55	MG	CJ	202	1/1	0.90	0.20	37,37,37,37	0
55	MG	CA	3694	1/1	0.90	0.18	76,76,76,76	0
55	MG	BA	1709	1/1	0.90	0.20	42,42,42,42	0
55	MG	AA	4557	1/1	0.90	0.37	70,70,70,70	0
55	MG	BA	1927	1/1	0.90	0.14	59,59,59,59	0
55	MG	CA	4066	1/1	0.90	0.60	54,54,54,54	0
55	MG	BE	203	1/1	0.90	0.59	91,91,91,91	0
55	MG	DA	1667	1/1	0.90	0.18	67,67,67,67	0
55	MG	AA	4242	1/1	0.90	0.44	32,32,32,32	0
55	MG	BW	101	1/1	0.90	0.23	106,106,106,106	0
55	MG	CA	3384	1/1	0.90	0.38	49,49,49,49	0
55	MG	BA	1959	1/1	0.90	0.26	49,49,49,49	0
55	MG	CA	3505	1/1	0.90	0.45	42,42,42,42	0
55	MG	AE	301	1/1	0.90	0.47	74,74,74,74	0
55	MG	AA	4787	1/1	0.90	0.26	77,77,77,77	0
55	MG	CA	3341	1/1	0.90	0.27	30,30,30,30	0
55	MG	CA	4251	1/1	0.90	0.31	56,56,56,56	0
55	MG	AA	5260	1/1	0.90	0.16	58,58,58,58	0
55	MG	DV	115	1/1	0.90	0.06	59,59,59,59	0
55	MG	AA	4008	1/1	0.90	0.30	79,79,79,79	0
55	MG	AA	4800	1/1	0.90	0.28	121,121,121,121	0
55	MG	AA	4256	1/1	0.90	0.17	59,59,59,59	0
55	MG	DA	2005	1/1	0.90	0.52	61,61,61,61	0
55	MG	CA	4125	1/1	0.90	0.36	76,76,76,76	0
55	MG	AA	4312	1/1	0.90	0.37	41,41,41,41	0
55	MG	AA	5104	1/1	0.90	0.29	54,54,54,54	0
55	MG	CA	3907	1/1	0.90	0.50	79,79,79,79	0
55	MG	AA	4920	1/1	0.90	0.15	75,75,75,75	0
55	MG	AB	230	1/1	0.90	0.16	74,74,74,74	0
55	MG	AA	4768	1/1	0.90	0.35	83,83,83,83	0
55	MG	AA	4938	1/1	0.90	0.31	45,45,45,45	0
55	MG	AA	4910	1/1	0.90	0.12	49,49,49,49	0
55	MG	AA	4233	1/1	0.90	0.39	29,29,29,29	0
55	MG	BA	1650	1/1	0.90	0.50	80,80,80,80	0
55	MG	CA	4033	1/1	0.90	0.41	45,45,45,45	0
55	MG	DA	1778	1/1	0.90	0.25	73,73,73,73	0
55	MG	CA	3154	1/1	0.90	0.31	29,29,29,29	0
55	MG	CA	3280	1/1	0.90	0.16	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4020	1/1	0.90	0.66	50,50,50,50	0
55	MG	AA	4091	1/1	0.90	0.14	41,41,41,41	0
55	MG	CA	3757	1/1	0.90	0.27	92,92,92,92	0
55	MG	AA	4399	1/1	0.90	0.23	35,35,35,35	0
55	MG	DA	2147	1/1	0.90	0.53	40,40,40,40	0
55	MG	CA	3573	1/1	0.90	0.76	51,51,51,51	0
55	MG	CA	3295	1/1	0.90	0.27	29,29,29,29	0
55	MG	AA	4583	1/1	0.90	0.25	68,68,68,68	0
55	MG	CA	3875	1/1	0.90	0.41	56,56,56,56	0
55	MG	AA	5217	1/1	0.91	0.47	66,66,66,66	0
55	MG	CA	3589	1/1	0.91	0.37	58,58,58,58	0
55	MG	AA	4820	1/1	0.91	0.25	44,44,44,44	0
55	MG	BA	1741	1/1	0.91	0.23	56,56,56,56	0
55	MG	CA	4260	1/1	0.91	0.34	46,46,46,46	0
55	MG	AA	4988	1/1	0.91	0.25	52,52,52,52	0
55	MG	CA	3098	1/1	0.91	0.41	98,98,98,98	0
55	MG	AA	5163	1/1	0.91	0.43	63,63,63,63	0
55	MG	BA	1811	1/1	0.91	0.17	68,68,68,68	0
55	MG	CA	3069	1/1	0.91	1.02	98,98,98,98	0
55	MG	CA	3867	1/1	0.91	0.20	53,53,53,53	0
55	MG	DA	1785	1/1	0.91	0.11	76,76,76,76	0
55	MG	AA	5218	1/1	0.91	0.29	51,51,51,51	0
55	MG	BA	1850	1/1	0.91	0.10	48,48,48,48	0
55	MG	AA	4489	1/1	0.91	0.14	94,94,94,94	0
55	MG	AA	4154	1/1	0.91	0.44	55,55,55,55	0
55	MG	CA	2932	1/1	0.91	0.22	58,58,58,58	0
55	MG	DA	1701	1/1	0.91	0.36	43,43,43,43	0
55	MG	CB	205	1/1	0.91	0.22	75,75,75,75	0
55	MG	BA	1668	1/1	0.91	0.35	57,57,57,57	0
55	MG	AA	4591	1/1	0.91	0.13	52,52,52,52	0
55	MG	AA	4671	1/1	0.91	0.19	122,122,122,122	0
55	MG	DA	2193	1/1	0.91	0.26	54,54,54,54	0
55	MG	BA	1778	1/1	0.91	0.27	64,64,64,64	0
55	MG	CA	3767	1/1	0.91	0.25	66,66,66,66	0
55	MG	CA	4056	1/1	0.91	0.18	61,61,61,61	0
55	MG	CA	3621	1/1	0.91	0.43	87,87,87,87	0
55	MG	CA	3354	1/1	0.91	1.08	52,52,52,52	0
55	MG	DA	1617	1/1	0.91	0.29	78,78,78,78	0
55	MG	CA	3778	1/1	0.91	0.30	106,106,106,106	0
55	MG	DA	2043	1/1	0.91	0.52	70,70,70,70	0
55	MG	CA	3345	1/1	0.91	0.49	48,48,48,48	0
55	MG	CA	4279	1/1	0.91	0.34	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	2115	1/1	0.91	1.32	92,92,92,92	0
55	MG	BA	1699	1/1	0.91	0.14	37,37,37,37	0
55	MG	BA	1729	1/1	0.91	0.33	53,53,53,53	0
55	MG	AA	4464	1/1	0.91	0.69	69,69,69,69	0
55	MG	DA	1634	1/1	0.91	0.75	79,79,79,79	0
55	MG	CA	3690	1/1	0.91	0.59	89,89,89,89	0
55	MG	AA	4599	1/1	0.91	0.28	61,61,61,61	0
55	MG	DA	1741	1/1	0.91	0.25	60,60,60,60	0
55	MG	CA	3600	1/1	0.91	0.85	54,54,54,54	0
55	MG	CA	4244	1/1	0.91	0.27	34,34,34,34	0
55	MG	AA	4231	1/1	0.91	0.38	48,48,48,48	0
55	MG	DA	1729	1/1	0.91	0.23	47,47,47,47	0
55	MG	AA	4334	1/1	0.91	0.33	53,53,53,53	0
55	MG	DA	2018	1/1	0.91	0.13	45,45,45,45	0
55	MG	CA	4288	1/1	0.91	0.59	53,53,53,53	0
55	MG	BA	1759	1/1	0.91	0.14	46,46,46,46	0
55	MG	AA	4598	1/1	0.91	0.28	104,104,104,104	0
55	MG	CB	210	1/1	0.91	0.24	81,81,81,81	0
55	MG	AA	4883	1/1	0.91	0.37	47,47,47,47	0
55	MG	DA	1782	1/1	0.91	0.25	54,54,54,54	0
55	MG	DA	1856	1/1	0.91	0.19	83,83,83,83	0
55	MG	CA	4040	1/1	0.91	0.34	36,36,36,36	0
55	MG	AA	4021	1/1	0.91	0.22	60,60,60,60	0
55	MG	DA	1881	1/1	0.91	0.40	92,92,92,92	0
55	MG	AA	4366	1/1	0.91	0.29	57,57,57,57	0
55	MG	CA	4159	1/1	0.91	0.19	36,36,36,36	0
55	MG	AA	4542	1/1	0.91	0.30	63,63,63,63	0
55	MG	CA	3784	1/1	0.91	0.21	82,82,82,82	0
55	MG	DA	1636	1/1	0.91	0.32	50,50,50,50	0
55	MG	CA	3924	1/1	0.91	0.29	44,44,44,44	0
55	MG	DA	2006	1/1	0.91	0.20	54,54,54,54	0
55	MG	CA	4152	1/1	0.91	0.21	77,77,77,77	0
55	MG	AA	5150	1/1	0.91	0.20	82,82,82,82	0
55	MG	DA	1802	1/1	0.91	0.41	77,77,77,77	0
55	MG	CA	4295	1/1	0.91	0.46	42,42,42,42	0
55	MG	BA	2122	1/1	0.91	0.49	44,44,44,44	0
55	MG	AA	4509	1/1	0.91	0.38	55,55,55,55	0
55	MG	CN	201	1/1	0.91	0.54	57,57,57,57	0
55	MG	AL	201	1/1	0.91	0.45	61,61,61,61	0
55	MG	AA	5272	1/1	0.91	0.34	58,58,58,58	0
55	MG	AB	234	1/1	0.91	0.10	44,44,44,44	0
55	MG	AA	4015	1/1	0.91	0.39	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4402	1/1	0.91	0.34	48,48,48,48	0
55	MG	CA	3509	1/1	0.91	0.35	49,49,49,49	0
55	MG	AA	5074	1/1	0.91	0.32	58,58,58,58	0
55	MG	BA	2037	1/1	0.91	0.32	55,55,55,55	0
55	MG	DA	1925	1/1	0.91	0.50	89,89,89,89	0
55	MG	AA	4898	1/1	0.91	0.24	67,67,67,67	0
55	MG	CA	3645	1/1	0.91	0.44	58,58,58,58	0
55	MG	AA	4704	1/1	0.91	0.55	78,78,78,78	0
55	MG	CA	4091	1/1	0.91	0.17	48,48,48,48	0
55	MG	BA	1747	1/1	0.91	0.12	56,56,56,56	0
55	MG	CA	3133	1/1	0.91	0.28	13,13,13,13	0
55	MG	AA	4520	1/1	0.91	0.19	67,67,67,67	0
55	MG	CA	3723	1/1	0.91	0.41	53,53,53,53	0
55	MG	AA	4778	1/1	0.91	0.25	69,69,69,69	0
55	MG	DA	2026	1/1	0.91	0.12	63,63,63,63	0
55	MG	AA	5022	1/1	0.91	0.47	55,55,55,55	0
55	MG	CA	4201	1/1	0.91	0.38	35,35,35,35	0
55	MG	CB	258	1/1	0.91	0.17	65,65,65,65	0
55	MG	CA	3660	1/1	0.91	0.15	60,60,60,60	0
55	MG	CA	3365	1/1	0.91	0.26	25,25,25,25	0
55	MG	CA	4014	1/1	0.91	0.16	37,37,37,37	0
55	MG	DA	1661	1/1	0.91	0.55	64,64,64,64	0
55	MG	AB	236	1/1	0.91	0.22	64,64,64,64	0
55	MG	BA	2067	1/1	0.91	0.13	66,66,66,66	0
55	MG	CA	3216	1/1	0.91	0.26	18,18,18,18	0
55	MG	BA	1754	1/1	0.91	0.22	68,68,68,68	0
55	MG	AA	4526	1/1	0.91	0.16	49,49,49,49	0
55	MG	CA	4108	1/1	0.91	1.00	57,57,57,57	0
55	MG	AA	5076	1/1	0.91	0.38	69,69,69,69	0
55	MG	CA	3274	1/1	0.91	0.47	40,40,40,40	0
55	MG	DA	1652	1/1	0.91	0.34	107,107,107,107	0
55	MG	DA	1853	1/1	0.91	0.10	87,87,87,87	0
55	MG	CY	101	1/1	0.91	0.40	58,58,58,58	0
55	MG	CQ	202	1/1	0.91	0.58	58,58,58,58	0
55	MG	CA	3077	1/1	0.91	0.36	91,91,91,91	0
55	MG	DA	2015	1/1	0.91	0.15	50,50,50,50	0
55	MG	CA	3940	1/1	0.91	0.79	44,44,44,44	0
55	MG	CA	2992	1/1	0.91	0.30	60,60,60,60	0
55	MG	CA	3896	1/1	0.91	0.45	120,120,120,120	0
55	MG	AA	4223	1/1	0.91	0.62	39,39,39,39	0
55	MG	BA	2167	1/1	0.91	0.12	52,52,52,52	0
55	MG	CA	4059	1/1	0.91	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1733	1/1	0.91	0.13	68,68,68,68	0
55	MG	AA	4722	1/1	0.91	0.26	56,56,56,56	0
55	MG	CA	4319	1/1	0.91	0.22	55,55,55,55	0
55	MG	CA	3681	1/1	0.91	0.19	58,58,58,58	0
55	MG	BE	201	1/1	0.91	0.41	86,86,86,86	0
55	MG	CB	234	1/1	0.91	0.34	74,74,74,74	0
55	MG	BA	1692	1/1	0.91	0.15	51,51,51,51	0
55	MG	BA	2020	1/1	0.91	0.21	61,61,61,61	0
55	MG	DW	118	1/1	0.91	0.40	157,157,157,157	0
55	MG	CA	2963	1/1	0.91	0.30	90,90,90,90	0
55	MG	CA	3101	1/1	0.91	0.60	21,21,21,21	0
55	MG	CA	3427	1/1	0.91	0.39	31,31,31,31	0
55	MG	AA	4801	1/1	0.91	0.12	61,61,61,61	0
55	MG	CA	3117	1/1	0.91	0.22	17,17,17,17	0
55	MG	CA	3006	1/1	0.91	0.64	50,50,50,50	0
55	MG	AA	4849	1/1	0.91	0.34	16,16,16,16	0
55	MG	AA	4049	1/1	0.91	0.13	60,60,60,60	0
55	MG	BA	1633	1/1	0.91	0.11	101,101,101,101	0
55	MG	CA	3268	1/1	0.91	0.52	35,35,35,35	0
55	MG	BA	1695	1/1	0.91	0.35	19,19,19,19	0
55	MG	AA	4079	1/1	0.91	0.35	76,76,76,76	0
55	MG	CA	2995	1/1	0.91	0.56	68,68,68,68	0
55	MG	BA	1693	1/1	0.91	0.18	43,43,43,43	0
55	MG	DA	1637	1/1	0.91	0.43	71,71,71,71	0
55	MG	CA	3966	1/1	0.91	0.54	49,49,49,49	0
55	MG	CA	3572	1/1	0.91	0.18	59,59,59,59	0
55	MG	AA	5156	1/1	0.91	0.08	52,52,52,52	0
55	MG	CE	301	1/1	0.91	0.38	47,47,47,47	0
55	MG	AA	4143	1/1	0.91	0.15	128,128,128,128	0
55	MG	AA	4368	1/1	0.91	0.20	38,38,38,38	0
55	MG	CA	4392	1/1	0.91	0.28	67,67,67,67	0
55	MG	AA	4281	1/1	0.91	0.38	44,44,44,44	0
55	MG	CA	4324	1/1	0.91	0.30	79,79,79,79	0
55	MG	AA	4287	1/1	0.91	0.40	40,40,40,40	0
55	MG	CA	3602	1/1	0.91	0.38	35,35,35,35	0
55	MG	AA	4682	1/1	0.91	0.30	71,71,71,71	0
55	MG	CA	3214	1/1	0.91	0.43	32,32,32,32	0
55	MG	AL	202	1/1	0.91	0.72	42,42,42,42	0
55	MG	CA	3953	1/1	0.91	0.32	36,36,36,36	0
55	MG	BA	1726	1/1	0.91	0.32	57,57,57,57	0
55	MG	DA	1674	1/1	0.91	0.22	85,85,85,85	0
55	MG	AA	4222	1/1	0.91	0.32	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	5210	1/1	0.91	0.48	83,83,83,83	0
55	MG	CA	3746	1/1	0.91	0.61	62,62,62,62	0
55	MG	DA	2094	1/1	0.91	0.55	44,44,44,44	0
55	MG	BA	1601	1/1	0.91	0.22	78,78,78,78	0
55	MG	BA	1797	1/1	0.91	0.21	53,53,53,53	0
55	MG	AA	4693	1/1	0.91	0.41	80,80,80,80	0
55	MG	BA	2162	1/1	0.91	0.07	38,38,38,38	0
55	MG	AA	5285	1/1	0.91	0.24	55,55,55,55	0
55	MG	CA	3363	1/1	0.91	0.36	22,22,22,22	0
55	MG	DA	1635	1/1	0.91	0.48	93,93,93,93	0
55	MG	CA	3113	1/1	0.91	0.22	9,9,9,9	0
55	MG	AA	4859	1/1	0.91	0.34	48,48,48,48	0
55	MG	CL	202	1/1	0.91	0.15	93,93,93,93	0
55	MG	CA	3712	1/1	0.91	0.21	32,32,32,32	0
55	MG	BA	1982	1/1	0.91	0.28	49,49,49,49	0
55	MG	AA	5213	1/1	0.91	0.32	60,60,60,60	0
55	MG	CA	3262	1/1	0.91	0.10	44,44,44,44	0
55	MG	AA	5036	1/1	0.91	0.29	45,45,45,45	0
55	MG	BA	2021	1/1	0.91	0.16	75,75,75,75	0
55	MG	DA	2040	1/1	0.91	0.67	53,53,53,53	0
55	MG	DA	1699	1/1	0.91	0.33	27,27,27,27	0
55	MG	AA	4504	1/1	0.91	0.36	67,67,67,67	0
55	MG	AA	4437	1/1	0.91	0.20	33,33,33,33	0
55	MG	DA	1756	1/1	0.91	0.09	106,106,106,106	0
55	MG	AA	4386	1/1	0.91	0.48	36,36,36,36	0
55	MG	BA	1606	1/1	0.91	0.46	82,82,82,82	0
55	MG	CA	3774	1/1	0.91	0.17	55,55,55,55	0
55	MG	BA	1869	1/1	0.91	0.23	66,66,66,66	0
55	MG	DA	2182	1/1	0.91	0.26	75,75,75,75	0
55	MG	CA	3390	1/1	0.91	0.26	37,37,37,37	0
55	MG	CA	4065	1/1	0.91	0.25	39,39,39,39	0
55	MG	AA	4940	1/1	0.91	0.94	48,48,48,48	0
55	MG	DA	1664	1/1	0.91	0.45	73,73,73,73	0
55	MG	AA	5030	1/1	0.91	0.18	45,45,45,45	0
55	MG	DA	1832	1/1	0.91	0.08	95,95,95,95	0
55	MG	DA	2190	1/1	0.91	0.24	59,59,59,59	0
55	MG	CA	4215	1/1	0.91	0.17	55,55,55,55	0
55	MG	AA	4586	1/1	0.91	0.12	84,84,84,84	0
55	MG	AA	4490	1/1	0.91	1.05	64,64,64,64	0
55	MG	CA	3238	1/1	0.91	0.40	29,29,29,29	0
55	MG	CA	3845	1/1	0.91	1.11	81,81,81,81	0
55	MG	BV	120	1/1	0.91	0.17	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3792	1/1	0.91	0.62	122,122,122,122	0
55	MG	CA	4317	1/1	0.91	0.41	70,70,70,70	0
55	MG	AA	4744	1/1	0.91	0.50	61,61,61,61	0
55	MG	AA	4321	1/1	0.91	0.50	53,53,53,53	0
55	MG	AA	4092	1/1	0.91	0.18	50,50,50,50	0
55	MG	CA	4002	1/1	0.91	0.21	34,34,34,34	0
55	MG	AA	4369	1/1	0.91	0.20	25,25,25,25	0
55	MG	CA	4219	1/1	0.91	0.81	78,78,78,78	0
55	MG	AA	4301	1/1	0.91	0.40	44,44,44,44	0
55	MG	AA	5241	1/1	0.91	0.30	91,91,91,91	0
55	MG	AA	4407	1/1	0.91	0.28	58,58,58,58	0
55	MG	CA	3143	1/1	0.91	0.47	24,24,24,24	0
55	MG	DA	2031	1/1	0.91	0.17	58,58,58,58	0
55	MG	AA	5197	1/1	0.91	0.22	73,73,73,73	0
55	MG	CA	3172	1/1	0.91	0.38	30,30,30,30	0
55	MG	CA	2988	1/1	0.91	0.26	87,87,87,87	0
55	MG	DW	121	1/1	0.91	0.25	62,62,62,62	0
55	MG	BA	1978	1/1	0.91	0.31	48,48,48,48	0
55	MG	CA	3810	1/1	0.91	0.34	43,43,43,43	0
55	MG	BW	107	1/1	0.91	0.08	78,78,78,78	0
55	MG	AA	5171	1/1	0.91	0.27	53,53,53,53	0
55	MG	CA	3671	1/1	0.91	0.33	87,87,87,87	0
55	MG	DA	1980	1/1	0.91	0.44	49,49,49,49	0
55	MG	DV	105	1/1	0.91	0.10	55,55,55,55	0
55	MG	CA	4164	1/1	0.91	0.27	44,44,44,44	0
55	MG	DA	1758	1/1	0.91	0.13	106,106,106,106	0
55	MG	DA	2048	1/1	0.91	0.38	52,52,52,52	0
55	MG	CA	3160	1/1	0.91	0.64	44,44,44,44	0
55	MG	CA	3872	1/1	0.91	0.66	55,55,55,55	0
55	MG	CA	3880	1/1	0.91	0.28	46,46,46,46	0
55	MG	CF	301	1/1	0.91	0.47	55,55,55,55	0
55	MG	CA	3140	1/1	0.91	0.25	8,8,8,8	0
55	MG	CA	3974	1/1	0.91	0.42	41,41,41,41	0
55	MG	CA	3575	1/1	0.91	0.22	36,36,36,36	0
55	MG	AA	4394	1/1	0.91	0.23	47,47,47,47	0
55	MG	AA	4984	1/1	0.91	0.28	39,39,39,39	0
55	MG	AA	5057	1/1	0.91	0.32	53,53,53,53	0
55	MG	AA	4385	1/1	0.91	0.23	54,54,54,54	0
55	MG	BA	1727	1/1	0.91	0.53	48,48,48,48	0
55	MG	DA	1707	1/1	0.91	0.26	41,41,41,41	0
55	MG	AA	4241	1/1	0.91	0.55	36,36,36,36	0
55	MG	AA	5175	1/1	0.91	0.54	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3094	1/1	0.92	0.35	41,41,41,41	0
55	MG	CA	4200	1/1	0.92	0.24	55,55,55,55	0
55	MG	CA	3538	1/1	0.92	0.35	50,50,50,50	0
55	MG	DA	1797	1/1	0.92	0.10	82,82,82,82	0
55	MG	CA	3134	1/1	0.92	0.26	14,14,14,14	0
55	MG	DA	1984	1/1	0.92	0.53	50,50,50,50	0
55	MG	AA	4176	1/1	0.92	0.59	21,21,21,21	0
55	MG	CA	3380	1/1	0.92	0.28	56,56,56,56	0
55	MG	CA	3377	1/1	0.92	0.09	44,44,44,44	0
55	MG	AA	4534	1/1	0.92	0.30	63,63,63,63	0
55	MG	BA	1996	1/1	0.92	0.11	61,61,61,61	0
55	MG	CA	3313	1/1	0.92	0.25	49,49,49,49	0
55	MG	CA	3403	1/1	0.92	0.45	45,45,45,45	0
55	MG	AA	4711	1/1	0.92	0.12	75,75,75,75	0
55	MG	DA	2025	1/1	0.92	0.12	40,40,40,40	0
55	MG	AA	4140	1/1	0.92	0.29	73,73,73,73	0
55	MG	BA	2041	1/1	0.92	0.08	66,66,66,66	0
55	MG	CD	304	1/1	0.92	0.25	55,55,55,55	0
55	MG	DA	1739	1/1	0.92	0.14	35,35,35,35	0
55	MG	DA	1861	1/1	0.92	0.26	95,95,95,95	0
55	MG	CA	3131	1/1	0.92	0.21	31,31,31,31	0
55	MG	CA	3969	1/1	0.92	0.58	31,31,31,31	0
55	MG	CA	3083	1/1	0.92	0.35	57,57,57,57	0
55	MG	DA	2053	1/1	0.92	0.20	92,92,92,92	0
55	MG	AB	248	1/1	0.92	0.26	50,50,50,50	0
55	MG	DA	2133	1/1	0.92	0.08	66,66,66,66	0
55	MG	CA	3585	1/1	0.92	0.33	43,43,43,43	0
55	MG	AA	4569	1/1	0.92	0.33	64,64,64,64	0
55	MG	AA	4641	1/1	0.92	0.31	66,66,66,66	0
55	MG	DA	1609	1/1	0.92	0.33	88,88,88,88	0
55	MG	AA	5283	1/1	0.92	0.92	87,87,87,87	0
55	MG	AA	4255	1/1	0.92	0.20	23,23,23,23	0
55	MG	BA	2050	1/1	0.92	0.22	62,62,62,62	0
55	MG	CA	3780	1/1	0.92	0.19	78,78,78,78	0
55	MG	AA	4339	1/1	0.92	0.21	33,33,33,33	0
55	MG	AA	4029	1/1	0.92	0.30	77,77,77,77	0
55	MG	AA	4148	1/1	0.92	0.30	71,71,71,71	0
55	MG	CA	3463	1/1	0.92	0.67	70,70,70,70	0
55	MG	CA	3991	1/1	0.92	0.14	21,21,21,21	0
55	MG	AA	4560	1/1	0.92	0.26	64,64,64,64	0
55	MG	AA	4712	1/1	0.92	1.18	69,69,69,69	0
55	MG	CA	3270	1/1	0.92	0.17	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3408	1/1	0.92	0.32	41,41,41,41	0
55	MG	AA	4043	1/1	0.92	0.27	52,52,52,52	0
55	MG	AA	4173	1/1	0.92	0.30	34,34,34,34	0
55	MG	CA	3025	1/1	0.92	0.22	46,46,46,46	0
55	MG	AA	4192	1/1	0.92	0.22	23,23,23,23	0
55	MG	CA	2957	1/1	0.92	0.22	73,73,73,73	0
55	MG	DA	1852	1/1	0.92	0.21	73,73,73,73	0
55	MG	CA	4315	1/1	0.92	0.19	58,58,58,58	0
55	MG	CA	3092	1/1	0.92	0.47	62,62,62,62	0
55	MG	BA	2108	1/1	0.92	0.34	56,56,56,56	0
55	MG	CA	4320	1/1	0.92	0.08	59,59,59,59	0
55	MG	CA	3733	1/1	0.92	0.97	156,156,156,156	0
55	MG	AA	4240	1/1	0.92	0.31	32,32,32,32	0
55	MG	AA	4789	1/1	0.92	0.17	81,81,81,81	0
55	MG	CA	3758	1/1	0.92	0.10	71,71,71,71	0
55	MG	AA	4439	1/1	0.92	1.02	66,66,66,66	0
55	MG	CA	3763	1/1	0.92	0.78	62,62,62,62	0
55	MG	BA	1944	1/1	0.92	0.25	77,77,77,77	0
55	MG	BA	1632	1/1	0.92	0.49	79,79,79,79	0
55	MG	AA	4005	1/1	0.92	0.61	64,64,64,64	0
55	MG	BA	1853	1/1	0.92	0.22	102,102,102,102	0
55	MG	CA	3618	1/1	0.92	0.24	56,56,56,56	0
55	MG	AA	4815	1/1	0.92	0.13	102,102,102,102	0
55	MG	AA	5176	1/1	0.92	0.42	61,61,61,61	0
55	MG	CA	3051	1/1	0.92	0.06	95,95,95,95	0
55	MG	AA	4156	1/1	0.92	0.50	72,72,72,72	0
55	MG	CA	3011	1/1	0.92	0.27	59,59,59,59	0
55	MG	AA	4578	1/1	0.92	0.14	60,60,60,60	0
55	MG	CA	3987	1/1	0.92	0.34	36,36,36,36	0
55	MG	CA	4169	1/1	0.92	0.36	46,46,46,46	0
55	MG	CA	2912	1/1	0.92	0.27	85,85,85,85	0
55	MG	BA	1636	1/1	0.92	0.20	56,56,56,56	0
55	MG	CA	4232	1/1	0.92	0.14	73,73,73,73	0
55	MG	DA	2022	1/1	0.92	0.23	39,39,39,39	0
55	MG	BW	112	1/1	0.92	0.24	97,97,97,97	0
55	MG	AA	5263	1/1	0.92	0.26	58,58,58,58	0
55	MG	BA	1751	1/1	0.92	0.48	91,91,91,91	0
55	MG	CA	3443	1/1	0.92	0.56	55,55,55,55	0
55	MG	CA	3236	1/1	0.92	0.43	31,31,31,31	0
55	MG	AJ	201	1/1	0.92	0.30	60,60,60,60	0
55	MG	CA	3711	1/1	0.92	0.31	67,67,67,67	0
55	MG	BA	2107	1/1	0.92	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4478	1/1	0.92	0.26	44,44,44,44	0
55	MG	DA	1624	1/1	0.92	0.29	127,127,127,127	0
55	MG	DA	1762	1/1	0.92	0.16	79,79,79,79	0
55	MG	CA	3047	1/1	0.92	0.68	48,48,48,48	0
55	MG	DA	1708	1/1	0.92	0.28	46,46,46,46	0
55	MG	BA	1844	1/1	0.92	0.64	74,74,74,74	0
55	MG	AA	4333	1/1	0.92	0.33	53,53,53,53	0
55	MG	DA	1969	1/1	0.92	0.36	46,46,46,46	0
55	MG	DA	2084	1/1	0.92	0.47	67,67,67,67	0
55	MG	CB	214	1/1	0.92	0.12	74,74,74,74	0
55	MG	CA	4281	1/1	0.92	0.30	68,68,68,68	0
55	MG	BA	1734	1/1	0.92	0.20	56,56,56,56	0
55	MG	DA	1825	1/1	0.92	0.23	66,66,66,66	0
55	MG	CA	4305	1/1	0.92	0.53	46,46,46,46	0
55	MG	CA	3292	1/1	0.92	0.26	35,35,35,35	0
55	MG	CA	3323	1/1	0.92	0.52	43,43,43,43	0
55	MG	CA	3263	1/1	0.92	0.19	36,36,36,36	0
55	MG	AA	5034	1/1	0.92	0.72	48,48,48,48	0
55	MG	AA	4060	1/1	0.92	0.42	84,84,84,84	0
55	MG	AA	5252	1/1	0.92	0.30	70,70,70,70	0
55	MG	AA	4206	1/1	0.92	0.18	19,19,19,19	0
55	MG	AA	4253	1/1	0.92	0.99	28,28,28,28	0
55	MG	AA	4388	1/1	0.92	0.15	66,66,66,66	0
55	MG	AA	4210	1/1	0.92	0.23	37,37,37,37	0
55	MG	AA	4996	1/1	0.92	0.31	65,65,65,65	0
55	MG	CA	3344	1/1	0.92	0.51	46,46,46,46	0
55	MG	DA	2142	1/1	0.92	0.34	45,45,45,45	0
55	MG	AA	4186	1/1	0.92	0.24	10,10,10,10	0
55	MG	CB	202	1/1	0.92	0.30	78,78,78,78	0
55	MG	AA	4066	1/1	0.92	0.47	65,65,65,65	0
55	MG	CA	3674	1/1	0.92	0.28	48,48,48,48	0
55	MG	DA	1836	1/1	0.92	0.47	80,80,80,80	0
55	MG	BA	1860	1/1	0.92	0.28	73,73,73,73	0
55	MG	CA	4342	1/1	0.92	0.54	60,60,60,60	0
55	MG	DA	1882	1/1	0.92	0.53	77,77,77,77	0
55	MG	BA	1740	1/1	0.92	0.20	51,51,51,51	0
55	MG	BA	1711	1/1	0.92	0.25	57,57,57,57	0
55	MG	CA	3762	1/1	0.92	0.27	78,78,78,78	0
55	MG	BA	1796	1/1	0.92	0.31	56,56,56,56	0
55	MG	AA	4207	1/1	0.92	0.16	25,25,25,25	0
55	MG	CA	3328	1/1	0.92	0.61	49,49,49,49	0
55	MG	AA	4327	1/1	0.92	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4012	1/1	0.92	0.19	40,40,40,40	0
55	MG	BA	2085	1/1	0.92	0.17	55,55,55,55	0
55	MG	CA	3315	1/1	0.92	0.62	29,29,29,29	0
55	MG	AA	4725	1/1	0.92	0.42	78,78,78,78	0
55	MG	BA	1735	1/1	0.92	0.07	47,47,47,47	0
55	MG	CA	2945	1/1	0.92	1.06	99,99,99,99	0
55	MG	CA	3312	1/1	0.92	0.44	38,38,38,38	0
55	MG	AA	4735	1/1	0.92	0.17	43,43,43,43	0
55	MG	CA	3373	1/1	0.92	0.13	53,53,53,53	0
55	MG	AA	4729	1/1	0.92	0.18	85,85,85,85	0
55	MG	BA	1806	1/1	0.92	0.17	56,56,56,56	0
55	MG	CA	3728	1/1	0.92	0.32	77,77,77,77	0
55	MG	AA	5084	1/1	0.92	0.13	57,57,57,57	0
55	MG	AA	5208	1/1	0.92	0.36	45,45,45,45	0
55	MG	AY	101	1/1	0.92	0.51	72,72,72,72	0
55	MG	AA	5015	1/1	0.92	0.19	46,46,46,46	0
55	MG	DA	1839	1/1	0.92	0.19	88,88,88,88	0
55	MG	CA	4370	1/1	0.92	0.26	61,61,61,61	0
55	MG	CA	4134	1/1	0.92	0.13	49,49,49,49	0
55	MG	CA	4011	1/1	0.92	0.14	30,30,30,30	0
55	MG	BA	1958	1/1	0.92	0.25	45,45,45,45	0
55	MG	CA	4007	1/1	0.92	0.17	29,29,29,29	0
55	MG	CA	3364	1/1	0.92	0.18	20,20,20,20	0
55	MG	AA	4387	1/1	0.92	0.41	35,35,35,35	0
55	MG	DA	1867	1/1	0.92	0.17	63,63,63,63	0
55	MG	AA	4836	1/1	0.92	0.36	52,52,52,52	0
55	MG	CA	3717	1/1	0.92	0.47	71,71,71,71	0
55	MG	AA	4673	1/1	0.92	0.26	49,49,49,49	0
55	MG	CA	3931	1/1	0.92	0.37	75,75,75,75	0
55	MG	CA	3196	1/1	0.92	0.21	23,23,23,23	0
55	MG	DA	1885	1/1	0.92	0.10	71,71,71,71	0
55	MG	AA	4427	1/1	0.92	0.11	68,68,68,68	0
55	MG	BE	205	1/1	0.92	0.48	56,56,56,56	0
55	MG	CF	302	1/1	0.92	0.20	43,43,43,43	0
55	MG	CA	3619	1/1	0.92	0.33	56,56,56,56	0
55	MG	CA	4118	1/1	0.92	0.58	58,58,58,58	0
55	MG	BA	1926	1/1	0.92	0.13	82,82,82,82	0
55	MG	BA	1670	1/1	0.92	0.10	78,78,78,78	0
55	MG	BA	1686	1/1	0.92	0.17	40,40,40,40	0
55	MG	CA	4009	1/1	0.92	0.25	34,34,34,34	0
55	MG	AA	5125	1/1	0.92	0.29	45,45,45,45	0
55	MG	CA	3811	1/1	0.92	0.28	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AB	240	1/1	0.92	0.11	65,65,65,65	0
55	MG	AA	4122	1/1	0.92	0.31	65,65,65,65	0
55	MG	CB	243	1/1	0.92	0.40	34,34,34,34	0
55	MG	BA	2091	1/1	0.92	0.18	70,70,70,70	0
55	MG	CA	4227	1/1	0.92	0.21	53,53,53,53	0
55	MG	CA	3199	1/1	0.92	0.31	41,41,41,41	0
55	MG	DA	1962	1/1	0.92	0.43	39,39,39,39	0
55	MG	AA	4070	1/1	0.92	0.37	60,60,60,60	0
55	MG	CA	3715	1/1	0.92	0.19	59,59,59,59	0
55	MG	CA	3571	1/1	0.92	0.90	88,88,88,88	0
55	MG	AA	4228	1/1	0.92	0.24	23,23,23,23	0
55	MG	BA	1825	1/1	0.92	0.15	62,62,62,62	0
55	MG	BA	1771	1/1	0.92	0.12	29,29,29,29	0
55	MG	BA	2027	1/1	0.92	0.32	63,63,63,63	0
55	MG	DA	1737	1/1	0.92	0.31	51,51,51,51	0
55	MG	CA	3971	1/1	0.92	0.36	36,36,36,36	0
55	MG	AA	4493	1/1	0.92	0.15	53,53,53,53	0
55	MG	CB	215	1/1	0.92	0.26	28,28,28,28	0
55	MG	DA	1614	1/1	0.92	0.31	91,91,91,91	0
55	MG	BG	201	1/1	0.92	0.30	46,46,46,46	0
55	MG	CA	2961	1/1	0.92	0.29	78,78,78,78	0
55	MG	BA	1981	1/1	0.92	0.11	74,74,74,74	0
55	MG	AA	4058	1/1	0.92	0.20	76,76,76,76	0
55	MG	DA	1810	1/1	0.92	0.09	67,67,67,67	0
55	MG	AA	4188	1/1	0.92	0.31	44,44,44,44	0
55	MG	AA	4163	1/1	0.92	0.43	72,72,72,72	0
55	MG	CA	3357	1/1	0.92	0.47	25,25,25,25	0
55	MG	CA	2931	1/1	0.92	0.26	105,105,105,105	0
55	MG	CA	3233	1/1	0.92	0.37	33,33,33,33	0
55	MG	AA	4685	1/1	0.92	0.24	63,63,63,63	0
55	MG	CA	3823	1/1	0.92	0.25	81,81,81,81	0
55	MG	AA	4341	1/1	0.92	0.21	38,38,38,38	0
55	MG	CA	4047	1/1	0.92	0.31	38,38,38,38	0
55	MG	AA	4141	1/1	0.92	0.41	65,65,65,65	0
55	MG	AB	242	1/1	0.92	0.20	62,62,62,62	0
55	MG	DA	2110	1/1	0.92	0.19	84,84,84,84	0
55	MG	BA	1912	1/1	0.92	0.30	57,57,57,57	0
55	MG	DA	2197	1/1	0.92	0.47	50,50,50,50	0
55	MG	CS	202	1/1	0.92	0.23	28,28,28,28	0
55	MG	CA	3038	1/1	0.92	0.54	52,52,52,52	0
55	MG	AA	4501	1/1	0.92	0.27	73,73,73,73	0
55	MG	CA	3109	1/1	0.92	0.51	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3193	1/1	0.92	0.60	38,38,38,38	0
55	MG	CA	3325	1/1	0.92	0.55	54,54,54,54	0
55	MG	CA	3150	1/1	0.92	0.46	23,23,23,23	0
55	MG	AA	5170	1/1	0.92	0.42	71,71,71,71	0
55	MG	CA	4018	1/1	0.92	0.69	56,56,56,56	0
55	MG	AA	4048	1/1	0.92	0.18	62,62,62,62	0
55	MG	CA	3829	1/1	0.92	0.42	68,68,68,68	0
55	MG	DA	1894	1/1	0.92	0.32	67,67,67,67	0
55	MG	CA	2906	1/1	0.92	0.43	66,66,66,66	0
55	MG	CA	2933	1/1	0.92	0.28	50,50,50,50	0
55	MG	BA	1635	1/1	0.92	0.41	63,63,63,63	0
55	MG	A4	104	1/1	0.92	0.28	99,99,99,99	0
55	MG	CA	3049	1/1	0.92	0.46	62,62,62,62	0
55	MG	CA	3290	1/1	0.92	0.42	28,28,28,28	0
55	MG	CA	3526	1/1	0.92	0.22	64,64,64,64	0
55	MG	BA	1891	1/1	0.92	0.36	56,56,56,56	0
55	MG	AF	302	1/1	0.92	0.22	49,49,49,49	0
55	MG	DA	2013	1/1	0.92	0.19	49,49,49,49	0
55	MG	CA	3260	1/1	0.92	0.23	25,25,25,25	0
55	MG	AA	4533	1/1	0.92	0.71	64,64,64,64	0
55	MG	CA	3284	1/1	0.92	0.22	42,42,42,42	0
55	MG	CA	3680	1/1	0.92	0.21	54,54,54,54	0
55	MG	AA	5234	1/1	0.92	0.31	61,61,61,61	0
55	MG	CA	3314	1/1	0.92	0.20	26,26,26,26	0
55	MG	DA	2149	1/1	0.92	0.37	74,74,74,74	0
55	MG	DV	104	1/1	0.92	0.33	92,92,92,92	0
55	MG	AA	4793	1/1	0.92	0.78	62,62,62,62	0
55	MG	DA	1975	1/1	0.92	0.15	43,43,43,43	0
55	MG	BA	1957	1/1	0.93	0.14	33,33,33,33	0
55	MG	CA	3822	1/1	0.93	0.49	57,57,57,57	0
55	MG	CA	3483	1/1	0.93	0.24	52,52,52,52	0
55	MG	CA	2956	1/1	0.93	1.05	59,59,59,59	0
55	MG	CA	3993	1/1	0.93	0.36	37,37,37,37	0
55	MG	CA	3141	1/1	0.93	0.16	9,9,9,9	0
55	MG	AB	209	1/1	0.93	0.35	30,30,30,30	0
55	MG	BA	1738	1/1	0.93	0.15	25,25,25,25	0
55	MG	AA	4683	1/1	0.93	0.16	53,53,53,53	0
55	MG	AA	5193	1/1	0.93	0.71	66,66,66,66	0
55	MG	CA	3765	1/1	0.93	0.24	77,77,77,77	0
55	MG	AA	4191	1/1	0.93	0.53	14,14,14,14	0
55	MG	AA	4237	1/1	0.93	0.32	17,17,17,17	0
55	MG	CA	2949	1/1	0.93	0.15	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3874	1/1	0.93	0.39	60,60,60,60	0
55	MG	DA	1974	1/1	0.93	0.20	62,62,62,62	0
55	MG	DA	1702	1/1	0.93	0.30	26,26,26,26	0
55	MG	DA	1808	1/1	0.93	0.29	61,61,61,61	0
55	MG	CA	4170	1/1	0.93	0.44	53,53,53,53	0
55	MG	AA	4950	1/1	0.93	0.17	51,51,51,51	0
55	MG	DA	1842	1/1	0.93	0.22	70,70,70,70	0
55	MG	DA	2175	1/1	0.93	0.23	35,35,35,35	0
55	MG	DA	1601	1/1	0.93	0.19	92,92,92,92	0
55	MG	CA	3847	1/1	0.93	0.36	71,71,71,71	0
55	MG	DA	1780	1/1	0.93	0.95	83,83,83,83	0
55	MG	AD	303	1/1	0.93	0.67	38,38,38,38	0
55	MG	AA	5107	1/1	0.93	0.25	38,38,38,38	0
55	MG	CA	4313	1/1	0.93	0.12	41,41,41,41	0
55	MG	BA	1725	1/1	0.93	0.12	27,27,27,27	0
55	MG	DA	2173	1/1	0.93	0.24	72,72,72,72	0
55	MG	AA	4010	1/1	0.93	0.57	64,64,64,64	0
55	MG	AP	201	1/1	0.93	0.22	55,55,55,55	0
55	MG	CA	3007	1/1	0.93	0.51	69,69,69,69	0
55	MG	AA	4296	1/1	0.93	0.16	25,25,25,25	0
55	MG	AA	4414	1/1	0.93	0.17	35,35,35,35	0
55	MG	BA	1622	1/1	0.93	0.45	122,122,122,122	0
55	MG	CA	3533	1/1	0.93	0.26	52,52,52,52	0
55	MG	BA	1804	1/1	0.93	0.57	39,39,39,39	0
55	MG	CA	3307	1/1	0.93	0.22	46,46,46,46	0
55	MG	AA	4356	1/1	0.93	0.38	33,33,33,33	0
55	MG	CA	3487	1/1	0.93	0.20	50,50,50,50	0
55	MG	CB	224	1/1	0.93	0.11	88,88,88,88	0
55	MG	CA	3484	1/1	0.93	0.36	49,49,49,49	0
55	MG	CA	3319	1/1	0.93	0.26	25,25,25,25	0
55	MG	CR	201	1/1	0.93	0.14	17,17,17,17	0
55	MG	DA	1770	1/1	0.93	0.54	46,46,46,46	0
55	MG	AB	235	1/1	0.93	0.36	53,53,53,53	0
55	MG	CA	4104	1/1	0.93	0.15	42,42,42,42	0
55	MG	BL	202	1/1	0.93	0.44	47,47,47,47	0
55	MG	BA	1884	1/1	0.93	0.18	76,76,76,76	0
55	MG	AA	5126	1/1	0.93	0.47	58,58,58,58	0
55	MG	AA	5262	1/1	0.93	0.48	64,64,64,64	0
55	MG	CA	4124	1/1	0.93	0.21	48,48,48,48	0
55	MG	CA	3852	1/1	0.93	0.16	30,30,30,30	0
55	MG	CA	4038	1/1	0.93	0.54	45,45,45,45	0
55	MG	AA	4538	1/1	0.93	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4733	1/1	0.93	0.12	20,20,20,20	0
55	MG	CA	3308	1/1	0.93	0.33	25,25,25,25	0
55	MG	DA	1930	1/1	0.93	0.11	95,95,95,95	0
55	MG	CA	3897	1/1	0.93	0.27	86,86,86,86	0
55	MG	CA	3206	1/1	0.93	0.34	24,24,24,24	0
55	MG	CA	3531	1/1	0.93	0.09	52,52,52,52	0
55	MG	DA	1820	1/1	0.93	0.59	102,102,102,102	0
55	MG	CA	3272	1/1	0.93	0.70	36,36,36,36	0
55	MG	BW	102	1/1	0.93	0.36	57,57,57,57	0
55	MG	BA	2031	1/1	0.93	0.18	55,55,55,55	0
55	MG	BA	2136	1/1	0.93	0.20	62,62,62,62	0
55	MG	DA	1722	1/1	0.93	0.10	73,73,73,73	0
55	MG	CA	3397	1/1	0.93	0.15	37,37,37,37	0
55	MG	CA	3643	1/1	0.93	0.27	48,48,48,48	0
55	MG	AA	4736	1/1	0.93	0.20	50,50,50,50	0
55	MG	AA	4580	1/1	0.93	0.45	90,90,90,90	0
55	MG	BA	2111	1/1	0.93	0.20	96,96,96,96	0
55	MG	DA	1817	1/1	0.93	0.13	34,34,34,34	0
55	MG	AA	4103	1/1	0.93	0.79	71,71,71,71	0
55	MG	AA	5280	1/1	0.93	0.17	85,85,85,85	0
55	MG	DA	1736	1/1	0.93	0.25	60,60,60,60	0
55	MG	BV	127	1/1	0.93	0.19	53,53,53,53	0
55	MG	CA	4399	1/1	0.93	0.30	70,70,70,70	0
55	MG	CA	3320	1/1	0.93	0.36	42,42,42,42	0
55	MG	DA	1640	1/1	0.93	0.34	91,91,91,91	0
55	MG	AA	4705	1/1	0.93	0.34	109,109,109,109	0
55	MG	CA	3282	1/1	0.93	0.19	25,25,25,25	0
55	MG	CA	3761	1/1	0.93	0.16	57,57,57,57	0
55	MG	CA	3112	1/1	0.93	0.45	14,14,14,14	0
55	MG	BA	1812	1/1	0.93	1.03	78,78,78,78	0
55	MG	CA	3534	1/1	0.93	0.39	47,47,47,47	0
55	MG	AA	4345	1/1	0.93	0.16	59,59,59,59	0
55	MG	CA	3629	1/1	0.93	0.38	106,106,106,106	0
55	MG	AA	4300	1/1	0.93	0.32	25,25,25,25	0
55	MG	AA	4247	1/1	0.93	0.44	33,33,33,33	0
55	MG	AS	203	1/1	0.93	0.73	75,75,75,75	0
55	MG	AX	102	1/1	0.93	0.23	25,25,25,25	0
55	MG	CA	4178	1/1	0.93	0.22	50,50,50,50	0
55	MG	AA	4785	1/1	0.93	0.20	68,68,68,68	0
55	MG	BC	303	1/1	0.93	0.26	49,49,49,49	0
55	MG	DA	1791	1/1	0.93	0.16	65,65,65,65	0
55	MG	CA	3506	1/1	0.93	0.30	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3249	1/1	0.93	0.21	40,40,40,40	0
55	MG	CA	4071	1/1	0.93	0.20	43,43,43,43	0
55	MG	AA	4306	1/1	0.93	0.30	42,42,42,42	0
55	MG	AB	222	1/1	0.93	0.22	62,62,62,62	0
55	MG	CA	3475	1/1	0.93	0.26	42,42,42,42	0
55	MG	CB	225	1/1	0.93	0.20	51,51,51,51	0
55	MG	BA	1758	1/1	0.93	0.17	49,49,49,49	0
55	MG	CA	3469	1/1	0.93	0.20	50,50,50,50	0
55	MG	AA	4252	1/1	0.93	0.16	37,37,37,37	0
55	MG	AA	4679	1/1	0.93	0.33	40,40,40,40	0
55	MG	DA	1653	1/1	0.93	0.13	47,47,47,47	0
55	MG	C4	101	1/1	0.93	1.17	63,63,63,63	0
55	MG	AA	4245	1/1	0.93	0.28	26,26,26,26	0
55	MG	AA	5079	1/1	0.93	0.36	53,53,53,53	0
55	MG	CA	3222	1/1	0.93	0.33	38,38,38,38	0
55	MG	AA	4946	1/1	0.93	0.26	49,49,49,49	0
55	MG	BA	1662	1/1	0.93	0.16	89,89,89,89	0
55	MG	AA	4440	1/1	0.93	0.07	60,60,60,60	0
55	MG	C5	103	1/1	0.93	0.15	44,44,44,44	0
55	MG	CA	3448	1/1	0.93	0.31	40,40,40,40	0
55	MG	CA	3329	1/1	0.93	0.20	21,21,21,21	0
55	MG	BA	1822	1/1	0.93	0.14	61,61,61,61	0
55	MG	AA	4936	1/1	0.93	0.12	46,46,46,46	0
55	MG	DA	1961	1/1	0.93	0.34	43,43,43,43	0
55	MG	AA	4346	1/1	0.93	0.52	49,49,49,49	0
55	MG	CA	3289	1/1	0.93	0.20	20,20,20,20	0
55	MG	AA	5278	1/1	0.93	0.33	56,56,56,56	0
55	MG	AA	5077	1/1	0.93	0.80	57,57,57,57	0
55	MG	CA	3104	1/1	0.93	0.60	19,19,19,19	0
55	MG	CD	301	1/1	0.93	0.22	61,61,61,61	0
55	MG	BP	101	1/1	0.93	0.23	88,88,88,88	0
55	MG	DA	1972	1/1	0.93	0.12	48,48,48,48	0
55	MG	CA	3973	1/1	0.93	0.18	23,23,23,23	0
55	MG	DA	1759	1/1	0.93	0.32	71,71,71,71	0
55	MG	CA	4277	1/1	0.93	0.23	72,72,72,72	0
55	MG	CA	3564	1/1	0.93	0.42	70,70,70,70	0
55	MG	CA	3303	1/1	0.93	0.46	28,28,28,28	0
55	MG	AA	4579	1/1	0.93	0.79	45,45,45,45	0
55	MG	CA	3224	1/1	0.93	0.14	36,36,36,36	0
55	MG	AA	4348	1/1	0.93	0.38	36,36,36,36	0
55	MG	CA	4311	1/1	0.93	0.27	65,65,65,65	0
55	MG	AA	4042	1/1	0.93	0.53	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4811	1/1	0.93	0.23	60,60,60,60	0
55	MG	AA	4277	1/1	0.93	0.19	41,41,41,41	0
55	MG	DA	1670	1/1	0.93	0.16	136,136,136,136	0
55	MG	BA	1910	1/1	0.93	0.30	51,51,51,51	0
55	MG	DA	1665	1/1	0.93	0.42	61,61,61,61	0
55	MG	DA	1880	1/1	0.93	0.51	104,104,104,104	0
55	MG	CA	3203	1/1	0.93	0.37	35,35,35,35	0
55	MG	AA	4271	1/1	0.93	0.31	28,28,28,28	0
55	MG	CA	3330	1/1	0.93	0.69	69,69,69,69	0
55	MG	DA	1960	1/1	0.93	0.16	20,20,20,20	0
55	MG	BA	1755	1/1	0.93	0.23	40,40,40,40	0
55	MG	DA	2057	1/1	0.93	0.13	49,49,49,49	0
55	MG	BA	1880	1/1	0.93	0.41	135,135,135,135	0
55	MG	AA	4104	1/1	0.93	0.30	91,91,91,91	0
55	MG	AA	4418	1/1	0.93	0.27	53,53,53,53	0
55	MG	DW	101	1/1	0.93	0.13	70,70,70,70	0
55	MG	CA	3221	1/1	0.93	0.42	37,37,37,37	0
55	MG	BA	2072	1/1	0.93	0.72	64,64,64,64	0
55	MG	CA	3294	1/1	0.93	0.13	31,31,31,31	0
55	MG	CA	3511	1/1	0.93	0.40	46,46,46,46	0
55	MG	DA	1936	1/1	0.93	0.15	60,60,60,60	0
55	MG	AA	4698	1/1	0.93	0.23	68,68,68,68	0
55	MG	AA	4132	1/1	0.93	0.18	63,63,63,63	0
55	MG	DW	110	1/1	0.93	0.06	58,58,58,58	0
55	MG	AA	4472	1/1	0.93	0.20	57,57,57,57	0
55	MG	BV	117	1/1	0.93	0.23	43,43,43,43	0
55	MG	CA	3175	1/1	0.93	0.25	28,28,28,28	0
55	MG	DA	1897	1/1	0.93	0.21	79,79,79,79	0
55	MG	CA	3257	1/1	0.93	0.26	32,32,32,32	0
55	MG	CA	3279	1/1	0.93	0.23	36,36,36,36	0
55	MG	AA	4792	1/1	0.93	0.18	74,74,74,74	0
55	MG	BA	1829	1/1	0.93	0.25	87,87,87,87	0
55	MG	AA	4349	1/1	0.93	0.47	56,56,56,56	0
55	MG	CA	3831	1/1	0.93	0.24	90,90,90,90	0
55	MG	DW	116	1/1	0.93	0.19	129,129,129,129	0
55	MG	CA	4267	1/1	0.93	0.42	56,56,56,56	0
55	MG	CA	3478	1/1	0.93	0.34	48,48,48,48	0
55	MG	CA	4143	1/1	0.93	0.20	57,57,57,57	0
55	MG	DA	2178	1/1	0.93	0.10	69,69,69,69	0
55	MG	CA	3909	1/1	0.93	0.46	62,62,62,62	0
55	MG	CA	4095	1/1	0.93	0.74	51,51,51,51	0
55	MG	CA	4268	1/1	0.93	0.72	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4053	1/1	0.93	0.54	45,45,45,45	0
55	MG	AA	4639	1/1	0.93	0.39	56,56,56,56	0
54	BLS	AA	4001	30/30	0.93	0.42	56,56,56,56	0
55	MG	BV	110	1/1	0.93	0.12	71,71,71,71	0
55	MG	AA	4260	1/1	0.93	0.49	35,35,35,35	0
55	MG	BA	2147	1/1	0.93	0.20	121,121,121,121	0
55	MG	AA	4559	1/1	0.93	0.15	87,87,87,87	0
55	MG	BA	1715	1/1	0.93	0.20	63,63,63,63	0
55	MG	AA	4547	1/1	0.93	0.30	83,83,83,83	0
55	MG	BV	128	1/1	0.93	0.06	63,63,63,63	0
55	MG	AA	4101	1/1	0.93	0.33	49,49,49,49	0
55	MG	CS	203	1/1	0.93	0.39	53,53,53,53	0
55	MG	AA	5183	1/1	0.93	0.19	58,58,58,58	0
55	MG	CA	4034	1/1	0.93	0.30	38,38,38,38	0
55	MG	CA	3158	1/1	0.93	0.19	9,9,9,9	0
55	MG	CA	3073	1/1	0.93	0.35	94,94,94,94	0
55	MG	CA	3201	1/1	0.93	0.45	24,24,24,24	0
55	MG	DA	1666	1/1	0.93	0.56	46,46,46,46	0
55	MG	AA	4230	1/1	0.93	0.23	19,19,19,19	0
55	MG	CA	3074	1/1	0.93	0.28	39,39,39,39	0
55	MG	BA	1674	1/1	0.93	0.38	118,118,118,118	0
55	MG	BA	2040	1/1	0.93	0.21	68,68,68,68	0
55	MG	BA	1951	1/1	0.93	0.14	29,29,29,29	0
55	MG	CA	3639	1/1	0.93	0.15	78,78,78,78	0
55	MG	AA	4724	1/1	0.93	0.09	59,59,59,59	0
55	MG	CA	3610	1/1	0.93	0.31	67,67,67,67	0
55	MG	CA	4383	1/1	0.93	0.16	58,58,58,58	0
55	MG	CA	3838	1/1	0.93	1.18	131,131,131,131	0
55	MG	AA	4036	1/1	0.93	0.32	64,64,64,64	0
55	MG	CA	3026	1/1	0.93	0.68	59,59,59,59	0
55	MG	CA	4094	1/1	0.93	0.36	39,39,39,39	0
55	MG	CA	3149	1/1	0.93	0.21	18,18,18,18	0
55	MG	BV	106	1/1	0.93	0.06	113,113,113,113	0
55	MG	BA	1698	1/1	0.93	0.13	51,51,51,51	0
55	MG	AA	5052	1/1	0.93	0.23	46,46,46,46	0
55	MG	AA	5237	1/1	0.93	0.45	37,37,37,37	0
55	MG	CA	3708	1/1	0.93	0.22	77,77,77,77	0
55	MG	BA	1691	1/1	0.94	0.26	20,20,20,20	0
55	MG	BA	1895	1/1	0.94	0.12	51,51,51,51	0
55	MG	CA	4127	1/1	0.94	0.34	49,49,49,49	0
55	MG	AA	5113	1/1	0.94	0.26	52,52,52,52	0
55	MG	AA	4050	1/1	0.94	0.19	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4812	1/1	0.94	0.17	62,62,62,62	0
55	MG	AA	4419	1/1	0.94	0.32	64,64,64,64	0
55	MG	BA	2035	1/1	0.94	0.33	61,61,61,61	0
55	MG	AA	4075	1/1	0.94	0.25	88,88,88,88	0
55	MG	AA	5270	1/1	0.94	0.17	47,47,47,47	0
55	MG	CA	4110	1/1	0.94	0.16	45,45,45,45	0
55	MG	CA	3574	1/1	0.94	1.10	91,91,91,91	0
55	MG	DA	2196	1/1	0.94	0.56	90,90,90,90	0
55	MG	AA	4211	1/1	0.94	0.20	21,21,21,21	0
55	MG	CA	3044	1/1	0.94	0.49	43,43,43,43	0
55	MG	BA	1856	1/1	0.94	0.24	85,85,85,85	0
55	MG	DA	1711	1/1	0.94	0.13	50,50,50,50	0
55	MG	AA	5114	1/1	0.94	0.13	53,53,53,53	0
55	MG	AA	4139	1/1	0.94	0.35	61,61,61,61	0
55	MG	AA	5035	1/1	0.94	0.36	65,65,65,65	0
55	MG	CA	3961	1/1	0.94	0.18	28,28,28,28	0
55	MG	CA	3371	1/1	0.94	0.50	51,51,51,51	0
55	MG	DA	2201	1/1	0.94	0.26	75,75,75,75	0
55	MG	BA	2144	1/1	0.94	0.15	92,92,92,92	0
55	MG	AA	4203	1/1	0.94	0.21	25,25,25,25	0
55	MG	AA	4380	1/1	0.94	0.23	50,50,50,50	0
55	MG	BA	1689	1/1	0.94	0.35	19,19,19,19	0
55	MG	DA	1618	1/1	0.94	0.18	85,85,85,85	0
55	MG	AA	4226	1/1	0.94	0.12	25,25,25,25	0
55	MG	CA	4274	1/1	0.94	0.34	42,42,42,42	0
55	MG	AA	4294	1/1	0.94	0.23	50,50,50,50	0
55	MG	CA	3707	1/1	0.94	0.14	49,49,49,49	0
55	MG	CA	4057	1/1	0.94	0.42	42,42,42,42	0
55	MG	CA	3132	1/1	0.94	0.25	16,16,16,16	0
55	MG	CA	4111	1/1	0.94	0.28	37,37,37,37	0
55	MG	CA	3208	1/1	0.94	0.08	46,46,46,46	0
55	MG	BA	1756	1/1	0.94	0.10	59,59,59,59	0
55	MG	BA	1892	1/1	0.94	0.53	83,83,83,83	0
55	MG	CL	206	1/1	0.94	0.43	55,55,55,55	0
55	MG	DA	2148	1/1	0.94	0.42	54,54,54,54	0
55	MG	CA	4166	1/1	0.94	0.49	59,59,59,59	0
55	MG	AA	4690	1/1	0.94	0.29	57,57,57,57	0
55	MG	AA	4687	1/1	0.94	0.11	58,58,58,58	0
55	MG	C2	102	1/1	0.94	0.54	49,49,49,49	0
55	MG	CA	3818	1/1	0.94	0.55	72,72,72,72	0
55	MG	CA	3180	1/1	0.94	0.18	18,18,18,18	0
55	MG	AA	4699	1/1	0.94	0.25	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3545	1/1	0.94	0.24	75,75,75,75	0
55	MG	AA	4847	1/1	0.94	0.47	37,37,37,37	0
55	MG	CA	3130	1/1	0.94	0.21	11,11,11,11	0
55	MG	DA	1968	1/1	0.94	0.17	56,56,56,56	0
55	MG	DA	1713	1/1	0.94	0.10	30,30,30,30	0
55	MG	AA	5068	1/1	0.94	0.29	51,51,51,51	0
55	MG	CA	3185	1/1	0.94	0.21	16,16,16,16	0
55	MG	CA	3212	1/1	0.94	0.23	26,26,26,26	0
55	MG	CA	3241	1/1	0.94	0.17	26,26,26,26	0
55	MG	CA	2904	1/1	0.94	0.27	49,49,49,49	0
55	MG	CL	205	1/1	0.94	0.36	35,35,35,35	0
55	MG	CA	3174	1/1	0.94	0.23	23,23,23,23	0
55	MG	BA	2153	1/1	0.94	0.14	38,38,38,38	0
55	MG	CA	3666	1/1	0.94	0.66	54,54,54,54	0
55	MG	AA	4330	1/1	0.94	0.11	72,72,72,72	0
55	MG	BA	2004	1/1	0.94	0.10	74,74,74,74	0
55	MG	CA	2913	1/1	0.94	0.48	77,77,77,77	0
55	MG	AA	4340	1/1	0.94	0.29	37,37,37,37	0
55	MG	AA	4105	1/1	0.94	0.41	52,52,52,52	0
55	MG	BA	1832	1/1	0.94	0.45	83,83,83,83	0
55	MG	CA	3225	1/1	0.94	0.27	23,23,23,23	0
55	MG	DW	112	1/1	0.94	0.40	71,71,71,71	0
55	MG	DA	1743	1/1	0.94	0.11	50,50,50,50	0
55	MG	AA	4911	1/1	0.94	0.55	45,45,45,45	0
55	MG	AA	4964	1/1	0.94	0.22	40,40,40,40	0
55	MG	AA	4474	1/1	0.94	0.13	42,42,42,42	0
55	MG	BA	1732	1/1	0.94	0.12	42,42,42,42	0
55	MG	BA	1894	1/1	0.94	0.13	86,86,86,86	0
55	MG	CA	3395	1/1	0.94	0.10	39,39,39,39	0
55	MG	CA	3148	1/1	0.94	0.33	17,17,17,17	0
55	MG	CA	3962	1/1	0.94	0.12	28,28,28,28	0
55	MG	AA	4022	1/1	0.94	0.24	66,66,66,66	0
55	MG	CA	3419	1/1	0.94	0.20	41,41,41,41	0
55	MG	CA	3305	1/1	0.94	0.67	50,50,50,50	0
55	MG	CA	3167	1/1	0.94	0.45	23,23,23,23	0
55	MG	CA	4001	1/1	0.94	0.42	11,11,11,11	0
55	MG	AK	201	1/1	0.94	0.34	56,56,56,56	0
55	MG	BA	1678	1/1	0.94	0.16	80,80,80,80	0
55	MG	BA	1603	1/1	0.94	0.21	65,65,65,65	0
55	MG	CA	3127	1/1	0.94	0.50	14,14,14,14	0
55	MG	AA	4232	1/1	0.94	0.04	40,40,40,40	0
55	MG	BQ	201	1/1	0.94	0.40	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3219	1/1	0.94	0.49	35,35,35,35	0
55	MG	CA	2971	1/1	0.94	0.28	60,60,60,60	0
55	MG	AA	4881	1/1	0.94	0.13	45,45,45,45	0
55	MG	BA	1704	1/1	0.94	0.30	41,41,41,41	0
55	MG	CA	2940	1/1	0.94	0.55	78,78,78,78	0
55	MG	AA	4846	1/1	0.94	0.18	13,13,13,13	0
55	MG	AA	4971	1/1	0.94	0.68	68,68,68,68	0
55	MG	CA	3173	1/1	0.94	0.26	14,14,14,14	0
55	MG	CA	3122	1/1	0.94	0.41	11,11,11,11	0
55	MG	CA	3278	1/1	0.94	0.23	36,36,36,36	0
55	MG	AA	4177	1/1	0.94	0.53	9,9,9,9	0
55	MG	AA	4880	1/1	0.94	0.20	34,34,34,34	0
55	MG	CA	3636	1/1	0.94	0.28	53,53,53,53	0
55	MG	CD	305	1/1	0.94	0.32	57,57,57,57	0
55	MG	BA	1776	1/1	0.94	0.14	66,66,66,66	0
55	MG	AR	203	1/1	0.94	0.21	19,19,19,19	0
55	MG	AA	4937	1/1	0.94	0.12	38,38,38,38	0
55	MG	CA	3687	1/1	0.94	0.66	67,67,67,67	0
55	MG	CA	4286	1/1	0.94	0.27	58,58,58,58	0
55	MG	BA	2045	1/1	0.94	0.31	56,56,56,56	0
55	MG	AA	4840	1/1	0.94	0.20	52,52,52,52	0
55	MG	CA	2969	1/1	0.94	0.28	73,73,73,73	0
55	MG	BA	1814	1/1	0.94	0.45	53,53,53,53	0
55	MG	CA	4230	1/1	0.94	0.31	53,53,53,53	0
55	MG	AA	4146	1/1	0.94	0.24	73,73,73,73	0
55	MG	AA	5128	1/1	0.94	0.27	50,50,50,50	0
55	MG	CA	3801	1/1	0.94	0.17	45,45,45,45	0
55	MG	CA	3135	1/1	0.94	0.12	17,17,17,17	0
55	MG	CB	246	1/1	0.94	0.15	53,53,53,53	0
55	MG	AA	4813	1/1	0.94	0.45	76,76,76,76	0
55	MG	AA	4382	1/1	0.94	0.20	48,48,48,48	0
55	MG	CA	3900	1/1	0.94	0.63	39,39,39,39	0
55	MG	DA	1615	1/1	0.94	0.21	104,104,104,104	0
54	BLS	CA	4405	30/30	0.94	0.43	53,53,54,54	0
55	MG	DA	1988	1/1	0.94	0.05	69,69,69,69	0
55	MG	AA	5026	1/1	0.94	0.30	40,40,40,40	0
55	MG	CA	4206	1/1	0.94	0.30	57,57,57,57	0
55	MG	AA	4862	1/1	0.94	0.19	30,30,30,30	0
55	MG	DA	1627	1/1	0.94	0.26	89,89,89,89	0
55	MG	CA	2947	1/1	0.94	0.27	38,38,38,38	0
55	MG	AA	4925	1/1	0.94	0.22	29,29,29,29	0
55	MG	CA	3129	1/1	0.94	0.48	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4054	1/1	0.94	0.89	33,33,33,33	0
55	MG	CB	219	1/1	0.94	0.26	52,52,52,52	0
55	MG	CA	3820	1/1	0.94	0.32	100,100,100,100	0
55	MG	CB	208	1/1	0.94	0.13	59,59,59,59	0
55	MG	BA	2006	1/1	0.94	0.25	144,144,144,144	0
55	MG	CB	256	1/1	0.94	0.35	59,59,59,59	0
55	MG	CA	3673	1/1	0.94	0.52	81,81,81,81	0
55	MG	AA	5274	1/1	0.94	0.23	66,66,66,66	0
55	MG	BA	1873	1/1	0.94	0.64	80,80,80,80	0
55	MG	CA	3189	1/1	0.94	0.09	25,25,25,25	0
55	MG	BA	2166	1/1	0.94	0.28	59,59,59,59	0
55	MG	AA	4781	1/1	0.94	0.18	46,46,46,46	0
55	MG	AA	4405	1/1	0.94	0.53	24,24,24,24	0
55	MG	CA	3617	1/1	0.94	0.35	88,88,88,88	0
55	MG	CA	3632	1/1	0.94	0.19	61,61,61,61	0
55	MG	BA	1746	1/1	0.94	0.19	48,48,48,48	0
55	MG	CB	216	1/1	0.94	0.27	21,21,21,21	0
55	MG	DA	1704	1/1	0.94	0.34	42,42,42,42	0
55	MG	DA	1959	1/1	0.94	0.21	45,45,45,45	0
55	MG	AX	103	1/1	0.94	0.77	62,62,62,62	0
55	MG	DA	1772	1/1	0.94	0.22	74,74,74,74	0
55	MG	DA	1675	1/1	0.94	0.67	49,49,49,49	0
55	MG	DA	1803	1/1	0.94	0.11	56,56,56,56	0
55	MG	AA	5073	1/1	0.94	0.20	36,36,36,36	0
55	MG	AA	4213	1/1	0.94	0.20	18,18,18,18	0
55	MG	CF	307	1/1	0.94	0.37	71,71,71,71	0
55	MG	CA	3407	1/1	0.94	0.28	36,36,36,36	0
55	MG	CA	3559	1/1	0.94	0.20	57,57,57,57	0
55	MG	CA	3588	1/1	0.94	0.29	57,57,57,57	0
55	MG	CA	3096	1/1	0.94	0.31	57,57,57,57	0
55	MG	CA	3663	1/1	0.94	0.12	44,44,44,44	0
55	MG	BA	2054	1/1	0.94	0.29	72,72,72,72	0
55	MG	CA	3151	1/1	0.94	0.63	42,42,42,42	0
55	MG	CA	4081	1/1	0.94	0.28	49,49,49,49	0
55	MG	AA	4674	1/1	0.94	0.32	50,50,50,50	0
55	MG	AA	4400	1/1	0.94	0.31	40,40,40,40	0
55	MG	CA	3985	1/1	0.94	0.31	22,22,22,22	0
55	MG	AB	239	1/1	0.94	0.13	49,49,49,49	0
55	MG	BA	1953	1/1	0.94	0.41	24,24,24,24	0
55	MG	DW	108	1/1	0.94	0.12	141,141,141,141	0
55	MG	AA	4900	1/1	0.94	0.33	47,47,47,47	0
55	MG	CA	4090	1/1	0.94	0.36	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3502	1/1	0.94	0.27	75,75,75,75	0
55	MG	CA	3659	1/1	0.94	0.06	52,52,52,52	0
55	MG	CA	3281	1/1	0.94	0.23	35,35,35,35	0
55	MG	CA	3404	1/1	0.94	0.17	36,36,36,36	0
55	MG	CA	3317	1/1	0.94	0.09	60,60,60,60	0
55	MG	DA	1956	1/1	0.94	0.18	40,40,40,40	0
55	MG	AA	4466	1/1	0.94	0.21	57,57,57,57	0
55	MG	AA	4617	1/1	0.94	0.22	51,51,51,51	0
55	MG	DA	1869	1/1	0.94	0.16	59,59,59,59	0
55	MG	CA	3213	1/1	0.94	0.12	14,14,14,14	0
55	MG	CN	203	1/1	0.94	0.52	65,65,65,65	0
55	MG	DA	1792	1/1	0.94	0.10	66,66,66,66	0
55	MG	CA	3590	1/1	0.94	0.29	42,42,42,42	0
55	MG	AA	5103	1/1	0.94	0.17	47,47,47,47	0
55	MG	AA	4307	1/1	0.94	0.67	34,34,34,34	0
55	MG	CA	3928	1/1	0.94	0.15	71,71,71,71	0
55	MG	DV	102	1/1	0.94	0.11	54,54,54,54	0
55	MG	CA	3144	1/1	0.94	0.29	29,29,29,29	0
55	MG	CA	4246	1/1	0.94	0.17	51,51,51,51	0
55	MG	AA	5277	1/1	0.94	0.23	72,72,72,72	0
55	MG	CA	3234	1/1	0.94	0.22	18,18,18,18	0
55	MG	CA	3992	1/1	0.94	0.21	26,26,26,26	0
55	MG	AA	4949	1/1	0.94	0.17	38,38,38,38	0
55	MG	BA	1961	1/1	0.94	0.21	51,51,51,51	0
55	MG	AR	201	1/1	0.94	0.28	61,61,61,61	0
55	MG	AA	4227	1/1	0.94	0.14	36,36,36,36	0
55	MG	DA	2030	1/1	0.94	0.11	26,26,26,26	0
55	MG	AS	204	1/1	0.94	0.30	43,43,43,43	0
55	MG	CA	3176	1/1	0.94	0.24	15,15,15,15	0
55	MG	AA	4236	1/1	0.94	0.39	23,23,23,23	0
55	MG	CA	3237	1/1	0.94	0.20	31,31,31,31	0
55	MG	CW	101	1/1	0.94	0.60	107,107,107,107	0
55	MG	DA	1846	1/1	0.94	0.34	133,133,133,133	0
55	MG	CA	3988	1/1	0.94	0.27	24,24,24,24	0
55	MG	CA	4101	1/1	0.94	0.21	46,46,46,46	0
55	MG	CA	4023	1/1	0.94	0.20	26,26,26,26	0
55	MG	CA	3110	1/1	0.94	0.40	15,15,15,15	0
55	MG	AA	4981	1/1	0.95	0.17	34,34,34,34	0
55	MG	AA	5153	1/1	0.95	0.31	44,44,44,44	0
55	MG	CA	2997	1/1	0.95	0.21	69,69,69,69	0
55	MG	AA	4894	1/1	0.95	0.17	93,93,93,93	0
55	MG	AA	4651	1/1	0.95	0.24	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	4303	1/1	0.95	0.19	50,50,50,50	0
55	MG	AA	4782	1/1	0.95	0.31	73,73,73,73	0
55	MG	DV	109	1/1	0.95	0.11	65,65,65,65	0
55	MG	CA	2942	1/1	0.95	0.28	56,56,56,56	0
55	MG	CA	4149	1/1	0.95	0.11	39,39,39,39	0
55	MG	DA	1844	1/1	0.95	0.28	164,164,164,164	0
55	MG	CA	2929	1/1	0.95	0.15	81,81,81,81	0
55	MG	BA	1998	1/1	0.95	0.32	52,52,52,52	0
55	MG	DA	1769	1/1	0.95	0.09	57,57,57,57	0
55	MG	DA	1997	1/1	0.95	0.29	50,50,50,50	0
55	MG	AG	201	1/1	0.95	0.80	78,78,78,78	0
55	MG	CA	3738	1/1	0.95	0.36	105,105,105,105	0
55	MG	CA	4250	1/1	0.95	0.64	48,48,48,48	0
55	MG	AA	4669	1/1	0.95	0.53	116,116,116,116	0
55	MG	DA	1868	1/1	0.95	0.51	58,58,58,58	0
55	MG	CA	2946	1/1	0.95	0.86	63,63,63,63	0
55	MG	CA	3980	1/1	0.95	0.27	39,39,39,39	0
55	MG	AA	4496	1/1	0.95	0.51	95,95,95,95	0
55	MG	BW	110	1/1	0.95	0.07	47,47,47,47	0
55	MG	AA	5242	1/1	0.95	0.19	70,70,70,70	0
55	MG	AA	4621	1/1	0.95	0.29	68,68,68,68	0
55	MG	AA	4205	1/1	0.95	0.46	18,18,18,18	0
55	MG	AA	4486	1/1	0.95	0.14	60,60,60,60	0
55	MG	CB	233	1/1	0.95	0.13	83,83,83,83	0
55	MG	BA	1677	1/1	0.95	0.28	71,71,71,71	0
55	MG	C2	101	1/1	0.95	0.25	15,15,15,15	0
55	MG	CA	4247	1/1	0.95	0.18	46,46,46,46	0
55	MG	CA	3360	1/1	0.95	0.41	53,53,53,53	0
55	MG	AA	4934	1/1	0.95	0.23	41,41,41,41	0
55	MG	DA	1905	1/1	0.95	0.20	113,113,113,113	0
55	MG	CA	3032	1/1	0.95	0.30	46,46,46,46	0
55	MG	DA	1765	1/1	0.95	0.54	50,50,50,50	0
55	MG	CA	4309	1/1	0.95	0.19	36,36,36,36	0
55	MG	CA	3461	1/1	0.95	0.60	45,45,45,45	0
55	MG	DA	2143	1/1	0.95	0.30	48,48,48,48	0
55	MG	BA	1935	1/1	0.95	0.19	73,73,73,73	0
55	MG	DA	1691	1/1	0.95	0.15	16,16,16,16	0
55	MG	CA	3773	1/1	0.95	0.17	67,67,67,67	0
55	MG	AA	4893	1/1	0.95	0.17	54,54,54,54	0
55	MG	CA	3676	1/1	0.95	0.22	61,61,61,61	0
55	MG	DA	1621	1/1	0.95	0.23	97,97,97,97	0
55	MG	DA	1892	1/1	0.95	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1864	1/1	0.95	0.11	92,92,92,92	0
55	MG	CA	3381	1/1	0.95	0.39	32,32,32,32	0
55	MG	CA	3808	1/1	0.95	0.40	88,88,88,88	0
55	MG	CA	4338	1/1	0.95	0.52	96,96,96,96	0
55	MG	AA	4608	1/1	0.95	0.09	81,81,81,81	0
55	MG	AA	4415	1/1	0.95	0.34	52,52,52,52	0
55	MG	BA	1617	1/1	0.95	0.20	99,99,99,99	0
55	MG	DA	2130	1/1	0.95	0.34	84,84,84,84	0
55	MG	CA	3311	1/1	0.95	0.14	20,20,20,20	0
55	MG	BA	1713	1/1	0.95	0.24	53,53,53,53	0
55	MG	CA	3701	1/1	0.95	0.09	66,66,66,66	0
55	MG	DA	1776	1/1	0.95	0.10	48,48,48,48	0
55	MG	AA	4726	1/1	0.95	0.55	59,59,59,59	0
55	MG	CA	3863	1/1	0.95	0.13	50,50,50,50	0
55	MG	AA	4637	1/1	0.95	0.15	79,79,79,79	0
55	MG	AA	4899	1/1	0.95	0.05	51,51,51,51	0
55	MG	AA	4961	1/1	0.95	0.26	44,44,44,44	0
55	MG	BA	1908	1/1	0.95	0.35	75,75,75,75	0
55	MG	CB	221	1/1	0.95	0.29	53,53,53,53	0
55	MG	AB	229	1/1	0.95	0.08	45,45,45,45	0
55	MG	CA	3194	1/1	0.95	0.20	9,9,9,9	0
55	MG	CA	3828	1/1	0.95	0.36	52,52,52,52	0
55	MG	CA	3332	1/1	0.95	0.29	45,45,45,45	0
55	MG	AA	4605	1/1	0.95	0.61	55,55,55,55	0
55	MG	CA	3934	1/1	0.95	0.14	55,55,55,55	0
55	MG	CA	3471	1/1	0.95	0.36	71,71,71,71	0
55	MG	AA	4357	1/1	0.95	0.23	56,56,56,56	0
55	MG	CA	3612	1/1	0.95	0.18	50,50,50,50	0
55	MG	CA	4256	1/1	0.95	0.12	70,70,70,70	0
55	MG	CA	3959	1/1	0.95	0.68	37,37,37,37	0
55	MG	CA	3751	1/1	0.95	0.63	50,50,50,50	0
55	MG	BA	2017	1/1	0.95	0.12	48,48,48,48	0
55	MG	AA	4422	1/1	0.95	0.47	50,50,50,50	0
55	MG	CA	3146	1/1	0.95	0.57	24,24,24,24	0
55	MG	CA	3700	1/1	0.95	0.53	79,79,79,79	0
55	MG	AA	4871	1/1	0.95	0.47	34,34,34,34	0
55	MG	AA	4200	1/1	0.95	0.22	8,8,8,8	0
55	MG	BV	119	1/1	0.95	0.84	142,142,142,142	0
55	MG	AA	5224	1/1	0.95	0.26	47,47,47,47	0
55	MG	BV	109	1/1	0.95	0.23	88,88,88,88	0
55	MG	DA	1840	1/1	0.95	0.13	68,68,68,68	0
55	MG	CE	303	1/1	0.95	0.32	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3615	1/1	0.95	0.11	50,50,50,50	0
55	MG	CA	4076	1/1	0.95	0.15	34,34,34,34	0
55	MG	BA	1748	1/1	0.95	0.55	57,57,57,57	0
55	MG	DA	1710	1/1	0.95	0.35	40,40,40,40	0
55	MG	DA	2024	1/1	0.95	0.45	63,63,63,63	0
55	MG	BA	1839	1/1	0.95	0.30	105,105,105,105	0
55	MG	BA	1800	1/1	0.95	0.16	73,73,73,73	0
55	MG	AA	4485	1/1	0.95	0.56	36,36,36,36	0
55	MG	AA	4264	1/1	0.95	0.43	32,32,32,32	0
55	MG	CA	2910	1/1	0.95	0.19	145,145,145,145	0
55	MG	CA	3819	1/1	0.95	0.24	68,68,68,68	0
55	MG	AA	4631	1/1	0.95	0.64	104,104,104,104	0
55	MG	CA	3624	1/1	0.95	0.37	33,33,33,33	0
55	MG	AA	4966	1/1	0.95	0.12	58,58,58,58	0
55	MG	AA	4323	1/1	0.95	0.30	31,31,31,31	0
55	MG	CA	3142	1/1	0.95	0.76	22,22,22,22	0
55	MG	AA	4303	1/1	0.95	0.23	41,41,41,41	0
55	MG	AA	5031	1/1	0.95	0.16	62,62,62,62	0
55	MG	DA	1716	1/1	0.95	0.16	51,51,51,51	0
55	MG	CA	3253	1/1	0.95	0.18	27,27,27,27	0
55	MG	AA	5070	1/1	0.95	0.16	79,79,79,79	0
55	MG	BA	1976	1/1	0.95	0.20	29,29,29,29	0
55	MG	AA	4902	1/1	0.95	0.21	35,35,35,35	0
55	MG	AA	4360	1/1	0.95	0.31	48,48,48,48	0
55	MG	AA	4888	1/1	0.95	0.35	36,36,36,36	0
55	MG	CA	3068	1/1	0.95	0.28	84,84,84,84	0
55	MG	AA	4875	1/1	0.95	0.22	57,57,57,57	0
55	MG	CA	3087	1/1	0.95	0.34	78,78,78,78	0
55	MG	AA	4302	1/1	0.95	0.06	28,28,28,28	0
55	MG	CA	3379	1/1	0.95	0.32	37,37,37,37	0
55	MG	AA	4221	1/1	0.95	0.31	43,43,43,43	0
55	MG	DA	1847	1/1	0.95	0.05	119,119,119,119	0
55	MG	DA	1801	1/1	0.95	0.10	79,79,79,79	0
55	MG	AA	5261	1/1	0.95	0.17	73,73,73,73	0
55	MG	DV	110	1/1	0.95	0.14	55,55,55,55	0
55	MG	AA	4276	1/1	0.95	0.39	39,39,39,39	0
55	MG	AA	4116	1/1	0.95	0.41	53,53,53,53	0
55	MG	CA	3414	1/1	0.95	0.12	42,42,42,42	0
55	MG	BA	1613	1/1	0.95	0.38	69,69,69,69	0
55	MG	AA	4235	1/1	0.95	0.24	59,59,59,59	0
55	MG	CA	3768	1/1	0.95	0.33	84,84,84,84	0
55	MG	CA	4357	1/1	0.95	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4298	1/1	0.95	0.56	47,47,47,47	0
55	MG	AA	4624	1/1	0.95	0.09	75,75,75,75	0
55	MG	AA	4172	1/1	0.95	0.46	14,14,14,14	0
55	MG	DA	2039	1/1	0.95	0.16	43,43,43,43	0
55	MG	CA	3114	1/1	0.95	0.39	17,17,17,17	0
55	MG	AA	4619	1/1	0.95	0.26	56,56,56,56	0
55	MG	CA	3848	1/1	0.95	0.30	70,70,70,70	0
55	MG	BA	2143	1/1	0.95	0.08	83,83,83,83	0
55	MG	AA	5102	1/1	0.95	0.42	50,50,50,50	0
55	MG	AN	202	1/1	0.95	0.62	48,48,48,48	0
55	MG	CA	3198	1/1	0.95	0.16	31,31,31,31	0
55	MG	AA	4216	1/1	0.95	0.13	18,18,18,18	0
55	MG	C4	102	1/1	0.95	0.77	70,70,70,70	0
55	MG	AA	4234	1/1	0.95	0.28	19,19,19,19	0
55	MG	AA	4195	1/1	0.95	0.16	21,21,21,21	0
55	MG	CA	4301	1/1	0.95	0.17	56,56,56,56	0
55	MG	CD	303	1/1	0.95	0.53	28,28,28,28	0
55	MG	DA	1645	1/1	0.95	0.21	131,131,131,131	0
55	MG	CA	4086	1/1	0.95	0.20	43,43,43,43	0
55	MG	BA	1791	1/1	0.95	0.10	60,60,60,60	0
55	MG	CA	4135	1/1	0.95	0.51	50,50,50,50	0
55	MG	BA	2074	1/1	0.95	0.28	46,46,46,46	0
55	MG	CA	4368	1/1	0.95	0.31	64,64,64,64	0
55	MG	BA	1707	1/1	0.95	0.59	38,38,38,38	0
55	MG	CA	4329	1/1	0.95	0.35	48,48,48,48	0
55	MG	DA	2136	1/1	0.95	0.15	52,52,52,52	0
55	MG	CA	3576	1/1	0.95	0.33	37,37,37,37	0
55	MG	BA	1620	1/1	0.95	0.43	62,62,62,62	0
55	MG	CA	3091	1/1	0.95	0.35	65,65,65,65	0
55	MG	CA	4032	1/1	0.95	0.36	49,49,49,49	0
55	MG	AA	4308	1/1	0.95	0.37	44,44,44,44	0
55	MG	DA	1606	1/1	0.95	0.45	83,83,83,83	0
55	MG	CA	3215	1/1	0.95	0.18	26,26,26,26	0
55	MG	CA	3029	1/1	0.95	0.13	79,79,79,79	0
55	MG	BA	1893	1/1	0.95	0.36	102,102,102,102	0
55	MG	AA	4209	1/1	0.95	0.17	47,47,47,47	0
55	MG	CA	4391	1/1	0.95	0.26	57,57,57,57	0
55	MG	CA	3413	1/1	0.95	0.74	48,48,48,48	0
55	MG	AA	4692	1/1	0.95	0.27	57,57,57,57	0
55	MG	BA	1768	1/1	0.95	0.15	89,89,89,89	0
55	MG	CA	3779	1/1	0.96	0.18	53,53,53,53	0
55	MG	AA	4194	1/1	0.96	0.26	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3190	1/1	0.96	0.23	11,11,11,11	0
55	MG	AA	4908	1/1	0.96	0.59	97,97,97,97	0
56	ZN	DN	101	1/1	0.96	0.13	94,94,94,94	0
55	MG	CA	3188	1/1	0.96	0.28	23,23,23,23	0
55	MG	AA	4544	1/1	0.96	0.38	69,69,69,69	0
55	MG	CA	3631	1/1	0.96	0.26	42,42,42,42	0
55	MG	CA	2967	1/1	0.96	0.32	73,73,73,73	0
55	MG	CA	3118	1/1	0.96	0.47	14,14,14,14	0
55	MG	BV	108	1/1	0.96	0.09	54,54,54,54	0
55	MG	CA	3261	1/1	0.96	0.45	48,48,48,48	0
55	MG	CA	3162	1/1	0.96	0.25	11,11,11,11	0
55	MG	AN	201	1/1	0.96	0.23	102,102,102,102	0
55	MG	AA	4170	1/1	0.96	0.41	22,22,22,22	0
55	MG	DA	1954	1/1	0.96	0.50	53,53,53,53	0
55	MG	CA	3725	1/1	0.96	0.20	67,67,67,67	0
55	MG	AA	4507	1/1	0.96	0.24	72,72,72,72	0
55	MG	CA	3147	1/1	0.96	0.46	12,12,12,12	0
55	MG	DA	1958	1/1	0.96	0.26	18,18,18,18	0
55	MG	AA	4764	1/1	0.96	0.21	112,112,112,112	0
55	MG	CS	201	1/1	0.96	0.46	44,44,44,44	0
55	MG	AA	4182	1/1	0.96	0.33	17,17,17,17	0
55	MG	AA	4175	1/1	0.96	0.40	14,14,14,14	0
55	MG	AA	4710	1/1	0.96	0.44	67,67,67,67	0
55	MG	AA	4649	1/1	0.96	0.55	58,58,58,58	0
55	MG	DA	1983	1/1	0.96	0.15	43,43,43,43	0
55	MG	CA	3297	1/1	0.96	0.58	37,37,37,37	0
55	MG	AA	4204	1/1	0.96	0.57	17,17,17,17	0
55	MG	AA	5291	1/1	0.96	0.26	78,78,78,78	0
55	MG	CA	3691	1/1	0.96	0.60	49,49,49,49	0
55	MG	AA	4220	1/1	0.96	0.11	36,36,36,36	0
55	MG	CW	102	1/1	0.96	0.22	32,32,32,32	0
55	MG	CA	3204	1/1	0.96	0.11	38,38,38,38	0
55	MG	AA	4636	1/1	0.96	0.30	102,102,102,102	0
55	MG	DA	1757	1/1	0.96	0.55	73,73,73,73	0
55	MG	AA	4056	1/1	0.96	0.60	87,87,87,87	0
55	MG	BA	2022	1/1	0.96	0.20	73,73,73,73	0
55	MG	BA	1651	1/1	0.96	0.27	64,64,64,64	0
55	MG	AA	4201	1/1	0.96	0.12	15,15,15,15	0
55	MG	AA	4199	1/1	0.96	0.41	10,10,10,10	0
55	MG	AA	4484	1/1	0.96	0.57	75,75,75,75	0
55	MG	AA	4444	1/1	0.96	0.19	23,23,23,23	0
55	MG	AA	4600	1/1	0.96	0.50	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	DA	1796	1/1	0.96	0.10	62,62,62,62	0
55	MG	AA	4161	1/1	0.96	0.19	46,46,46,46	0
55	MG	CD	302	1/1	0.96	0.40	15,15,15,15	0
55	MG	CA	3485	1/1	0.96	0.24	63,63,63,63	0
55	MG	DA	1851	1/1	0.96	0.28	102,102,102,102	0
55	MG	CA	3336	1/1	0.96	0.19	36,36,36,36	0
55	MG	AA	4960	1/1	0.96	0.07	55,55,55,55	0
55	MG	BA	1938	1/1	0.96	0.74	78,78,78,78	0
55	MG	AA	4892	1/1	0.96	0.07	45,45,45,45	0
55	MG	AA	5135	1/1	0.96	0.34	75,75,75,75	0
55	MG	CA	3679	1/1	0.96	0.39	90,90,90,90	0
55	MG	CA	3444	1/1	0.96	0.23	48,48,48,48	0
55	MG	AA	4969	1/1	0.96	0.17	68,68,68,68	0
55	MG	CA	3020	1/1	0.96	0.34	139,139,139,139	0
55	MG	CA	2930	1/1	0.96	0.33	92,92,92,92	0
55	MG	AA	4406	1/1	0.96	0.22	28,28,28,28	0
55	MG	AB	208	1/1	0.96	0.22	77,77,77,77	0
55	MG	CA	3490	1/1	0.96	0.44	146,146,146,146	0
55	MG	AA	4274	1/1	0.96	0.12	50,50,50,50	0
55	MG	AA	4467	1/1	0.96	0.10	36,36,36,36	0
55	MG	AA	5199	1/1	0.96	0.18	49,49,49,49	0
55	MG	DA	1692	1/1	0.96	0.32	11,11,11,11	0
55	MG	DA	1709	1/1	0.96	0.12	36,36,36,36	0
55	MG	DV	107	1/1	0.96	0.19	69,69,69,69	0
55	MG	DA	1976	1/1	0.96	0.15	47,47,47,47	0
55	MG	CA	3182	1/1	0.96	0.33	33,33,33,33	0
55	MG	CA	3202	1/1	0.96	0.31	28,28,28,28	0
55	MG	CA	3045	1/1	0.96	0.40	53,53,53,53	0
55	MG	AA	4286	1/1	0.96	0.11	35,35,35,35	0
55	MG	CA	4387	1/1	0.96	0.46	50,50,50,50	0
55	MG	BA	2164	1/1	0.96	0.15	40,40,40,40	0
55	MG	DA	1633	1/1	0.96	0.32	94,94,94,94	0
55	MG	AA	4053	1/1	0.96	0.22	107,107,107,107	0
55	MG	CA	3772	1/1	0.96	0.77	58,58,58,58	0
55	MG	CA	3794	1/1	0.96	0.53	106,106,106,106	0
55	MG	BA	1690	1/1	0.96	0.49	38,38,38,38	0
55	MG	CA	3611	1/1	0.96	0.42	49,49,49,49	0
55	MG	CA	3128	1/1	0.96	0.14	8,8,8,8	0
55	MG	BA	1887	1/1	0.96	0.11	51,51,51,51	0
55	MG	CA	4097	1/1	0.96	0.35	57,57,57,57	0
55	MG	AA	4610	1/1	0.96	0.14	74,74,74,74	0
55	MG	AA	4118	1/1	0.96	0.19	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4410	1/1	0.96	0.45	65,65,65,65	0
55	MG	AA	4498	1/1	0.96	0.28	77,77,77,77	0
55	MG	DA	1694	1/1	0.96	0.21	22,22,22,22	0
55	MG	BA	1997	1/1	0.96	0.34	58,58,58,58	0
55	MG	CX	102	1/1	0.96	0.15	18,18,18,18	0
55	MG	CA	3579	1/1	0.96	0.06	53,53,53,53	0
55	MG	CA	3184	1/1	0.96	0.26	13,13,13,13	0
55	MG	DA	1788	1/1	0.96	0.12	70,70,70,70	0
55	MG	DA	1610	1/1	0.96	0.17	59,59,59,59	0
55	MG	BA	1871	1/1	0.96	0.12	71,71,71,71	0
55	MG	AA	4367	1/1	0.96	0.33	35,35,35,35	0
55	MG	AA	4672	1/1	0.96	0.24	57,57,57,57	0
55	MG	AA	4280	1/1	0.96	0.21	51,51,51,51	0
55	MG	CA	3001	1/1	0.96	0.17	40,40,40,40	0
55	MG	CA	4024	1/1	0.96	0.17	48,48,48,48	0
55	MG	AA	4202	1/1	0.96	0.27	20,20,20,20	0
55	MG	CA	4386	1/1	0.96	0.72	59,59,59,59	0
55	MG	CQ	203	1/1	0.96	0.44	80,80,80,80	0
55	MG	CA	3392	1/1	0.96	0.23	25,25,25,25	0
55	MG	DA	1821	1/1	0.96	0.32	82,82,82,82	0
55	MG	CA	3604	1/1	0.96	0.33	57,57,57,57	0
55	MG	DA	1824	1/1	0.96	0.51	63,63,63,63	0
55	MG	AA	5191	1/1	0.96	0.13	41,41,41,41	0
55	MG	CA	4078	1/1	0.96	0.44	44,44,44,44	0
55	MG	CA	3587	1/1	0.96	0.27	44,44,44,44	0
55	MG	CA	4016	1/1	0.96	0.23	42,42,42,42	0
55	MG	AA	5003	1/1	0.96	0.14	69,69,69,69	0
55	MG	CA	3724	1/1	0.96	0.26	60,60,60,60	0
55	MG	CA	3124	1/1	0.96	0.29	17,17,17,17	0
55	MG	BA	1965	1/1	0.96	0.07	61,61,61,61	0
55	MG	CA	3299	1/1	0.96	0.22	21,21,21,21	0
55	MG	AA	4164	1/1	0.96	0.33	83,83,83,83	0
55	MG	CA	3685	1/1	0.96	0.33	86,86,86,86	0
55	MG	A4	101	1/1	0.96	0.27	117,117,117,117	0
55	MG	AA	4149	1/1	0.96	0.27	104,104,104,104	0
55	MG	BA	1685	1/1	0.96	0.60	34,34,34,34	0
55	MG	AA	4661	1/1	0.96	0.67	97,97,97,97	0
55	MG	DA	1719	1/1	0.96	0.25	42,42,42,42	0
55	MG	BA	2064	1/1	0.96	0.39	79,79,79,79	0
55	MG	AA	4288	1/1	0.96	0.41	35,35,35,35	0
55	MG	AA	4647	1/1	0.96	0.49	59,59,59,59	0
55	MG	CA	3695	1/1	0.96	0.14	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	BA	1888	1/1	0.96	0.12	75,75,75,75	0
55	MG	AA	4891	1/1	0.96	0.20	25,25,25,25	0
55	MG	CA	3385	1/1	0.96	0.38	69,69,69,69	0
55	MG	AA	4977	1/1	0.96	0.21	33,33,33,33	0
55	MG	CA	3806	1/1	0.96	0.39	86,86,86,86	0
55	MG	CA	3239	1/1	0.96	0.20	29,29,29,29	0
55	MG	AA	4033	1/1	0.96	0.25	47,47,47,47	0
55	MG	AA	4179	1/1	0.96	0.28	14,14,14,14	0
55	MG	CA	3682	1/1	0.96	0.06	93,93,93,93	0
55	MG	BA	1760	1/1	0.96	0.17	53,53,53,53	0
55	MG	AA	5122	1/1	0.96	0.16	52,52,52,52	0
55	MG	AV	202	1/1	0.97	0.26	56,56,56,56	0
55	MG	AA	5209	1/1	0.97	0.31	51,51,51,51	0
55	MG	CA	3726	1/1	0.97	0.67	160,160,160,160	0
55	MG	CA	3195	1/1	0.97	0.14	20,20,20,20	0
55	MG	AA	4183	1/1	0.97	0.63	13,13,13,13	0
55	MG	DA	1884	1/1	0.97	0.15	71,71,71,71	0
55	MG	BA	2095	1/1	0.97	0.18	68,68,68,68	0
55	MG	AA	4190	1/1	0.97	0.47	23,23,23,23	0
55	MG	AA	4558	1/1	0.97	0.24	48,48,48,48	0
55	MG	DA	1940	1/1	0.97	0.06	94,94,94,94	0
55	MG	CA	3976	1/1	0.97	0.09	14,14,14,14	0
55	MG	AA	4171	1/1	0.97	0.37	21,21,21,21	0
55	MG	CA	3963	1/1	0.97	0.32	24,24,24,24	0
55	MG	CA	3137	1/1	0.97	0.26	16,16,16,16	0
55	MG	CA	2975	1/1	0.97	0.30	59,59,59,59	0
55	MG	CA	3086	1/1	0.97	0.36	57,57,57,57	0
55	MG	DV	121	1/1	0.97	0.14	62,62,62,62	0
55	MG	DA	2132	1/1	0.97	0.08	60,60,60,60	0
55	MG	CA	3111	1/1	0.97	0.32	12,12,12,12	0
55	MG	BA	2018	1/1	0.97	0.12	46,46,46,46	0
55	MG	CQ	201	1/1	0.97	0.29	33,33,33,33	0
55	MG	AA	4738	1/1	0.97	0.23	19,19,19,19	0
55	MG	CA	3982	1/1	0.97	0.12	57,57,57,57	0
55	MG	AA	4450	1/1	0.97	0.18	62,62,62,62	0
55	MG	CA	3960	1/1	0.97	0.43	6,6,6,6	0
55	MG	AA	4611	1/1	0.97	0.23	98,98,98,98	0
55	MG	CA	3361	1/1	0.97	0.36	42,42,42,42	0
55	MG	CA	4138	1/1	0.97	0.24	49,49,49,49	0
55	MG	AA	4324	1/1	0.97	0.47	46,46,46,46	0
55	MG	CA	3171	1/1	0.97	0.29	30,30,30,30	0
55	MG	AA	4457	1/1	0.97	0.26	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3787	1/1	0.97	0.15	52,52,52,52	0
55	MG	AA	4452	1/1	0.97	0.06	42,42,42,42	0
55	MG	CA	4354	1/1	0.97	0.23	60,60,60,60	0
55	MG	DA	1887	1/1	0.97	0.82	113,113,113,113	0
55	MG	CA	3668	1/1	0.97	0.30	84,84,84,84	0
55	MG	AA	4522	1/1	0.97	0.18	76,76,76,76	0
55	MG	CA	3486	1/1	0.97	0.07	61,61,61,61	0
55	MG	CA	3840	1/1	0.97	0.32	63,63,63,63	0
55	MG	CA	3139	1/1	0.97	0.25	19,19,19,19	0
55	MG	AX	106	1/1	0.97	0.16	50,50,50,50	0
55	MG	AA	4371	1/1	0.97	0.28	44,44,44,44	0
55	MG	AF	304	1/1	0.97	0.54	73,73,73,73	0
55	MG	AA	4359	1/1	0.97	0.10	50,50,50,50	0
55	MG	AA	4475	1/1	0.97	0.05	53,53,53,53	0
55	MG	AA	4771	1/1	0.97	0.21	25,25,25,25	0
55	MG	CA	4113	1/1	0.97	0.23	32,32,32,32	0
55	MG	CA	3741	1/1	0.97	0.20	59,59,59,59	0
55	MG	DA	2097	1/1	0.97	0.36	61,61,61,61	0
55	MG	AB	217	1/1	0.97	0.17	84,84,84,84	0
55	MG	BA	1718	1/1	0.97	0.23	30,30,30,30	0
55	MG	CA	3246	1/1	0.97	0.23	46,46,46,46	0
55	MG	AA	4331	1/1	0.97	0.30	34,34,34,34	0
55	MG	CA	4029	1/1	0.97	0.08	58,58,58,58	0
55	MG	AA	4582	1/1	0.97	0.12	62,62,62,62	0
55	MG	AA	4886	1/1	0.97	0.11	42,42,42,42	0
55	MG	DA	1641	1/1	0.97	0.51	86,86,86,86	0
55	MG	BA	1769	1/1	0.97	0.16	50,50,50,50	0
55	MG	AA	4225	1/1	0.97	0.15	44,44,44,44	0
55	MG	AE	302	1/1	0.97	0.25	77,77,77,77	0
55	MG	BA	1858	1/1	0.97	0.13	88,88,88,88	0
55	MG	CA	3106	1/1	0.97	0.36	11,11,11,11	0
55	MG	CA	3337	1/1	0.97	0.13	58,58,58,58	0
55	MG	CA	3543	1/1	0.97	0.18	47,47,47,47	0
55	MG	CA	3581	1/1	0.97	0.09	49,49,49,49	0
55	MG	CA	3103	1/1	0.97	0.75	18,18,18,18	0
55	MG	BA	1694	1/1	0.97	0.59	44,44,44,44	0
55	MG	DA	2185	1/1	0.97	0.35	62,62,62,62	0
55	MG	AA	5021	1/1	0.97	0.29	61,61,61,61	0
55	MG	CA	3232	1/1	0.97	0.20	32,32,32,32	0
55	MG	CA	3170	1/1	0.97	0.23	24,24,24,24	0
55	MG	BA	1688	1/1	0.97	0.11	11,11,11,11	0
55	MG	CA	3183	1/1	0.97	0.27	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	4336	1/1	0.97	0.48	51,51,51,51	0
55	MG	CA	3536	1/1	0.97	0.12	72,72,72,72	0
55	MG	CA	3019	1/1	0.97	0.20	130,130,130,130	0
55	MG	AA	4370	1/1	0.97	0.11	51,51,51,51	0
55	MG	CA	3107	1/1	0.97	0.62	20,20,20,20	0
55	MG	AA	4178	1/1	0.97	0.37	9,9,9,9	0
55	MG	CA	3304	1/1	0.97	0.23	13,13,13,13	0
55	MG	CA	4197	1/1	0.97	0.42	64,64,64,64	0
55	MG	CK	201	1/1	0.97	0.58	105,105,105,105	0
55	MG	CA	4171	1/1	0.97	0.18	26,26,26,26	0
55	MG	CA	3565	1/1	0.97	0.14	65,65,65,65	0
55	MG	DA	1985	1/1	0.97	0.21	58,58,58,58	0
55	MG	CA	3105	1/1	0.97	0.41	18,18,18,18	0
55	MG	AA	4851	1/1	0.97	0.27	16,16,16,16	0
55	MG	AA	4250	1/1	0.97	0.11	24,24,24,24	0
55	MG	CA	2965	1/1	0.97	0.76	74,74,74,74	0
55	MG	AA	4658	1/1	0.97	0.28	56,56,56,56	0
55	MG	BA	1623	1/1	0.97	0.16	47,47,47,47	0
55	MG	AA	4869	1/1	0.97	0.10	61,61,61,61	0
55	MG	AA	4269	1/1	0.97	0.25	34,34,34,34	0
55	MG	CA	4374	1/1	0.97	0.73	41,41,41,41	0
55	MG	CA	3465	1/1	0.97	0.33	48,48,48,48	0
55	MG	DA	2049	1/1	0.97	0.16	56,56,56,56	0
55	MG	BA	1643	1/1	0.97	0.10	81,81,81,81	0
55	MG	BA	1786	1/1	0.97	0.35	60,60,60,60	0
55	MG	CA	3155	1/1	0.97	0.25	18,18,18,18	0
55	MG	DA	1879	1/1	0.97	0.21	80,80,80,80	0
55	MG	AA	4613	1/1	0.97	0.15	41,41,41,41	0
55	MG	AA	4263	1/1	0.97	0.15	38,38,38,38	0
55	MG	AA	4344	1/1	0.97	0.24	33,33,33,33	0
55	MG	AA	4456	1/1	0.97	0.16	61,61,61,61	0
55	MG	BA	1710	1/1	0.97	0.18	43,43,43,43	0
55	MG	CA	3267	1/1	0.97	0.04	56,56,56,56	0
55	MG	CA	3333	1/1	0.97	0.17	49,49,49,49	0
55	MG	AA	4187	1/1	0.97	0.84	30,30,30,30	0
55	MG	CA	3530	1/1	0.97	0.05	57,57,57,57	0
55	MG	AA	4727	1/1	0.97	0.06	75,75,75,75	0
55	MG	CA	3369	1/1	0.97	0.24	67,67,67,67	0
55	MG	CA	3152	1/1	0.97	0.49	22,22,22,22	0
55	MG	BA	1684	1/1	0.97	0.52	29,29,29,29	0
55	MG	CB	201	1/1	0.97	0.12	61,61,61,61	0
55	MG	CA	3136	1/1	0.97	0.17	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	AA	5196	1/1	0.97	0.32	48,48,48,48	0
55	MG	AD	302	1/1	0.97	0.39	79,79,79,79	0
55	MG	AA	4845	1/1	0.97	0.42	35,35,35,35	0
55	MG	CA	3231	1/1	0.97	0.23	19,19,19,19	0
55	MG	AA	4028	1/1	0.97	0.39	88,88,88,88	0
55	MG	AA	4455	1/1	0.97	0.28	72,72,72,72	0
55	MG	CA	3028	1/1	0.98	1.27	56,56,56,56	0
55	MG	AA	4530	1/1	0.98	0.52	64,64,64,64	0
55	MG	AA	4652	1/1	0.98	0.29	74,74,74,74	0
55	MG	BL	201	1/1	0.98	0.60	78,78,78,78	0
55	MG	AA	4174	1/1	0.98	0.24	14,14,14,14	0
55	MG	CA	3508	1/1	0.98	0.13	89,89,89,89	0
55	MG	CA	3790	1/1	0.98	0.48	111,111,111,111	0
55	MG	CA	3102	1/1	0.98	0.53	20,20,20,20	0
55	MG	CA	3120	1/1	0.98	0.36	11,11,11,11	0
55	MG	AA	4016	1/1	0.98	0.35	99,99,99,99	0
55	MG	AA	4413	1/1	0.98	0.22	40,40,40,40	0
55	MG	AA	4491	1/1	0.98	0.09	74,74,74,74	0
55	MG	CA	3121	1/1	0.98	0.28	11,11,11,11	0
55	MG	AA	4434	1/1	0.98	0.17	54,54,54,54	0
55	MG	CA	2911	1/1	0.98	0.44	64,64,64,64	0
55	MG	CA	4083	1/1	0.98	0.08	37,37,37,37	0
55	MG	CA	3693	1/1	0.98	0.33	59,59,59,59	0
55	MG	CA	2909	1/1	0.98	0.26	67,67,67,67	0
55	MG	AA	4180	1/1	0.98	0.25	22,22,22,22	0
55	MG	CA	3157	1/1	0.98	0.31	8,8,8,8	0
55	MG	CA	3265	1/1	0.98	0.06	35,35,35,35	0
55	MG	AA	4921	1/1	0.98	0.47	74,74,74,74	0
55	MG	BA	2087	1/1	0.98	0.24	94,94,94,94	0
55	MG	CA	3123	1/1	0.98	0.22	6,6,6,6	0
55	MG	CA	3116	1/1	0.98	0.27	14,14,14,14	0
55	MG	CA	3316	1/1	0.98	0.07	61,61,61,61	0
55	MG	BA	1831	1/1	0.98	0.20	124,124,124,124	0
55	MG	AA	4193	1/1	0.98	0.27	11,11,11,11	0
55	MG	BA	1851	1/1	0.98	0.43	66,66,66,66	0
55	MG	BA	1700	1/1	0.98	0.22	41,41,41,41	0
55	MG	AD	301	1/1	0.98	0.31	28,28,28,28	0
55	MG	CB	222	1/1	0.98	0.15	29,29,29,29	0
55	MG	CA	3737	1/1	0.98	0.44	91,91,91,91	0
55	MG	AA	4224	1/1	0.98	0.19	14,14,14,14	0
55	MG	AA	4320	1/1	0.98	0.53	46,46,46,46	0
55	MG	CA	3220	1/1	0.98	0.16	12,12,12,12	0

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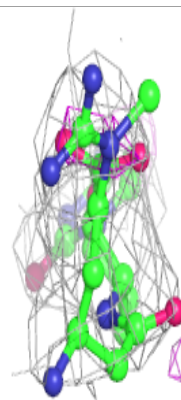
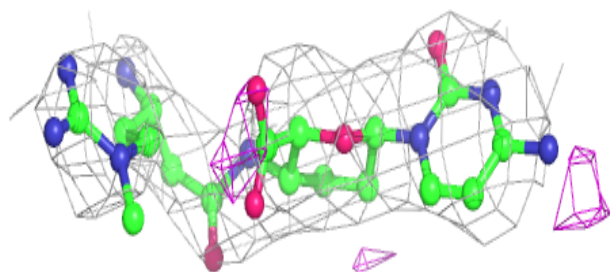
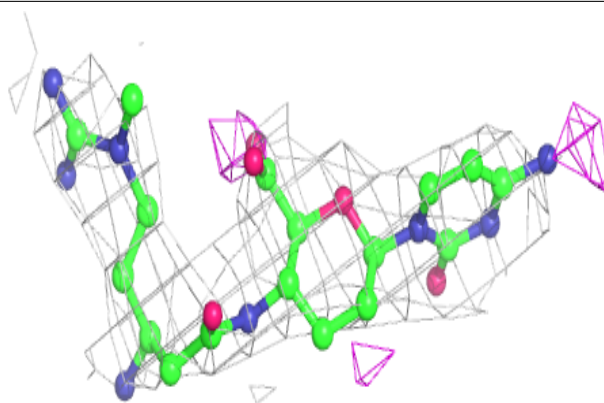
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	CA	3630	1/1	0.98	0.12	47,47,47,47	0
56	ZN	DD	303	1/1	0.98	0.24	80,80,80,80	0
55	MG	AA	4872	1/1	0.98	0.14	32,32,32,32	0
55	MG	BA	2120	1/1	0.98	0.33	65,65,65,65	0
55	MG	AA	4285	1/1	0.98	0.12	23,23,23,23	0
55	MG	AA	4249	1/1	0.98	0.46	25,25,25,25	0
55	MG	AA	4082	1/1	0.98	0.52	77,77,77,77	0
55	MG	CA	3742	1/1	0.98	0.56	112,112,112,112	0
55	MG	CA	3386	1/1	0.98	0.19	43,43,43,43	0
55	MG	CA	3568	1/1	0.98	0.09	75,75,75,75	0
55	MG	AA	4867	1/1	0.98	0.30	44,44,44,44	0
55	MG	AA	4383	1/1	0.98	0.16	54,54,54,54	0
55	MG	CA	3093	1/1	0.98	0.41	69,69,69,69	0
55	MG	AA	4527	1/1	0.98	0.11	43,43,43,43	0
55	MG	CA	3451	1/1	0.99	0.08	35,35,35,35	0
56	ZN	BD	301	1/1	0.99	0.28	38,38,38,38	0
55	MG	CA	3302	1/1	0.99	0.42	50,50,50,50	0
55	MG	AA	4088	1/1	0.99	0.47	120,120,120,120	0
55	MG	CA	3156	1/1	0.99	0.20	17,17,17,17	0
55	MG	AA	4251	1/1	0.99	0.25	27,27,27,27	0
55	MG	AA	4215	1/1	0.99	0.29	19,19,19,19	0
55	MG	CA	3119	1/1	0.99	0.58	8,8,8,8	0
55	MG	CA	3108	1/1	0.99	0.29	8,8,8,8	0
56	ZN	BN	101	1/1	0.99	0.14	76,76,76,76	0
55	MG	CA	3785	1/1	0.99	0.31	69,69,69,69	0
55	MG	CA	2901	1/1	0.99	0.45	20,20,20,20	0
55	MG	CA	3843	1/1	0.99	0.36	68,68,68,68	0
55	MG	AA	4585	1/1	0.99	0.41	72,72,72,72	0
55	MG	CA	3523	1/1	0.99	0.39	59,59,59,59	0
55	MG	CA	3393	1/1	0.99	0.24	36,36,36,36	0
55	MG	DA	1647	1/1	0.99	0.09	57,57,57,57	0
55	MG	AR	205	1/1	0.99	0.31	110,110,110,110	0
55	MG	CA	3662	1/1	0.99	0.67	76,76,76,76	0
55	MG	AA	4196	1/1	0.99	0.34	24,24,24,24	0

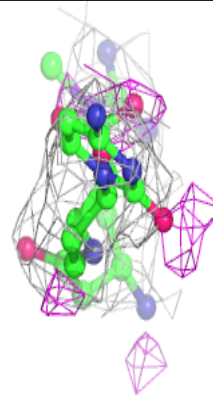
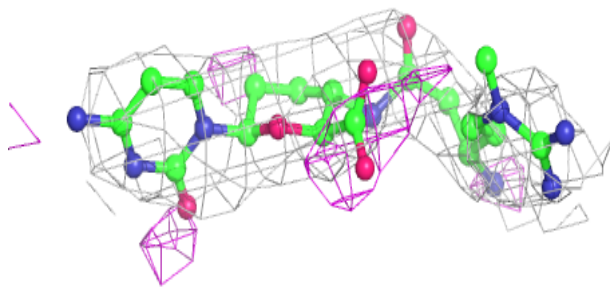
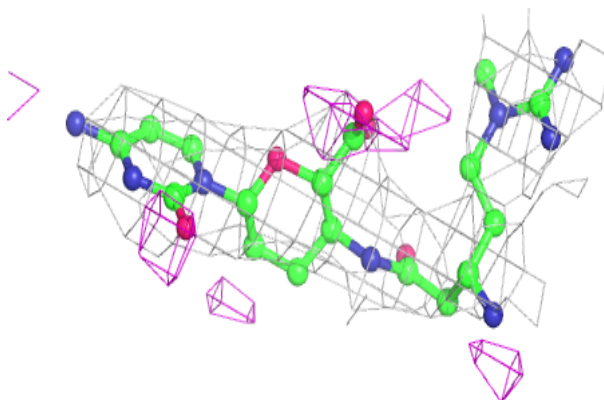
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BLS AA 4001:

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

**Electron density around BLS CA 4405:**

$2mF_o-DF_c$ (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.