



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 04:39 am BST

PDB ID : 4V9N
Title : Crystal structure of the 70S ribosome bound with the Q253P mutant of release factor RF2.
Authors : Santos, N.; Zhu, J.; Donohue, J.P.; Korostelev, A.A.; Noller, H.F.
Deposited on : 2013-04-26
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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

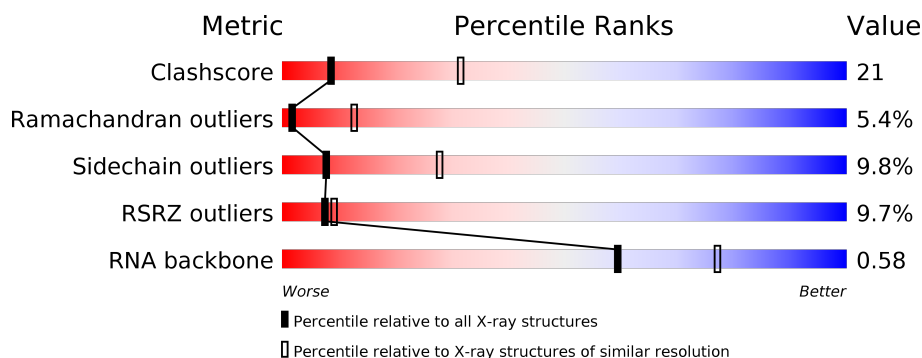
1 Overall quality at a glance

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))
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	1504	<div> <div>2%</div> <div> <div>44%</div> <div>46%</div> <div>10%</div> </div> </div>
1	CA	1504	<div> <div>3%</div> <div> <div>44%</div> <div>46%</div> <div>10%</div> </div> </div>
2	AV	10	<div> <div>10%</div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	CV	10	<div> <div>30%</div> <div> <div>40%</div> <div>60%</div> </div> </div>
3	AW	77	<div> <div>%</div> <div> <div>60%</div> <div>35%</div> <div>5%</div> </div> </div>
3	CW	77	<div> <div>%</div> <div> <div>58%</div> <div>36%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	AY	362	
4	CY	362	
5	AB	234	
5	CB	234	
6	AC	206	
6	CC	206	
7	AD	208	
7	CD	208	
8	AE	151	
8	CE	151	
9	AF	101	
9	CF	101	
10	AG	155	
10	CG	155	
11	AH	138	
11	CH	138	
12	AI	127	
12	CI	127	
13	AJ	98	
13	CJ	98	
14	AK	114	
14	CK	114	
15	AL	122	
15	CL	122	
16	AM	117	

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Mol	Chain	Length	Quality of chain
16	CM	117	
17	AN	60	
17	CN	60	
18	AO	88	
18	CO	88	
19	AP	83	
19	CP	83	
20	AQ	99	
20	CQ	99	
21	AR	70	
21	CR	70	
22	AS	78	
22	CS	78	
23	AT	99	
23	CT	99	
24	AU	24	
24	CU	24	
25	BA	2879	
25	DA	2879	
26	BB	119	
26	DB	119	
27	BD	271	
27	DD	271	
28	BE	204	
28	DE	204	

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Mol	Chain	Length	Quality of chain
29	BF	202	
29	DF	202	
30	BG	181	
30	DG	181	
31	BH	159	
31	DH	159	
32	BI	145	
32	DI	145	
33	BK	147	
33	DK	147	
34	BN	137	
34	DN	137	
35	BO	122	
35	DO	122	
36	BP	146	
36	DP	146	
37	BQ	134	
37	DQ	134	
38	BR	117	
38	DR	117	
39	BS	98	
39	DS	98	
40	BT	137	
40	DT	137	
41	BU	117	

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Mol	Chain	Length	Quality of chain
41	DU	117	
42	BV	101	
42	DV	101	
43	BW	112	
43	DW	112	
44	BX	92	
44	DX	92	
45	BY	100	
45	DY	100	
46	BZ	187	
46	DZ	187	
47	B0	76	
47	D0	76	
48	B1	88	
48	D1	88	
49	B2	62	
49	D2	62	
50	B3	59	
50	D3	59	
51	B4	30	
51	D4	30	
52	B5	52	
52	D5	52	
53	B6	44	
53	D6	44	

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Mol	Chain	Length	Quality of chain
54	B7	48	
54	D7	48	
55	B8	63	
55	D8	63	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1607	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1619	-	-	-	X
56	MG	AA	1622	-	-	-	X
56	MG	AA	1625	-	-	-	X
56	MG	AA	1629	-	-	-	X
56	MG	AA	1631	-	-	-	X
56	MG	AA	1632	-	-	-	X
56	MG	AA	1639	-	-	-	X
56	MG	AA	1672	-	-	-	X
56	MG	AA	1675	-	-	-	X
56	MG	AA	1686	-	-	-	X
56	MG	AA	1699	-	-	-	X
56	MG	AA	1702	-	-	-	X
56	MG	AA	1714	-	-	-	X
56	MG	AA	1725	-	-	-	X
56	MG	AA	1726	-	-	-	X
56	MG	AA	1727	-	-	-	X
56	MG	AA	1742	-	-	-	X
56	MG	AA	1744	-	-	-	X
56	MG	AA	1764	-	-	-	X
56	MG	AA	1765	-	-	-	X
56	MG	AA	1767	-	-	-	X
56	MG	AA	1772	-	-	-	X
56	MG	AA	1780	-	-	-	X
56	MG	AA	1782	-	-	-	X
56	MG	AA	1783	-	-	-	X
56	MG	AA	1786	-	-	-	X
56	MG	AA	1790	-	-	-	X
56	MG	AA	1796	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1804	-	-	-	X
56	MG	AA	1824	-	-	-	X
56	MG	AA	1825	-	-	-	X
56	MG	AA	1829	-	-	-	X
56	MG	AA	1831	-	-	-	X
56	MG	AA	1835	-	-	-	X
56	MG	AA	1839	-	-	-	X
56	MG	AA	1846	-	-	-	X
56	MG	AA	1854	-	-	-	X
56	MG	AA	1860	-	-	-	X
56	MG	AA	1874	-	-	-	X
56	MG	AA	1879	-	-	-	X
56	MG	AA	1897	-	-	-	X
56	MG	AA	1934	-	-	-	X
56	MG	AA	1941	-	-	-	X
56	MG	AA	1945	-	-	-	X
56	MG	AA	1947	-	-	-	X
56	MG	AA	1950	-	-	-	X
56	MG	AA	1951	-	-	-	X
56	MG	AA	1957	-	-	-	X
56	MG	AA	1979	-	-	-	X
56	MG	AC	301	-	-	-	X
56	MG	AG	201	-	-	-	X
56	MG	AT	203	-	-	-	X
56	MG	AW	102	-	-	-	X
56	MG	AW	104	-	-	-	X
56	MG	AW	107	-	-	-	X
56	MG	AW	109	-	-	-	X
56	MG	AW	112	-	-	-	X
56	MG	AY	401	-	-	-	X
56	MG	AY	403	-	-	-	X
56	MG	B0	102	-	-	-	X
56	MG	BA	2917	-	-	-	X
56	MG	BA	2918	-	-	-	X
56	MG	BA	2920	-	-	-	X
56	MG	BA	2922	-	-	-	X
56	MG	BA	2925	-	-	-	X
56	MG	BA	2926	-	-	-	X
56	MG	BA	2929	-	-	-	X
56	MG	BA	2930	-	-	-	X
56	MG	BA	2934	-	-	-	X
56	MG	BA	2935	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	2939	-	-	-	X
56	MG	BA	2943	-	-	-	X
56	MG	BA	2946	-	-	-	X
56	MG	BA	2949	-	-	-	X
56	MG	BA	2950	-	-	-	X
56	MG	BA	2959	-	-	-	X
56	MG	BA	2972	-	-	-	X
56	MG	BA	2973	-	-	-	X
56	MG	BA	2976	-	-	-	X
56	MG	BA	2992	-	-	-	X
56	MG	BA	2994	-	-	-	X
56	MG	BA	3003	-	-	-	X
56	MG	BA	3004	-	-	-	X
56	MG	BA	3011	-	-	-	X
56	MG	BA	3012	-	-	-	X
56	MG	BA	3020	-	-	-	X
56	MG	BA	3022	-	-	-	X
56	MG	BA	3032	-	-	-	X
56	MG	BA	3043	-	-	-	X
56	MG	BA	3053	-	-	-	X
56	MG	BA	3064	-	-	-	X
56	MG	BA	3073	-	-	-	X
56	MG	BA	3078	-	-	-	X
56	MG	BA	3084	-	-	-	X
56	MG	BA	3085	-	-	-	X
56	MG	BA	3092	-	-	-	X
56	MG	BA	3093	-	-	-	X
56	MG	BA	3095	-	-	-	X
56	MG	BA	3097	-	-	-	X
56	MG	BA	3098	-	-	-	X
56	MG	BA	3119	-	-	-	X
56	MG	BA	3121	-	-	-	X
56	MG	BA	3128	-	-	-	X
56	MG	BA	3130	-	-	-	X
56	MG	BA	3139	-	-	-	X
56	MG	BA	3141	-	-	-	X
56	MG	BA	3143	-	-	-	X
56	MG	BA	3147	-	-	-	X
56	MG	BA	3156	-	-	-	X
56	MG	BA	3157	-	-	-	X
56	MG	BA	3168	-	-	-	X
56	MG	BA	3173	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3175	-	-	-	X
56	MG	BA	3180	-	-	-	X
56	MG	BA	3182	-	-	-	X
56	MG	BA	3185	-	-	-	X
56	MG	BA	3186	-	-	-	X
56	MG	BA	3188	-	-	-	X
56	MG	BA	3189	-	-	-	X
56	MG	BA	3205	-	-	-	X
56	MG	BA	3211	-	-	-	X
56	MG	BA	3213	-	-	-	X
56	MG	BA	3218	-	-	-	X
56	MG	BA	3224	-	-	-	X
56	MG	BA	3229	-	-	-	X
56	MG	BA	3230	-	-	-	X
56	MG	BA	3237	-	-	-	X
56	MG	BA	3239	-	-	-	X
56	MG	BA	3244	-	-	-	X
56	MG	BA	3247	-	-	-	X
56	MG	BA	3248	-	-	-	X
56	MG	BA	3252	-	-	-	X
56	MG	BA	3256	-	-	-	X
56	MG	BA	3257	-	-	-	X
56	MG	BA	3261	-	-	-	X
56	MG	BA	3264	-	-	-	X
56	MG	BA	3267	-	-	-	X
56	MG	BA	3270	-	-	-	X
56	MG	BA	3275	-	-	-	X
56	MG	BA	3278	-	-	-	X
56	MG	BA	3284	-	-	-	X
56	MG	BA	3297	-	-	-	X
56	MG	BA	3299	-	-	-	X
56	MG	BA	3332	-	-	-	X
56	MG	BA	3369	-	-	-	X
56	MG	BA	3377	-	-	-	X
56	MG	BA	3403	-	-	-	X
56	MG	BA	3407	-	-	-	X
56	MG	BA	3414	-	-	-	X
56	MG	BA	3435	-	-	-	X
56	MG	BA	3450	-	-	-	X
56	MG	BA	3462	-	-	-	X
56	MG	BA	3465	-	-	-	X
56	MG	BA	3479	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	BA	3482	-	-	-	X
56	MG	BA	3496	-	-	-	X
56	MG	BA	3514	-	-	-	X
56	MG	BA	3517	-	-	-	X
56	MG	BA	3536	-	-	-	X
56	MG	BA	3540	-	-	-	X
56	MG	BA	3546	-	-	-	X
56	MG	BA	3548	-	-	-	X
56	MG	BA	3553	-	-	-	X
56	MG	BA	3563	-	-	-	X
56	MG	BA	3569	-	-	-	X
56	MG	BA	3577	-	-	-	X
56	MG	BA	3583	-	-	-	X
56	MG	BA	3584	-	-	-	X
56	MG	BA	3588	-	-	-	X
56	MG	BA	3591	-	-	-	X
56	MG	BA	3597	-	-	-	X
56	MG	BA	3599	-	-	-	X
56	MG	BA	3600	-	-	-	X
56	MG	BA	3602	-	-	-	X
56	MG	BA	3612	-	-	-	X
56	MG	BA	3613	-	-	-	X
56	MG	BA	3616	-	-	-	X
56	MG	BA	3618	-	-	-	X
56	MG	BA	3622	-	-	-	X
56	MG	BA	3628	-	-	-	X
56	MG	BA	3629	-	-	-	X
56	MG	BA	3639	-	-	-	X
56	MG	BA	3641	-	-	-	X
56	MG	BA	3650	-	-	-	X
56	MG	BA	3655	-	-	-	X
56	MG	BA	3661	-	-	-	X
56	MG	BA	3672	-	-	-	X
56	MG	BA	3676	-	-	-	X
56	MG	BA	3713	-	-	-	X
56	MG	BB	208	-	-	-	X
56	MG	BB	211	-	-	-	X
56	MG	BB	216	-	-	-	X
56	MG	BB	223	-	-	-	X
56	MG	BE	301	-	-	-	X
56	MG	CA	1607	-	-	-	X
56	MG	CA	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	1614	-	-	-	X
56	MG	CA	1626	-	-	-	X
56	MG	CA	1631	-	-	-	X
56	MG	CA	1644	-	-	-	X
56	MG	CA	1645	-	-	-	X
56	MG	CA	1647	-	-	-	X
56	MG	CA	1658	-	-	-	X
56	MG	CA	1663	-	-	-	X
56	MG	CA	1665	-	-	-	X
56	MG	CA	1669	-	-	-	X
56	MG	CA	1675	-	-	-	X
56	MG	CA	1677	-	-	-	X
56	MG	CA	1678	-	-	-	X
56	MG	CA	1681	-	-	-	X
56	MG	CA	1683	-	-	-	X
56	MG	CA	1693	-	-	-	X
56	MG	CA	1699	-	-	-	X
56	MG	CA	1704	-	-	-	X
56	MG	CA	1710	-	-	-	X
56	MG	CA	1719	-	-	-	X
56	MG	CA	1720	-	-	-	X
56	MG	CA	1725	-	-	-	X
56	MG	CA	1732	-	-	-	X
56	MG	CA	1735	-	-	-	X
56	MG	CA	1737	-	-	-	X
56	MG	CA	1747	-	-	-	X
56	MG	CA	1748	-	-	-	X
56	MG	CA	1752	-	-	-	X
56	MG	CA	1772	-	-	-	X
56	MG	CA	1780	-	-	-	X
56	MG	CA	1790	-	-	-	X
56	MG	CA	1792	-	-	-	X
56	MG	CA	1800	-	-	-	X
56	MG	CA	1807	-	-	-	X
56	MG	CA	1808	-	-	-	X
56	MG	CA	1809	-	-	-	X
56	MG	CA	1810	-	-	-	X
56	MG	CA	1812	-	-	-	X
56	MG	CA	1816	-	-	-	X
56	MG	CA	1820	-	-	-	X
56	MG	CA	1833	-	-	-	X
56	MG	CA	1840	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	1842	-	-	-	X
56	MG	CA	1854	-	-	-	X
56	MG	CA	1874	-	-	-	X
56	MG	CA	1877	-	-	-	X
56	MG	CA	1882	-	-	-	X
56	MG	CA	1884	-	-	-	X
56	MG	CA	1887	-	-	-	X
56	MG	CA	1900	-	-	-	X
56	MG	CA	1902	-	-	-	X
56	MG	CA	1907	-	-	-	X
56	MG	CA	1911	-	-	-	X
56	MG	CA	1912	-	-	-	X
56	MG	CA	1926	-	-	-	X
56	MG	CD	302	-	-	-	X
56	MG	CM	201	-	-	-	X
56	MG	CW	102	-	-	-	X
56	MG	CW	105	-	-	-	X
56	MG	CY	401	-	-	-	X
56	MG	D7	101	-	-	-	X
56	MG	DA	2903	-	-	-	X
56	MG	DA	2911	-	-	-	X
56	MG	DA	2914	-	-	-	X
56	MG	DA	2915	-	-	-	X
56	MG	DA	2916	-	-	-	X
56	MG	DA	2917	-	-	-	X
56	MG	DA	2930	-	-	-	X
56	MG	DA	2936	-	-	-	X
56	MG	DA	2937	-	-	-	X
56	MG	DA	2948	-	-	-	X
56	MG	DA	2949	-	-	-	X
56	MG	DA	2964	-	-	-	X
56	MG	DA	2972	-	-	-	X
56	MG	DA	2975	-	-	-	X
56	MG	DA	2989	-	-	-	X
56	MG	DA	3001	-	-	-	X
56	MG	DA	3003	-	-	-	X
56	MG	DA	3004	-	-	-	X
56	MG	DA	3008	-	-	-	X
56	MG	DA	3009	-	-	-	X
56	MG	DA	3016	-	-	-	X
56	MG	DA	3030	-	-	-	X
56	MG	DA	3033	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3044	-	-	-	X
56	MG	DA	3052	-	-	-	X
56	MG	DA	3054	-	-	-	X
56	MG	DA	3062	-	-	-	X
56	MG	DA	3066	-	-	-	X
56	MG	DA	3070	-	-	-	X
56	MG	DA	3072	-	-	-	X
56	MG	DA	3073	-	-	-	X
56	MG	DA	3086	-	-	-	X
56	MG	DA	3092	-	-	-	X
56	MG	DA	3097	-	-	-	X
56	MG	DA	3107	-	-	-	X
56	MG	DA	3119	-	-	-	X
56	MG	DA	3188	-	-	-	X
56	MG	DA	3243	-	-	-	X
56	MG	DA	3248	-	-	-	X
56	MG	DA	3270	-	-	-	X
56	MG	DA	3287	-	-	-	X
56	MG	DA	3308	-	-	-	X
56	MG	DA	3325	-	-	-	X
56	MG	DA	3326	-	-	-	X
56	MG	DA	3338	-	-	-	X
56	MG	DA	3343	-	-	-	X
56	MG	DA	3348	-	-	-	X
56	MG	DA	3351	-	-	-	X
56	MG	DA	3375	-	-	-	X
56	MG	DA	3381	-	-	-	X
56	MG	DA	3385	-	-	-	X
56	MG	DA	3398	-	-	-	X
56	MG	DA	3403	-	-	-	X
56	MG	DA	3427	-	-	-	X
56	MG	DA	3428	-	-	-	X
56	MG	DA	3484	-	-	-	X
56	MG	DA	3498	-	-	-	X
56	MG	DA	3502	-	-	-	X
56	MG	DA	3510	-	-	-	X
56	MG	DA	3516	-	-	-	X
56	MG	DA	3517	-	-	-	X
56	MG	DA	3519	-	-	-	X
56	MG	DA	3531	-	-	-	X
56	MG	DA	3541	-	-	-	X
56	MG	DA	3544	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3548	-	-	-	X
56	MG	DA	3568	-	-	-	X
56	MG	DA	3577	-	-	-	X
56	MG	DA	3586	-	-	-	X
56	MG	DA	3611	-	-	-	X
56	MG	DB	206	-	-	-	X
56	MG	DB	209	-	-	-	X
56	MG	DB	218	-	-	-	X
56	MG	DF	301	-	-	-	X
56	MG	DV	201	-	-	-	X
56	MG	DW	201	-	-	-	X

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 294074 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 16S rRNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

- Molecule 2 is a RNA chain called messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			
2	CV	10	Total	C	N	O	P	0	0	0
			214	98	44	63	9			

- Molecule 3 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
3	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 4 is a protein called Bacterial peptide chain release factor 2 (RF-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AY	362	Total	C	N	O	S	0	0	0
			2874	1794	517	555	8			
4	CY	362	Total	C	N	O	S	0	0	0
			2874	1794	517	555	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	253	PRO	GLN	ENGINEERED MUTATION	UNP Q72GJ6
CY	253	PRO	GLN	ENGINEERED MUTATION	UNP Q72GJ6

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
5	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
6	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
7	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			
8	CE	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
9	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
10	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
11	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
12	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
13	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			
14	CK	114	Total	C	N	O	S	0	0	0
			843	522	159	159	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			
15	CL	122	Total	C	N	O	S	0	0	0
			957	603	193	160	1			

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			
16	CM	117	Total	C	N	O	S	0	0	0
			934	577	192	163	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
17	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
18	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
19	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CQ	99	Total	C	N	O	S	0	0	0
			824	528	152	142	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AR	70	Total	C	N	O		0	0	0
			574	367	112	95				
21	CR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
22	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
23	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2789	Total	C	N	O	P	0	0	0
			60059	26734	11225	19312	2788			
25	DA	2789	Total	C	N	O	P	0	0	0
			60059	26734	11225	19312	2788			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	276	C	A	CONFLICT	GB AE017221.1
BA	277	A	C	CONFLICT	GB AE017221.1
BA	1141A	U	C	CONFLICT	GB AE017221.1
BA	2825	U	G	CONFLICT	GB AE017221.1
DA	276	C	A	CONFLICT	GB AE017221.1
DA	277	A	C	CONFLICT	GB AE017221.1
DA	1141A	U	C	CONFLICT	GB AE017221.1
DA	2825	U	G	CONFLICT	GB AE017221.1

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
26	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
27	DD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
28	DE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
29	DF	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
31	DH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
32	DI	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			
33	DK	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
34	DN	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			
37	DQ	134	Total	C	N	O	S	0	0	0
			1065	680	201	179	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	98	Total	C	N	O		0	0	0
			771	486	154	131				
39	DS	98	Total	C	N	O		0	0	0
			771	486	154	131				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DT	137	Total	C	N	O	S	0	0	0
			1144	713	234	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
43	DW	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BX	92	Total	C	N	O	0	0	0
			726	471	131	124			
44	DX	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
45	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			
46	DZ	187	Total	C	N	O	S	0	0	0
			1483	945	264	272	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
47	D0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	88	Total	C	N	O	0	0	0
			695	435	141	119			
48	D1	88	Total	C	N	O	0	0	0
			695	435	141	119			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			
49	D2	62	Total	C	N	O	S	0	0	0
			521	325	102	92	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
50	D3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
51	D4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			
52	D5	52	Total	C	N	O	S	0	0	0
			405	255	79	66	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
53	D6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
54	D7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
55	D8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	824	Total	Mg	0	0
			824	824		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CA	326	Total 326	Mg 326	0	0
56	DQ	4	Total 4	Mg 4	0	0
56	DF	2	Total 2	Mg 2	0	0
56	CV	2	Total 2	Mg 2	0	0
56	B8	2	Total 2	Mg 2	0	0
56	BE	1	Total 1	Mg 1	0	0
56	AW	18	Total 18	Mg 18	0	0
56	B1	1	Total 1	Mg 1	0	0
56	CD	1	Total 1	Mg 1	0	0
56	BP	1	Total 1	Mg 1	0	0
56	CR	1	Total 1	Mg 1	0	0
56	DN	1	Total 1	Mg 1	0	0
56	CY	2	Total 2	Mg 2	0	0
56	B5	1	Total 1	Mg 1	0	0
56	BB	23	Total 23	Mg 23	0	0
56	BT	1	Total 1	Mg 1	0	0
56	BF	1	Total 1	Mg 1	0	0
56	AV	1	Total 1	Mg 1	0	0
56	BX	2	Total 2	Mg 2	0	0
56	AA	393	Total 393	Mg 393	0	0
56	D7	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DV	1	Total 1	Mg 1	0	0
56	DI	2	Total 2	Mg 2	0	0
56	DD	1	Total 1	Mg 1	0	0
56	CM	1	Total 1	Mg 1	0	0
56	D0	1	Total 1	Mg 1	0	0
56	BY	1	Total 1	Mg 1	0	0
56	B3	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	DA	732	Total 732	Mg 732	0	0
56	DW	2	Total 2	Mg 2	0	0
56	DH	1	Total 1	Mg 1	0	0
56	AG	1	Total 1	Mg 1	0	0
56	DE	1	Total 1	Mg 1	0	0
56	AQ	1	Total 1	Mg 1	0	0
56	D1	1	Total 1	Mg 1	0	0
56	DP	2	Total 2	Mg 2	0	0
56	AC	1	Total 1	Mg 1	0	0
56	CW	16	Total 16	Mg 16	0	0
56	D5	3	Total 3	Mg 3	0	0
56	BD	1	Total 1	Mg 1	0	0
56	AT	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B0	2	Total 2	Mg 2	0	0
56	AO	1	Total 1	Mg 1	0	0
56	AY	3	Total 3	Mg 3	0	0
56	DB	20	Total 20	Mg 20	0	0

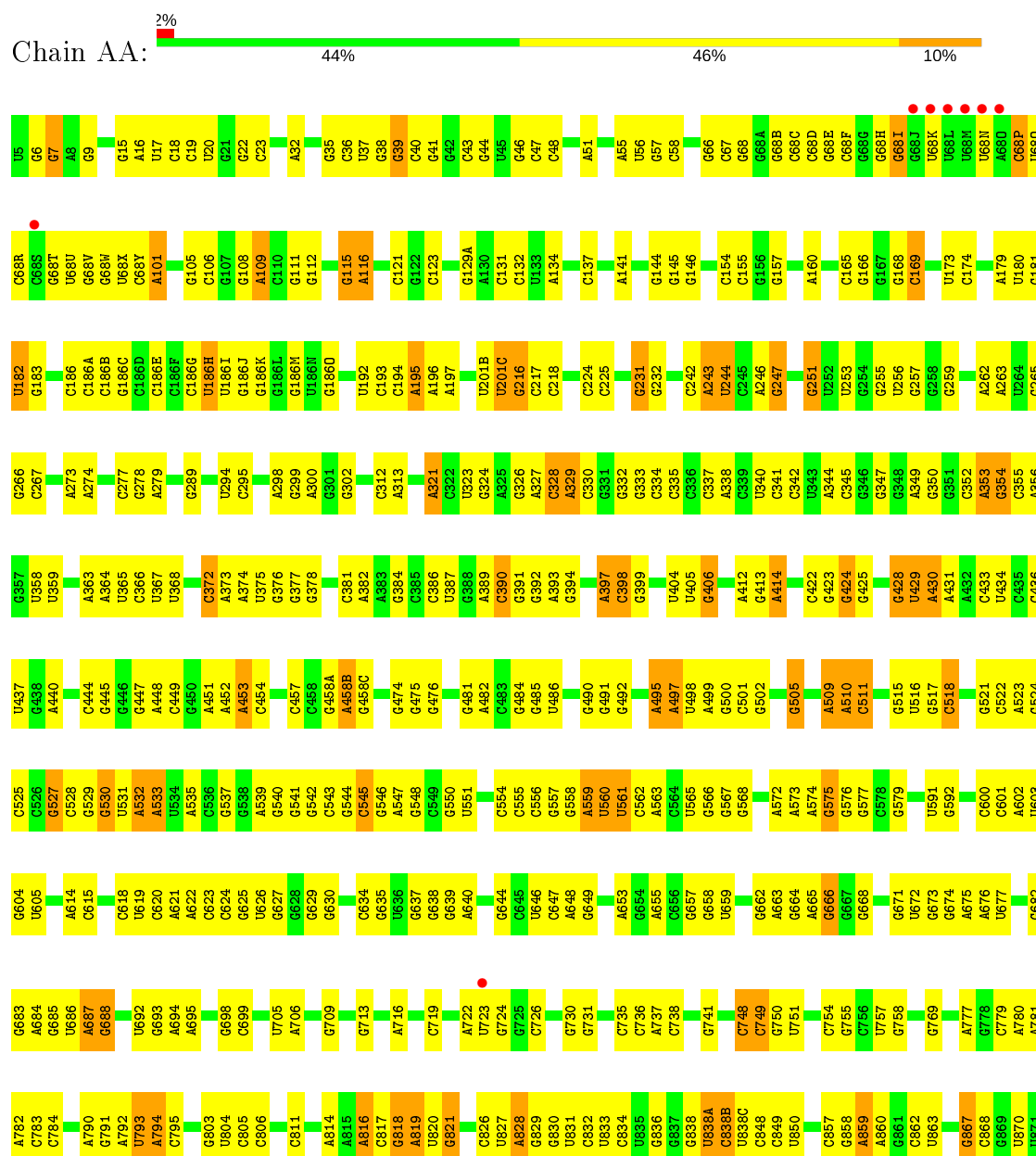
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

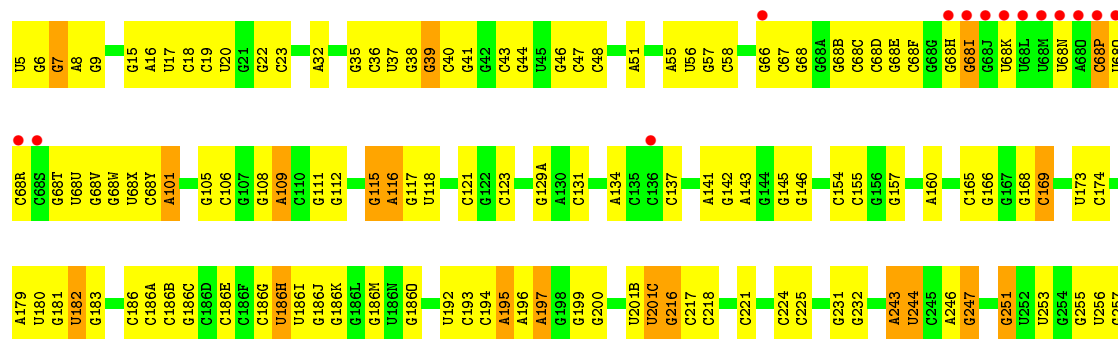
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CN	1	Total 1	Zn 1	0	0
57	AD	1	Total 1	Zn 1	0	0
57	CD	1	Total 1	Zn 1	0	0
57	AN	1	Total 1	Zn 1	0	0

3 Residue-property plots

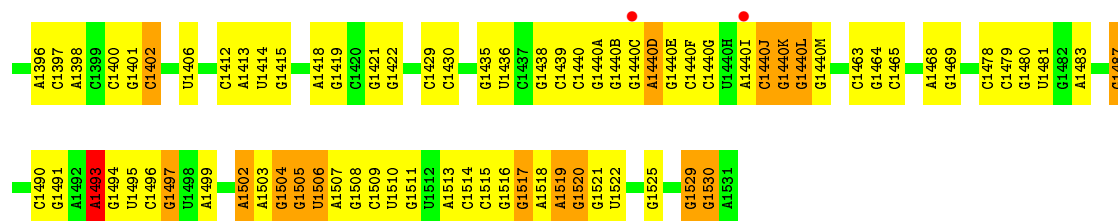
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S rRNA (1504-MER)

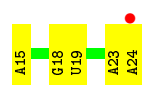




G1322	G1323	A1324	C1325	G1326	G1327	G1328	A1329	U1330	G1331	G1332	G1337	G1338	C1342	G1343	G1344	U1345	A1346	G1347	U1348	A1349	U1350	U1351	G1352	G1353	G1354	G1355	G1356	A1357	U1358	C1359	G1360	G1361	G1362	G1362A	A1363	U1364	G1365	G1366	C1367	G1368	C1369	G1370	G1371	U1372	G1373	A1374	U1375	U1376	A1377	C1378	G1379	U1380	G1386	G1387	U1390
G1253	C1254	G1255	A1256	U1257	G1258	C1259	A1260	G1261	C1262	C1263	G1264	G1265	A1269	G1270	G1271	G1272	U1273	G1274	U1278	A1279	A1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	G1290	G1291	G1292	G1293	G1294	G1295	C1298	A1299	G1300	U1301	C1302	C1303	G1304	G1305	A1306	G1309	U1313	C1314	G1315	G1316	C1317	C1320	C1321				
G1182	G1186	G1187	A1188	C1189	G1190	G1193	U1194	C1195	U1196	G1197	C1200	A1201	G1202	C1203	A1204	U1205	G1206	G1207	U1211	U1212	A1213	C1214	G1215	G1216	G1220	G1221	C1228	C1229	G1230	G1231	U1232	G1233	U1234	A1235	C1236	C1237	A1238	G1241	C1242	G1246	U1247	A1248	C1249	A1250	C1320	C1321									
C1109	A1110	A1111	C1112	G1115	C1116	G1117	C1118	C1119	G1120	A1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	U1136	C1137	G1138	G1139	C1140	G1141	G1142	C1145	A1146	C1147	U1148	C1149	A1152	C1153	G1154	G1155	G1156	A1157	C1158	U1159	G1160	G1164	A1169	A1170	G1171	C1172	G1173	A1176	G1177	U1178	A1179	A1180	G1181				
G1033	C1038	A1039	U1040	A1041	G1042	C1043	A1044	C1045	A1046	G1047	G1048	C1051	U1052	G1053	C1054	A1055	U1056	G1057	C1060	G1061	U1062	C1063	G1064	U1065	U1070	C1071	G1072	U1073	G1074	C1075	C1076	G1077	A1080	G1081	G1082	U1083	G1084	U1085	U1086	G1094	U1095	C1096	C1097	C1100	A1101	A1102	C1103	G1104	A1105	C1106	C1107	G1108			
U956	U957	A958	A959	U960	U961	A965	A968	A969	C970	G971	C972	G973	A974	G975	G976	A977	A978	C979	C980	U981	U982	C984	C985	A986	C989	C990	U991	U992	G993	A1000	G1001	G1002	G1003	A1004	G1009	G1010	G1013	A1014	A1015	A1016	G1017	U1025	G1026	C1027	C1028	C1028A	C1028D	G1028E	G1028H						
A872	C875	G878	G879	C880	G881	C882	U884	G885	U892	G893	C896	A900	A901	G902	A908	A909	C910	A913	A914	A915	U916	A919	U920	U921	G922	A923	C924	G925	G926	G927	C932	G933	C934	A935	C936	C937	G938A	C938B	U938C	C943	C949	U950	C957	G958	A959	A960	G961	C962	U963	G967	C968	G969	U991	U995	
A780	A781	A782	C783	C784	A786	U787	G788	A789	C795	G803	U804	C805	C806	C811	A814	A815	C817	G818	A819	U820	C821	C826	U827	A828	G829	C830	U831	C832	U833	C834	U835	C836	G837	G838	U838A	C838B	U838C	C843	C849	U850	C857	G858	A859	A860	G861	C862	U863	G867	C868	G869	U871				
C600	C601	A602	G603	G604	C613	C614	C615	C618	U619	C620	A621	G622	A623	C624	G625	U626	G627	G628	G629	C630	C634	G635	U636	G637	U638	G639	A640	C644	C645	U646	C647	A648	C649	A653	G654	A655	C656	G657	G658	U659	G662	A663	G664	A665	G666	G667	G668	G671	U672	G673	G674				
G521	C522	A523	G524	C525	C526	G527	G528	G529	G530	U531	A532	A533	U534	A535	C536	G537	G538	A539	G540	G541	C542	C543	G544	C545	C546	A547	G548	C549	G550	U551	C554	C555	C556	G557	G558	A559	U560	U561	C562	A563	C564	G565	G566	G567	G568	A572	A573	A574	G575	G576	G577	C578	G579	U591	G592
A430	A431	A432	C433	U434	C435	C436	U437	A438	A440	C444	C445	G446	G447	A448	C449	G450	A451	A452	A453	C454	G456A	A456B	G456C	G474	G475	G476	G481	G484	C485	U486	G490	G491	A495	A497	U498	A499	C501	G502	G505	A509	A510	C511	G515	U516	G517	C518	U529								
G350	G351	C352	A353	G354	C355	A356	A363	A364	C366	U367	C372	A373	A374	U375	G376	G377	G378	A381	A382	A383	C384	C385	C386	G387	A389	C390	G391	U392	G393	G394	A397	C398	G399	U404	U405	G406	G407	A408	G409	G410	A411	A412	G413	A414	C422	G423	A424	G425	G428	U429					
G258	G259	A262	G263	U264	G265	G266	C267	A273	A274	C277	G278	A279	G289	U294	C295	A298	G299	A300	G301	G302	A321	C322	U323	G324	A325	G326	A327	C328	A329	C330	G331	G332	G333	C334	C335	C336	C337	A338	C339	U340	C341	C342	U343	A344	C345	G346	G347	G348	A349						



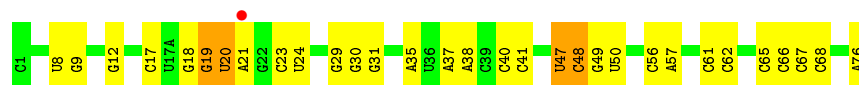
- Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')



- Molecule 2: messenger RNA (5'-R(*AP*AP*UP*GP*UP*AP*G)-3')



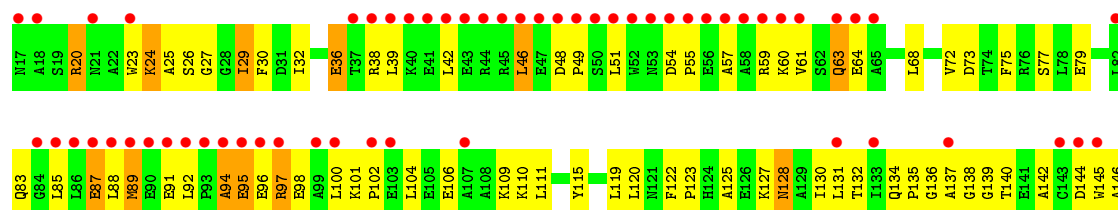
- Molecule 3: P-site tRNA-fMet

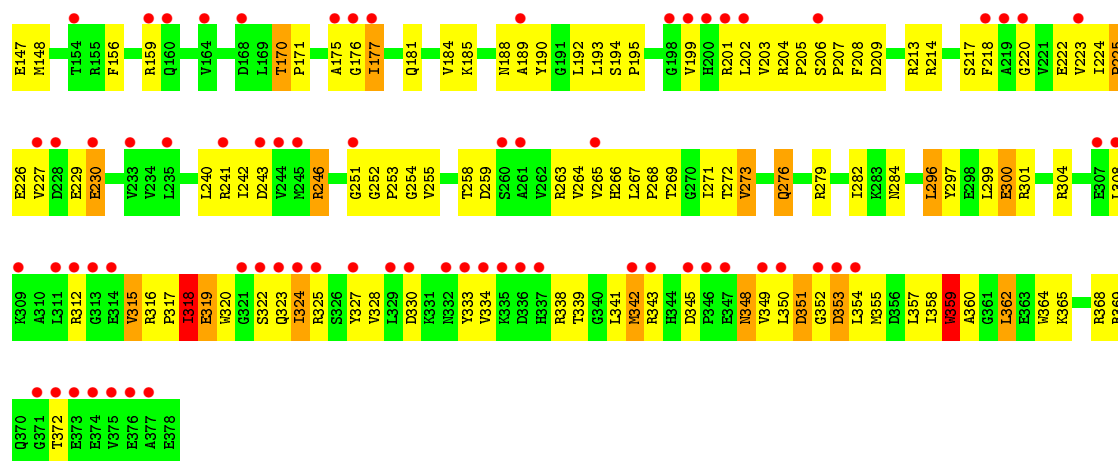


- Molecule 3: P-site tRNA-fMet

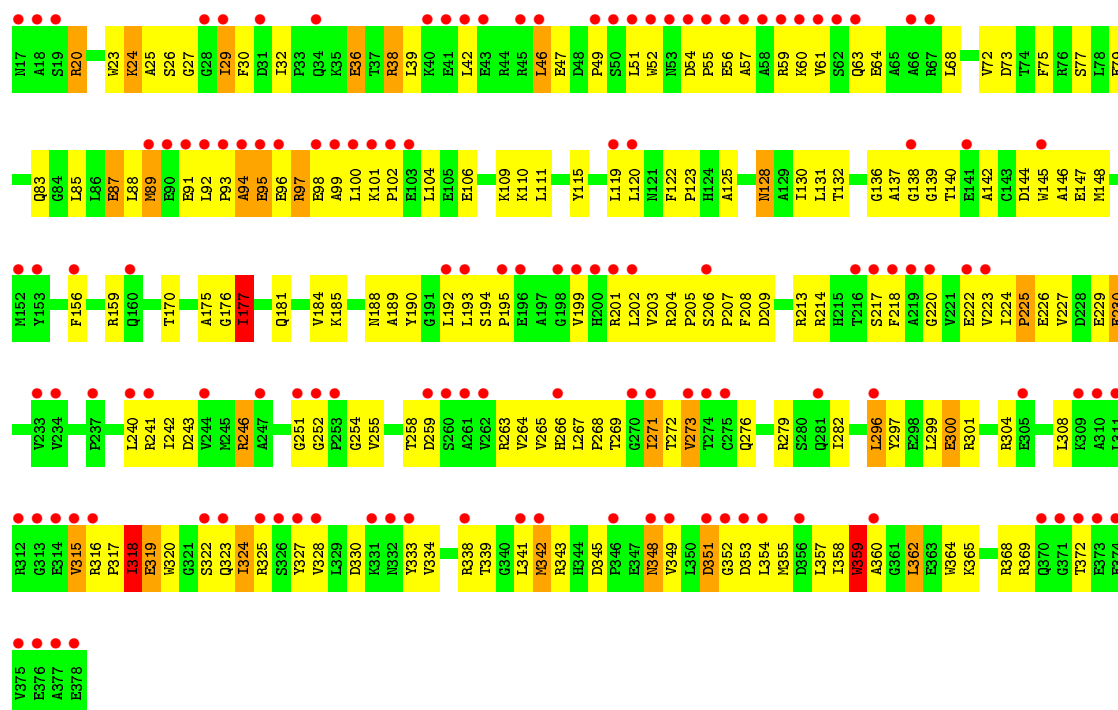


- Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

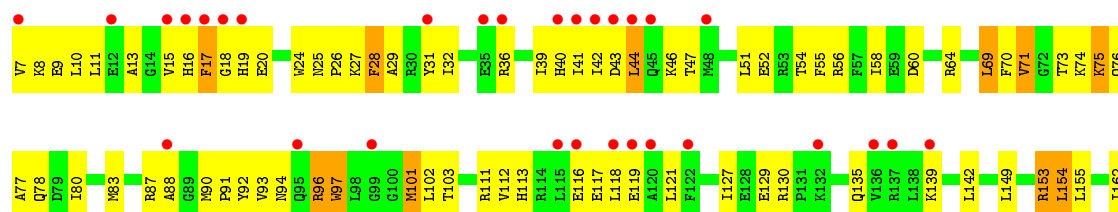


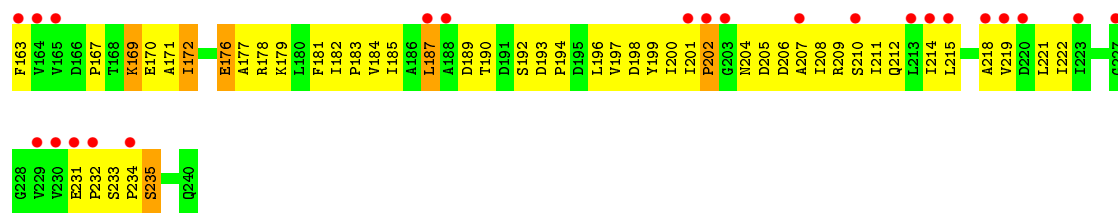


• Molecule 4: Bacterial peptide chain release factor 2 (RF-2)

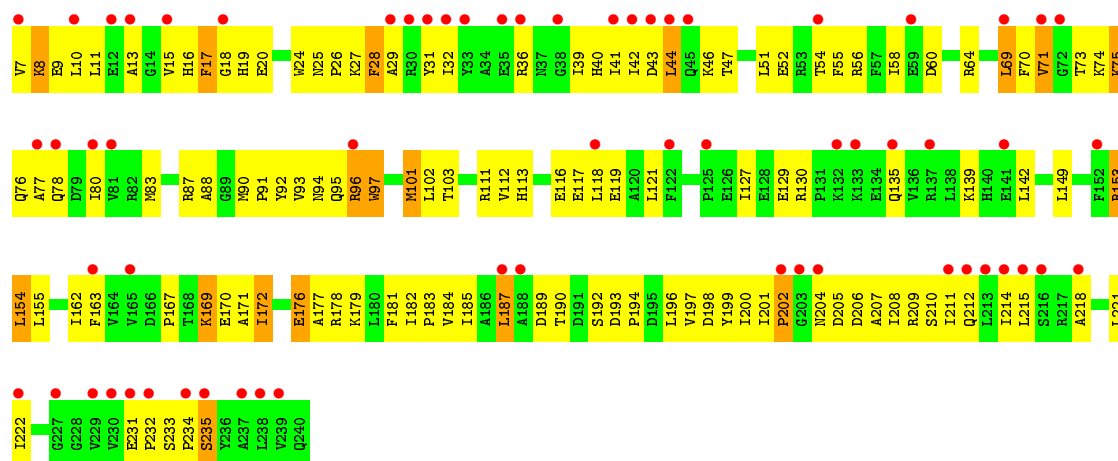


• Molecule 5: 30S ribosomal protein S2

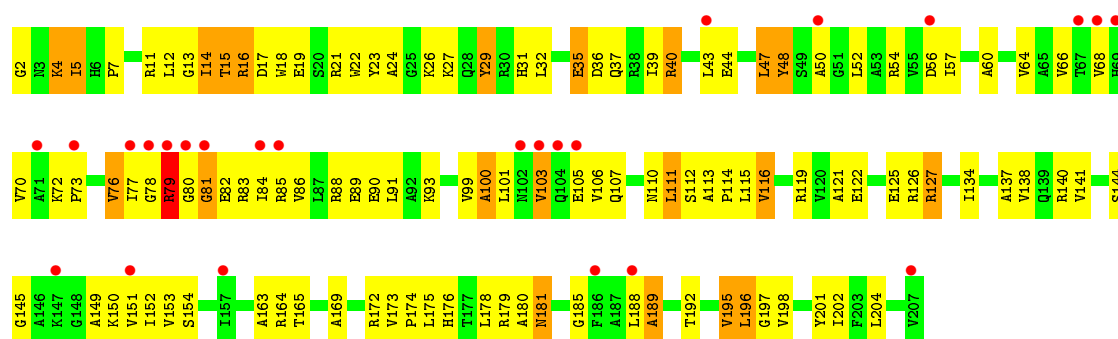




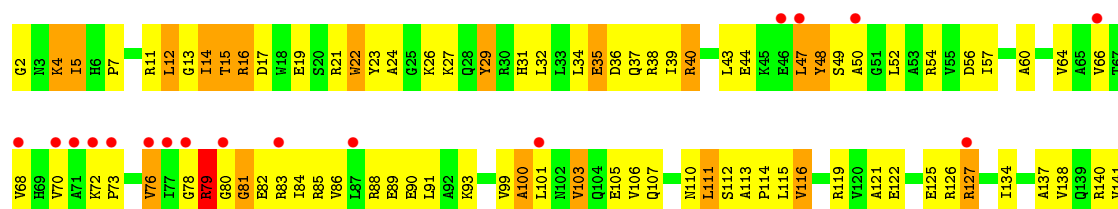
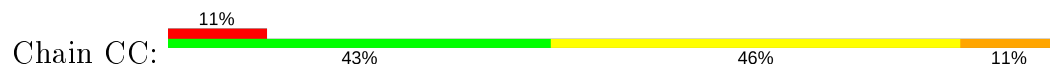
• Molecule 5: 30S ribosomal protein S2

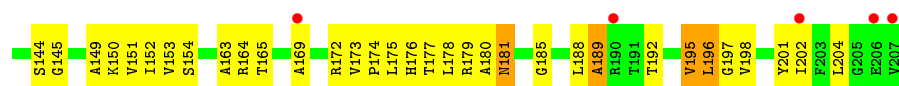


• Molecule 6: 30S ribosomal protein S3

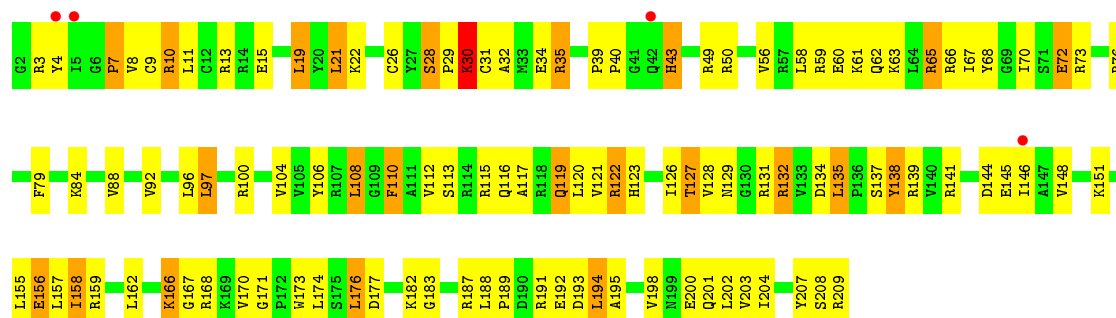


• Molecule 6: 30S ribosomal protein S3

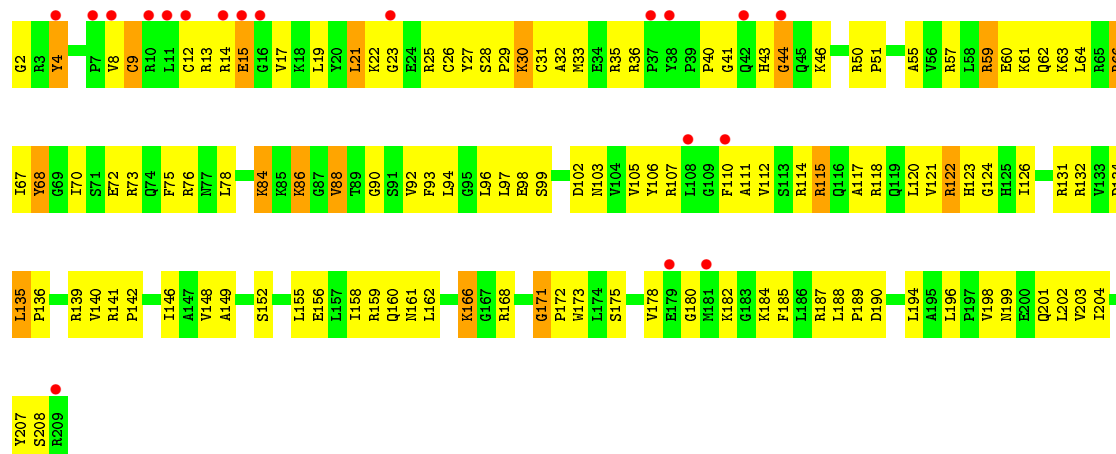




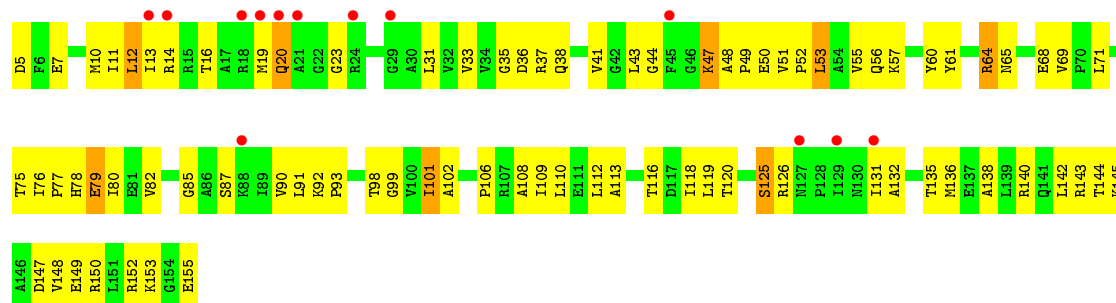
• Molecule 7: 30S ribosomal protein S4



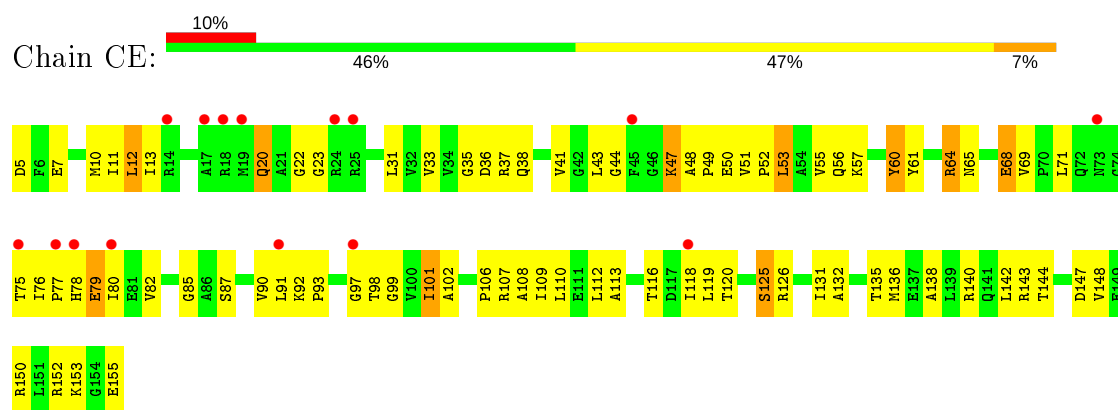
• Molecule 7: 30S ribosomal protein S4



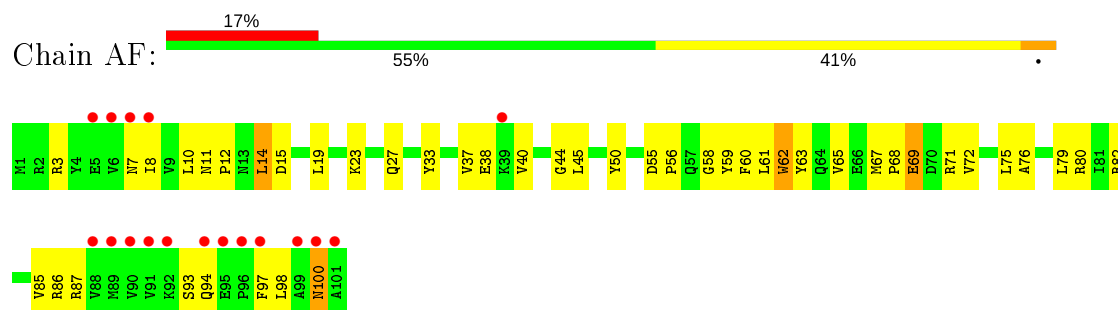
• Molecule 8: 30S ribosomal protein S5



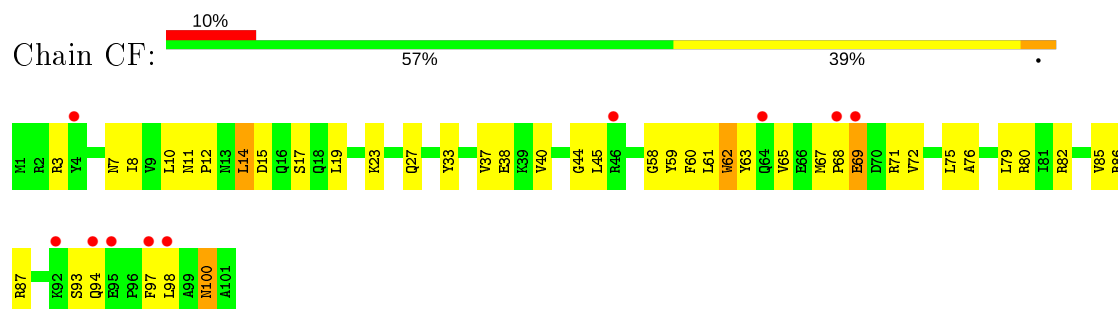
• Molecule 8: 30S ribosomal protein S5



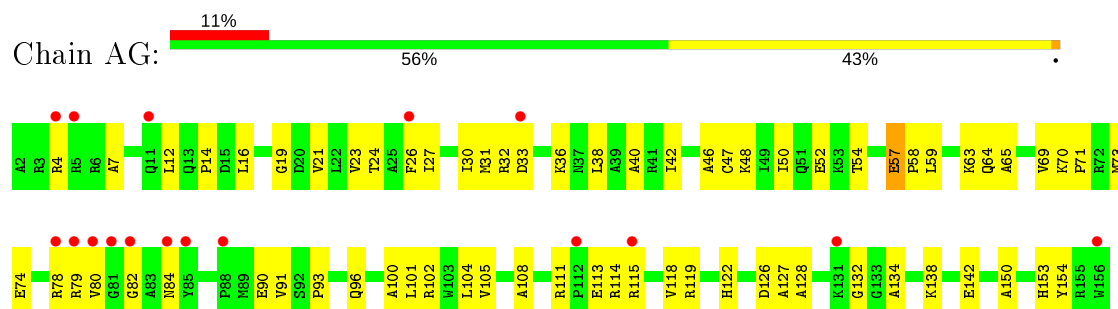
• Molecule 9: 30S ribosomal protein S6



• Molecule 9: 30S ribosomal protein S6

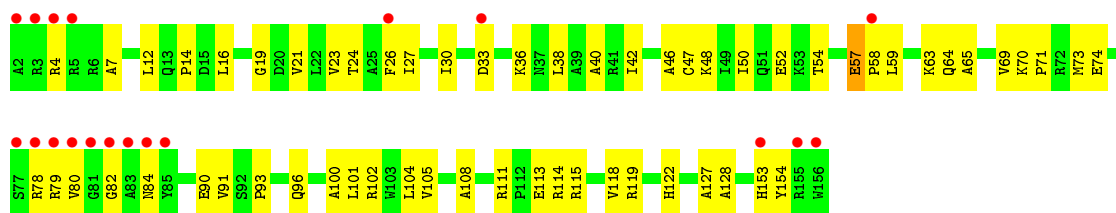


• Molecule 10: 30S ribosomal protein S7

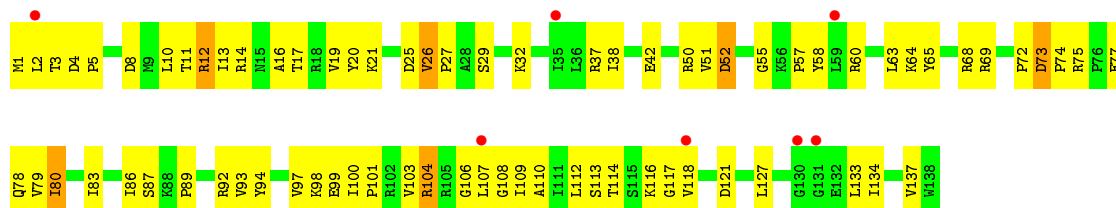


• Molecule 10: 30S ribosomal protein S7

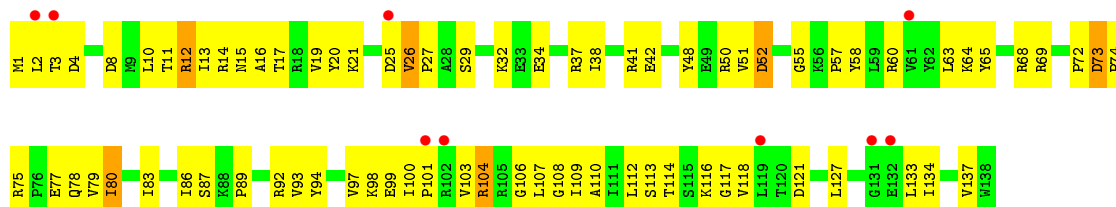




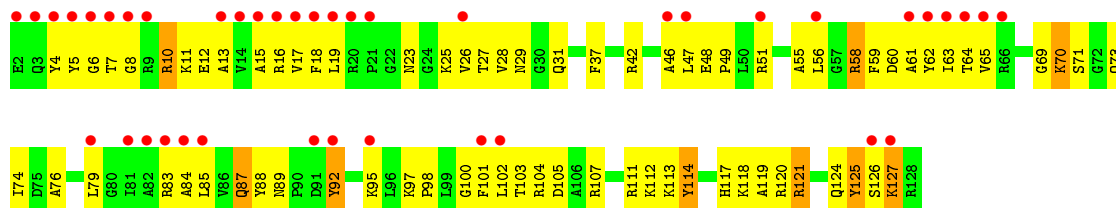
• Molecule 11: 30S ribosomal protein S8



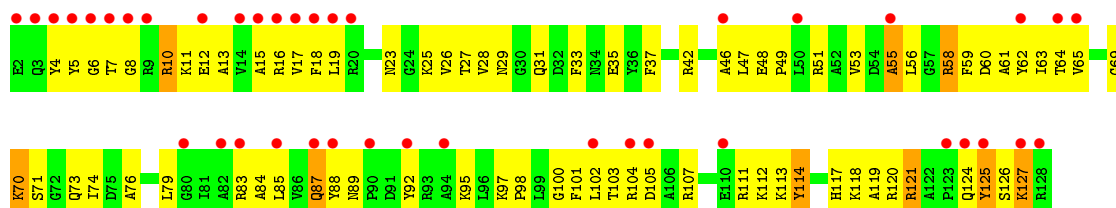
• Molecule 11: 30S ribosomal protein S8



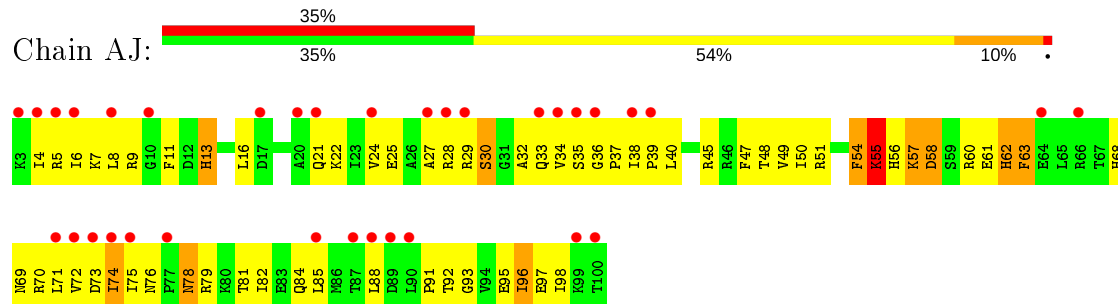
• Molecule 12: 30S ribosomal protein S9



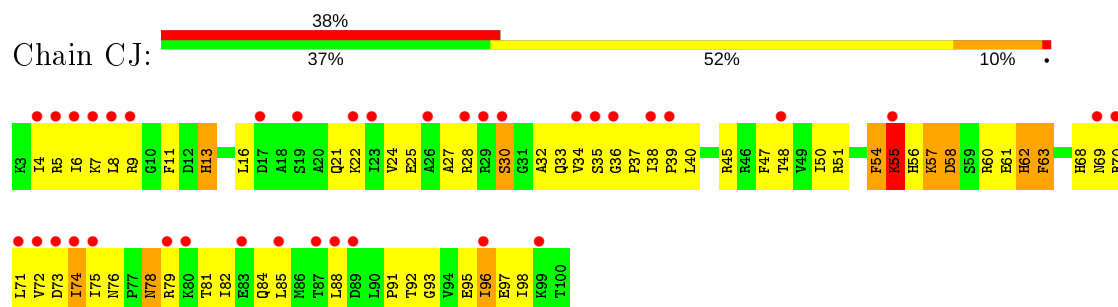
• Molecule 12: 30S ribosomal protein S9



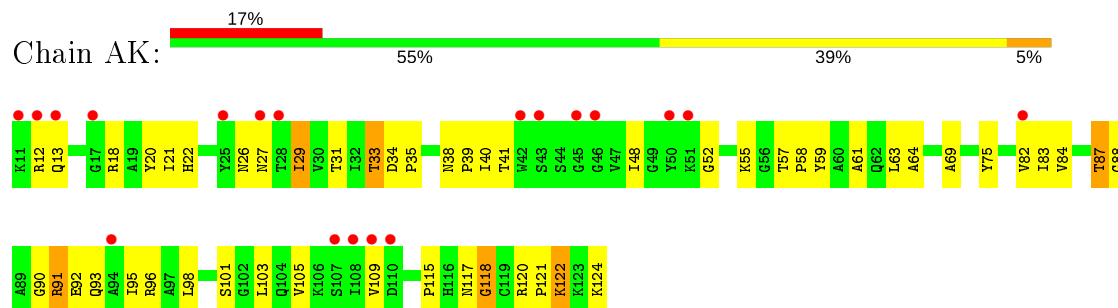
- Molecule 13: 30S ribosomal protein S10



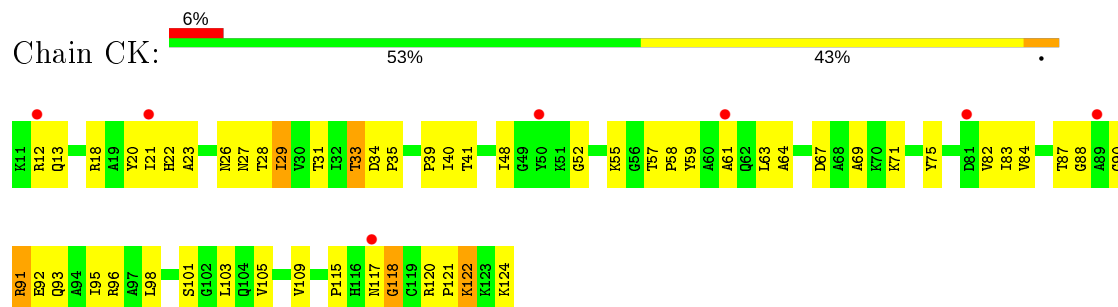
- Molecule 13: 30S ribosomal protein S10



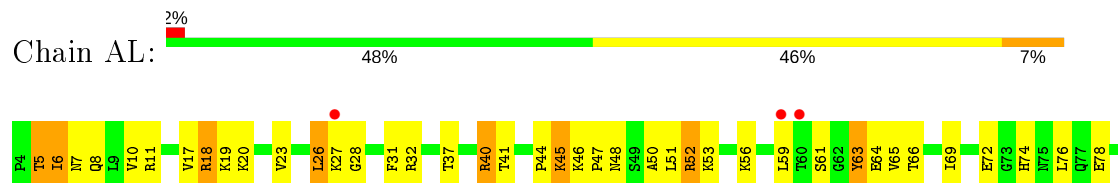
- Molecule 14: 30S ribosomal protein S11



- Molecule 14: 30S ribosomal protein S11



- Molecule 15: 30S ribosomal protein S12

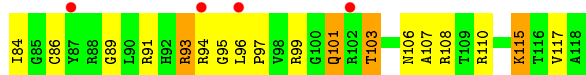




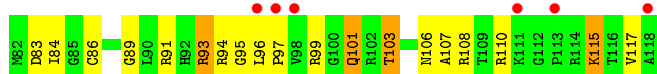
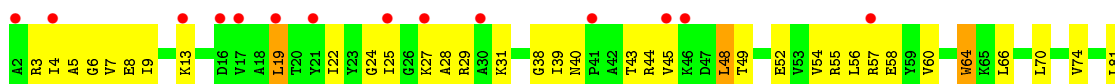
- Molecule 15: 30S ribosomal protein S12



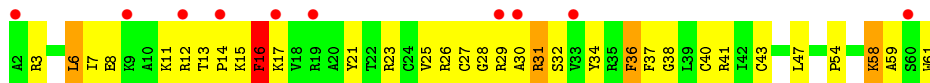
- Molecule 16: 30S ribosomal protein S13



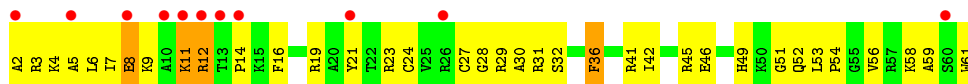
- Molecule 16: 30S ribosomal protein S13



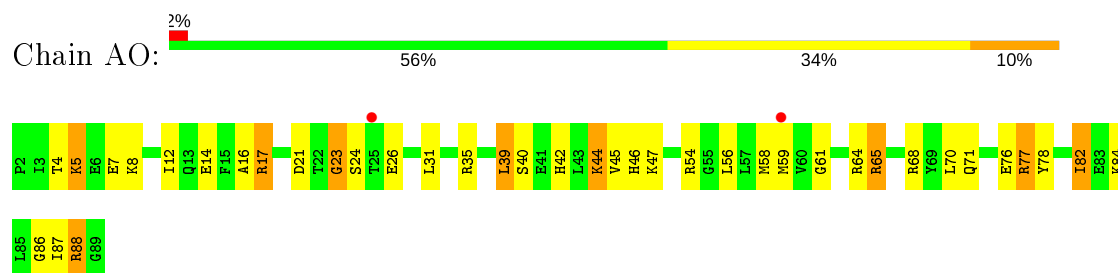
- Molecule 17: 30S ribosomal protein S14



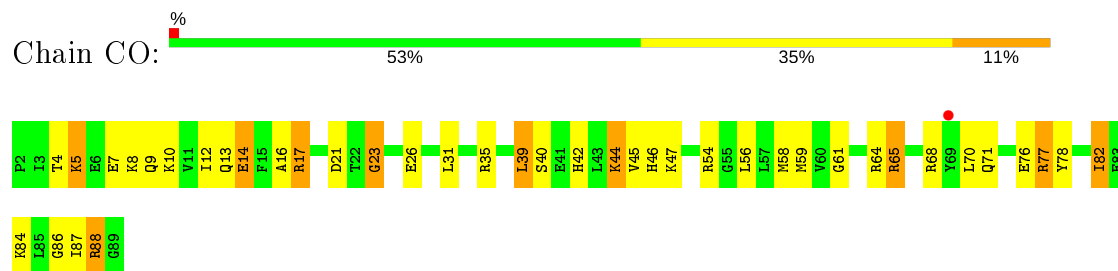
- Molecule 17: 30S ribosomal protein S14



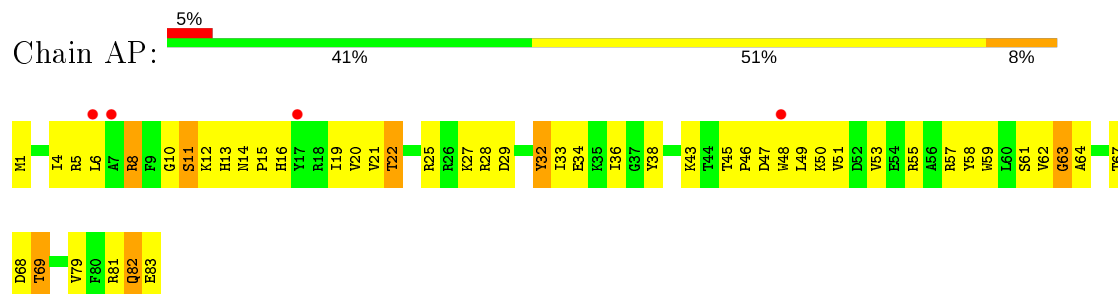
- Molecule 18: 30S ribosomal protein S15



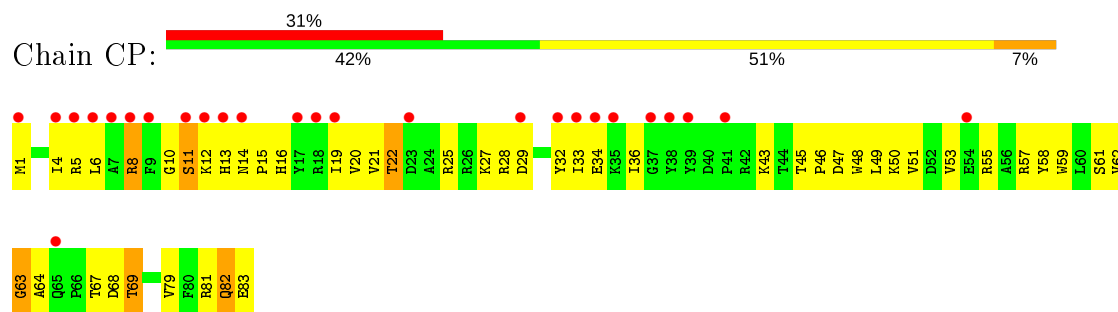
- Molecule 18: 30S ribosomal protein S15



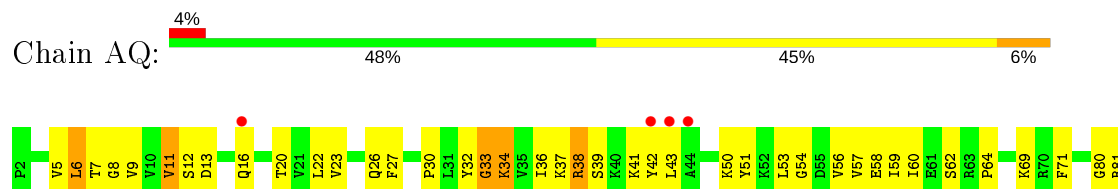
- Molecule 19: 30S ribosomal protein S16



- Molecule 19: 30S ribosomal protein S16

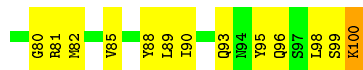
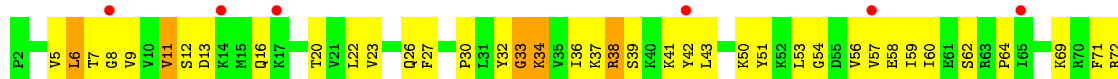


- Molecule 20: 30S ribosomal protein S17

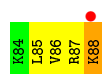
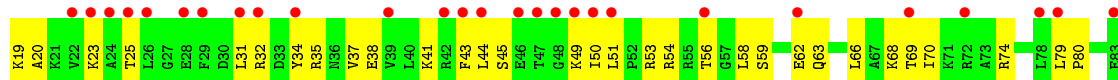
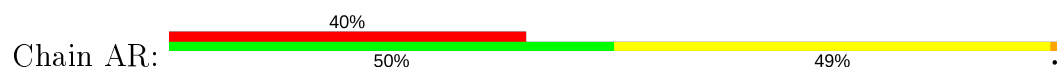




- Molecule 20: 30S ribosomal protein S17



- Molecule 21: 30S ribosomal protein S18



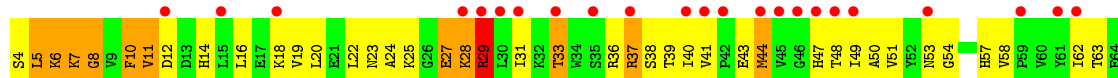
- Molecule 21: 30S ribosomal protein S18

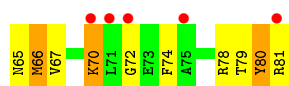


- Molecule 22: 30S ribosomal protein S19

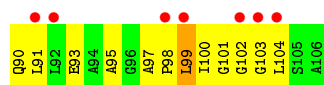
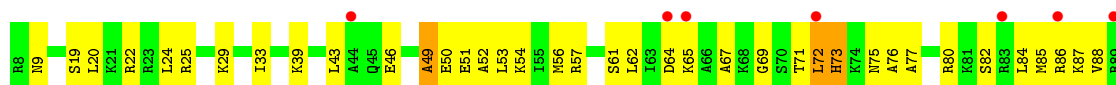


- Molecule 22: 30S ribosomal protein S19

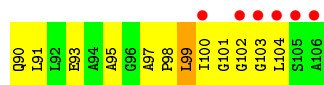




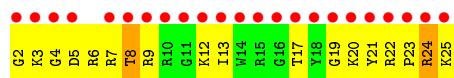
- Molecule 23: 30S ribosomal protein S20



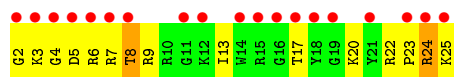
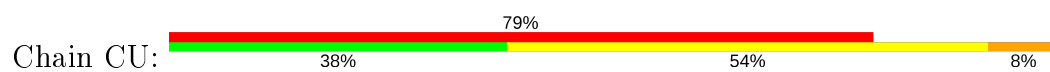
- Molecule 23: 30S ribosomal protein S20



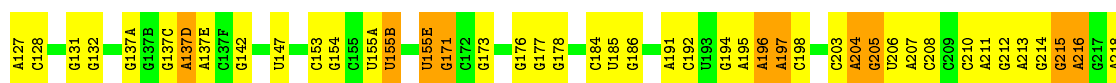
- Molecule 24: 30S ribosomal protein Thx

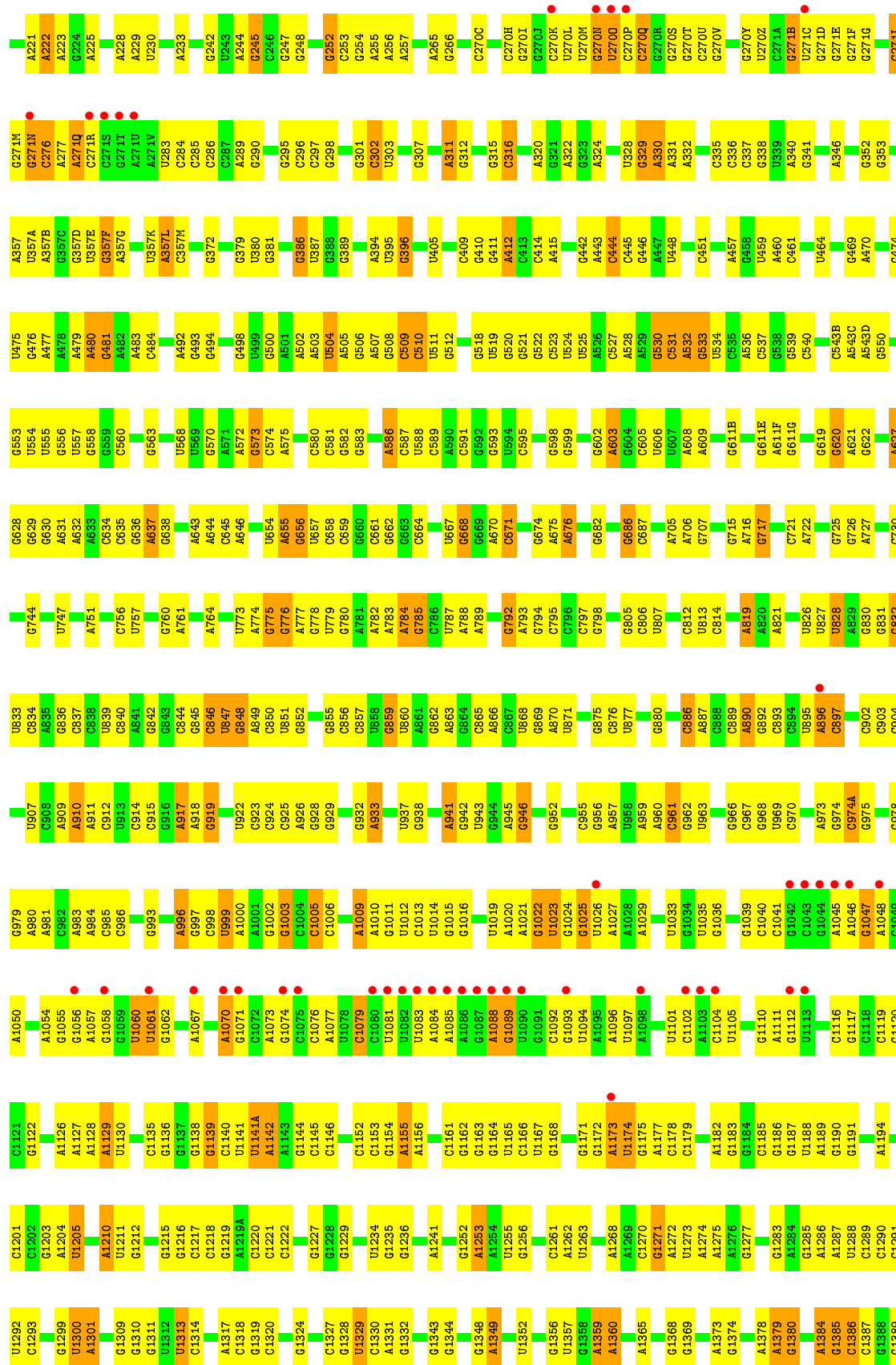


- Molecule 24: 30S ribosomal protein Thx

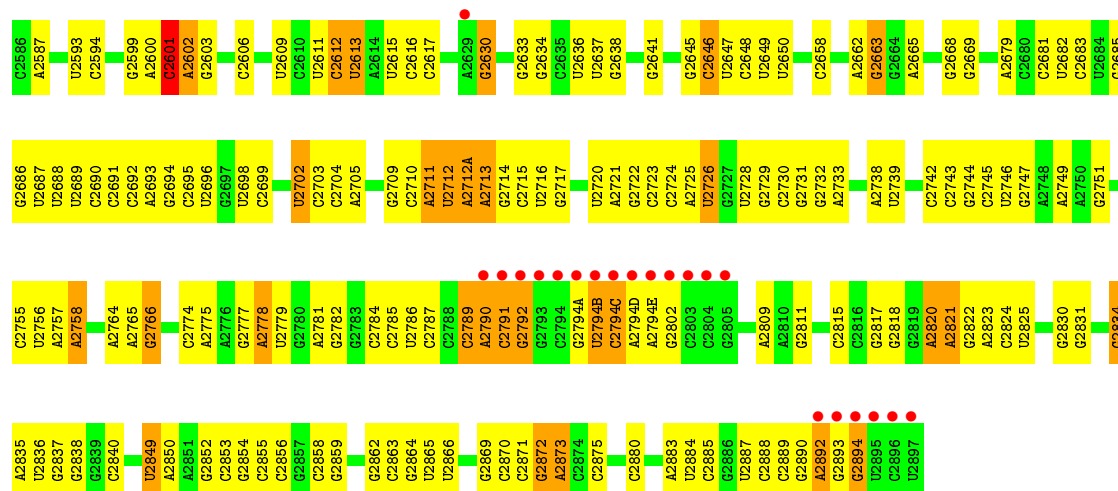


- Molecule 25: 23S ribosomal RNA

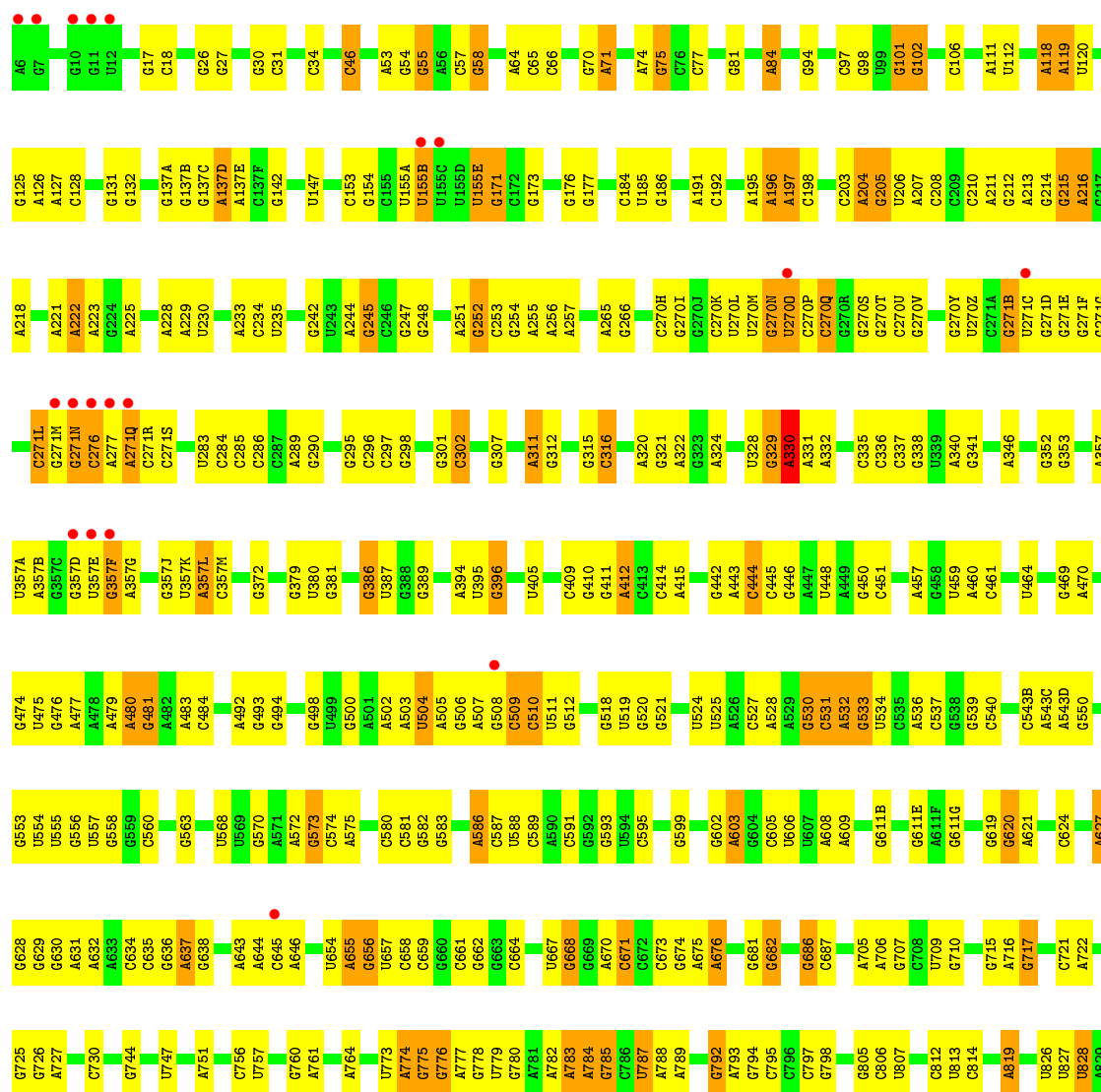




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	C2424			G2038		G1856	U1775		C1577	C1411	
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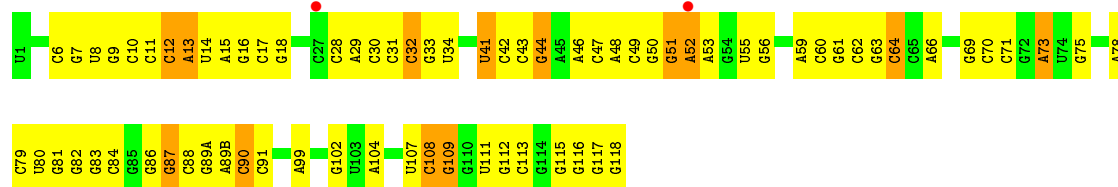
• Molecule 25: 23S ribosomal RNA



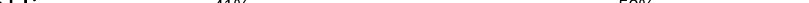


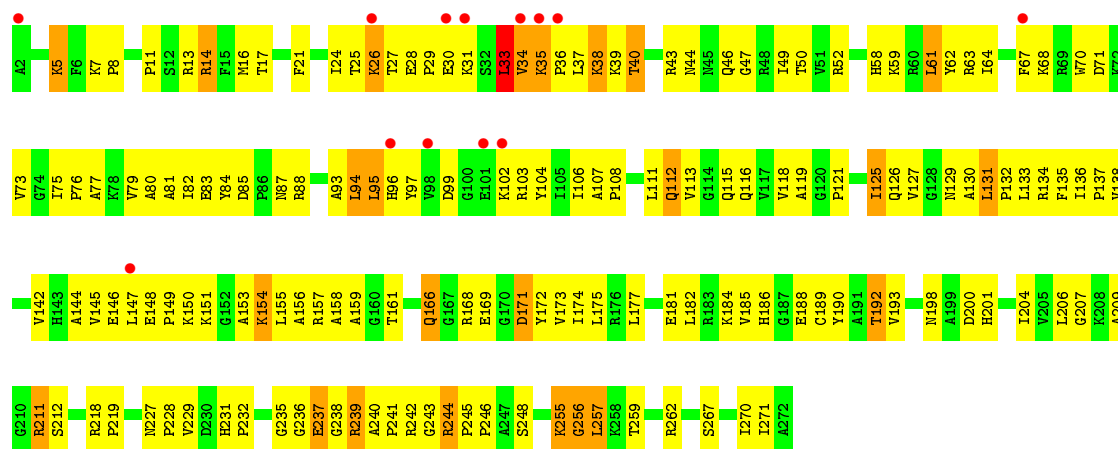


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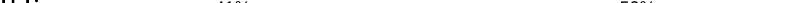


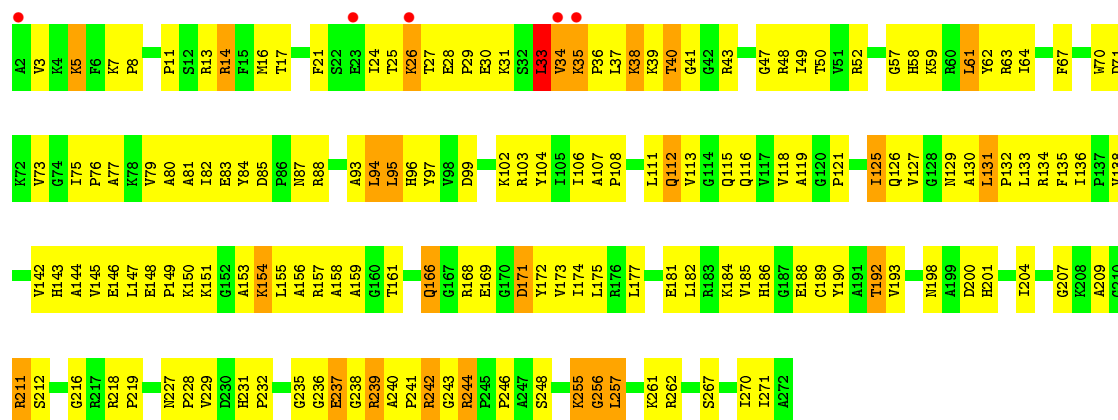
- Molecule 27: 50S ribosomal protein L2

Chain BD: 



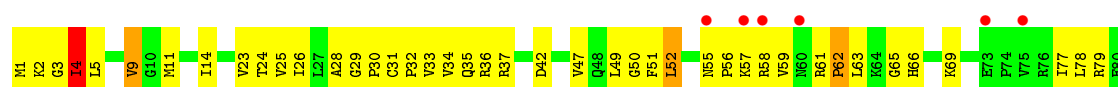
- Molecule 27: 50S ribosomal protein L2

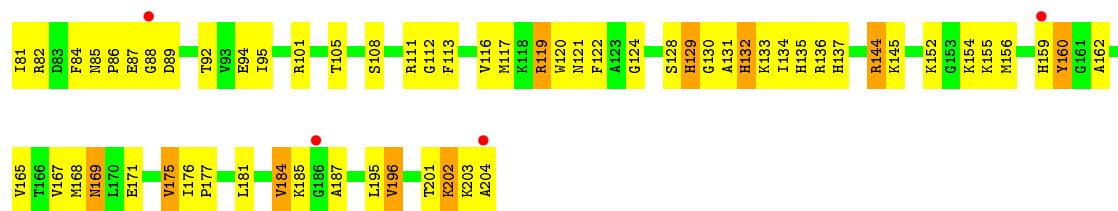
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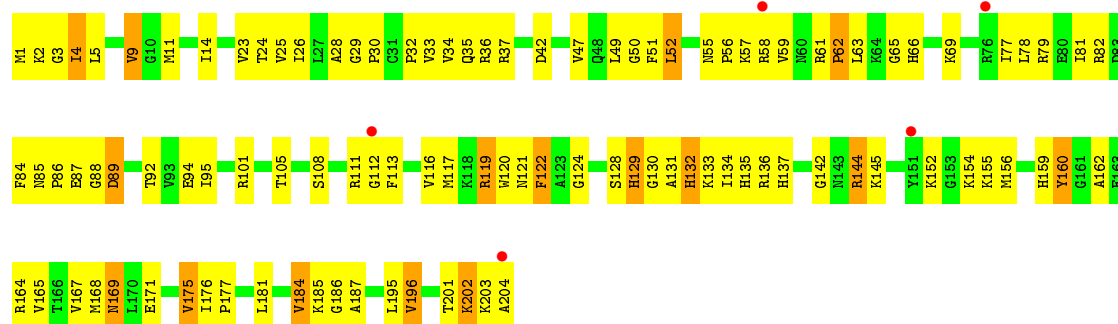
- Molecule 28: 50S ribosomal protein L3

Chain BE: 

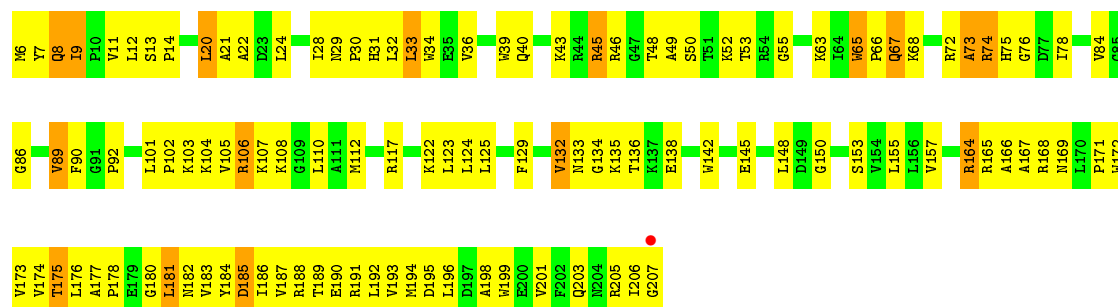




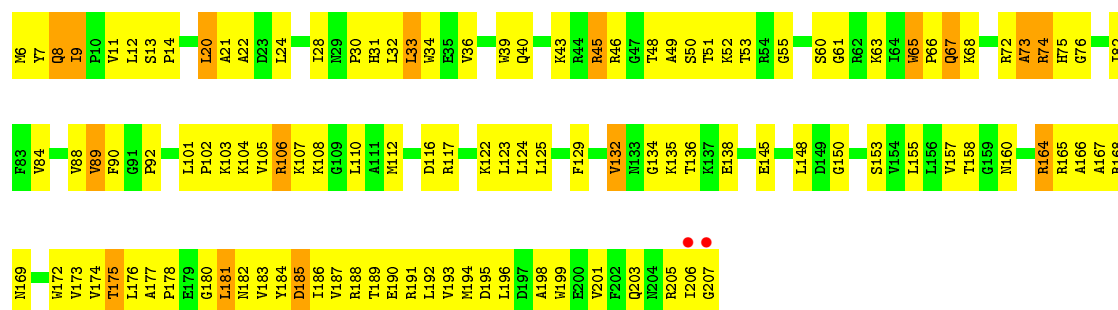
• Molecule 28: 50S ribosomal protein L3



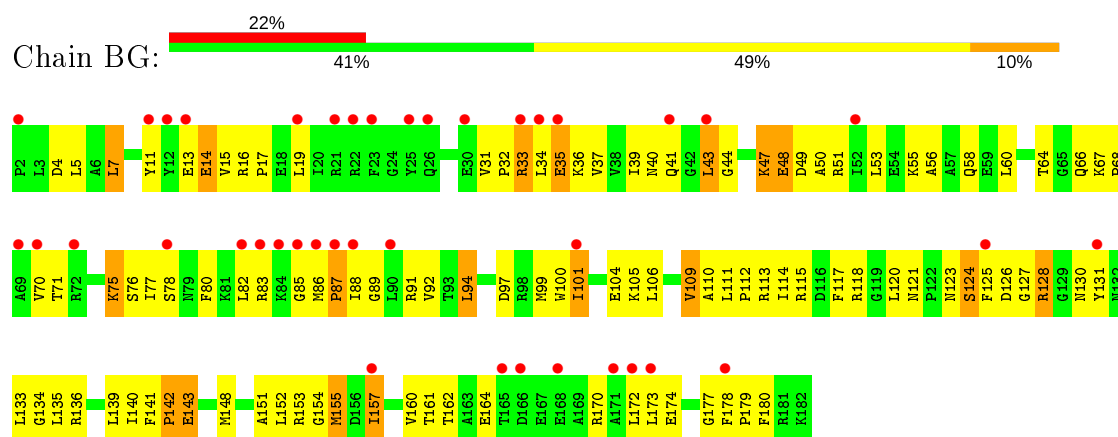
• Molecule 29: 50S ribosomal protein L4



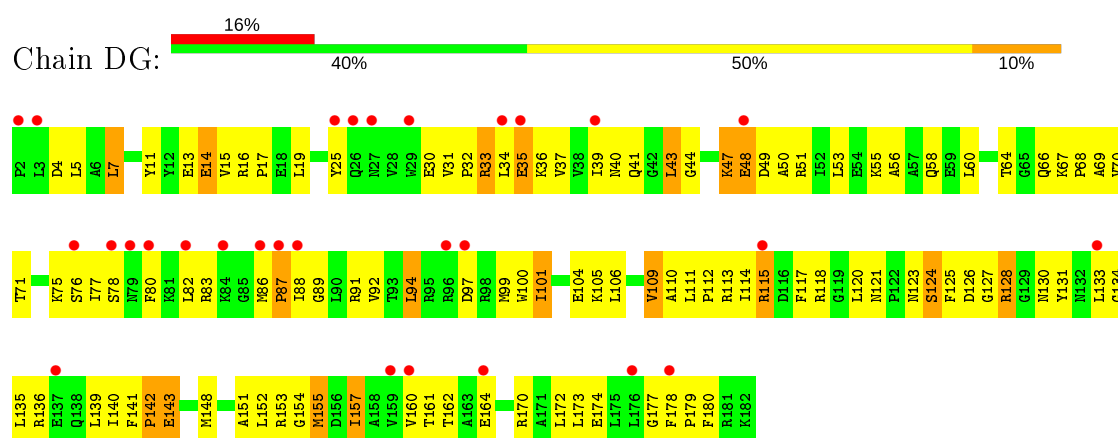
• Molecule 29: 50S ribosomal protein L4



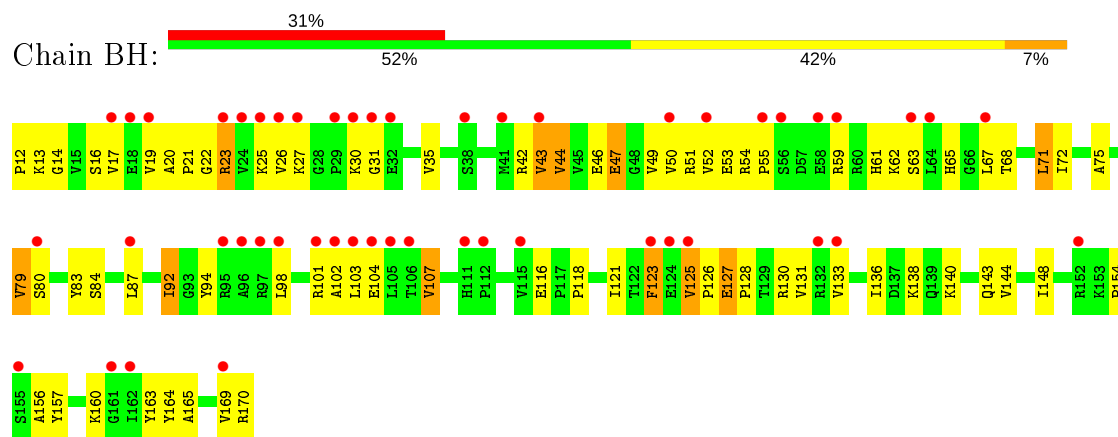
• Molecule 30: 50S ribosomal protein L5



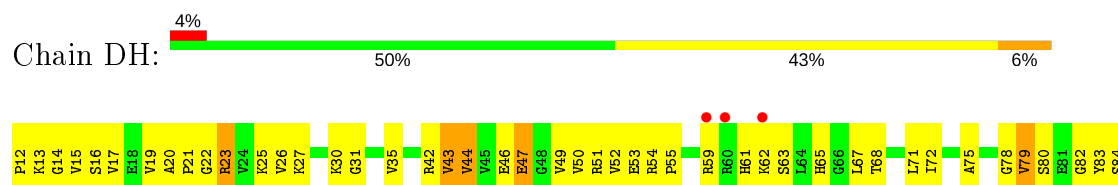
• Molecule 30: 50S ribosomal protein L5

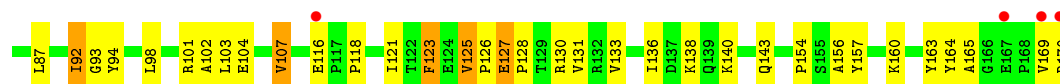


• Molecule 31: 50S ribosomal protein L6

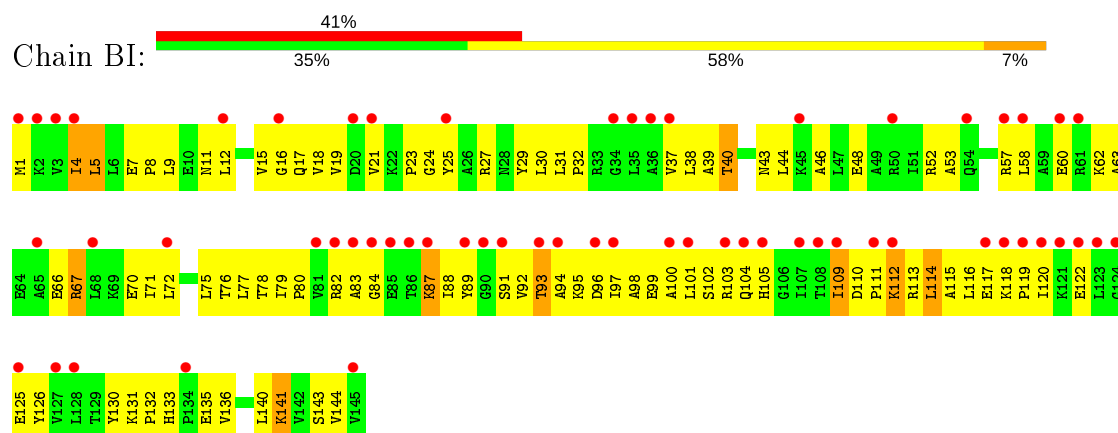


• Molecule 31: 50S ribosomal protein L6

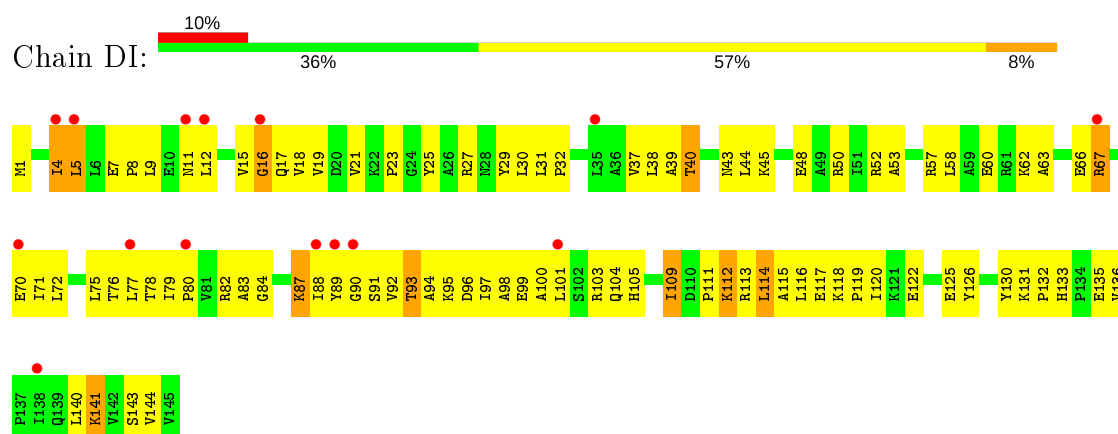




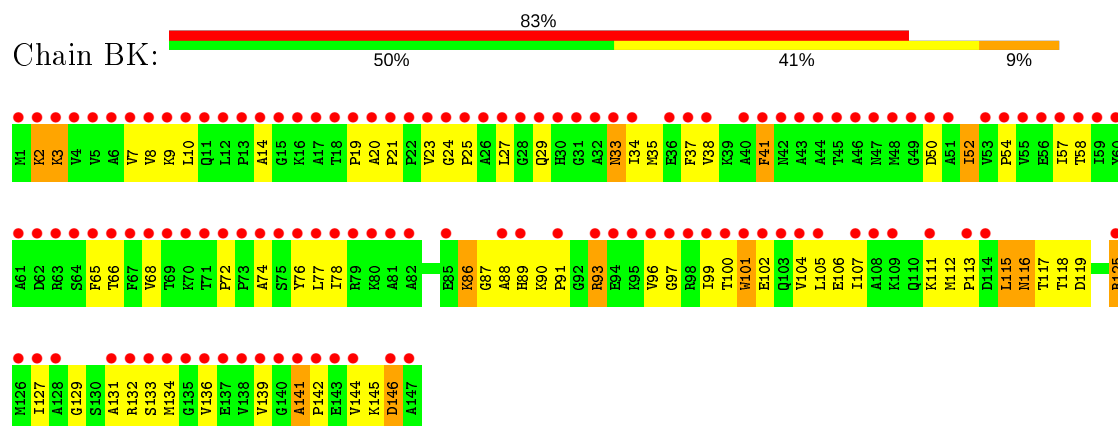
- Molecule 32: 50S ribosomal protein L9



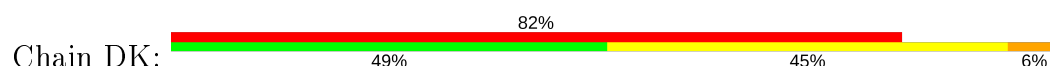
- Molecule 32: 50S ribosomal protein L9

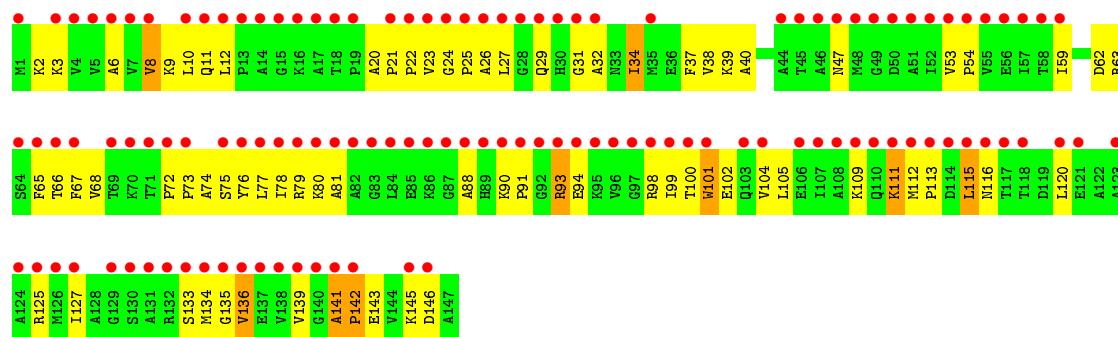


- Molecule 33: 50S ribosomal protein L11

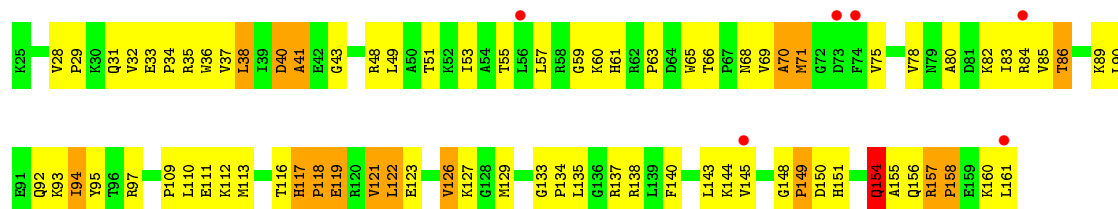


- Molecule 33: 50S ribosomal protein L11

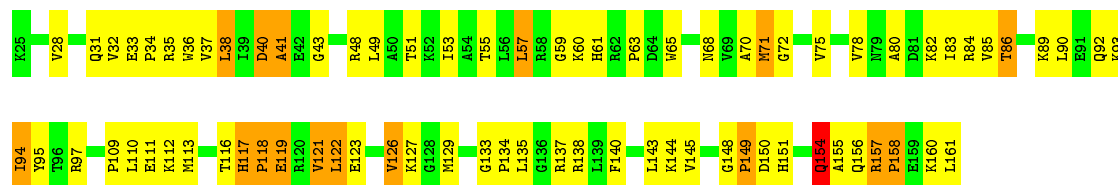




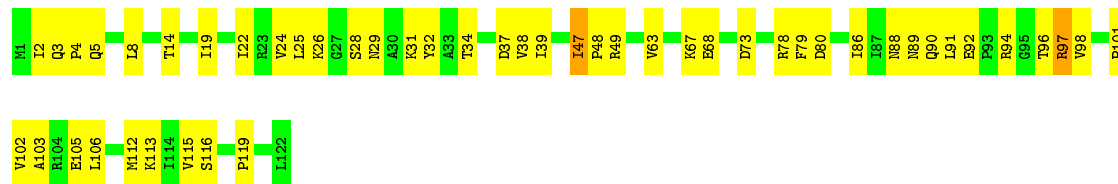
• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13

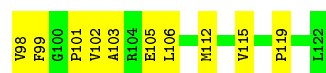


• Molecule 35: 50S ribosomal protein L14

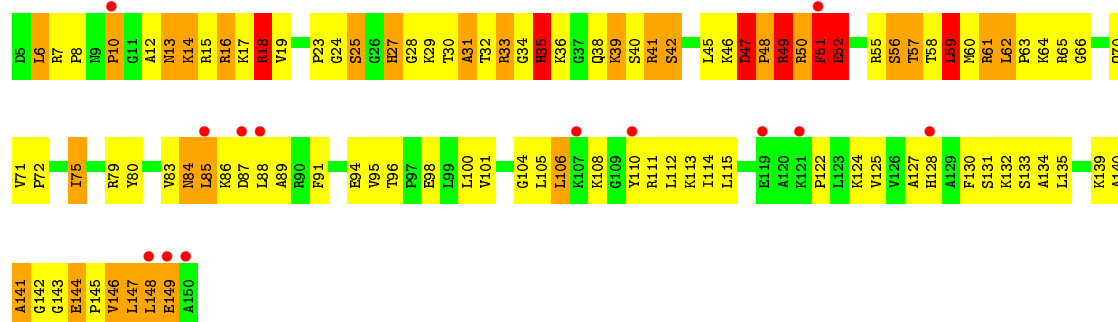


• Molecule 35: 50S ribosomal protein L14

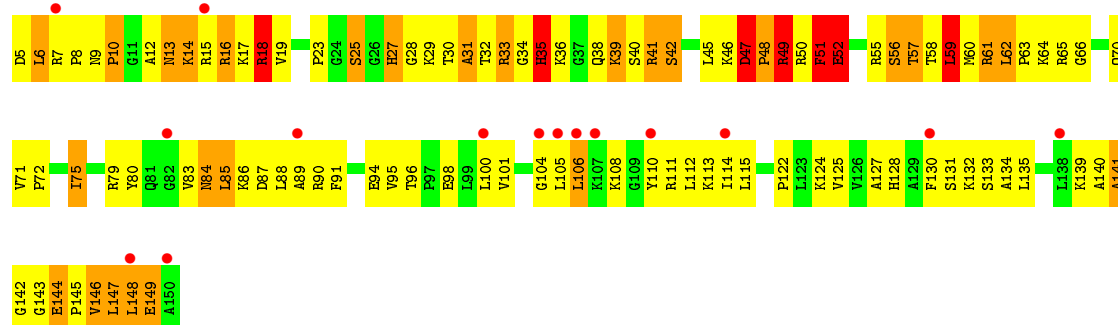




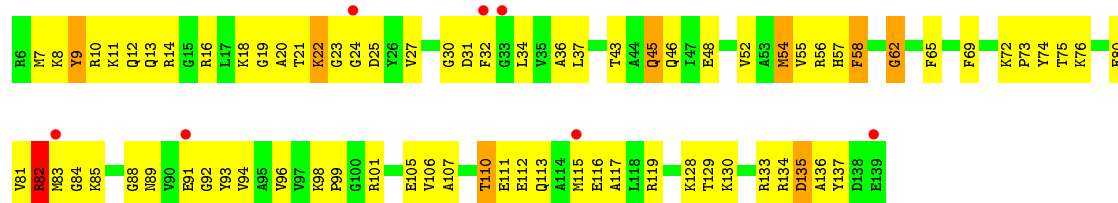
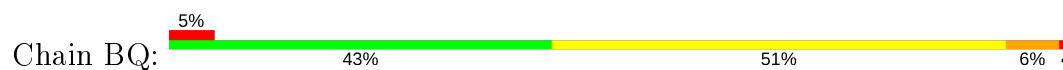
• Molecule 36: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L15

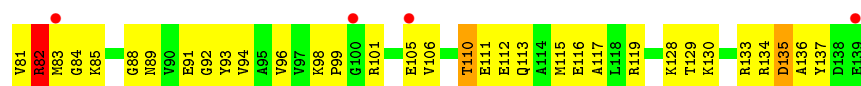


• Molecule 37: 50S ribosomal protein L16

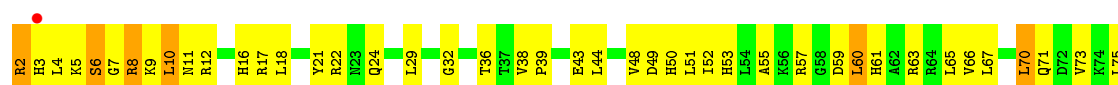


• Molecule 37: 50S ribosomal protein L16

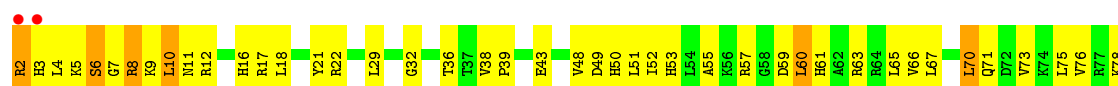
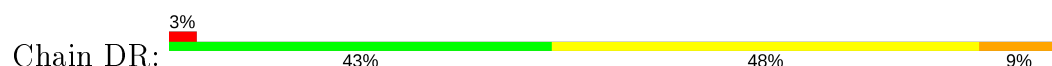




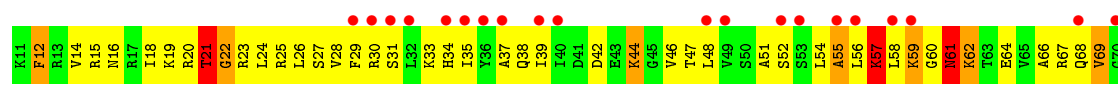
- Molecule 38: 50S ribosomal protein L17



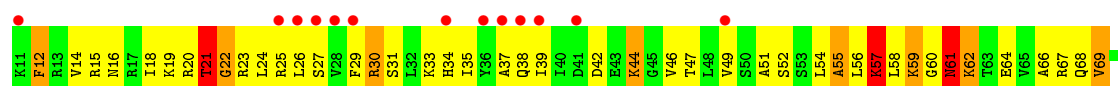
- Molecule 38: 50S ribosomal protein L17



- Molecule 39: 50S ribosomal protein L18

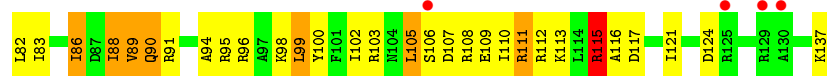


- Molecule 39: 50S ribosomal protein L18

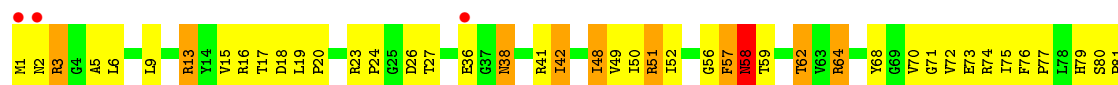


- Molecule 40: 50S ribosomal protein L19

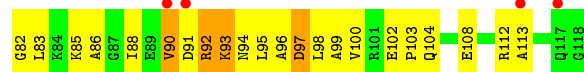




• Molecule 40: 50S ribosomal protein L19



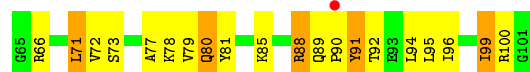
• Molecule 41: 50S ribosomal protein L20



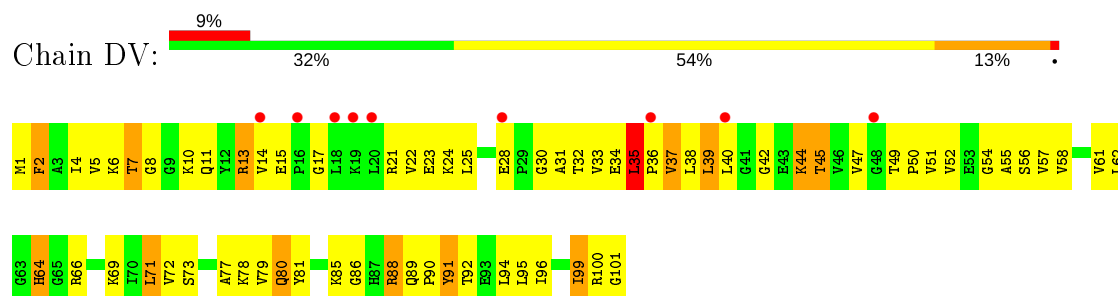
• Molecule 41: 50S ribosomal protein L20



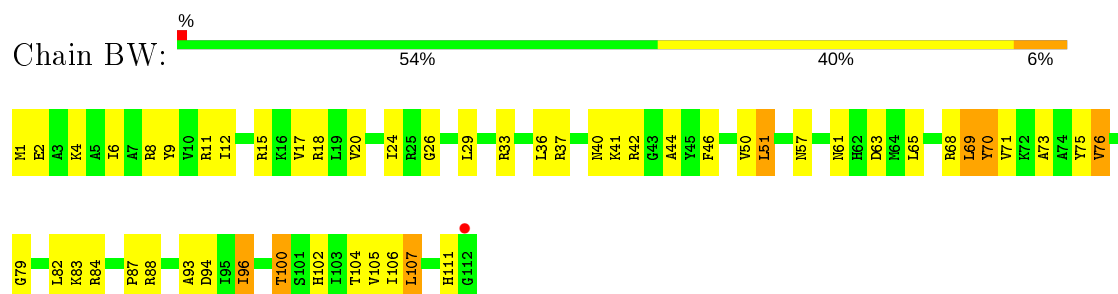
• Molecule 42: 50S ribosomal protein L21



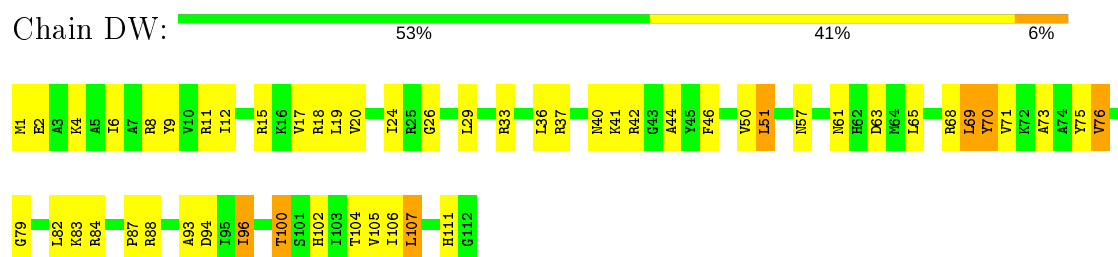
- Molecule 42: 50S ribosomal protein L21



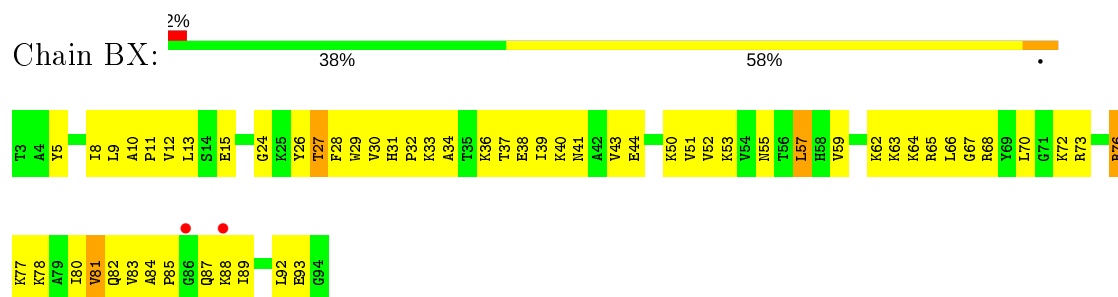
- Molecule 43: 50S ribosomal protein L22



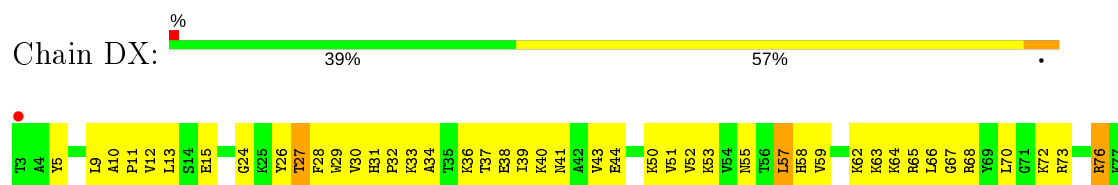
- Molecule 43: 50S ribosomal protein L22



- Molecule 44: 50S ribosomal protein L23

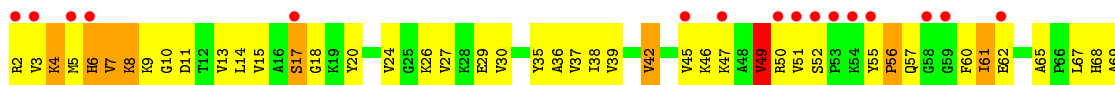


- Molecule 44: 50S ribosomal protein L23

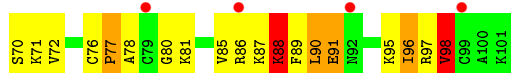
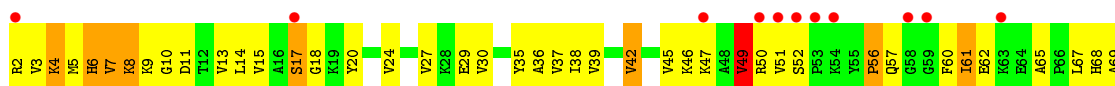
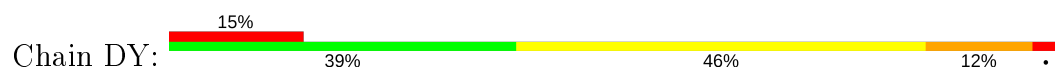




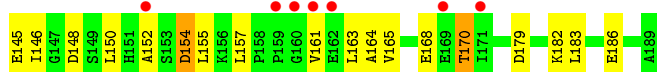
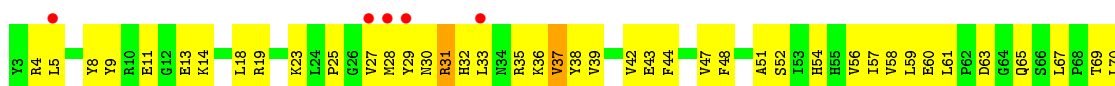
- Molecule 45: 50S ribosomal protein L24



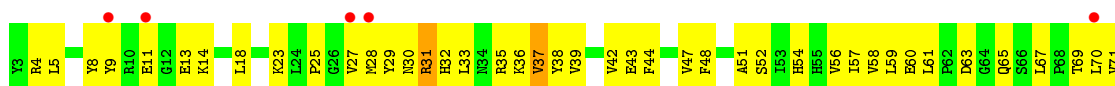
- Molecule 45: 50S ribosomal protein L24



- Molecule 46: 50S ribosomal protein L25

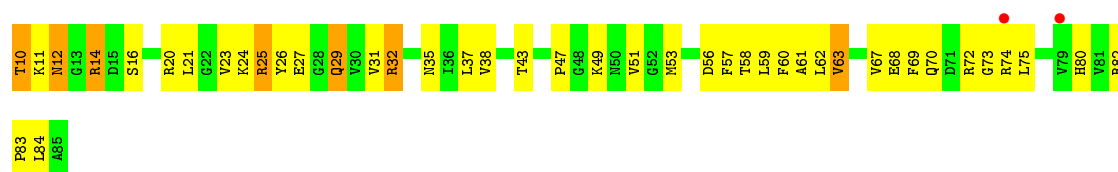
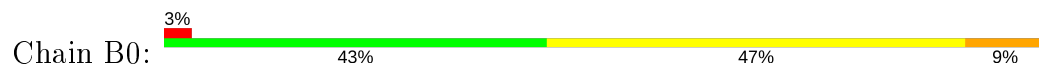


- Molecule 46: 50S ribosomal protein L25





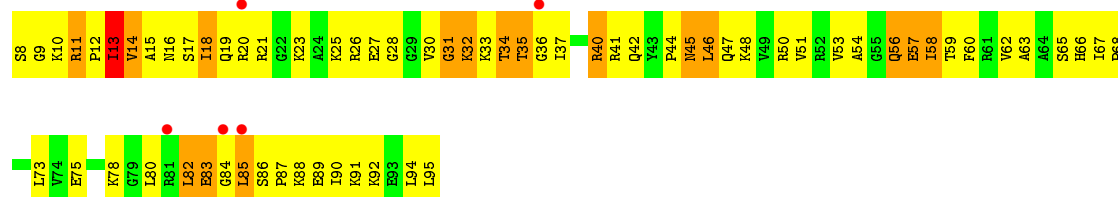
- Molecule 47: 50S ribosomal protein L27



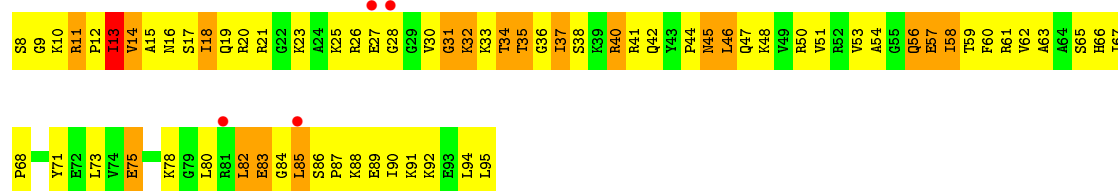
- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



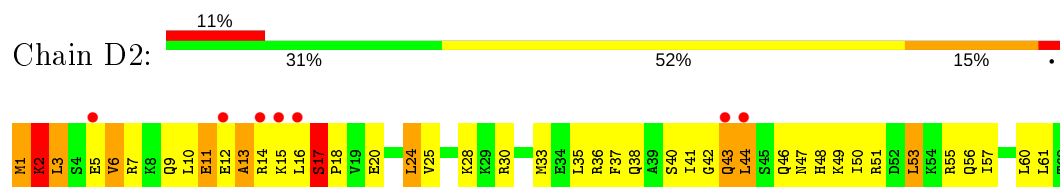
- Molecule 48: 50S ribosomal protein L28



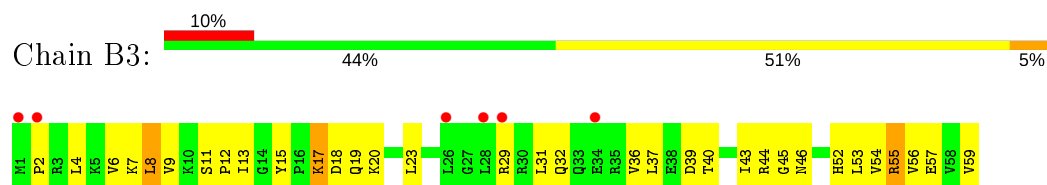
- Molecule 49: 50S ribosomal protein L29



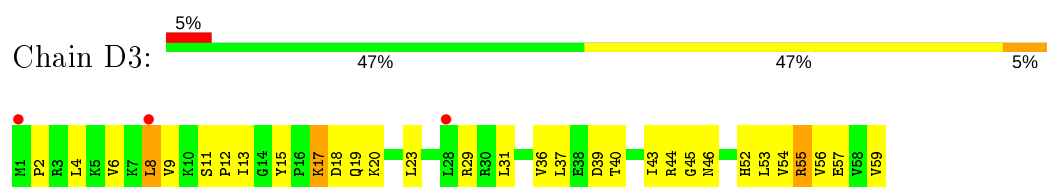
• Molecule 49: 50S ribosomal protein L29



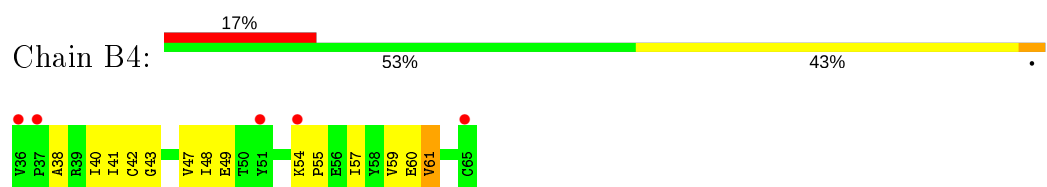
• Molecule 50: 50S ribosomal protein L30



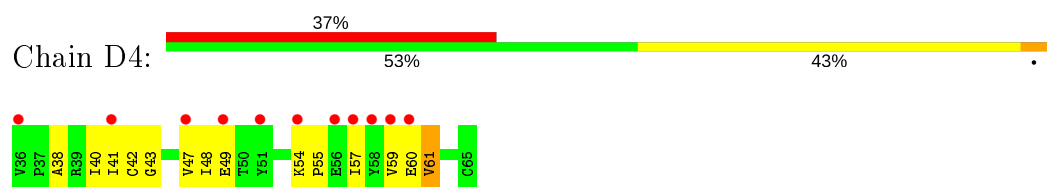
• Molecule 50: 50S ribosomal protein L30



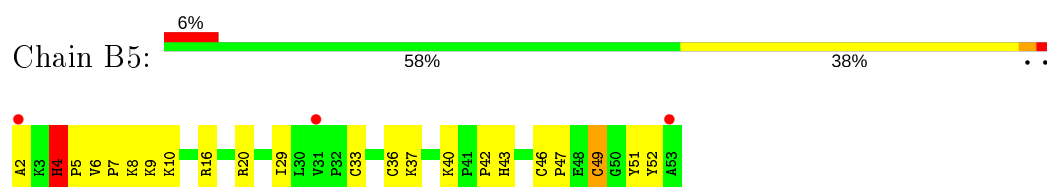
• Molecule 51: 50S ribosomal protein L31



• Molecule 51: 50S ribosomal protein L31



• Molecule 52: 50S ribosomal protein L32

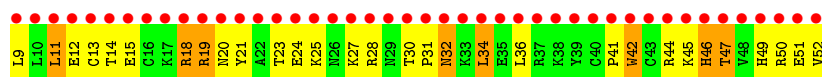


• Molecule 52: 50S ribosomal protein L32

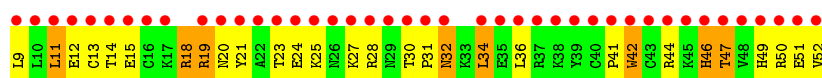




- Molecule 53: 50S ribosomal protein L33



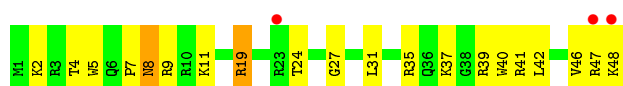
- Molecule 53: 50S ribosomal protein L33



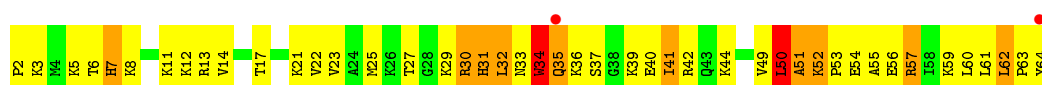
- Molecule 54: 50S ribosomal protein L34



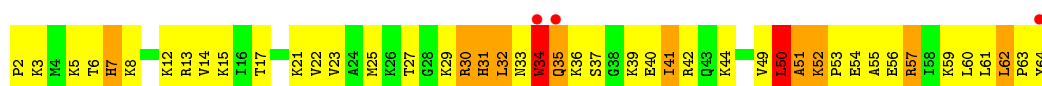
- Molecule 54: 50S ribosomal protein L34



- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	212.07Å 454.40Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.40 49.78 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.67-3.40) 99.7 (49.78-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486), CNS	Depositor
R, R_{free}	0.234 , 0.268 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 97.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	294074	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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

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	0.27	2/36194 (0.0%)	0.55	0/56493
1	CA	0.27	2/36194 (0.0%)	0.54	0/56493
2	AV	0.26	0/241	0.53	0/374
2	CV	0.23	0/241	0.54	0/374
3	AW	0.25	0/1832	0.52	0/2855
3	CW	0.26	0/1832	0.53	0/2855
4	AY	0.21	0/2925	0.39	0/3953
4	CY	0.21	0/2925	0.39	0/3953
5	AB	0.22	0/1936	0.40	0/2609
5	CB	0.22	0/1936	0.39	0/2609
6	AC	0.22	0/1637	0.39	0/2205
6	CC	0.22	0/1637	0.39	0/2205
7	AD	0.25	0/1733	0.44	0/2318
7	CD	0.24	0/1733	0.41	0/2318
8	AE	0.24	0/1172	0.44	0/1576
8	CE	0.24	0/1172	0.43	0/1576
9	AF	0.23	0/856	0.42	0/1154
9	CF	0.24	0/856	0.43	0/1154
10	AG	0.22	0/1276	0.37	0/1709
10	CG	0.22	0/1276	0.37	0/1709
11	AH	0.23	0/1136	0.44	0/1527
11	CH	0.22	0/1136	0.43	0/1527
12	AI	0.23	0/1029	0.40	0/1378
12	CI	0.22	0/1029	0.40	0/1378
13	AJ	0.21	0/808	0.41	0/1085
13	CJ	0.21	0/808	0.41	0/1085
14	AK	0.24	0/857	0.43	0/1157
14	CK	0.24	0/857	0.43	0/1157
15	AL	0.27	0/973	0.47	0/1301
15	CL	0.26	0/973	0.47	0/1301
16	AM	0.20	0/944	0.40	0/1265
16	CM	0.20	0/944	0.40	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AN	0.24	0/501	0.41	0/664
17	CN	0.25	0/501	0.39	0/664
18	AO	0.24	0/745	0.39	0/992
18	CO	0.24	0/745	0.39	0/992
19	AP	0.24	0/717	0.43	0/963
19	CP	0.22	0/717	0.43	0/963
20	AQ	0.25	0/837	0.41	0/1117
20	CQ	0.23	0/837	0.41	0/1117
21	AR	0.24	0/579	0.43	0/768
21	CR	0.24	0/579	0.43	0/768
22	AS	0.21	0/643	0.40	0/865
22	CS	0.22	0/643	0.40	0/865
23	AT	0.23	0/764	0.39	0/1006
23	CT	0.22	0/764	0.39	0/1006
24	AU	0.21	0/213	0.40	0/277
24	CU	0.21	0/213	0.41	0/277
25	BA	0.38	6/67268 (0.0%)	0.67	12/105011 (0.0%)
25	DA	0.42	6/67268 (0.0%)	0.70	21/105011 (0.0%)
26	BB	0.25	0/2853	0.55	0/4451
26	DB	0.26	0/2853	0.56	0/4451
27	BD	0.33	0/2155	0.53	0/2905
27	DD	0.35	0/2155	0.53	1/2905 (0.0%)
28	BE	0.28	0/1597	0.49	0/2153
28	DE	0.29	0/1597	0.49	0/2153
29	BF	0.29	0/1622	0.48	0/2194
29	DF	0.31	0/1622	0.48	0/2194
30	BG	0.23	0/1500	0.42	0/2017
30	DG	0.23	0/1500	0.43	0/2017
31	BH	0.22	0/1246	0.44	0/1682
31	DH	0.24	0/1246	0.45	0/1682
32	BI	0.22	0/1148	0.42	0/1552
32	DI	0.23	0/1148	0.43	0/1552
33	BK	0.21	0/1108	0.40	0/1500
33	DK	0.20	0/1108	0.39	0/1500
34	BN	0.27	0/1124	0.46	0/1515
34	DN	0.29	0/1124	0.47	0/1515
35	BO	0.28	0/942	0.47	0/1268
35	DO	0.30	0/942	0.48	0/1268
36	BP	0.34	0/1131	0.62	1/1504 (0.1%)
36	DP	0.36	0/1131	0.63	1/1504 (0.1%)
37	BQ	0.30	0/1085	0.52	0/1449
37	DQ	0.31	0/1085	0.52	0/1449
38	BR	0.28	0/974	0.48	0/1302

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/974	0.49	0/1302
39	BS	0.24	0/779	0.44	0/1036
39	DS	0.25	0/779	0.44	0/1036
40	BT	0.27	0/1158	0.47	0/1544
40	DT	0.28	0/1158	0.48	0/1544
41	BU	0.31	0/982	0.47	0/1306
41	DU	0.32	0/982	0.46	0/1306
42	BV	0.28	0/790	0.49	0/1057
42	DV	0.29	0/790	0.49	0/1057
43	BW	0.30	0/902	0.47	0/1209
43	DW	0.29	0/902	0.47	0/1209
44	BX	0.30	0/740	0.46	0/993
44	DX	0.33	0/740	0.48	0/993
45	BY	0.28	0/789	0.49	0/1051
45	DY	0.30	0/789	0.49	0/1051
46	BZ	0.22	0/1515	0.42	0/2056
46	DZ	0.23	0/1515	0.42	0/2056
47	B0	0.27	0/613	0.53	0/816
47	D0	0.29	0/613	0.52	0/816
48	B1	0.34	0/702	0.59	1/932 (0.1%)
48	D1	0.36	0/702	0.61	1/932 (0.1%)
49	B2	0.27	0/523	0.50	0/690
49	D2	0.32	0/523	0.53	0/690
50	B3	0.25	0/473	0.43	0/634
50	D3	0.27	0/473	0.43	0/634
51	B4	0.24	0/229	0.40	0/309
51	D4	0.23	0/229	0.42	0/309
52	B5	0.27	0/419	0.51	0/567
52	D5	0.29	0/419	0.50	0/567
53	B6	0.21	0/388	0.41	0/518
53	D6	0.21	0/388	0.42	0/518
54	B7	0.34	0/427	0.54	0/561
54	D7	0.38	0/427	0.56	0/561
55	B8	0.32	0/516	0.49	0/679
55	D8	0.35	0/516	0.50	0/679
All	All	0.33	16/316492 (0.0%)	0.59	38/472144 (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
36	BP	0	1
36	DP	0	1
38	BR	0	1
38	DR	0	1
48	B1	0	1
48	D1	0	1
52	B5	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1913	A	P-OP1	-9.19	1.33	1.49
1	AA	1493	A	P-OP2	-9.00	1.33	1.49
25	BA	1912	A	P-OP2	-9.00	1.33	1.49
25	DA	1912	A	P-OP1	-8.94	1.33	1.49
1	CA	1493	A	P-OP1	-8.80	1.33	1.49

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2061	G	N1-C6-O6	8.50	125.00	119.90
25	DA	2447	G	N1-C6-O6	6.34	123.71	119.90
25	DA	2061	G	N1-C6-O6	6.02	123.51	119.90
25	DA	1899	G	C2-N3-C4	-6.02	108.89	111.90
25	DA	2447	G	C6-C5-N7	-5.97	126.82	130.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	B1	26	ARG	Peptide
52	B5	4	HIS	Peptide
36	BP	51	PHE	Peptide
38	BR	10	LEU	Peptide
36	DP	51	PHE	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	32332	0	16318	783	0
1	CA	32332	0	16318	798	0
2	AV	214	0	110	7	0
2	CV	214	0	110	8	0
3	AW	1640	0	837	26	0
3	CW	1640	0	837	24	0
4	AY	2874	0	2866	173	0
4	CY	2874	0	2866	164	0
5	AB	1901	0	1951	118	0
5	CB	1901	0	1951	119	0
6	AC	1613	0	1677	100	0
6	CC	1613	0	1677	101	0
7	AD	1703	0	1764	102	0
7	CD	1703	0	1765	121	0
8	AE	1156	0	1213	80	0
8	CE	1156	0	1213	80	0
9	AF	843	0	857	36	0
9	CF	843	0	857	36	0
10	AG	1257	0	1296	46	0
10	CG	1257	0	1296	42	0
11	AH	1116	0	1177	72	0
11	CH	1116	0	1177	77	0
12	AI	1011	0	1043	69	0
12	CI	1011	0	1043	70	0
13	AJ	795	0	840	74	0
13	CJ	795	0	840	72	0
14	AK	843	0	859	39	0
14	CK	843	0	859	40	0
15	AL	957	0	1046	73	0
15	CL	957	0	1046	71	0
16	AM	934	0	992	50	0
16	CM	934	0	992	55	0
17	AN	492	0	530	47	0
17	CN	492	0	530	39	0
18	AO	734	0	771	34	0
18	CO	734	0	771	34	0
19	AP	701	0	720	51	0
19	CP	701	0	720	49	0
20	AQ	824	0	893	38	0
20	CQ	824	0	893	40	0
21	AR	574	0	644	37	0
21	CR	574	0	644	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AS	630	0	652	55	0
22	CS	630	0	652	56	0
23	AT	762	0	859	38	0
23	CT	762	0	859	40	0
24	AU	209	0	221	16	0
24	CU	209	0	221	17	0
25	BA	60059	0	30274	1273	0
25	DA	60059	0	30274	1280	0
26	BB	2551	0	1295	81	0
26	DB	2551	0	1295	83	0
27	BD	2105	0	2182	176	0
27	DD	2105	0	2182	179	0
28	BE	1564	0	1629	122	0
28	DE	1564	0	1629	123	0
29	BF	1587	0	1632	100	0
29	DF	1587	0	1632	108	0
30	BG	1475	0	1537	110	0
30	DG	1475	0	1537	114	0
31	BH	1223	0	1282	76	0
31	DH	1223	0	1282	77	0
32	BI	1133	0	1220	100	0
32	DI	1133	0	1220	110	0
33	BK	1088	0	1138	58	0
33	DK	1088	0	1138	61	0
34	BN	1097	0	1168	80	0
34	DN	1097	0	1168	74	0
35	BO	932	0	994	45	0
35	DO	932	0	994	46	0
36	BP	1114	0	1187	184	0
36	DP	1114	0	1187	194	0
37	BQ	1065	0	1114	82	0
37	DQ	1065	0	1114	83	0
38	BR	960	0	1021	84	0
38	DR	960	0	1021	77	0
39	BS	771	0	832	60	0
39	DS	771	0	832	60	0
40	BT	1144	0	1211	76	0
40	DT	1144	0	1211	74	0
41	BU	964	0	1022	83	0
41	DU	964	0	1022	78	0
42	BV	779	0	852	83	0
42	DV	779	0	852	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BW	891	0	951	58	0
43	DW	891	0	951	61	0
44	BX	726	0	778	64	0
44	DX	726	0	778	65	0
45	BY	776	0	870	80	0
45	DY	776	0	870	81	0
46	BZ	1483	0	1507	89	0
46	DZ	1483	0	1507	89	0
47	B0	605	0	628	36	0
47	D0	605	0	628	32	0
48	B1	695	0	764	67	0
48	D1	695	0	764	77	0
49	B2	521	0	575	52	0
49	D2	521	0	575	56	0
50	B3	468	0	523	27	0
50	D3	468	0	523	24	0
51	B4	226	0	227	13	0
51	D4	226	0	225	15	0
52	B5	405	0	420	27	0
52	D5	405	0	420	31	0
53	B6	381	0	391	28	0
53	D6	381	0	391	26	0
54	B7	419	0	467	22	0
54	D7	419	0	467	22	0
55	B8	508	0	576	58	0
55	D8	508	0	576	60	0
56	AA	393	0	0	0	0
56	AC	1	0	0	0	0
56	AG	1	0	0	0	0
56	AO	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AT	3	0	0	0	0
56	AV	1	0	0	0	0
56	AW	18	0	0	0	0
56	AY	3	0	0	0	0
56	B0	2	0	0	0	0
56	B1	1	0	0	0	0
56	B3	1	0	0	0	0
56	B5	1	0	0	0	0
56	B8	2	0	0	0	0
56	BA	824	0	0	0	0
56	BB	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BD	1	0	0	0	0
56	BE	1	0	0	0	0
56	BF	1	0	0	0	0
56	BP	1	0	0	0	0
56	BT	1	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	326	0	0	0	0
56	CD	1	0	0	0	0
56	CM	1	0	0	0	0
56	CR	1	0	0	0	0
56	CV	2	0	0	0	0
56	CW	16	0	0	0	0
56	CY	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	1	0	0	0	0
56	D5	3	0	0	0	0
56	D7	2	0	0	0	0
56	DA	732	0	0	0	0
56	DB	20	0	0	0	0
56	DD	1	0	0	0	0
56	DE	1	0	0	0	0
56	DF	2	0	0	0	0
56	DH	1	0	0	0	0
56	DI	2	0	0	0	0
56	DN	1	0	0	0	0
56	DP	2	0	0	0	0
56	DQ	4	0	0	0	0
56	DV	1	0	0	0	0
56	DW	2	0	0	0	0
56	DX	1	0	0	0	0
57	AD	1	0	0	0	0
57	AN	1	0	0	0	0
57	CD	1	0	0	0	0
57	CN	1	0	0	0	0
All	All	294074	0	200805	10187	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 10187 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:CA:559:A:H4'	1:CA:560:U:H3'	1.26	1.16
25:BA:1899:G:N2	25:BA:1902:C:H41	1.43	1.15
45:DY:76:CYS:SG	45:DY:77:PRO:HD2	1.91	1.11
25:DA:1899:G:N2	25:DA:1902:C:H41	1.48	1.10
1:AA:559:A:H4'	1:AA:560:U:H3'	1.26	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AY	360/362 (99%)	301 (84%)	41 (11%)	18 (5%)	2	14
4	CY	360/362 (99%)	301 (84%)	42 (12%)	17 (5%)	2	15
5	AB	232/234 (99%)	185 (80%)	37 (16%)	10 (4%)	2	17
5	CB	232/234 (99%)	184 (79%)	38 (16%)	10 (4%)	2	17
6	AC	204/206 (99%)	144 (71%)	40 (20%)	20 (10%)	0	4
6	CC	204/206 (99%)	145 (71%)	38 (19%)	21 (10%)	0	3
7	AD	206/208 (99%)	165 (80%)	32 (16%)	9 (4%)	2	16
7	CD	206/208 (99%)	166 (81%)	29 (14%)	11 (5%)	2	13
8	AE	149/151 (99%)	113 (76%)	32 (22%)	4 (3%)	5	26
8	CE	149/151 (99%)	116 (78%)	29 (20%)	4 (3%)	5	26
9	AF	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15	46
9	CF	99/101 (98%)	82 (83%)	16 (16%)	1 (1%)	15	46
10	AG	153/155 (99%)	136 (89%)	13 (8%)	4 (3%)	5	26
10	CG	153/155 (99%)	136 (89%)	13 (8%)	4 (3%)	5	26
11	AH	136/138 (99%)	111 (82%)	23 (17%)	2 (2%)	10	36
11	CH	136/138 (99%)	113 (83%)	21 (15%)	2 (2%)	10	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AI	125/127 (98%)	90 (72%)	27 (22%)	8 (6%)	1	9
12	CI	125/127 (98%)	90 (72%)	27 (22%)	8 (6%)	1	9
13	AJ	96/98 (98%)	72 (75%)	18 (19%)	6 (6%)	1	9
13	CJ	96/98 (98%)	72 (75%)	18 (19%)	6 (6%)	1	9
14	AK	112/114 (98%)	93 (83%)	14 (12%)	5 (4%)	2	16
14	CK	112/114 (98%)	93 (83%)	15 (13%)	4 (4%)	3	21
15	AL	120/122 (98%)	94 (78%)	21 (18%)	5 (4%)	3	18
15	CL	120/122 (98%)	93 (78%)	22 (18%)	5 (4%)	3	18
16	AM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	26
16	CM	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	5	26
17	AN	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	3	21
17	CN	58/60 (97%)	43 (74%)	11 (19%)	4 (7%)	1	8
18	AO	86/88 (98%)	75 (87%)	8 (9%)	3 (4%)	3	21
18	CO	86/88 (98%)	75 (87%)	8 (9%)	3 (4%)	3	21
19	AP	81/83 (98%)	62 (76%)	16 (20%)	3 (4%)	3	20
19	CP	81/83 (98%)	61 (75%)	17 (21%)	3 (4%)	3	20
20	AQ	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	18
20	CQ	97/99 (98%)	83 (86%)	10 (10%)	4 (4%)	3	18
21	AR	68/70 (97%)	49 (72%)	17 (25%)	2 (3%)	4	24
21	CR	68/70 (97%)	50 (74%)	16 (24%)	2 (3%)	4	24
22	AS	76/78 (97%)	53 (70%)	15 (20%)	8 (10%)	0	3
22	CS	76/78 (97%)	53 (70%)	15 (20%)	8 (10%)	0	3
23	AT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	5
23	CT	97/99 (98%)	75 (77%)	14 (14%)	8 (8%)	1	5
24	AU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	4
24	CU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	4
27	BD	269/271 (99%)	227 (84%)	29 (11%)	13 (5%)	2	15
27	DD	269/271 (99%)	227 (84%)	29 (11%)	13 (5%)	2	15
28	BE	202/204 (99%)	167 (83%)	26 (13%)	9 (4%)	2	16
28	DE	202/204 (99%)	165 (82%)	27 (13%)	10 (5%)	2	14
29	BF	200/202 (99%)	172 (86%)	21 (10%)	7 (4%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DF	200/202 (99%)	171 (86%)	24 (12%)	5 (2%)	5	26
30	BG	179/181 (99%)	141 (79%)	28 (16%)	10 (6%)	2	12
30	DG	179/181 (99%)	141 (79%)	28 (16%)	10 (6%)	2	12
31	BH	157/159 (99%)	130 (83%)	19 (12%)	8 (5%)	2	14
31	DH	157/159 (99%)	131 (83%)	18 (12%)	8 (5%)	2	14
32	BI	143/145 (99%)	113 (79%)	25 (18%)	5 (4%)	3	21
32	DI	143/145 (99%)	115 (80%)	23 (16%)	5 (4%)	3	21
33	BK	145/147 (99%)	99 (68%)	41 (28%)	5 (3%)	3	21
33	DK	145/147 (99%)	103 (71%)	31 (21%)	11 (8%)	1	6
34	BN	135/137 (98%)	96 (71%)	29 (22%)	10 (7%)	1	7
34	DN	135/137 (98%)	96 (71%)	29 (22%)	10 (7%)	1	7
35	BO	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	5	26
35	DO	120/122 (98%)	103 (86%)	14 (12%)	3 (2%)	5	26
36	BP	144/146 (99%)	91 (63%)	32 (22%)	21 (15%)	0	1
36	DP	144/146 (99%)	93 (65%)	31 (22%)	20 (14%)	0	1
37	BQ	132/134 (98%)	104 (79%)	22 (17%)	6 (4%)	2	16
37	DQ	132/134 (98%)	105 (80%)	22 (17%)	5 (4%)	3	19
38	BR	115/117 (98%)	96 (84%)	17 (15%)	2 (2%)	9	34
38	DR	115/117 (98%)	97 (84%)	16 (14%)	2 (2%)	9	34
39	BS	96/98 (98%)	62 (65%)	20 (21%)	14 (15%)	0	1
39	DS	96/98 (98%)	60 (62%)	22 (23%)	14 (15%)	0	1
40	BT	135/137 (98%)	100 (74%)	24 (18%)	11 (8%)	1	5
40	DT	135/137 (98%)	101 (75%)	23 (17%)	11 (8%)	1	5
41	BU	115/117 (98%)	99 (86%)	13 (11%)	3 (3%)	5	26
41	DU	115/117 (98%)	101 (88%)	11 (10%)	3 (3%)	5	26
42	BV	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	1	10
42	DV	99/101 (98%)	74 (75%)	19 (19%)	6 (6%)	1	10
43	BW	110/112 (98%)	98 (89%)	12 (11%)	0	100	100
43	DW	110/112 (98%)	95 (86%)	15 (14%)	0	100	100
44	BX	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	14	44
44	DX	90/92 (98%)	81 (90%)	8 (9%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BY	98/100 (98%)	68 (69%)	14 (14%)	16 (16%)	0	0
45	DY	98/100 (98%)	68 (69%)	13 (13%)	17 (17%)	0	0
46	BZ	185/187 (99%)	158 (85%)	21 (11%)	6 (3%)	4	22
46	DZ	185/187 (99%)	158 (85%)	21 (11%)	6 (3%)	4	22
47	B0	74/76 (97%)	63 (85%)	7 (10%)	4 (5%)	2	13
47	D0	74/76 (97%)	63 (85%)	7 (10%)	4 (5%)	2	13
48	B1	86/88 (98%)	59 (69%)	14 (16%)	13 (15%)	0	0
48	D1	86/88 (98%)	59 (69%)	14 (16%)	13 (15%)	0	0
49	B2	60/62 (97%)	45 (75%)	7 (12%)	8 (13%)	0	1
49	D2	60/62 (97%)	45 (75%)	7 (12%)	8 (13%)	0	1
50	B3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	8	32
50	D3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	8	32
51	B4	28/30 (93%)	16 (57%)	10 (36%)	2 (7%)	1	7
51	D4	28/30 (93%)	16 (57%)	10 (36%)	2 (7%)	1	7
52	B5	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	1	10
52	D5	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	1	10
53	B6	42/44 (96%)	29 (69%)	8 (19%)	5 (12%)	0	3
53	D6	42/44 (96%)	29 (69%)	8 (19%)	5 (12%)	0	3
54	B7	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
54	D7	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
55	B8	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	0	3
55	D8	61/63 (97%)	47 (77%)	7 (12%)	7 (12%)	0	3
All	All	12130/12330 (98%)	9635 (79%)	1836 (15%)	659 (5%)	2	13

5 of 659 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AY	55	PRO
4	AY	95	GLU
4	AY	175	ALA
4	AY	225	PRO
4	AY	315	VAL

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	
4	AY	305/305 (100%)	278 (91%)	27 (9%)	9	33
4	CY	305/305 (100%)	277 (91%)	28 (9%)	9	31
5	AB	202/202 (100%)	189 (94%)	13 (6%)	17	47
5	CB	202/202 (100%)	188 (93%)	14 (7%)	15	45
6	AC	160/160 (100%)	147 (92%)	13 (8%)	11	38
6	CC	160/160 (100%)	147 (92%)	13 (8%)	11	38
7	AD	180/180 (100%)	149 (83%)	31 (17%)	2	8
7	CD	180/180 (100%)	162 (90%)	18 (10%)	7	27
8	AE	116/116 (100%)	108 (93%)	8 (7%)	15	45
8	CE	116/116 (100%)	108 (93%)	8 (7%)	15	45
9	AF	90/90 (100%)	85 (94%)	5 (6%)	21	51
9	CF	90/90 (100%)	85 (94%)	5 (6%)	21	51
10	AG	126/126 (100%)	123 (98%)	3 (2%)	49	74
10	CG	126/126 (100%)	123 (98%)	3 (2%)	49	74
11	AH	119/119 (100%)	111 (93%)	8 (7%)	16	46
11	CH	119/119 (100%)	110 (92%)	9 (8%)	13	41
12	AI	98/98 (100%)	88 (90%)	10 (10%)	7	26
12	CI	98/98 (100%)	88 (90%)	10 (10%)	7	26
13	AJ	88/88 (100%)	78 (89%)	10 (11%)	5	21
13	CJ	88/88 (100%)	78 (89%)	10 (11%)	5	21
14	AK	86/86 (100%)	82 (95%)	4 (5%)	26	57
14	CK	86/86 (100%)	82 (95%)	4 (5%)	26	57
15	AL	103/103 (100%)	95 (92%)	8 (8%)	12	39
15	CL	103/103 (100%)	95 (92%)	8 (8%)	12	39
16	AM	94/94 (100%)	86 (92%)	8 (8%)	10	35
16	CM	94/94 (100%)	86 (92%)	8 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AN	49/49 (100%)	44 (90%)	5 (10%)	7	26
17	CN	49/49 (100%)	47 (96%)	2 (4%)	30	59
18	AO	79/79 (100%)	71 (90%)	8 (10%)	7	27
18	CO	79/79 (100%)	71 (90%)	8 (10%)	7	27
19	AP	72/72 (100%)	65 (90%)	7 (10%)	8	28
19	CP	72/72 (100%)	66 (92%)	6 (8%)	11	36
20	AQ	94/94 (100%)	89 (95%)	5 (5%)	22	52
20	CQ	94/94 (100%)	89 (95%)	5 (5%)	22	52
21	AR	61/61 (100%)	60 (98%)	1 (2%)	62	81
21	CR	61/61 (100%)	60 (98%)	1 (2%)	62	81
22	AS	69/69 (100%)	57 (83%)	12 (17%)	2	7
22	CS	69/69 (100%)	57 (83%)	12 (17%)	2	7
23	AT	76/76 (100%)	72 (95%)	4 (5%)	22	52
23	CT	76/76 (100%)	72 (95%)	4 (5%)	22	52
24	AU	19/19 (100%)	18 (95%)	1 (5%)	22	52
24	CU	19/19 (100%)	18 (95%)	1 (5%)	22	52
27	BD	213/213 (100%)	188 (88%)	25 (12%)	5	20
27	DD	213/213 (100%)	188 (88%)	25 (12%)	5	20
28	BE	165/165 (100%)	149 (90%)	16 (10%)	8	28
28	DE	165/165 (100%)	150 (91%)	15 (9%)	9	32
29	BF	161/161 (100%)	145 (90%)	16 (10%)	8	27
29	DF	161/161 (100%)	145 (90%)	16 (10%)	8	27
30	BG	155/155 (100%)	140 (90%)	15 (10%)	8	28
30	DG	155/155 (100%)	140 (90%)	15 (10%)	8	28
31	BH	132/132 (100%)	123 (93%)	9 (7%)	16	45
31	DH	132/132 (100%)	124 (94%)	8 (6%)	18	48
32	BI	122/122 (100%)	111 (91%)	11 (9%)	9	32
32	DI	122/122 (100%)	111 (91%)	11 (9%)	9	32
33	BK	111/111 (100%)	98 (88%)	13 (12%)	5	20
33	DK	111/111 (100%)	105 (95%)	6 (5%)	22	52
34	BN	116/116 (100%)	99 (85%)	17 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DN	116/116 (100%)	99 (85%)	17 (15%)	3	12
35	BO	100/100 (100%)	95 (95%)	5 (5%)	24	54
35	DO	100/100 (100%)	94 (94%)	6 (6%)	19	49
36	BP	112/112 (100%)	87 (78%)	25 (22%)	1	2
36	DP	112/112 (100%)	87 (78%)	25 (22%)	1	2
37	BQ	105/105 (100%)	94 (90%)	11 (10%)	7	25
37	DQ	105/105 (100%)	95 (90%)	10 (10%)	8	29
38	BR	100/100 (100%)	86 (86%)	14 (14%)	3	13
38	DR	100/100 (100%)	85 (85%)	15 (15%)	3	12
39	BS	77/77 (100%)	66 (86%)	11 (14%)	3	13
39	DS	77/77 (100%)	66 (86%)	11 (14%)	3	13
40	BT	121/121 (100%)	101 (84%)	20 (16%)	2	9
40	DT	121/121 (100%)	99 (82%)	22 (18%)	1	6
41	BU	93/93 (100%)	85 (91%)	8 (9%)	10	35
41	DU	93/93 (100%)	85 (91%)	8 (9%)	10	35
42	BV	82/82 (100%)	67 (82%)	15 (18%)	1	5
42	DV	82/82 (100%)	67 (82%)	15 (18%)	1	5
43	BW	91/91 (100%)	81 (89%)	10 (11%)	6	23
43	DW	91/91 (100%)	81 (89%)	10 (11%)	6	23
44	BX	74/74 (100%)	69 (93%)	5 (7%)	16	45
44	DX	74/74 (100%)	69 (93%)	5 (7%)	16	45
45	BY	84/84 (100%)	78 (93%)	6 (7%)	14	44
45	DY	84/84 (100%)	78 (93%)	6 (7%)	14	44
46	BZ	162/162 (100%)	153 (94%)	9 (6%)	21	51
46	DZ	162/162 (100%)	153 (94%)	9 (6%)	21	51
47	B0	61/61 (100%)	52 (85%)	9 (15%)	3	12
47	D0	61/61 (100%)	52 (85%)	9 (15%)	3	12
48	B1	73/73 (100%)	58 (80%)	15 (20%)	1	3
48	D1	73/73 (100%)	58 (80%)	15 (20%)	1	3
49	B2	58/58 (100%)	52 (90%)	6 (10%)	7	26
49	D2	58/58 (100%)	51 (88%)	7 (12%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B3	51/51 (100%)	46 (90%)	5 (10%)	8	28
50	D3	51/51 (100%)	46 (90%)	5 (10%)	8	28
51	B4	27/27 (100%)	26 (96%)	1 (4%)	34	62
51	D4	27/27 (100%)	26 (96%)	1 (4%)	34	62
52	B5	45/45 (100%)	42 (93%)	3 (7%)	16	46
52	D5	45/45 (100%)	42 (93%)	3 (7%)	16	46
53	B6	43/43 (100%)	37 (86%)	6 (14%)	3	13
53	D6	43/43 (100%)	37 (86%)	6 (14%)	3	13
54	B7	41/41 (100%)	34 (83%)	7 (17%)	2	8
54	D7	41/41 (100%)	34 (83%)	7 (17%)	2	8
55	B8	53/53 (100%)	45 (85%)	8 (15%)	3	12
55	D8	53/53 (100%)	45 (85%)	8 (15%)	3	12
All	All	10228/10228 (100%)	9223 (90%)	1005 (10%)	8	28

5 of 1005 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	20	ARG
6	CC	107	GLN
44	DX	81	VAL
48	B1	37	ILE
55	B8	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 268 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	19	GLN
7	CD	160	GLN
44	DX	87	GLN
51	B4	46	ASN
5	CB	40	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	216 (14%)	20 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	CA	1503/1504 (99%)	217 (14%)	20 (1%)
2	AV	9/10 (90%)	2 (22%)	0
2	CV	9/10 (90%)	2 (22%)	0
25	BA	2787/2879 (96%)	431 (15%)	19 (0%)
25	DA	2787/2879 (96%)	432 (15%)	19 (0%)
26	BB	118/119 (99%)	15 (12%)	0
26	DB	118/119 (99%)	15 (12%)	0
3	AW	76/77 (98%)	7 (9%)	0
3	CW	76/77 (98%)	7 (9%)	0
All	All	8986/9178 (97%)	1344 (14%)	78 (0%)

5 of 1344 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	41	G

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2225	A
1	CA	428	G
25	DA	1912	A
25	BA	2447	G
1	CA	115	G

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 2414 ligands modelled in this entry, 2414 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1504/1504 (100%)	0.20	37 (2%) 57 55	46, 108, 215, 381	0
1	CA	1504/1504 (100%)	0.36	40 (2%) 54 53	48, 122, 235, 451	0
2	AV	10/10 (100%)	1.06	1 (10%) 7 8	76, 120, 198, 250	0
2	CV	10/10 (100%)	0.97	3 (30%) 0 0	74, 123, 204, 230	0
3	AW	77/77 (100%)	0.28	1 (1%) 77 76	73, 106, 160, 212	0
3	CW	77/77 (100%)	0.14	1 (1%) 77 76	65, 104, 140, 219	0
4	AY	362/362 (100%)	1.93	128 (35%) 0 0	72, 164, 304, 366	0
4	CY	362/362 (100%)	2.14	131 (36%) 0 0	69, 180, 326, 473	0
5	AB	234/234 (100%)	1.25	53 (22%) 0 1	84, 152, 249, 335	0
5	CB	234/234 (100%)	1.23	63 (26%) 0 0	84, 173, 267, 348	0
6	AC	206/206 (100%)	0.57	25 (12%) 4 5	69, 141, 224, 325	0
6	CC	206/206 (100%)	0.53	22 (10%) 6 7	88, 154, 252, 385	0
7	AD	208/208 (100%)	0.25	4 (1%) 66 65	46, 104, 158, 201	0
7	CD	208/208 (100%)	0.59	19 (9%) 9 10	78, 146, 224, 346	0
8	AE	151/151 (100%)	0.29	13 (8%) 10 12	61, 102, 156, 274	0
8	CE	151/151 (100%)	0.62	15 (9%) 7 8	84, 125, 202, 274	0
9	AF	101/101 (100%)	0.72	17 (16%) 1 2	92, 150, 222, 283	0
9	CF	101/101 (100%)	0.28	10 (9%) 7 8	60, 104, 157, 216	0
10	AG	155/155 (100%)	0.60	17 (10%) 5 6	81, 147, 220, 290	0
10	CG	155/155 (100%)	0.56	19 (12%) 4 5	91, 147, 209, 352	0
11	AH	138/138 (100%)	0.27	7 (5%) 28 28	58, 110, 163, 235	0
11	CH	138/138 (100%)	0.54	9 (6%) 18 20	74, 130, 191, 271	0
12	AI	127/127 (100%)	1.61	41 (32%) 0 0	94, 172, 247, 329	0
12	CI	127/127 (100%)	1.65	40 (31%) 0 0	85, 174, 242, 307	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AJ	98/98 (100%)	1.79	34 (34%) 0 0	85, 172, 278, 357	0
13	CJ	98/98 (100%)	2.15	37 (37%) 0 0	86, 197, 311, 435	0
14	AK	114/114 (100%)	0.84	19 (16%) 1 2	59, 110, 172, 233	0
14	CK	114/114 (100%)	0.47	7 (6%) 21 22	55, 99, 165, 372	0
15	AL	122/122 (100%)	0.23	3 (2%) 57 55	44, 85, 148, 192	0
15	CL	122/122 (100%)	0.25	3 (2%) 57 55	48, 99, 149, 268	0
16	AM	117/117 (100%)	0.64	15 (12%) 3 4	81, 166, 258, 377	0
16	CM	117/117 (100%)	1.12	20 (17%) 1 2	109, 159, 244, 340	0
17	AN	60/60 (100%)	0.82	10 (16%) 1 2	72, 128, 174, 224	0
17	CN	60/60 (100%)	1.05	11 (18%) 1 1	80, 151, 191, 265	0
18	AO	88/88 (100%)	0.46	2 (2%) 60 59	67, 109, 157, 188	0
18	CO	88/88 (100%)	0.12	1 (1%) 80 79	58, 106, 146, 168	0
19	AP	83/83 (100%)	0.62	4 (4%) 30 31	65, 99, 135, 245	0
19	CP	83/83 (100%)	1.39	26 (31%) 0 0	78, 139, 192, 243	0
20	AQ	99/99 (100%)	0.33	4 (4%) 38 37	63, 102, 157, 211	0
20	CQ	99/99 (100%)	0.67	6 (6%) 21 22	76, 116, 167, 283	0
21	AR	70/70 (100%)	2.07	28 (40%) 0 0	76, 134, 215, 266	0
21	CR	70/70 (100%)	0.90	10 (14%) 2 3	70, 112, 182, 225	0
22	AS	78/78 (100%)	1.44	25 (32%) 0 0	113, 164, 229, 318	0
22	CS	78/78 (100%)	1.62	28 (35%) 0 0	112, 174, 250, 339	0
23	AT	99/99 (100%)	0.84	14 (14%) 2 3	68, 115, 202, 272	0
23	CT	99/99 (100%)	0.80	17 (17%) 1 1	84, 134, 222, 336	0
24	AU	24/24 (100%)	3.89	23 (95%) 0 0	102, 150, 217, 233	0
24	CU	24/24 (100%)	3.60	19 (79%) 0 0	126, 169, 229, 236	0
25	BA	2789/2879 (96%)	0.12	72 (2%) 56 54	36, 76, 211, 411	0
25	DA	2789/2879 (96%)	0.06	84 (3%) 50 49	27, 65, 189, 401	0
26	BB	119/119 (100%)	0.27	0 100 100	63, 129, 186, 245	0
26	DB	119/119 (100%)	0.30	2 (1%) 70 68	73, 119, 167, 276	0
27	BD	271/271 (100%)	0.30	13 (4%) 30 31	31, 66, 114, 224	0
27	DD	271/271 (100%)	-0.01	5 (1%) 68 67	14, 56, 107, 221	0
28	BE	204/204 (100%)	0.40	10 (4%) 29 29	35, 82, 148, 377	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	204/204 (100%)	0.09	5 (2%) 57 55	29, 74, 138, 256	0
29	BF	202/202 (100%)	0.01	1 (0%) 91 90	28, 81, 163, 345	0
29	DF	202/202 (100%)	0.10	2 (0%) 82 81	13, 69, 145, 300	0
30	BG	181/181 (100%)	1.06	40 (22%) 0 1	78, 147, 221, 323	0
30	DG	181/181 (100%)	0.75	29 (16%) 1 2	73, 136, 220, 288	0
31	BH	159/159 (100%)	1.37	49 (30%) 0 0	86, 172, 263, 376	0
31	DH	159/159 (100%)	0.07	7 (4%) 34 34	48, 100, 157, 286	0
32	BI	145/145 (100%)	2.16	60 (41%) 0 0	74, 188, 473, 559	0
32	DI	145/145 (100%)	0.76	15 (10%) 6 8	47, 118, 209, 462	0
33	BK	147/147 (100%)	5.37	122 (82%) 0 0	155, 266, 359, 430	0
33	DK	147/147 (100%)	4.51	120 (81%) 0 0	115, 275, 372, 435	0
34	BN	137/137 (100%)	0.44	6 (4%) 34 34	51, 89, 139, 220	0
34	DN	137/137 (100%)	0.02	0 100 100	37, 84, 149, 192	0
35	BO	122/122 (100%)	-0.15	0 100 100	44, 77, 121, 158	0
35	DO	122/122 (100%)	-0.15	0 100 100	31, 67, 117, 149	0
36	BP	146/146 (100%)	0.75	13 (8%) 9 11	27, 100, 201, 293	0
36	DP	146/146 (100%)	0.55	15 (10%) 6 8	23, 85, 172, 304	0
37	BQ	134/134 (100%)	0.39	7 (5%) 27 27	45, 86, 159, 419	0
37	DQ	134/134 (100%)	0.25	7 (5%) 27 27	41, 83, 175, 469	0
38	BR	117/117 (100%)	0.21	1 (0%) 84 83	37, 83, 141, 190	0
38	DR	117/117 (100%)	0.13	4 (3%) 45 44	32, 74, 137, 174	0
39	BS	98/98 (100%)	1.15	25 (25%) 0 0	61, 135, 212, 245	0
39	DS	98/98 (100%)	0.70	14 (14%) 2 3	72, 116, 180, 203	0
40	BT	137/137 (100%)	0.51	7 (5%) 28 28	54, 95, 195, 362	0
40	DT	137/137 (100%)	0.44	14 (10%) 6 8	34, 90, 194, 343	0
41	BU	117/117 (100%)	0.47	6 (5%) 28 28	36, 73, 137, 173	0
41	DU	117/117 (100%)	0.57	4 (3%) 45 44	35, 74, 125, 363	0
42	BV	101/101 (100%)	0.16	2 (1%) 65 64	49, 93, 159, 283	0
42	DV	101/101 (100%)	0.44	9 (8%) 9 11	34, 96, 153, 283	0
43	BW	112/112 (100%)	-0.09	1 (0%) 84 83	28, 66, 124, 378	0
43	DW	112/112 (100%)	-0.11	0 100 100	38, 66, 125, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	92/92 (100%)	0.08	2 (2%) 62 60	61, 87, 139, 179	0
44	DX	92/92 (100%)	0.09	1 (1%) 80 79	34, 66, 106, 168	0
45	BY	100/100 (100%)	1.41	23 (23%) 0 1	46, 112, 248, 418	0
45	DY	100/100 (100%)	1.11	15 (15%) 2 2	50, 92, 223, 452	0
46	BZ	187/187 (100%)	0.67	17 (9%) 9 10	75, 130, 200, 267	0
46	DZ	187/187 (100%)	0.46	11 (5%) 22 23	56, 123, 182, 260	0
47	B0	76/76 (100%)	0.30	2 (2%) 56 54	54, 84, 150, 259	0
47	D0	76/76 (100%)	0.33	3 (3%) 39 38	37, 80, 115, 238	0
48	B1	88/88 (100%)	0.44	5 (5%) 23 24	46, 90, 156, 264	0
48	D1	88/88 (100%)	0.36	4 (4%) 33 33	23, 69, 147, 267	0
49	B2	62/62 (100%)	0.50	6 (9%) 7 9	67, 119, 210, 257	0
49	D2	62/62 (100%)	0.61	7 (11%) 5 6	33, 75, 176, 304	0
50	B3	59/59 (100%)	0.86	6 (10%) 6 8	52, 80, 144, 224	0
50	D3	59/59 (100%)	0.42	3 (5%) 28 28	42, 81, 143, 236	0
51	B4	30/30 (100%)	0.75	5 (16%) 1 2	107, 184, 297, 335	0
51	D4	30/30 (100%)	1.43	11 (36%) 0 0	125, 215, 272, 361	0
52	B5	52/52 (100%)	0.33	3 (5%) 23 24	32, 75, 181, 213	0
52	D5	52/52 (100%)	-0.14	1 (1%) 66 65	20, 77, 172, 269	0
53	B6	44/44 (100%)	8.21	44 (100%) 0 0	118, 225, 304, 330	0
53	D6	44/44 (100%)	7.05	42 (95%) 0 0	136, 208, 276, 330	0
54	B7	48/48 (100%)	0.89	6 (12%) 3 4	35, 60, 131, 156	0
54	D7	48/48 (100%)	0.27	3 (6%) 20 21	19, 36, 94, 156	0
55	B8	63/63 (100%)	0.39	2 (3%) 47 46	38, 78, 155, 190	0
55	D8	63/63 (100%)	0.24	3 (4%) 30 31	33, 62, 142, 213	0
All	All	21328/21508 (99%)	0.56	2078 (9%) 7 9	13, 103, 238, 559	0

The worst 5 of 2078 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DK	6	ALA	23.8
53	B6	40	CYS	20.9
33	DK	1	MET	20.5
33	BK	135	GLY	18.7
53	D6	13	CYS	18.6

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
56	MG	BA	3022	1/1	-0.48	0.79	168,168,168,168	0
56	MG	AA	1831	1/1	-0.15	1.10	203,203,203,203	0
56	MG	BA	2918	1/1	-0.08	1.68	191,191,191,191	0
56	MG	CA	1792	1/1	-0.04	1.12	122,122,122,122	0
56	MG	AA	1854	1/1	-0.03	0.48	187,187,187,187	0
56	MG	BA	3197	1/1	0.01	0.14	215,215,215,215	0
56	MG	CA	1746	1/1	0.01	0.15	255,255,255,255	0
56	MG	CA	1626	1/1	0.04	0.43	109,109,109,109	0
56	MG	DA	2921	1/1	0.04	0.21	113,113,113,113	0
56	MG	AA	1764	1/1	0.06	0.91	103,103,103,103	0
56	MG	CA	1898	1/1	0.07	0.36	126,126,126,126	0
56	MG	AA	1780	1/1	0.07	1.15	105,105,105,105	0
56	MG	AT	201	1/1	0.09	0.32	117,117,117,117	0
56	MG	CA	1736	1/1	0.10	0.39	193,193,193,193	0
56	MG	CA	1677	1/1	0.11	1.25	138,138,138,138	0
56	MG	DA	3348	1/1	0.14	0.71	165,165,165,165	0
56	MG	BA	3078	1/1	0.14	0.76	117,117,117,117	0
56	MG	AC	301	1/1	0.17	1.50	98,98,98,98	0
56	MG	BA	3435	1/1	0.22	1.05	112,112,112,112	0
56	MG	DA	3484	1/1	0.26	0.59	98,98,98,98	0
56	MG	BA	3717	1/1	0.27	0.16	100,100,100,100	0
56	MG	CA	1633	1/1	0.28	0.33	143,143,143,143	0
56	MG	DB	218	1/1	0.28	0.51	111,111,111,111	0
56	MG	BB	223	1/1	0.28	0.41	242,242,242,242	0
56	MG	BA	3713	1/1	0.29	0.98	123,123,123,123	0
56	MG	DA	3072	1/1	0.30	0.63	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1979	1/1	0.31	0.77	118,118,118,118	0
56	MG	BA	3153	1/1	0.32	0.33	81,81,81,81	0
56	MG	CA	1631	1/1	0.32	1.38	119,119,119,119	0
56	MG	CA	1809	1/1	0.35	1.24	117,117,117,117	0
56	MG	AA	1765	1/1	0.35	0.61	74,74,74,74	0
56	MG	BA	3369	1/1	0.35	1.02	74,74,74,74	0
56	MG	CA	1613	1/1	0.36	0.87	71,71,71,71	0
56	MG	DA	3004	1/1	0.37	0.41	100,100,100,100	0
56	MG	CA	1912	1/1	0.38	0.43	152,152,152,152	0
56	MG	CA	1605	1/1	0.38	0.31	159,159,159,159	0
56	MG	BA	3672	1/1	0.38	0.47	88,88,88,88	0
56	MG	AA	1612	1/1	0.38	0.67	87,87,87,87	0
56	MG	CA	1748	1/1	0.38	0.52	78,78,78,78	0
56	MG	BA	3718	1/1	0.38	0.25	163,163,163,163	0
56	MG	DB	209	1/1	0.39	0.73	143,143,143,143	0
56	MG	DA	3541	1/1	0.39	0.79	70,70,70,70	0
56	MG	AA	1717	1/1	0.40	0.31	99,99,99,99	0
56	MG	AA	1629	1/1	0.40	0.90	83,83,83,83	0
56	MG	CA	1806	1/1	0.40	0.32	95,95,95,95	0
56	MG	AA	1950	1/1	0.41	0.41	102,102,102,102	0
56	MG	CA	1833	1/1	0.41	0.82	65,65,65,65	0
56	MG	CA	1741	1/1	0.41	0.30	104,104,104,104	0
56	MG	CA	1606	1/1	0.42	0.37	115,115,115,115	0
56	MG	BA	3592	1/1	0.42	0.24	132,132,132,132	0
56	MG	BA	2922	1/1	0.42	0.75	108,108,108,108	0
56	MG	BA	3186	1/1	0.42	0.47	98,98,98,98	0
56	MG	DA	3092	1/1	0.43	1.39	200,200,200,200	0
56	MG	BA	3607	1/1	0.43	0.18	105,105,105,105	0
56	MG	BA	3450	1/1	0.43	0.97	83,83,83,83	0
56	MG	CA	1800	1/1	0.43	0.63	124,124,124,124	0
56	MG	AA	1723	1/1	0.44	0.31	106,106,106,106	0
56	MG	AA	1945	1/1	0.44	0.41	115,115,115,115	0
56	MG	AA	1642	1/1	0.44	0.30	120,120,120,120	0
56	MG	AA	1697	1/1	0.46	0.20	148,148,148,148	0
56	MG	CY	401	1/1	0.46	0.53	103,103,103,103	0
56	MG	DA	3401	1/1	0.46	0.39	81,81,81,81	0
56	MG	BA	3588	1/1	0.46	0.80	120,120,120,120	0
56	MG	CA	1699	1/1	0.46	0.44	152,152,152,152	0
56	MG	CA	1860	1/1	0.47	0.27	133,133,133,133	0
56	MG	AA	1639	1/1	0.47	0.79	114,114,114,114	0
56	MG	DA	2948	1/1	0.47	0.64	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3591	1/1	0.47	1.28	102,102,102,102	0
56	MG	BA	3618	1/1	0.48	0.58	79,79,79,79	0
56	MG	CA	1772	1/1	0.48	0.64	66,66,66,66	0
56	MG	CA	1681	1/1	0.48	0.56	136,136,136,136	0
56	MG	DA	3054	1/1	0.49	0.64	93,93,93,93	0
56	MG	CA	1643	1/1	0.49	0.10	126,126,126,126	0
56	MG	CA	1794	1/1	0.50	0.34	60,60,60,60	0
56	MG	AA	1770	1/1	0.50	0.36	86,86,86,86	0
56	MG	BA	3247	1/1	0.50	0.55	105,105,105,105	0
56	MG	CA	1750	1/1	0.50	0.25	222,222,222,222	0
56	MG	BB	206	1/1	0.50	0.23	188,188,188,188	0
56	MG	AA	1957	1/1	0.50	0.79	109,109,109,109	0
56	MG	BA	3542	1/1	0.50	0.40	116,116,116,116	0
56	MG	DA	3044	1/1	0.51	0.42	87,87,87,87	0
56	MG	CA	1712	1/1	0.51	0.21	106,106,106,106	0
56	MG	AA	1653	1/1	0.52	0.26	105,105,105,105	0
56	MG	DV	201	1/1	0.52	0.43	85,85,85,85	0
56	MG	CA	1732	1/1	0.52	0.77	131,131,131,131	0
56	MG	CA	1777	1/1	0.52	0.29	98,98,98,98	0
56	MG	CA	1856	1/1	0.52	0.40	136,136,136,136	0
56	MG	BA	3261	1/1	0.52	0.72	89,89,89,89	0
56	MG	CA	1842	1/1	0.52	0.79	137,137,137,137	0
56	MG	BA	3003	1/1	0.53	0.59	113,113,113,113	0
56	MG	AA	1687	1/1	0.53	0.13	85,85,85,85	0
56	MG	BA	3606	1/1	0.53	0.38	72,72,72,72	0
56	MG	BA	3569	1/1	0.53	0.48	87,87,87,87	0
56	MG	BA	3213	1/1	0.53	0.48	125,125,125,125	0
56	MG	BA	3548	1/1	0.54	0.64	88,88,88,88	0
56	MG	DB	204	1/1	0.54	0.28	78,78,78,78	0
56	MG	CA	1914	1/1	0.54	0.27	96,96,96,96	0
56	MG	AA	1846	1/1	0.54	0.42	118,118,118,118	0
56	MG	CA	1725	1/1	0.54	0.90	78,78,78,78	0
56	MG	AA	1796	1/1	0.54	0.68	129,129,129,129	0
56	MG	BA	3665	1/1	0.55	0.24	117,117,117,117	0
56	MG	DA	3351	1/1	0.55	0.45	116,116,116,116	0
56	MG	BA	3119	1/1	0.55	1.15	133,133,133,133	0
56	MG	DA	3350	1/1	0.55	0.19	76,76,76,76	0
56	MG	CA	1907	1/1	0.55	0.54	77,77,77,77	0
56	MG	AA	1804	1/1	0.55	1.32	108,108,108,108	0
56	MG	DA	3405	1/1	0.55	0.21	91,91,91,91	0
56	MG	CA	1817	1/1	0.55	0.32	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	2950	1/1	0.56	0.85	87,87,87,87	0
56	MG	DA	3060	1/1	0.56	0.20	77,77,77,77	0
56	MG	BA	3583	1/1	0.56	0.69	87,87,87,87	0
56	MG	DA	3582	1/1	0.56	0.38	95,95,95,95	0
56	MG	BA	3600	1/1	0.56	0.59	73,73,73,73	0
56	MG	CA	1706	1/1	0.56	0.18	88,88,88,88	0
56	MG	BA	3263	1/1	0.57	0.40	66,66,66,66	0
56	MG	CA	1820	1/1	0.57	0.85	193,193,193,193	0
56	MG	BA	3173	1/1	0.57	0.81	67,67,67,67	0
56	MG	BA	2935	1/1	0.57	0.53	89,89,89,89	0
56	MG	BA	2974	1/1	0.57	0.29	85,85,85,85	0
56	MG	DA	2949	1/1	0.57	1.12	94,94,94,94	0
56	MG	BA	2997	1/1	0.57	0.21	104,104,104,104	0
56	MG	AA	1790	1/1	0.57	0.40	53,53,53,53	0
56	MG	BA	3064	1/1	0.57	0.44	63,63,63,63	0
56	MG	DA	3244	1/1	0.58	0.22	59,59,59,59	0
56	MG	DA	3548	1/1	0.58	0.43	85,85,85,85	0
56	MG	BA	3599	1/1	0.58	0.59	93,93,93,93	0
56	MG	BA	3236	1/1	0.58	0.34	132,132,132,132	0
56	MG	AA	1728	1/1	0.58	0.21	130,130,130,130	0
56	MG	DA	3248	1/1	0.58	1.19	66,66,66,66	0
56	MG	AA	1783	1/1	0.58	0.41	127,127,127,127	0
56	MG	BB	211	1/1	0.59	1.35	132,132,132,132	0
56	MG	BA	2958	1/1	0.59	0.15	103,103,103,103	0
56	MG	AA	1699	1/1	0.59	0.42	85,85,85,85	0
56	MG	BA	2915	1/1	0.59	0.27	102,102,102,102	0
56	MG	DA	3339	1/1	0.59	0.32	63,63,63,63	0
56	MG	CA	1724	1/1	0.59	0.30	108,108,108,108	0
56	MG	BA	2959	1/1	0.59	0.71	81,81,81,81	0
56	MG	BA	3012	1/1	0.59	0.99	91,91,91,91	0
56	MG	BA	2939	1/1	0.59	0.45	79,79,79,79	0
56	MG	AA	1631	1/1	0.59	0.81	76,76,76,76	0
56	MG	CA	1710	1/1	0.59	1.27	97,97,97,97	0
56	MG	AA	1767	1/1	0.60	0.56	102,102,102,102	0
56	MG	CA	1682	1/1	0.60	0.14	152,152,152,152	0
56	MG	AA	1689	1/1	0.60	0.14	169,169,169,169	0
56	MG	CA	1687	1/1	0.60	0.20	58,58,58,58	0
56	MG	DA	3531	1/1	0.60	0.42	92,92,92,92	0
56	MG	CA	1837	1/1	0.60	0.24	66,66,66,66	0
56	MG	AW	107	1/1	0.60	0.46	102,102,102,102	0
56	MG	AW	109	1/1	0.60	0.69	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1753	1/1	0.60	0.28	63,63,63,63	0
56	MG	BA	2943	1/1	0.60	1.09	98,98,98,98	0
56	MG	CA	1836	1/1	0.60	0.33	94,94,94,94	0
56	MG	BA	3584	1/1	0.61	0.49	96,96,96,96	0
56	MG	BA	3175	1/1	0.61	0.54	109,109,109,109	0
56	MG	CA	1752	1/1	0.61	0.44	83,83,83,83	0
56	MG	BA	3011	1/1	0.61	0.58	82,82,82,82	0
56	MG	DA	3381	1/1	0.61	0.44	43,43,43,43	0
56	MG	BA	3465	1/1	0.61	0.60	114,114,114,114	0
56	MG	BA	2926	1/1	0.61	0.56	80,80,80,80	0
56	MG	BA	3158	1/1	0.61	0.28	150,150,150,150	0
56	MG	BA	3697	1/1	0.61	0.12	64,64,64,64	0
56	MG	AT	203	1/1	0.61	1.74	99,99,99,99	0
56	MG	BA	3168	1/1	0.62	1.18	78,78,78,78	0
56	MG	AA	1726	1/1	0.62	0.51	141,141,141,141	0
56	MG	BA	3602	1/1	0.62	0.46	117,117,117,117	0
56	MG	DA	3632	1/1	0.62	0.19	135,135,135,135	0
56	MG	CA	1640	1/1	0.62	0.33	78,78,78,78	0
56	MG	DA	2914	1/1	0.62	0.46	97,97,97,97	0
56	MG	DA	3577	1/1	0.62	0.64	80,80,80,80	0
56	MG	CA	1816	1/1	0.62	0.64	77,77,77,77	0
56	MG	BA	3589	1/1	0.62	0.20	135,135,135,135	0
56	MG	CA	1669	1/1	0.62	1.73	118,118,118,118	0
56	MG	DA	3626	1/1	0.62	0.29	117,117,117,117	0
56	MG	DB	205	1/1	0.62	0.33	94,94,94,94	0
56	MG	CA	1647	1/1	0.62	0.43	98,98,98,98	0
56	MG	BA	3085	1/1	0.63	0.49	116,116,116,116	0
56	MG	CA	1735	1/1	0.63	0.84	108,108,108,108	0
56	MG	CA	1603	1/1	0.63	0.23	255,255,255,255	0
56	MG	DA	3398	1/1	0.63	0.79	107,107,107,107	0
56	MG	BA	3722	1/1	0.63	0.26	80,80,80,80	0
56	MG	AY	403	1/1	0.63	0.87	87,87,87,87	0
56	MG	DB	208	1/1	0.63	0.31	83,83,83,83	0
56	MG	BA	3081	1/1	0.63	0.18	79,79,79,79	0
56	MG	DA	3497	1/1	0.63	0.28	61,61,61,61	0
56	MG	AA	1947	1/1	0.63	0.49	89,89,89,89	0
56	MG	CA	1920	1/1	0.63	0.13	138,138,138,138	0
56	MG	DA	2903	1/1	0.63	0.45	77,77,77,77	0
56	MG	DA	3308	1/1	0.64	0.90	72,72,72,72	0
56	MG	DA	3527	1/1	0.64	0.27	77,77,77,77	0
56	MG	DA	3428	1/1	0.64	0.65	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3573	1/1	0.64	0.24	81,81,81,81	0
56	MG	AA	1742	1/1	0.64	1.36	197,197,197,197	0
56	MG	BA	3482	1/1	0.64	1.30	74,74,74,74	0
56	MG	DA	3097	1/1	0.64	0.51	68,68,68,68	0
56	MG	CA	1926	1/1	0.64	0.73	101,101,101,101	0
56	MG	AA	1855	1/1	0.64	0.15	103,103,103,103	0
56	MG	DA	3516	1/1	0.64	0.42	70,70,70,70	0
56	MG	AA	1727	1/1	0.64	0.48	93,93,93,93	0
56	MG	DA	2953	1/1	0.64	0.17	151,151,151,151	0
56	MG	DA	3489	1/1	0.64	0.33	51,51,51,51	0
56	MG	CA	1796	1/1	0.65	0.16	41,41,41,41	0
56	MG	AA	1702	1/1	0.65	0.65	97,97,97,97	0
56	MG	CA	1645	1/1	0.65	1.03	113,113,113,113	0
56	MG	CA	1828	1/1	0.65	0.28	135,135,135,135	0
56	MG	DA	3052	1/1	0.65	0.52	76,76,76,76	0
56	MG	AA	1645	1/1	0.65	0.32	82,82,82,82	0
56	MG	AA	1890	1/1	0.66	0.15	124,124,124,124	0
56	MG	CA	1740	1/1	0.66	0.21	101,101,101,101	0
56	MG	DA	3118	1/1	0.66	0.18	61,61,61,61	0
56	MG	DA	3122	1/1	0.66	0.35	67,67,67,67	0
56	MG	CA	1884	1/1	0.66	0.53	79,79,79,79	0
56	MG	AY	401	1/1	0.66	0.54	119,119,119,119	0
56	MG	BA	2949	1/1	0.66	0.43	70,70,70,70	0
56	MG	CA	1646	1/1	0.66	0.12	113,113,113,113	0
56	MG	BA	3577	1/1	0.66	0.91	88,88,88,88	0
56	MG	DA	3001	1/1	0.66	0.53	79,79,79,79	0
56	MG	DA	3088	1/1	0.66	0.38	86,86,86,86	0
56	MG	AA	1782	1/1	0.66	0.56	77,77,77,77	0
56	MG	BA	3105	1/1	0.66	0.24	122,122,122,122	0
56	MG	CA	1874	1/1	0.67	1.45	89,89,89,89	0
56	MG	CA	1790	1/1	0.67	0.84	86,86,86,86	0
56	MG	BA	3123	1/1	0.67	0.25	156,156,156,156	0
56	MG	CA	1854	1/1	0.67	0.41	98,98,98,98	0
56	MG	BA	3212	1/1	0.67	0.36	109,109,109,109	0
56	MG	BA	2946	1/1	0.67	0.46	61,61,61,61	0
56	MG	AA	1688	1/1	0.67	0.24	80,80,80,80	0
56	MG	CA	1877	1/1	0.67	0.84	154,154,154,154	0
56	MG	CA	1671	1/1	0.67	0.31	92,92,92,92	0
56	MG	AW	104	1/1	0.67	1.33	95,95,95,95	0
56	MG	CA	1843	1/1	0.67	0.32	103,103,103,103	0
56	MG	BA	2976	1/1	0.67	0.44	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BB	216	1/1	0.67	0.54	109,109,109,109	0
56	MG	CA	1882	1/1	0.67	0.52	81,81,81,81	0
56	MG	BA	3255	1/1	0.67	0.38	66,66,66,66	0
56	MG	AA	1952	1/1	0.67	0.09	53,53,53,53	0
56	MG	AW	102	1/1	0.67	0.48	94,94,94,94	0
56	MG	BA	3062	1/1	0.67	0.21	110,110,110,110	0
56	MG	BA	3111	1/1	0.67	0.12	96,96,96,96	0
56	MG	CA	1658	1/1	0.67	0.49	93,93,93,93	0
56	MG	BA	3639	1/1	0.68	0.41	79,79,79,79	0
56	MG	DA	2940	1/1	0.68	0.18	94,94,94,94	0
56	MG	DA	3544	1/1	0.68	0.41	73,73,73,73	0
56	MG	CA	1698	1/1	0.68	0.27	100,100,100,100	0
56	MG	BA	3073	1/1	0.68	0.51	124,124,124,124	0
56	MG	CA	1703	1/1	0.68	0.19	89,89,89,89	0
56	MG	DA	2975	1/1	0.68	0.91	79,79,79,79	0
56	MG	AA	1917	1/1	0.68	0.15	86,86,86,86	0
56	MG	DA	3532	1/1	0.68	0.25	72,72,72,72	0
56	MG	CA	1801	1/1	0.68	0.31	76,76,76,76	0
56	MG	AW	115	1/1	0.68	0.35	111,111,111,111	0
56	MG	BA	3284	1/1	0.68	0.46	82,82,82,82	0
56	MG	CW	113	1/1	0.68	0.20	89,89,89,89	0
56	MG	AA	1619	1/1	0.68	0.74	69,69,69,69	0
56	MG	AW	113	1/1	0.68	0.31	96,96,96,96	0
56	MG	DA	3373	1/1	0.68	0.19	86,86,86,86	0
56	MG	BA	3065	1/1	0.68	0.23	90,90,90,90	0
56	MG	DA	3343	1/1	0.68	0.49	76,76,76,76	0
56	MG	BA	3218	1/1	0.68	0.60	82,82,82,82	0
56	MG	BA	3290	1/1	0.68	0.25	77,77,77,77	0
56	MG	DA	2964	1/1	0.68	0.41	65,65,65,65	0
56	MG	AA	1879	1/1	0.69	0.48	99,99,99,99	0
56	MG	BA	3536	1/1	0.69	0.64	66,66,66,66	0
56	MG	DA	3073	1/1	0.69	0.46	80,80,80,80	0
56	MG	DA	3119	1/1	0.69	0.50	82,82,82,82	0
56	MG	BA	3663	1/1	0.69	0.28	105,105,105,105	0
56	MG	DA	2911	1/1	0.69	1.04	84,84,84,84	0
56	MG	AA	1829	1/1	0.69	1.54	232,232,232,232	0
56	MG	BA	2932	1/1	0.69	0.16	78,78,78,78	0
56	MG	DA	3075	1/1	0.69	0.38	75,75,75,75	0
56	MG	DA	3128	1/1	0.69	0.27	101,101,101,101	0
56	MG	CA	1783	1/1	0.69	0.10	82,82,82,82	0
56	MG	AA	1934	1/1	0.69	0.40	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1731	1/1	0.69	0.11	139,139,139,139	0
56	MG	BA	2941	1/1	0.69	0.37	87,87,87,87	0
56	MG	BA	3596	1/1	0.69	0.38	140,140,140,140	0
56	MG	DA	3353	1/1	0.69	0.11	66,66,66,66	0
56	MG	BA	3393	1/1	0.69	0.17	99,99,99,99	0
56	MG	AA	1794	1/1	0.69	0.15	151,151,151,151	0
56	MG	AA	1772	1/1	0.69	0.41	94,94,94,94	0
56	MG	CA	1743	1/1	0.69	0.34	169,169,169,169	0
56	MG	DA	3511	1/1	0.69	0.36	64,64,64,64	0
56	MG	BA	3202	1/1	0.69	0.20	205,205,205,205	0
56	MG	DA	3338	1/1	0.69	0.79	76,76,76,76	0
56	MG	AA	1824	1/1	0.69	0.68	108,108,108,108	0
56	MG	AA	1672	1/1	0.70	0.66	73,73,73,73	0
56	MG	DA	3326	1/1	0.70	0.42	47,47,47,47	0
56	MG	AA	1981	1/1	0.70	0.18	90,90,90,90	0
56	MG	CA	1719	1/1	0.70	0.50	106,106,106,106	0
56	MG	DA	3439	1/1	0.70	0.34	66,66,66,66	0
56	MG	BA	2920	1/1	0.70	0.41	70,70,70,70	0
56	MG	AA	1615	1/1	0.70	0.17	87,87,87,87	0
56	MG	CA	1822	1/1	0.70	0.27	112,112,112,112	0
56	MG	BA	3533	1/1	0.70	0.17	97,97,97,97	0
56	MG	CA	1739	1/1	0.70	0.16	122,122,122,122	0
56	MG	CA	1734	1/1	0.70	0.22	196,196,196,196	0
56	MG	BB	208	1/1	0.70	0.70	82,82,82,82	0
56	MG	CA	1607	1/1	0.70	0.43	138,138,138,138	0
56	MG	AW	110	1/1	0.70	0.27	145,145,145,145	0
56	MG	DA	2983	1/1	0.70	0.33	77,77,77,77	0
56	MG	DA	3086	1/1	0.70	0.77	120,120,120,120	0
56	MG	BA	3239	1/1	0.70	0.45	99,99,99,99	0
56	MG	BA	3332	1/1	0.70	0.83	58,58,58,58	0
56	MG	BA	3676	1/1	0.71	0.43	181,181,181,181	0
56	MG	BA	3709	1/1	0.71	0.34	97,97,97,97	0
56	MG	DA	3243	1/1	0.71	0.55	77,77,77,77	0
56	MG	BA	3004	1/1	0.71	0.46	99,99,99,99	0
56	MG	AA	1892	1/1	0.71	0.24	108,108,108,108	0
56	MG	AA	1839	1/1	0.71	0.52	88,88,88,88	0
56	MG	BA	3224	1/1	0.71	0.64	85,85,85,85	0
56	MG	BA	3080	1/1	0.71	0.31	112,112,112,112	0
56	MG	BA	3553	1/1	0.71	0.46	92,92,92,92	0
56	MG	DA	2910	1/1	0.71	0.10	90,90,90,90	0
56	MG	BA	2973	1/1	0.71	0.53	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3540	1/1	0.71	0.59	84,84,84,84	0
56	MG	CA	1614	1/1	0.71	0.42	122,122,122,122	0
56	MG	AA	1621	1/1	0.71	0.17	74,74,74,74	0
56	MG	DA	3284	1/1	0.71	0.36	53,53,53,53	0
56	MG	AA	1990	1/1	0.71	0.24	58,58,58,58	0
56	MG	AA	1632	1/1	0.71	0.45	87,87,87,87	0
56	MG	AA	1786	1/1	0.71	0.46	71,71,71,71	0
56	MG	AA	1605	1/1	0.71	0.19	142,142,142,142	0
56	MG	DA	3023	1/1	0.71	0.40	71,71,71,71	0
56	MG	CA	1807	1/1	0.71	0.70	195,195,195,195	0
56	MG	CA	1902	1/1	0.71	0.63	128,128,128,128	0
56	MG	BA	2993	1/1	0.71	0.30	57,57,57,57	0
56	MG	DA	2917	1/1	0.71	0.45	83,83,83,83	0
56	MG	DA	3385	1/1	0.71	0.40	77,77,77,77	0
56	MG	DA	3016	1/1	0.71	0.41	99,99,99,99	0
56	MG	CA	1675	1/1	0.71	0.45	75,75,75,75	0
56	MG	DA	3059	1/1	0.71	0.30	82,82,82,82	0
56	MG	DA	3346	1/1	0.71	0.26	90,90,90,90	0
56	MG	AA	1660	1/1	0.71	0.27	105,105,105,105	0
56	MG	AA	1951	1/1	0.71	0.50	73,73,73,73	0
56	MG	BA	3230	1/1	0.71	0.58	103,103,103,103	0
56	MG	BA	2917	1/1	0.71	0.59	188,188,188,188	0
56	MG	BA	3605	1/1	0.71	0.09	72,72,72,72	0
56	MG	BA	3170	1/1	0.71	0.37	60,60,60,60	0
56	MG	BA	2996	1/1	0.71	0.19	209,209,209,209	0
56	MG	BA	3131	1/1	0.71	0.36	65,65,65,65	0
56	MG	BA	3098	1/1	0.72	0.59	94,94,94,94	0
56	MG	AA	1942	1/1	0.72	0.16	92,92,92,92	0
56	MG	DA	3009	1/1	0.72	0.62	130,130,130,130	0
56	MG	BA	3055	1/1	0.72	0.28	71,71,71,71	0
56	MG	CA	1802	1/1	0.72	0.31	61,61,61,61	0
56	MG	BA	3448	1/1	0.72	0.35	72,72,72,72	0
56	MG	BA	2951	1/1	0.72	0.16	50,50,50,50	0
56	MG	AG	201	1/1	0.72	0.88	78,78,78,78	0
56	MG	BA	3092	1/1	0.72	0.46	99,99,99,99	0
56	MG	BA	3711	1/1	0.72	0.16	104,104,104,104	0
56	MG	CA	1904	1/1	0.72	0.26	80,80,80,80	0
56	MG	AA	1714	1/1	0.72	0.58	114,114,114,114	0
56	MG	BA	3148	1/1	0.72	0.19	111,111,111,111	0
56	MG	BA	2907	1/1	0.72	0.38	129,129,129,129	0
56	MG	CA	1676	1/1	0.72	0.21	88,88,88,88	0
56	MG	BA	3252	1/1	0.72	0.48	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3597	1/1	0.72	0.54	91,91,91,91	0
56	MG	CA	1840	1/1	0.72	0.56	101,101,101,101	0
56	MG	BA	3093	1/1	0.72	0.43	55,55,55,55	0
56	MG	AA	1725	1/1	0.72	0.66	121,121,121,121	0
56	MG	BA	3612	1/1	0.72	0.40	96,96,96,96	0
56	MG	BA	3002	1/1	0.72	0.40	91,91,91,91	0
56	MG	CD	302	1/1	0.72	0.43	111,111,111,111	0
56	MG	BA	3307	1/1	0.72	0.20	83,83,83,83	0
56	MG	DA	2944	1/1	0.72	0.18	94,94,94,94	0
56	MG	AA	1860	1/1	0.72	0.41	62,62,62,62	0
56	MG	BA	3189	1/1	0.72	0.45	105,105,105,105	0
56	MG	BA	3194	1/1	0.72	0.34	91,91,91,91	0
56	MG	DA	3449	1/1	0.72	0.25	53,53,53,53	0
56	MG	DA	3430	1/1	0.72	0.16	80,80,80,80	0
56	MG	BA	3147	1/1	0.72	0.42	88,88,88,88	0
56	MG	CW	102	1/1	0.73	0.57	105,105,105,105	0
56	MG	DA	3510	1/1	0.73	0.76	69,69,69,69	0
56	MG	DA	3287	1/1	0.73	0.84	44,44,44,44	0
56	MG	BA	2981	1/1	0.73	0.36	79,79,79,79	0
56	MG	BA	2930	1/1	0.73	0.60	89,89,89,89	0
56	MG	DA	3416	1/1	0.73	0.18	60,60,60,60	0
56	MG	BA	3053	1/1	0.73	0.45	95,95,95,95	0
56	MG	BE	301	1/1	0.73	0.56	60,60,60,60	0
56	MG	BA	2927	1/1	0.73	0.25	82,82,82,82	0
56	MG	AA	1778	1/1	0.73	0.19	159,159,159,159	0
56	MG	BA	3668	1/1	0.73	0.20	71,71,71,71	0
56	MG	DA	3522	1/1	0.73	0.19	77,77,77,77	0
56	MG	BA	3529	1/1	0.73	0.31	79,79,79,79	0
56	MG	BA	3084	1/1	0.73	0.50	73,73,73,73	0
56	MG	DA	2905	1/1	0.73	0.14	87,87,87,87	0
56	MG	DA	3070	1/1	0.73	0.60	69,69,69,69	0
56	MG	BA	3300	1/1	0.73	0.39	89,89,89,89	0
56	MG	CA	1720	1/1	0.73	0.45	84,84,84,84	0
56	MG	CA	1670	1/1	0.73	0.29	61,61,61,61	0
56	MG	AA	1622	1/1	0.73	0.66	70,70,70,70	0
56	MG	AA	1750	1/1	0.73	0.31	77,77,77,77	0
56	MG	BA	3309	1/1	0.73	0.35	68,68,68,68	0
56	MG	D0	101	1/1	0.73	0.33	42,42,42,42	0
56	MG	CA	1674	1/1	0.73	0.20	107,107,107,107	0
56	MG	BA	3574	1/1	0.73	0.40	70,70,70,70	0
56	MG	BA	3020	1/1	0.73	0.55	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3273	1/1	0.73	0.30	110,110,110,110	0
56	MG	BA	2925	1/1	0.73	0.59	76,76,76,76	0
56	MG	BA	3035	1/1	0.73	0.13	158,158,158,158	0
56	MG	DA	3325	1/1	0.73	0.48	46,46,46,46	0
56	MG	BA	3629	1/1	0.73	0.88	129,129,129,129	0
56	MG	AA	1811	1/1	0.73	0.38	91,91,91,91	0
56	MG	AA	1874	1/1	0.73	0.41	59,59,59,59	0
56	MG	BA	3278	1/1	0.73	0.51	115,115,115,115	0
56	MG	DA	3117	1/1	0.73	0.24	72,72,72,72	0
56	MG	BA	3229	1/1	0.74	0.53	92,92,92,92	0
56	MG	CA	1905	1/1	0.74	0.39	84,84,84,84	0
56	MG	AA	1858	1/1	0.74	0.28	132,132,132,132	0
56	MG	CA	1678	1/1	0.74	1.80	128,128,128,128	0
56	MG	CW	112	1/1	0.74	0.27	103,103,103,103	0
56	MG	BA	3139	1/1	0.74	0.41	73,73,73,73	0
56	MG	DA	3630	1/1	0.74	0.15	76,76,76,76	0
56	MG	CA	1717	1/1	0.74	0.25	121,121,121,121	0
56	MG	CA	1667	1/1	0.74	0.28	118,118,118,118	0
56	MG	CA	1780	1/1	0.74	0.53	72,72,72,72	0
56	MG	AA	1975	1/1	0.74	0.26	121,121,121,121	0
56	MG	DA	3329	1/1	0.74	0.34	46,46,46,46	0
56	MG	AA	1850	1/1	0.74	0.23	98,98,98,98	0
56	MG	BA	3267	1/1	0.74	0.41	123,123,123,123	0
56	MG	BA	3054	1/1	0.74	0.30	91,91,91,91	0
56	MG	DA	3586	1/1	0.74	0.77	133,133,133,133	0
56	MG	BA	3389	1/1	0.74	0.31	47,47,47,47	0
56	MG	DA	3375	1/1	0.74	0.49	78,78,78,78	0
56	MG	DA	3292	1/1	0.74	0.31	34,34,34,34	0
56	MG	DA	2930	1/1	0.74	0.45	86,86,86,86	0
56	MG	DA	3066	1/1	0.74	1.50	90,90,90,90	0
56	MG	DA	2936	1/1	0.74	0.50	82,82,82,82	0
56	MG	BA	3517	1/1	0.74	0.53	55,55,55,55	0
56	MG	D7	101	1/1	0.74	0.48	62,62,62,62	0
56	MG	CA	1644	1/1	0.74	1.32	120,120,120,120	0
56	MG	BA	3359	1/1	0.74	0.10	106,106,106,106	0
56	MG	BA	3130	1/1	0.75	0.50	82,82,82,82	0
56	MG	CW	116	1/1	0.75	0.14	70,70,70,70	0
56	MG	BA	3256	1/1	0.75	0.57	91,91,91,91	0
56	MG	BA	3496	1/1	0.75	0.43	63,63,63,63	0
56	MG	BA	3299	1/1	0.75	0.65	102,102,102,102	0
56	MG	BA	3479	1/1	0.75	0.47	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3441	1/1	0.75	0.38	46,46,46,46	0
56	MG	BA	3501	1/1	0.75	0.19	52,52,52,52	0
56	MG	BA	3433	1/1	0.75	0.37	97,97,97,97	0
56	MG	BA	3455	1/1	0.75	0.26	64,64,64,64	0
56	MG	BB	202	1/1	0.75	0.19	98,98,98,98	0
56	MG	DF	301	1/1	0.75	0.45	37,37,37,37	0
56	MG	BA	3156	1/1	0.75	0.50	74,74,74,74	0
56	MG	BA	3442	1/1	0.75	0.39	79,79,79,79	0
56	MG	CA	1887	1/1	0.75	0.43	116,116,116,116	0
56	MG	AA	1681	1/1	0.75	0.22	68,68,68,68	0
56	MG	BA	3264	1/1	0.75	0.48	89,89,89,89	0
56	MG	DA	2937	1/1	0.75	0.67	104,104,104,104	0
56	MG	BA	3082	1/1	0.75	0.34	119,119,119,119	0
56	MG	CA	1738	1/1	0.75	0.38	123,123,123,123	0
56	MG	DA	2972	1/1	0.75	0.62	187,187,187,187	0
56	MG	BA	3225	1/1	0.75	0.28	96,96,96,96	0
56	MG	CA	1850	1/1	0.75	0.40	93,93,93,93	0
56	MG	BA	3117	1/1	0.75	0.21	92,92,92,92	0
56	MG	DA	3403	1/1	0.75	0.81	77,77,77,77	0
56	MG	DA	3521	1/1	0.75	0.30	93,93,93,93	0
56	MG	DA	3386	1/1	0.75	0.22	102,102,102,102	0
56	MG	DA	3427	1/1	0.75	1.15	84,84,84,84	0
56	MG	CW	101	1/1	0.75	0.35	96,96,96,96	0
56	MG	BA	3494	1/1	0.75	0.18	73,73,73,73	0
56	MG	BA	3557	1/1	0.75	0.15	97,97,97,97	0
56	MG	AW	112	1/1	0.75	0.57	82,82,82,82	0
56	MG	BA	3403	1/1	0.76	0.50	79,79,79,79	0
56	MG	DA	3453	1/1	0.76	0.19	85,85,85,85	0
56	MG	BA	3298	1/1	0.76	0.38	101,101,101,101	0
56	MG	AA	1977	1/1	0.76	0.37	126,126,126,126	0
56	MG	BA	3550	1/1	0.76	0.12	68,68,68,68	0
56	MG	BA	3196	1/1	0.76	0.09	84,84,84,84	0
56	MG	DB	201	1/1	0.76	0.34	62,62,62,62	0
56	MG	AA	1835	1/1	0.76	0.99	76,76,76,76	0
56	MG	BA	3546	1/1	0.76	0.63	200,200,200,200	0
56	MG	BA	3407	1/1	0.76	0.61	78,78,78,78	0
56	MG	DA	3033	1/1	0.76	0.41	93,93,93,93	0
56	MG	BA	3655	1/1	0.76	0.41	87,87,87,87	0
56	MG	DW	201	1/1	0.76	0.53	76,76,76,76	0
56	MG	CA	1918	1/1	0.76	0.15	107,107,107,107	0
56	MG	BA	3137	1/1	0.76	0.28	83,83,83,83	0
56	MG	DA	3342	1/1	0.76	0.09	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1747	1/1	0.76	1.26	122,122,122,122	0
56	MG	AA	1722	1/1	0.76	0.24	72,72,72,72	0
56	MG	BA	2929	1/1	0.76	0.53	64,64,64,64	0
56	MG	CA	1863	1/1	0.76	0.30	69,69,69,69	0
56	MG	DA	3364	1/1	0.76	0.10	80,80,80,80	0
56	MG	DA	2915	1/1	0.76	0.42	78,78,78,78	0
56	MG	BA	3114	1/1	0.76	0.20	119,119,119,119	0
56	MG	BA	2934	1/1	0.76	0.72	79,79,79,79	0
56	MG	CA	1718	1/1	0.76	0.12	136,136,136,136	0
56	MG	CA	1663	1/1	0.76	0.63	210,210,210,210	0
56	MG	BA	3297	1/1	0.76	0.63	122,122,122,122	0
56	MG	BA	3049	1/1	0.76	0.30	90,90,90,90	0
56	MG	BA	3257	1/1	0.76	0.51	69,69,69,69	0
56	MG	AA	1652	1/1	0.76	0.19	98,98,98,98	0
56	MG	DA	2938	1/1	0.76	0.38	71,71,71,71	0
56	MG	DB	206	1/1	0.76	0.41	121,121,121,121	0
56	MG	AA	1748	1/1	0.76	0.24	54,54,54,54	0
56	MG	CA	1808	1/1	0.76	0.56	74,74,74,74	0
56	MG	BA	3016	1/1	0.76	0.28	168,168,168,168	0
56	MG	DA	3491	1/1	0.76	0.35	71,71,71,71	0
56	MG	AA	1607	1/1	0.76	0.47	97,97,97,97	0
56	MG	BA	3696	1/1	0.77	0.17	96,96,96,96	0
56	MG	BA	3570	1/1	0.77	0.15	83,83,83,83	0
56	MG	CA	1810	1/1	0.77	0.71	121,121,121,121	0
56	MG	BB	215	1/1	0.77	0.34	94,94,94,94	0
56	MG	DA	3501	1/1	0.77	0.09	96,96,96,96	0
56	MG	AA	1825	1/1	0.77	0.43	138,138,138,138	0
56	MG	BA	2999	1/1	0.77	0.09	92,92,92,92	0
56	MG	CA	1911	1/1	0.77	1.07	107,107,107,107	0
56	MG	BA	3514	1/1	0.77	1.15	80,80,80,80	0
56	MG	BB	222	1/1	0.77	0.19	206,206,206,206	0
56	MG	AA	1891	1/1	0.77	0.19	67,67,67,67	0
56	MG	BA	3303	1/1	0.77	0.27	69,69,69,69	0
56	MG	DA	3528	1/1	0.77	0.33	54,54,54,54	0
56	MG	BB	203	1/1	0.77	0.37	78,78,78,78	0
56	MG	DA	3456	1/1	0.77	0.20	116,116,116,116	0
56	MG	BA	3270	1/1	0.77	0.40	70,70,70,70	0
56	MG	AA	1721	1/1	0.77	0.40	128,128,128,128	0
56	MG	AA	1909	1/1	0.77	0.18	65,65,65,65	0
56	MG	DA	3568	1/1	0.77	0.41	65,65,65,65	0
56	MG	BA	2972	1/1	0.77	0.53	122,122,122,122	0
56	MG	DA	3436	1/1	0.77	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3593	1/1	0.77	0.32	57,57,57,57	0
56	MG	DA	2999	1/1	0.77	0.19	102,102,102,102	0
56	MG	BA	3193	1/1	0.77	0.31	79,79,79,79	0
56	MG	DA	3107	1/1	0.77	0.60	139,139,139,139	0
56	MG	AA	1967	1/1	0.77	0.27	61,61,61,61	0
56	MG	CA	1756	1/1	0.77	0.37	60,60,60,60	0
56	MG	DA	3627	1/1	0.77	0.28	81,81,81,81	0
56	MG	BA	3141	1/1	0.77	0.71	62,62,62,62	0
56	MG	CA	1885	1/1	0.77	0.27	270,270,270,270	0
56	MG	BA	3306	1/1	0.77	0.39	68,68,68,68	0
56	MG	BA	3414	1/1	0.77	0.67	47,47,47,47	0
56	MG	DA	2989	1/1	0.77	0.47	53,53,53,53	0
56	MG	DA	3380	1/1	0.77	0.28	85,85,85,85	0
56	MG	BA	3538	1/1	0.77	0.37	82,82,82,82	0
56	MG	BA	2913	1/1	0.77	0.35	77,77,77,77	0
56	MG	DA	3432	1/1	0.77	0.30	104,104,104,104	0
56	MG	DA	3003	1/1	0.77	0.43	59,59,59,59	0
56	MG	CA	1704	1/1	0.77	0.71	88,88,88,88	0
56	MG	BA	3211	1/1	0.77	0.49	71,71,71,71	0
56	MG	BA	3110	1/1	0.77	0.37	72,72,72,72	0
56	MG	BA	3601	1/1	0.77	0.15	50,50,50,50	0
56	MG	BA	3720	1/1	0.77	0.22	85,85,85,85	0
56	MG	BA	3067	1/1	0.78	0.17	142,142,142,142	0
56	MG	AA	1625	1/1	0.78	0.48	85,85,85,85	0
56	MG	DA	3007	1/1	0.78	0.13	70,70,70,70	0
56	MG	DA	3517	1/1	0.78	0.42	62,62,62,62	0
56	MG	AA	1953	1/1	0.78	0.38	51,51,51,51	0
56	MG	BA	3661	1/1	0.78	0.69	56,56,56,56	0
56	MG	BA	3248	1/1	0.78	0.49	102,102,102,102	0
56	MG	BA	3650	1/1	0.78	0.48	95,95,95,95	0
56	MG	AA	1866	1/1	0.78	0.18	118,118,118,118	0
56	MG	CA	1869	1/1	0.78	0.38	95,95,95,95	0
56	MG	DA	3320	1/1	0.78	0.11	78,78,78,78	0
56	MG	AA	1900	1/1	0.78	0.30	213,213,213,213	0
56	MG	DA	3519	1/1	0.78	1.54	78,78,78,78	0
56	MG	BA	3610	1/1	0.78	0.40	95,95,95,95	0
56	MG	AW	116	1/1	0.78	0.19	86,86,86,86	0
56	MG	DA	3270	1/1	0.78	0.64	69,69,69,69	0
56	MG	DA	3502	1/1	0.78	1.32	73,73,73,73	0
56	MG	AA	1757	1/1	0.78	0.32	74,74,74,74	0
56	MG	BA	3377	1/1	0.78	0.46	56,56,56,56	0
56	MG	CA	1686	1/1	0.78	0.27	286,286,286,286	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3395	1/1	0.78	0.13	95,95,95,95	0
56	MG	BA	3115	1/1	0.78	0.20	62,62,62,62	0
56	MG	BA	3112	1/1	0.78	0.18	83,83,83,83	0
56	MG	DA	3030	1/1	0.78	1.40	78,78,78,78	0
56	MG	AA	1777	1/1	0.78	0.17	101,101,101,101	0
56	MG	AA	1826	1/1	0.78	0.36	78,78,78,78	0
56	MG	CA	1812	1/1	0.78	0.58	75,75,75,75	0
56	MG	DA	3611	1/1	0.78	0.88	60,60,60,60	0
56	MG	CA	1693	1/1	0.78	0.42	67,67,67,67	0
56	MG	BA	3143	1/1	0.78	0.43	81,81,81,81	0
56	MG	CA	1793	1/1	0.78	0.26	114,114,114,114	0
56	MG	CA	1617	1/1	0.78	0.38	69,69,69,69	0
56	MG	DA	3095	1/1	0.78	0.13	100,100,100,100	0
56	MG	CA	1691	1/1	0.78	0.32	161,161,161,161	0
56	MG	AA	1686	1/1	0.78	0.42	85,85,85,85	0
56	MG	CA	1900	1/1	0.78	0.49	112,112,112,112	0
56	MG	BA	3182	1/1	0.78	0.60	70,70,70,70	0
56	MG	BA	3462	1/1	0.78	0.41	95,95,95,95	0
56	MG	BA	3140	1/1	0.78	0.34	55,55,55,55	0
56	MG	BA	3185	1/1	0.78	0.65	66,66,66,66	0
56	MG	BA	2983	1/1	0.78	0.17	44,44,44,44	0
56	MG	AA	1946	1/1	0.79	0.30	86,86,86,86	0
56	MG	DA	3008	1/1	0.79	0.52	70,70,70,70	0
56	MG	DA	3257	1/1	0.79	0.28	90,90,90,90	0
56	MG	AA	1941	1/1	0.79	0.75	100,100,100,100	0
56	MG	BA	2910	1/1	0.79	0.11	79,79,79,79	0
56	MG	AA	1752	1/1	0.79	0.37	183,183,183,183	0
56	MG	CA	1872	1/1	0.79	0.31	88,88,88,88	0
56	MG	BA	3097	1/1	0.79	0.73	73,73,73,73	0
56	MG	BA	3128	1/1	0.79	0.99	111,111,111,111	0
56	MG	BA	3568	1/1	0.79	0.17	84,84,84,84	0
56	MG	B0	102	1/1	0.79	0.45	68,68,68,68	0
56	MG	DA	3367	1/1	0.79	0.21	74,74,74,74	0
56	MG	BA	3244	1/1	0.79	1.33	67,67,67,67	0
56	MG	AA	1646	1/1	0.79	0.10	73,73,73,73	0
56	MG	DA	3621	1/1	0.79	0.40	77,77,77,77	0
56	MG	DA	3618	1/1	0.79	0.27	69,69,69,69	0
56	MG	CA	1892	1/1	0.79	0.14	150,150,150,150	0
56	MG	DA	2931	1/1	0.79	0.22	87,87,87,87	0
56	MG	DA	3371	1/1	0.79	0.39	65,65,65,65	0
56	MG	DA	3161	1/1	0.79	0.21	10,10,10,10	0
56	MG	BA	3032	1/1	0.79	0.67	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1797	1/1	0.79	0.36	60,60,60,60	0
56	MG	DA	3062	1/1	0.79	0.47	75,75,75,75	0
56	MG	CA	1819	1/1	0.79	0.10	59,59,59,59	0
56	MG	BA	3234	1/1	0.79	0.12	83,83,83,83	0
56	MG	CW	110	1/1	0.79	0.11	90,90,90,90	0
56	MG	AA	1937	1/1	0.79	0.26	51,51,51,51	0
56	MG	BA	3237	1/1	0.79	0.59	90,90,90,90	0
56	MG	BA	3048	1/1	0.79	0.33	54,54,54,54	0
56	MG	CA	1602	1/1	0.79	0.25	112,112,112,112	0
56	MG	BA	2994	1/1	0.79	0.51	71,71,71,71	0
56	MG	DA	3463	1/1	0.79	0.36	60,60,60,60	0
56	MG	BA	3265	1/1	0.79	0.21	114,114,114,114	0
56	MG	CA	1879	1/1	0.79	0.35	53,53,53,53	0
56	MG	BA	2992	1/1	0.79	0.51	73,73,73,73	0
56	MG	CA	1728	1/1	0.79	0.20	195,195,195,195	0
56	MG	AA	1823	1/1	0.79	0.29	96,96,96,96	0
56	MG	BA	3188	1/1	0.79	0.40	78,78,78,78	0
56	MG	DA	2988	1/1	0.79	0.22	85,85,85,85	0
56	MG	DA	2916	1/1	0.79	0.49	57,57,57,57	0
56	MG	BA	3507	1/1	0.79	0.27	56,56,56,56	0
56	MG	DA	3498	1/1	0.79	0.43	80,80,80,80	0
56	MG	BA	3628	1/1	0.79	0.67	82,82,82,82	0
56	MG	AA	1815	1/1	0.79	0.35	74,74,74,74	0
56	MG	BA	3205	1/1	0.79	0.45	95,95,95,95	0
56	MG	CA	1683	1/1	0.79	0.58	62,62,62,62	0
56	MG	BA	3275	1/1	0.79	0.44	102,102,102,102	0
56	MG	AA	1744	1/1	0.80	0.48	103,103,103,103	0
56	MG	AA	1912	1/1	0.80	0.23	87,87,87,87	0
56	MG	DA	3188	1/1	0.80	0.47	50,50,50,50	0
56	MG	AA	1675	1/1	0.80	0.89	96,96,96,96	0
56	MG	BA	2954	1/1	0.80	0.46	77,77,77,77	0
56	MG	CA	1665	1/1	0.80	0.58	94,94,94,94	0
56	MG	BA	3292	1/1	0.80	0.64	40,40,40,40	0
56	MG	BA	2988	1/1	0.80	0.37	77,77,77,77	0
56	MG	CA	1871	1/1	0.80	0.13	56,56,56,56	0
56	MG	DA	3583	1/1	0.80	0.16	68,68,68,68	0
56	MG	DA	3576	1/1	0.80	0.28	102,102,102,102	0
56	MG	BA	3241	1/1	0.80	0.62	77,77,77,77	0
56	MG	BA	3616	1/1	0.80	0.61	62,62,62,62	0
56	MG	DA	3585	1/1	0.80	0.26	66,66,66,66	0
56	MG	BA	3121	1/1	0.80	0.81	137,137,137,137	0
56	MG	BA	3008	1/1	0.80	0.47	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CW	105	1/1	0.80	0.64	65,65,65,65	0
56	MG	BA	3180	1/1	0.80	0.72	113,113,113,113	0
56	MG	BA	3422	1/1	0.80	0.55	42,42,42,42	0
56	MG	DA	2980	1/1	0.80	0.38	57,57,57,57	0
56	MG	BA	3157	1/1	0.80	0.72	57,57,57,57	0
56	MG	AA	1635	1/1	0.80	0.36	106,106,106,106	0
56	MG	BA	3563	1/1	0.80	0.69	83,83,83,83	0
56	MG	BA	3488	1/1	0.80	0.33	62,62,62,62	0
56	MG	BA	3206	1/1	0.80	0.24	176,176,176,176	0
56	MG	CA	1737	1/1	0.80	0.93	98,98,98,98	0
56	MG	AV	101	1/1	0.80	0.75	109,109,109,109	0
56	MG	AA	1929	1/1	0.80	0.36	79,79,79,79	0
56	MG	AA	1897	1/1	0.80	1.14	80,80,80,80	0
56	MG	DB	214	1/1	0.80	0.13	110,110,110,110	0
56	MG	DA	3362	1/1	0.80	0.99	83,83,83,83	0
56	MG	DA	3426	1/1	0.80	0.50	63,63,63,63	0
56	MG	BA	3287	1/1	0.80	0.29	55,55,55,55	0
56	MG	DA	3026	1/1	0.80	0.24	78,78,78,78	0
56	MG	DA	3349	1/1	0.80	0.58	56,56,56,56	0
56	MG	BA	3641	1/1	0.80	0.61	60,60,60,60	0
56	MG	CA	1709	1/1	0.80	0.26	61,61,61,61	0
56	MG	BA	3259	1/1	0.80	0.27	77,77,77,77	0
56	MG	DA	3109	1/1	0.80	0.33	65,65,65,65	0
56	MG	DA	3120	1/1	0.80	0.37	76,76,76,76	0
56	MG	BA	2985	1/1	0.80	0.34	61,61,61,61	0
56	MG	BA	3095	1/1	0.80	0.41	90,90,90,90	0
56	MG	BA	3613	1/1	0.80	0.60	76,76,76,76	0
56	MG	DA	3352	1/1	0.80	0.13	86,86,86,86	0
56	MG	DA	3471	1/1	0.80	0.33	55,55,55,55	0
56	MG	AA	1644	1/1	0.80	0.23	57,57,57,57	0
56	MG	CA	1896	1/1	0.80	0.38	95,95,95,95	0
56	MG	BA	3215	1/1	0.80	0.18	88,88,88,88	0
56	MG	BA	3622	1/1	0.80	0.97	68,68,68,68	0
56	MG	BA	3532	1/1	0.80	0.29	58,58,58,58	0
56	MG	CM	201	1/1	0.80	1.20	84,84,84,84	0
56	MG	BA	3404	1/1	0.80	1.16	82,82,82,82	0
56	MG	DA	3238	1/1	0.80	0.30	89,89,89,89	0
56	MG	BA	3245	1/1	0.80	0.58	185,185,185,185	0
56	MG	DA	3010	1/1	0.80	0.79	54,54,54,54	0
56	MG	DA	3027	1/1	0.80	0.15	94,94,94,94	0
56	MG	BA	3043	1/1	0.80	0.46	155,155,155,155	0
56	MG	BA	2940	1/1	0.80	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1610	1/1	0.81	0.27	78,78,78,78	0
56	MG	AA	1830	1/1	0.81	0.73	179,179,179,179	0
56	MG	BA	3242	1/1	0.81	0.52	63,63,63,63	0
56	MG	BA	3585	1/1	0.81	0.48	87,87,87,87	0
56	MG	CA	1866	1/1	0.81	0.71	85,85,85,85	0
56	MG	DA	3106	1/1	0.81	0.32	79,79,79,79	0
56	MG	BA	3364	1/1	0.81	0.14	82,82,82,82	0
56	MG	CA	1630	1/1	0.81	0.22	177,177,177,177	0
56	MG	DA	3290	1/1	0.81	0.29	38,38,38,38	0
56	MG	DA	2956	1/1	0.81	0.32	59,59,59,59	0
56	MG	CA	1708	1/1	0.81	0.37	63,63,63,63	0
56	MG	BA	3086	1/1	0.81	0.55	64,64,64,64	0
56	MG	AT	202	1/1	0.81	0.40	100,100,100,100	0
56	MG	DA	3595	1/1	0.81	0.42	106,106,106,106	0
56	MG	BA	3436	1/1	0.81	0.30	86,86,86,86	0
56	MG	DA	2979	1/1	0.81	0.39	81,81,81,81	0
56	MG	AA	1872	1/1	0.81	0.69	67,67,67,67	0
56	MG	AA	1716	1/1	0.81	0.46	103,103,103,103	0
56	MG	BA	3419	1/1	0.81	0.35	57,57,57,57	0
56	MG	BA	3543	1/1	0.81	0.29	53,53,53,53	0
56	MG	DA	3447	1/1	0.81	0.64	89,89,89,89	0
56	MG	AA	1971	1/1	0.81	0.18	60,60,60,60	0
56	MG	DA	3074	1/1	0.81	1.36	99,99,99,99	0
56	MG	AA	1700	1/1	0.81	0.51	158,158,158,158	0
56	MG	BA	3331	1/1	0.81	0.69	121,121,121,121	0
56	MG	DA	3064	1/1	0.81	0.19	62,62,62,62	0
56	MG	BB	213	1/1	0.81	0.35	93,93,93,93	0
56	MG	DA	3317	1/1	0.81	0.17	48,48,48,48	0
56	MG	BA	3571	1/1	0.81	0.49	68,68,68,68	0
56	MG	BA	2964	1/1	0.81	0.25	74,74,74,74	0
56	MG	BA	3060	1/1	0.81	0.53	80,80,80,80	0
56	MG	DA	3327	1/1	0.81	0.20	58,58,58,58	0
56	MG	BA	3712	1/1	0.81	0.50	52,52,52,52	0
56	MG	DA	3043	1/1	0.81	1.55	77,77,77,77	0
56	MG	BA	3391	1/1	0.81	0.64	78,78,78,78	0
56	MG	BA	3096	1/1	0.81	0.79	173,173,173,173	0
56	MG	DA	3421	1/1	0.81	0.35	76,76,76,76	0
56	MG	CA	1766	1/1	0.81	0.39	49,49,49,49	0
56	MG	BA	2991	1/1	0.81	0.36	80,80,80,80	0
56	MG	AA	1828	1/1	0.81	0.10	97,97,97,97	0
56	MG	AA	1738	1/1	0.81	0.65	71,71,71,71	0
56	MG	AA	1733	1/1	0.81	1.05	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DX	101	1/1	0.81	0.41	99,99,99,99	0
56	MG	AA	1774	1/1	0.81	0.41	68,68,68,68	0
56	MG	BA	3346	1/1	0.81	0.12	111,111,111,111	0
56	MG	AA	1873	1/1	0.81	0.23	110,110,110,110	0
56	MG	CA	1895	1/1	0.81	0.31	126,126,126,126	0
56	MG	BA	3520	1/1	0.81	0.46	51,51,51,51	0
56	MG	AA	1989	1/1	0.81	0.21	70,70,70,70	0
56	MG	DA	3178	1/1	0.82	0.31	40,40,40,40	0
56	MG	BA	3523	1/1	0.82	0.59	47,47,47,47	0
56	MG	DA	2963	1/1	0.82	0.34	62,62,62,62	0
56	MG	CA	1662	1/1	0.82	0.55	90,90,90,90	0
56	MG	CA	1831	1/1	0.82	0.48	62,62,62,62	0
56	MG	DA	3578	1/1	0.82	0.55	57,57,57,57	0
56	MG	BA	2960	1/1	0.82	0.50	74,74,74,74	0
56	MG	BA	3279	1/1	0.82	0.34	80,80,80,80	0
56	MG	DA	3571	1/1	0.82	0.94	70,70,70,70	0
56	MG	CA	1811	1/1	0.82	0.27	54,54,54,54	0
56	MG	DA	3601	1/1	0.82	0.33	61,61,61,61	0
56	MG	CA	1650	1/1	0.82	0.18	170,170,170,170	0
56	MG	BA	3477	1/1	0.82	0.32	54,54,54,54	0
56	MG	CA	1722	1/1	0.82	0.72	168,168,168,168	0
56	MG	CA	1921	1/1	0.82	0.26	108,108,108,108	0
56	MG	DA	2950	1/1	0.82	0.15	61,61,61,61	0
56	MG	DA	3121	1/1	0.82	0.19	41,41,41,41	0
56	MG	DA	3535	1/1	0.82	0.31	67,67,67,67	0
56	MG	BA	3276	1/1	0.82	0.56	107,107,107,107	0
56	MG	CA	1823	1/1	0.82	0.30	166,166,166,166	0
56	MG	DQ	201	1/1	0.82	0.22	49,49,49,49	0
56	MG	AA	1931	1/1	0.82	0.24	102,102,102,102	0
56	MG	DA	3459	1/1	0.82	0.26	76,76,76,76	0
56	MG	BA	3151	1/1	0.82	0.30	80,80,80,80	0
56	MG	DA	3307	1/1	0.82	0.18	82,82,82,82	0
56	MG	DA	2991	1/1	0.82	0.68	80,80,80,80	0
56	MG	DB	213	1/1	0.82	0.21	76,76,76,76	0
56	MG	BA	2923	1/1	0.82	1.32	85,85,85,85	0
56	MG	CA	1696	1/1	0.82	0.30	66,66,66,66	0
56	MG	AA	1679	1/1	0.82	0.13	112,112,112,112	0
56	MG	CA	1795	1/1	0.82	0.62	84,84,84,84	0
56	MG	BA	3068	1/1	0.82	0.44	115,115,115,115	0
56	MG	CA	1798	1/1	0.82	0.32	79,79,79,79	0
56	MG	DA	2926	1/1	0.82	0.54	91,91,91,91	0
56	MG	AA	1751	1/1	0.82	0.58	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3112	1/1	0.82	0.21	141,141,141,141	0
56	MG	BA	3258	1/1	0.82	0.56	67,67,67,67	0
56	MG	BA	3083	1/1	0.82	0.22	69,69,69,69	0
56	MG	CA	1916	1/1	0.82	0.62	77,77,77,77	0
56	MG	BA	3491	1/1	0.82	0.25	85,85,85,85	0
56	MG	DA	3589	1/1	0.82	0.18	74,74,74,74	0
56	MG	AA	1746	1/1	0.82	0.38	93,93,93,93	0
56	MG	CA	1689	1/1	0.82	0.21	52,52,52,52	0
56	MG	BA	3087	1/1	0.82	0.49	82,82,82,82	0
56	MG	BA	3674	1/1	0.82	0.32	55,55,55,55	0
56	MG	BA	3135	1/1	0.82	0.45	55,55,55,55	0
56	MG	DA	3424	1/1	0.82	0.40	52,52,52,52	0
56	MG	AA	1753	1/1	0.82	0.52	72,72,72,72	0
56	MG	CA	1649	1/1	0.82	0.15	63,63,63,63	0
56	MG	DA	3369	1/1	0.82	0.59	86,86,86,86	0
56	MG	DA	3539	1/1	0.82	0.31	98,98,98,98	0
56	MG	AA	1616	1/1	0.82	0.46	87,87,87,87	0
56	MG	DA	3089	1/1	0.82	0.10	70,70,70,70	0
56	MG	AA	1713	1/1	0.82	0.14	84,84,84,84	0
56	MG	BA	3561	1/1	0.82	0.33	58,58,58,58	0
56	MG	DA	3266	1/1	0.82	0.55	64,64,64,64	0
56	MG	BA	3701	1/1	0.82	0.34	74,74,74,74	0
56	MG	AA	1973	1/1	0.82	0.64	65,65,65,65	0
56	MG	BA	3560	1/1	0.82	0.37	47,47,47,47	0
56	MG	BA	3664	1/1	0.82	0.21	82,82,82,82	0
56	MG	BA	3587	1/1	0.82	0.93	104,104,104,104	0
56	MG	DA	3035	1/1	0.82	0.36	71,71,71,71	0
56	MG	DA	3038	1/1	0.82	0.37	77,77,77,77	0
56	MG	DA	3063	1/1	0.83	0.18	99,99,99,99	0
56	MG	DA	3579	1/1	0.83	0.36	36,36,36,36	0
56	MG	CA	1844	1/1	0.83	0.82	104,104,104,104	0
56	MG	BA	3069	1/1	0.83	0.23	69,69,69,69	0
56	MG	BA	3176	1/1	0.83	0.29	52,52,52,52	0
56	MG	BA	3500	1/1	0.83	0.38	72,72,72,72	0
56	MG	DA	3616	1/1	0.83	0.23	65,65,65,65	0
56	MG	DA	3542	1/1	0.83	0.51	70,70,70,70	0
56	MG	CA	1789	1/1	0.83	0.93	184,184,184,184	0
56	MG	AA	1641	1/1	0.83	0.12	121,121,121,121	0
56	MG	BA	3304	1/1	0.83	0.45	167,167,167,167	0
56	MG	AA	1992	1/1	0.83	0.27	84,84,84,84	0
56	MG	DA	3130	1/1	0.83	0.61	69,69,69,69	0
56	MG	CA	1622	1/1	0.83	0.40	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3581	1/1	0.83	0.45	94,94,94,94	0
56	MG	CA	1653	1/1	0.83	0.15	53,53,53,53	0
56	MG	AA	1903	1/1	0.83	0.22	51,51,51,51	0
56	MG	BA	3473	1/1	0.83	0.81	70,70,70,70	0
56	MG	DA	3478	1/1	0.83	0.17	67,67,67,67	0
56	MG	BA	3405	1/1	0.83	0.70	64,64,64,64	0
56	MG	AA	1705	1/1	0.83	0.28	101,101,101,101	0
56	MG	DA	3162	1/1	0.83	0.15	23,23,23,23	0
56	MG	DA	3454	1/1	0.83	0.34	62,62,62,62	0
56	MG	CA	1727	1/1	0.83	0.14	112,112,112,112	0
56	MG	DA	2907	1/1	0.83	0.10	75,75,75,75	0
56	MG	BB	209	1/1	0.83	0.27	91,91,91,91	0
56	MG	BA	2975	1/1	0.83	0.23	77,77,77,77	0
56	MG	CA	1890	1/1	0.83	0.26	59,59,59,59	0
56	MG	AA	1986	1/1	0.83	0.79	69,69,69,69	0
56	MG	BA	3460	1/1	0.83	0.24	51,51,51,51	0
56	MG	BA	3326	1/1	0.83	0.63	56,56,56,56	0
56	MG	AA	1921	1/1	0.83	0.34	68,68,68,68	0
56	MG	AA	1740	1/1	0.83	0.40	105,105,105,105	0
56	MG	BA	3522	1/1	0.83	1.09	96,96,96,96	0
56	MG	BA	3693	1/1	0.83	0.18	65,65,65,65	0
56	MG	DA	3594	1/1	0.83	0.30	50,50,50,50	0
56	MG	AA	1609	1/1	0.83	0.21	46,46,46,46	0
56	MG	AA	1640	1/1	0.83	0.12	102,102,102,102	0
56	MG	BA	3698	1/1	0.83	0.32	55,55,55,55	0
56	MG	AA	1938	1/1	0.83	0.13	72,72,72,72	0
56	MG	CA	1660	1/1	0.83	0.41	94,94,94,94	0
56	MG	BA	3010	1/1	0.83	0.48	93,93,93,93	0
56	MG	BA	3209	1/1	0.83	0.33	96,96,96,96	0
56	MG	BA	3075	1/1	0.83	0.69	73,73,73,73	0
56	MG	CW	111	1/1	0.83	0.30	82,82,82,82	0
56	MG	AA	1925	1/1	0.83	0.52	63,63,63,63	0
56	MG	BA	3480	1/1	0.83	0.29	77,77,77,77	0
56	MG	BA	3318	1/1	0.83	0.18	93,93,93,93	0
56	MG	DA	3429	1/1	0.83	0.78	59,59,59,59	0
56	MG	DA	3470	1/1	0.83	0.22	81,81,81,81	0
56	MG	CA	1642	1/1	0.83	0.73	82,82,82,82	0
56	MG	DA	3390	1/1	0.83	0.74	53,53,53,53	0
56	MG	BA	3074	1/1	0.83	0.09	108,108,108,108	0
56	MG	BA	3367	1/1	0.83	0.36	84,84,84,84	0
56	MG	AA	1864	1/1	0.83	0.20	116,116,116,116	0
56	MG	AA	1650	1/1	0.83	0.16	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1870	1/1	0.83	0.11	73,73,73,73	0
56	MG	BA	3541	1/1	0.83	0.21	44,44,44,44	0
56	MG	BA	3222	1/1	0.83	0.46	70,70,70,70	0
56	MG	DA	3082	1/1	0.83	0.09	67,67,67,67	0
56	MG	CA	1893	1/1	0.83	0.46	125,125,125,125	0
56	MG	BA	3608	1/1	0.83	0.95	54,54,54,54	0
56	MG	BB	205	1/1	0.83	0.30	64,64,64,64	0
56	MG	BX	102	1/1	0.83	0.35	50,50,50,50	0
56	MG	BA	3223	1/1	0.83	0.24	58,58,58,58	0
56	MG	BA	3487	1/1	0.83	0.40	51,51,51,51	0
56	MG	DA	3077	1/1	0.83	0.35	77,77,77,77	0
56	MG	BA	3179	1/1	0.83	0.88	98,98,98,98	0
56	MG	DA	3081	1/1	0.83	0.40	87,87,87,87	0
56	MG	DA	3098	1/1	0.84	0.28	57,57,57,57	0
56	MG	BA	3050	1/1	0.84	0.34	60,60,60,60	0
56	MG	BA	3524	1/1	0.84	0.26	95,95,95,95	0
56	MG	BA	3715	1/1	0.84	0.44	75,75,75,75	0
56	MG	CA	1865	1/1	0.84	0.48	108,108,108,108	0
56	MG	DA	3068	1/1	0.84	0.28	69,69,69,69	0
56	MG	DA	3067	1/1	0.84	0.58	83,83,83,83	0
56	MG	BA	3638	1/1	0.84	0.31	73,73,73,73	0
56	MG	CV	102	1/1	0.84	0.70	78,78,78,78	0
56	MG	AA	1993	1/1	0.84	0.36	73,73,73,73	0
56	MG	DA	3455	1/1	0.84	0.20	72,72,72,72	0
56	MG	DA	3083	1/1	0.84	0.76	125,125,125,125	0
56	MG	DA	3090	1/1	0.84	0.25	47,47,47,47	0
56	MG	AA	1775	1/1	0.84	0.95	66,66,66,66	0
56	MG	BA	3191	1/1	0.84	0.32	64,64,64,64	0
56	MG	BA	3582	1/1	0.84	0.57	72,72,72,72	0
56	MG	BA	3537	1/1	0.84	0.32	60,60,60,60	0
56	MG	BA	2987	1/1	0.84	0.40	79,79,79,79	0
56	MG	D1	101	1/1	0.84	0.17	66,66,66,66	0
56	MG	DA	2997	1/1	0.84	0.89	132,132,132,132	0
56	MG	BA	3409	1/1	0.84	0.19	115,115,115,115	0
56	MG	BA	3654	1/1	0.84	0.24	86,86,86,86	0
56	MG	BA	3138	1/1	0.84	0.28	82,82,82,82	0
56	MG	CA	1901	1/1	0.84	0.24	54,54,54,54	0
56	MG	CW	115	1/1	0.84	0.30	81,81,81,81	0
56	MG	BA	3199	1/1	0.84	0.29	69,69,69,69	0
56	MG	BA	3208	1/1	0.84	0.40	87,87,87,87	0
56	MG	DA	2976	1/1	0.84	0.39	71,71,71,71	0
56	MG	CW	104	1/1	0.84	0.28	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	2921	1/1	0.84	0.66	95,95,95,95	0
56	MG	BA	3653	1/1	0.84	0.16	62,62,62,62	0
56	MG	BA	3077	1/1	0.84	0.23	50,50,50,50	0
56	MG	CA	1908	1/1	0.84	0.27	84,84,84,84	0
56	MG	CA	1776	1/1	0.84	0.68	125,125,125,125	0
56	MG	DA	2934	1/1	0.84	0.29	76,76,76,76	0
56	MG	BA	3554	1/1	0.84	0.39	62,62,62,62	0
56	MG	DA	3376	1/1	0.84	0.42	43,43,43,43	0
56	MG	AA	1676	1/1	0.84	0.32	152,152,152,152	0
56	MG	DA	3158	1/1	0.84	0.46	18,18,18,18	0
56	MG	BA	3451	1/1	0.84	0.60	83,83,83,83	0
56	MG	DA	3560	1/1	0.84	0.42	55,55,55,55	0
56	MG	BA	3390	1/1	0.84	0.41	44,44,44,44	0
56	MG	BA	3071	1/1	0.84	0.24	52,52,52,52	0
56	MG	AA	1966	1/1	0.84	0.29	51,51,51,51	0
56	MG	CA	1604	1/1	0.84	0.47	99,99,99,99	0
56	MG	CA	1690	1/1	0.84	0.16	69,69,69,69	0
56	MG	BA	3397	1/1	0.84	0.89	67,67,67,67	0
56	MG	BA	3039	1/1	0.84	0.78	176,176,176,176	0
56	MG	BA	3162	1/1	0.84	0.51	60,60,60,60	0
56	MG	BA	3503	1/1	0.84	0.69	195,195,195,195	0
56	MG	CA	1761	1/1	0.84	0.48	49,49,49,49	0
56	MG	CA	1851	1/1	0.84	0.36	94,94,94,94	0
56	MG	BA	3702	1/1	0.84	0.20	61,61,61,61	0
56	MG	DA	3609	1/1	0.84	0.24	27,27,27,27	0
56	MG	CA	1714	1/1	0.84	0.18	104,104,104,104	0
56	MG	DA	2967	1/1	0.84	0.90	86,86,86,86	0
56	MG	DA	3591	1/1	0.84	0.15	129,129,129,129	0
56	MG	DA	3402	1/1	0.84	0.65	28,28,28,28	0
56	MG	CA	1897	1/1	0.84	0.24	227,227,227,227	0
56	MG	BA	3122	1/1	0.84	0.14	89,89,89,89	0
56	MG	DA	3297	1/1	0.84	0.42	64,64,64,64	0
56	MG	DA	2993	1/1	0.84	0.41	85,85,85,85	0
56	MG	DA	3574	1/1	0.84	0.44	67,67,67,67	0
56	MG	AA	1787	1/1	0.84	0.31	79,79,79,79	0
56	MG	DA	3564	1/1	0.84	0.54	25,25,25,25	0
56	MG	AA	1680	1/1	0.84	0.17	87,87,87,87	0
56	MG	DA	3261	1/1	0.85	0.26	32,32,32,32	0
56	MG	CA	1788	1/1	0.85	0.19	66,66,66,66	0
56	MG	AA	1822	1/1	0.85	0.17	69,69,69,69	0
56	MG	DA	3494	1/1	0.85	0.28	112,112,112,112	0
56	MG	CA	1861	1/1	0.85	0.50	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3132	1/1	0.85	0.40	53,53,53,53	0
56	MG	BA	3059	1/1	0.85	0.36	43,43,43,43	0
56	MG	DA	3425	1/1	0.85	0.55	52,52,52,52	0
56	MG	BA	2967	1/1	0.85	0.59	77,77,77,77	0
56	MG	BA	3240	1/1	0.85	0.22	75,75,75,75	0
56	MG	BA	3567	1/1	0.85	0.40	75,75,75,75	0
56	MG	BA	3124	1/1	0.85	0.54	79,79,79,79	0
56	MG	AA	1745	1/1	0.85	0.21	80,80,80,80	0
56	MG	CA	1711	1/1	0.85	0.66	88,88,88,88	0
56	MG	DQ	202	1/1	0.85	0.28	31,31,31,31	0
56	MG	DA	3629	1/1	0.85	0.23	67,67,67,67	0
56	MG	CA	1782	1/1	0.85	0.54	56,56,56,56	0
56	MG	CA	1755	1/1	0.85	0.91	120,120,120,120	0
56	MG	DA	3029	1/1	0.85	0.29	73,73,73,73	0
56	MG	BA	3154	1/1	0.85	0.84	169,169,169,169	0
56	MG	BA	3468	1/1	0.85	0.26	67,67,67,67	0
56	MG	CA	1857	1/1	0.85	0.59	73,73,73,73	0
56	MG	BA	3623	1/1	0.85	0.28	79,79,79,79	0
56	MG	AA	1817	1/1	0.85	0.55	175,175,175,175	0
56	MG	AA	1809	1/1	0.85	0.18	106,106,106,106	0
56	MG	BA	3310	1/1	0.85	0.50	117,117,117,117	0
56	MG	DA	3356	1/1	0.85	0.13	107,107,107,107	0
56	MG	DA	3434	1/1	0.85	0.45	61,61,61,61	0
56	MG	DA	3336	1/1	0.85	0.18	51,51,51,51	0
56	MG	BA	2965	1/1	0.85	0.47	167,167,167,167	0
56	MG	DA	3486	1/1	0.85	0.37	62,62,62,62	0
56	MG	BA	3343	1/1	0.85	0.24	73,73,73,73	0
56	MG	BA	3492	1/1	0.85	0.60	102,102,102,102	0
56	MG	BA	2966	1/1	0.85	0.36	49,49,49,49	0
56	MG	DF	302	1/1	0.85	0.25	25,25,25,25	0
56	MG	DA	3499	1/1	0.85	0.17	98,98,98,98	0
56	MG	DD	301	1/1	0.85	0.19	62,62,62,62	0
56	MG	BA	3485	1/1	0.85	0.49	53,53,53,53	0
56	MG	AA	1867	1/1	0.85	1.19	96,96,96,96	0
56	MG	BA	3486	1/1	0.85	0.27	47,47,47,47	0
56	MG	BA	2971	1/1	0.85	1.04	89,89,89,89	0
56	MG	DA	3530	1/1	0.85	0.29	70,70,70,70	0
56	MG	BA	2904	1/1	0.85	0.22	48,48,48,48	0
56	MG	CA	1688	1/1	0.85	0.26	45,45,45,45	0
56	MG	AA	1724	1/1	0.85	0.46	133,133,133,133	0
56	MG	AA	1848	1/1	0.85	0.26	125,125,125,125	0
56	MG	BA	3472	1/1	0.85	0.48	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1657	1/1	0.85	0.24	95,95,95,95	0
56	MG	BA	3031	1/1	0.85	0.50	255,255,255,255	0
56	MG	CW	107	1/1	0.85	0.10	50,50,50,50	0
56	MG	DA	2995	1/1	0.85	0.18	65,65,65,65	0
56	MG	DB	210	1/1	0.85	0.25	82,82,82,82	0
56	MG	AA	1939	1/1	0.85	0.11	61,61,61,61	0
56	MG	DA	3057	1/1	0.85	0.11	107,107,107,107	0
56	MG	DA	3014	1/1	0.85	0.19	54,54,54,54	0
56	MG	AA	1668	1/1	0.85	0.35	90,90,90,90	0
56	MG	BA	3519	1/1	0.85	0.64	93,93,93,93	0
56	MG	BA	3204	1/1	0.85	0.33	65,65,65,65	0
56	MG	BA	3611	1/1	0.85	0.23	67,67,67,67	0
56	MG	BA	3508	1/1	0.85	0.30	67,67,67,67	0
56	MG	DA	3604	1/1	0.85	0.42	58,58,58,58	0
56	MG	CA	1909	1/1	0.85	0.16	133,133,133,133	0
56	MG	BA	3617	1/1	0.85	0.16	88,88,88,88	0
56	MG	AA	1604	1/1	0.85	0.21	91,91,91,91	0
56	MG	AA	1758	1/1	0.85	0.17	48,48,48,48	0
56	MG	CA	1922	1/1	0.85	0.32	67,67,67,67	0
56	MG	BA	3167	1/1	0.85	0.38	60,60,60,60	0
56	MG	AA	1882	1/1	0.85	0.48	32,32,32,32	0
56	MG	AW	105	1/1	0.85	0.07	55,55,55,55	0
56	MG	CA	1659	1/1	0.85	0.38	57,57,57,57	0
56	MG	AA	1729	1/1	0.85	0.49	99,99,99,99	0
56	MG	BA	3190	1/1	0.85	0.27	49,49,49,49	0
56	MG	AA	1819	1/1	0.85	0.96	84,84,84,84	0
56	MG	CA	1730	1/1	0.85	0.16	80,80,80,80	0
56	MG	AA	1678	1/1	0.85	0.16	101,101,101,101	0
56	MG	BA	3723	1/1	0.86	0.20	71,71,71,71	0
56	MG	BA	3370	1/1	0.86	0.36	50,50,50,50	0
56	MG	DA	3504	1/1	0.86	0.34	68,68,68,68	0
56	MG	BA	3089	1/1	0.86	0.58	72,72,72,72	0
56	MG	BA	2962	1/1	0.86	0.70	78,78,78,78	0
56	MG	DA	3392	1/1	0.86	0.13	38,38,38,38	0
56	MG	DA	3407	1/1	0.86	0.11	62,62,62,62	0
56	MG	DA	3145	1/1	0.86	0.26	39,39,39,39	0
56	MG	DA	3423	1/1	0.86	0.20	35,35,35,35	0
56	MG	DA	3047	1/1	0.86	0.71	69,69,69,69	0
56	MG	AA	1684	1/1	0.86	0.86	62,62,62,62	0
56	MG	BA	3166	1/1	0.86	0.29	70,70,70,70	0
56	MG	DA	3250	1/1	0.86	0.61	77,77,77,77	0
56	MG	DA	3592	1/1	0.86	0.19	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3411	1/1	0.86	0.56	59,59,59,59	0
56	MG	BA	3040	1/1	0.86	0.27	85,85,85,85	0
56	MG	BF	1901	1/1	0.86	0.28	74,74,74,74	0
56	MG	CA	1835	1/1	0.86	0.57	61,61,61,61	0
56	MG	CA	1619	1/1	0.86	0.11	128,128,128,128	0
56	MG	DA	3610	1/1	0.86	0.52	56,56,56,56	0
56	MG	CA	1841	1/1	0.86	0.77	77,77,77,77	0
56	MG	BA	2957	1/1	0.86	0.46	71,71,71,71	0
56	MG	CA	1754	1/1	0.86	1.40	162,162,162,162	0
56	MG	BA	3361	1/1	0.86	0.19	106,106,106,106	0
56	MG	AA	1606	1/1	0.86	0.13	77,77,77,77	0
56	MG	CA	1729	1/1	0.86	0.21	139,139,139,139	0
56	MG	BA	3070	1/1	0.86	0.55	159,159,159,159	0
56	MG	AA	1658	1/1	0.86	0.16	76,76,76,76	0
56	MG	DA	3002	1/1	0.86	0.33	139,139,139,139	0
56	MG	DA	3017	1/1	0.86	0.17	60,60,60,60	0
56	MG	BA	2952	1/1	0.86	0.08	55,55,55,55	0
56	MG	BA	3302	1/1	0.86	0.69	63,63,63,63	0
56	MG	AA	1881	1/1	0.86	0.46	54,54,54,54	0
56	MG	DA	3091	1/1	0.86	0.57	96,96,96,96	0
56	MG	DA	3196	1/1	0.86	0.35	30,30,30,30	0
56	MG	BA	3423	1/1	0.86	0.28	38,38,38,38	0
56	MG	AA	1827	1/1	0.86	0.41	98,98,98,98	0
56	MG	BA	2995	1/1	0.86	0.22	92,92,92,92	0
56	MG	BA	3640	1/1	0.86	0.51	60,60,60,60	0
56	MG	CA	1695	1/1	0.86	0.41	108,108,108,108	0
56	MG	AA	1637	1/1	0.86	0.12	67,67,67,67	0
56	MG	AA	1643	1/1	0.86	0.25	114,114,114,114	0
56	MG	BA	3700	1/1	0.86	0.37	60,60,60,60	0
56	MG	BA	3721	1/1	0.86	0.19	86,86,86,86	0
56	MG	CA	1611	1/1	0.86	0.32	71,71,71,71	0
56	MG	BA	3604	1/1	0.86	0.37	72,72,72,72	0
56	MG	AA	1923	1/1	0.86	0.11	72,72,72,72	0
56	MG	CA	1919	1/1	0.86	0.24	39,39,39,39	0
56	MG	DA	2996	1/1	0.86	0.22	65,65,65,65	0
56	MG	BB	214	1/1	0.86	0.20	68,68,68,68	0
56	MG	AA	1759	1/1	0.86	0.88	88,88,88,88	0
56	MG	DA	2952	1/1	0.86	0.69	68,68,68,68	0
56	MG	BA	3559	1/1	0.86	0.31	76,76,76,76	0
56	MG	BA	3088	1/1	0.86	0.18	167,167,167,167	0
56	MG	DA	3400	1/1	0.86	0.35	88,88,88,88	0
56	MG	DA	3058	1/1	0.86	0.10	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3614	1/1	0.86	0.16	107,107,107,107	0
56	MG	CA	1886	1/1	0.86	0.18	100,100,100,100	0
56	MG	DA	3055	1/1	0.86	0.12	75,75,75,75	0
56	MG	BA	3305	1/1	0.86	0.16	62,62,62,62	0
56	MG	AA	1651	1/1	0.86	0.30	84,84,84,84	0
56	MG	CA	1839	1/1	0.86	0.13	38,38,38,38	0
56	MG	AA	1898	1/1	0.86	0.23	70,70,70,70	0
56	MG	BA	3308	1/1	0.86	0.16	88,88,88,88	0
56	MG	BA	3024	1/1	0.86	0.31	65,65,65,65	0
56	MG	AA	1763	1/1	0.86	0.27	88,88,88,88	0
56	MG	BA	3227	1/1	0.86	0.22	90,90,90,90	0
56	MG	DA	3260	1/1	0.86	0.27	58,58,58,58	0
56	MG	BA	3478	1/1	0.86	0.12	63,63,63,63	0
56	MG	DA	3013	1/1	0.86	0.39	55,55,55,55	0
56	MG	DA	3028	1/1	0.86	0.35	55,55,55,55	0
56	MG	AA	1762	1/1	0.86	0.25	95,95,95,95	0
56	MG	DA	3365	1/1	0.86	0.37	55,55,55,55	0
56	MG	DA	3300	1/1	0.86	0.27	69,69,69,69	0
56	MG	AA	1913	1/1	0.86	0.39	35,35,35,35	0
56	MG	CA	1637	1/1	0.86	0.29	53,53,53,53	0
56	MG	DA	3559	1/1	0.86	0.61	51,51,51,51	0
56	MG	DB	212	1/1	0.86	0.09	84,84,84,84	0
56	MG	BA	3152	1/1	0.86	0.13	72,72,72,72	0
56	MG	DA	3046	1/1	0.86	0.35	48,48,48,48	0
56	MG	DA	3271	1/1	0.86	0.27	65,65,65,65	0
56	MG	CA	1618	1/1	0.86	0.48	49,49,49,49	0
56	MG	DA	3294	1/1	0.86	0.53	64,64,64,64	0
56	MG	DA	3289	1/1	0.86	0.26	45,45,45,45	0
56	MG	BA	3149	1/1	0.86	0.17	44,44,44,44	0
56	MG	AA	1734	1/1	0.86	0.24	66,66,66,66	0
56	MG	AA	1732	1/1	0.86	0.23	60,60,60,60	0
56	MG	BA	3708	1/1	0.86	0.19	61,61,61,61	0
56	MG	DA	3049	1/1	0.86	0.61	52,52,52,52	0
56	MG	DA	3612	1/1	0.86	0.18	52,52,52,52	0
56	MG	CR	101	1/1	0.86	1.59	182,182,182,182	0
56	MG	BA	3590	1/1	0.86	0.26	90,90,90,90	0
56	MG	DA	2951	1/1	0.86	0.20	78,78,78,78	0
56	MG	DA	2986	1/1	0.87	0.36	110,110,110,110	0
56	MG	CA	1881	1/1	0.87	0.19	111,111,111,111	0
56	MG	BA	3017	1/1	0.87	0.36	27,27,27,27	0
56	MG	B0	101	1/1	0.87	0.27	33,33,33,33	0
56	MG	AA	1956	1/1	0.87	0.32	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1770	1/1	0.87	0.31	39,39,39,39	0
56	MG	BA	3415	1/1	0.87	0.24	47,47,47,47	0
56	MG	DA	3045	1/1	0.87	0.40	62,62,62,62	0
56	MG	DA	3309	1/1	0.87	0.27	81,81,81,81	0
56	MG	CA	1684	1/1	0.87	0.48	87,87,87,87	0
56	MG	CA	1672	1/1	0.87	0.25	78,78,78,78	0
56	MG	DA	2945	1/1	0.87	0.50	88,88,88,88	0
56	MG	CA	1615	1/1	0.87	0.50	110,110,110,110	0
56	MG	AA	1894	1/1	0.87	0.27	124,124,124,124	0
56	MG	DH	201	1/1	0.87	0.26	64,64,64,64	0
56	MG	DA	3080	1/1	0.87	0.38	84,84,84,84	0
56	MG	DA	2909	1/1	0.87	0.60	85,85,85,85	0
56	MG	DA	3104	1/1	0.87	0.33	70,70,70,70	0
56	MG	BA	3200	1/1	0.87	0.95	63,63,63,63	0
56	MG	BA	3013	1/1	0.87	0.81	81,81,81,81	0
56	MG	BA	3221	1/1	0.87	0.22	77,77,77,77	0
56	MG	DA	3160	1/1	0.87	0.57	45,45,45,45	0
56	MG	BA	3387	1/1	0.87	0.18	49,49,49,49	0
56	MG	DA	3094	1/1	0.87	0.26	30,30,30,30	0
56	MG	DA	3500	1/1	0.87	0.76	72,72,72,72	0
56	MG	DA	3037	1/1	0.87	0.42	77,77,77,77	0
56	MG	BA	3107	1/1	0.87	0.56	87,87,87,87	0
56	MG	DB	207	1/1	0.87	0.14	87,87,87,87	0
56	MG	BA	3666	1/1	0.87	0.28	67,67,67,67	0
56	MG	BA	3564	1/1	0.87	0.42	28,28,28,28	0
56	MG	BA	3662	1/1	0.87	0.42	87,87,87,87	0
56	MG	CA	1636	1/1	0.87	0.97	56,56,56,56	0
56	MG	CA	1849	1/1	0.87	0.23	75,75,75,75	0
56	MG	CA	1700	1/1	0.87	0.81	180,180,180,180	0
56	MG	BA	3322	1/1	0.87	0.28	46,46,46,46	0
56	MG	BA	3163	1/1	0.87	0.53	93,93,93,93	0
56	MG	CA	1705	1/1	0.87	0.24	94,94,94,94	0
56	MG	DA	3368	1/1	0.87	0.14	83,83,83,83	0
56	MG	AA	1868	1/1	0.87	0.24	49,49,49,49	0
56	MG	DA	3288	1/1	0.87	0.37	57,57,57,57	0
56	MG	AA	1634	1/1	0.87	0.28	78,78,78,78	0
56	MG	DA	3472	1/1	0.87	0.24	52,52,52,52	0
56	MG	BA	3079	1/1	0.87	0.41	48,48,48,48	0
56	MG	BA	3497	1/1	0.87	0.17	78,78,78,78	0
56	MG	AA	1698	1/1	0.87	0.70	97,97,97,97	0
56	MG	DA	3079	1/1	0.87	0.38	62,62,62,62	0
56	MG	DA	3304	1/1	0.87	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	2903	1/1	0.87	0.41	83,83,83,83	0
56	MG	BA	3291	1/1	0.87	0.48	94,94,94,94	0
56	MG	BA	3380	1/1	0.87	0.69	49,49,49,49	0
56	MG	AA	1806	1/1	0.87	0.47	111,111,111,111	0
56	MG	BA	3469	1/1	0.87	0.16	82,82,82,82	0
56	MG	BA	3626	1/1	0.87	0.57	62,62,62,62	0
56	MG	BA	2936	1/1	0.87	0.10	65,65,65,65	0
56	MG	DA	3189	1/1	0.87	0.52	27,27,27,27	0
56	MG	AA	1935	1/1	0.87	0.18	39,39,39,39	0
56	MG	CA	1779	1/1	0.87	0.36	72,72,72,72	0
56	MG	BA	3366	1/1	0.87	0.45	31,31,31,31	0
56	MG	DA	3482	1/1	0.87	0.54	50,50,50,50	0
56	MG	AA	1920	1/1	0.87	0.11	71,71,71,71	0
56	MG	CA	1621	1/1	0.87	0.36	48,48,48,48	0
56	MG	AA	1638	1/1	0.87	0.81	132,132,132,132	0
56	MG	AA	1988	1/1	0.87	0.40	53,53,53,53	0
56	MG	CA	1917	1/1	0.87	0.33	123,123,123,123	0
56	MG	BA	3281	1/1	0.87	0.23	73,73,73,73	0
56	MG	BA	3644	1/1	0.87	0.32	106,106,106,106	0
56	MG	AA	1801	1/1	0.87	0.16	88,88,88,88	0
56	MG	AA	1914	1/1	0.87	0.14	53,53,53,53	0
56	MG	DA	3569	1/1	0.87	0.34	52,52,52,52	0
56	MG	BA	3146	1/1	0.87	0.28	57,57,57,57	0
56	MG	DA	3384	1/1	0.87	0.31	62,62,62,62	0
56	MG	CA	1847	1/1	0.87	0.28	84,84,84,84	0
56	MG	DA	3216	1/1	0.87	0.30	23,23,23,23	0
56	MG	BA	3164	1/1	0.87	0.29	62,62,62,62	0
56	MG	DA	3042	1/1	0.87	0.62	50,50,50,50	0
56	MG	BA	3192	1/1	0.87	0.26	90,90,90,90	0
56	MG	AA	1666	1/1	0.87	0.43	91,91,91,91	0
56	MG	BA	3181	1/1	0.87	0.51	56,56,56,56	0
56	MG	AA	1667	1/1	0.87	0.30	53,53,53,53	0
56	MG	BA	3150	1/1	0.88	0.32	79,79,79,79	0
56	MG	DA	3275	1/1	0.88	0.83	52,52,52,52	0
56	MG	BA	3531	1/1	0.88	0.30	71,71,71,71	0
56	MG	CA	1868	1/1	0.88	0.25	69,69,69,69	0
56	MG	DB	219	1/1	0.88	0.80	66,66,66,66	0
56	MG	DA	3302	1/1	0.88	0.40	83,83,83,83	0
56	MG	B8	101	1/1	0.88	0.28	38,38,38,38	0
56	MG	CA	1668	1/1	0.88	0.37	118,118,118,118	0
56	MG	AA	1916	1/1	0.88	0.48	49,49,49,49	0
56	MG	CA	1655	1/1	0.88	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3165	1/1	0.88	0.26	59,59,59,59	0
56	MG	AA	1808	1/1	0.88	0.20	70,70,70,70	0
56	MG	AA	1852	1/1	0.88	0.13	89,89,89,89	0
56	MG	DA	3331	1/1	0.88	0.24	93,93,93,93	0
56	MG	AA	1760	1/1	0.88	0.16	172,172,172,172	0
56	MG	AA	1617	1/1	0.88	0.24	108,108,108,108	0
56	MG	DA	3318	1/1	0.88	0.46	42,42,42,42	0
56	MG	DA	3490	1/1	0.88	0.26	96,96,96,96	0
56	MG	DA	3032	1/1	0.88	0.18	82,82,82,82	0
56	MG	DA	3322	1/1	0.88	0.21	46,46,46,46	0
56	MG	AA	1739	1/1	0.88	0.10	88,88,88,88	0
56	MG	BA	3246	1/1	0.88	0.42	47,47,47,47	0
56	MG	BA	2968	1/1	0.88	0.22	46,46,46,46	0
56	MG	BA	2908	1/1	0.88	0.37	235,235,235,235	0
56	MG	CA	1767	1/1	0.88	0.49	50,50,50,50	0
56	MG	CA	1702	1/1	0.88	0.43	75,75,75,75	0
56	MG	AA	1907	1/1	0.88	0.49	45,45,45,45	0
56	MG	BA	3076	1/1	0.88	0.10	48,48,48,48	0
56	MG	DA	3223	1/1	0.88	0.18	75,75,75,75	0
56	MG	DA	3201	1/1	0.88	0.34	25,25,25,25	0
56	MG	BA	2928	1/1	0.88	0.24	80,80,80,80	0
56	MG	BA	3282	1/1	0.88	0.52	78,78,78,78	0
56	MG	BA	2919	1/1	0.88	0.09	127,127,127,127	0
56	MG	DA	2912	1/1	0.88	0.30	78,78,78,78	0
56	MG	BA	3685	1/1	0.88	1.06	79,79,79,79	0
56	MG	CA	1825	1/1	0.88	0.21	80,80,80,80	0
56	MG	CA	1876	1/1	0.88	0.31	127,127,127,127	0
56	MG	DA	3321	1/1	0.88	0.36	66,66,66,66	0
56	MG	DA	2966	1/1	0.88	0.31	42,42,42,42	0
56	MG	DA	3379	1/1	0.88	0.26	54,54,54,54	0
56	MG	AA	1695	1/1	0.88	0.11	71,71,71,71	0
56	MG	CA	1616	1/1	0.88	0.41	61,61,61,61	0
56	MG	DA	2970	1/1	0.88	0.66	69,69,69,69	0
56	MG	DA	3015	1/1	0.88	0.53	91,91,91,91	0
56	MG	BA	3371	1/1	0.88	0.74	55,55,55,55	0
56	MG	DA	3467	1/1	0.88	0.22	60,60,60,60	0
56	MG	BA	3651	1/1	0.88	0.30	92,92,92,92	0
56	MG	BA	3539	1/1	0.88	0.53	71,71,71,71	0
56	MG	DQ	204	1/1	0.88	0.40	41,41,41,41	0
56	MG	BA	3406	1/1	0.88	0.44	28,28,28,28	0
56	MG	BA	3444	1/1	0.88	0.52	65,65,65,65	0
56	MG	DA	3116	1/1	0.88	0.17	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1680	1/1	0.88	0.88	77,77,77,77	0
56	MG	CA	1867	1/1	0.88	0.23	82,82,82,82	0
56	MG	BA	3217	1/1	0.88	0.20	65,65,65,65	0
56	MG	AA	1792	1/1	0.88	0.32	84,84,84,84	0
56	MG	DA	3461	1/1	0.88	0.13	73,73,73,73	0
56	MG	BA	3432	1/1	0.88	0.43	69,69,69,69	0
56	MG	BA	3358	1/1	0.88	0.50	150,150,150,150	0
56	MG	BA	3682	1/1	0.88	0.27	64,64,64,64	0
56	MG	DA	3319	1/1	0.88	0.17	34,34,34,34	0
56	MG	AA	1836	1/1	0.88	0.39	139,139,139,139	0
56	MG	CA	1815	1/1	0.88	0.18	80,80,80,80	0
56	MG	DA	3285	1/1	0.88	0.21	63,63,63,63	0
56	MG	CA	1634	1/1	0.88	0.26	74,74,74,74	0
56	MG	AA	1613	1/1	0.88	0.11	83,83,83,83	0
56	MG	DA	2955	1/1	0.88	0.26	30,30,30,30	0
56	MG	BA	3178	1/1	0.88	0.42	52,52,52,52	0
56	MG	DA	3496	1/1	0.88	0.33	40,40,40,40	0
56	MG	DA	3019	1/1	0.88	0.29	67,67,67,67	0
56	MG	CA	1813	1/1	0.88	0.38	99,99,99,99	0
56	MG	DA	3508	1/1	0.88	0.36	37,37,37,37	0
56	MG	AA	1970	1/1	0.88	0.29	62,62,62,62	0
56	MG	DA	3481	1/1	0.88	0.17	73,73,73,73	0
56	MG	CA	1764	1/1	0.88	0.38	50,50,50,50	0
56	MG	BA	2924	1/1	0.88	1.07	64,64,64,64	0
56	MG	AA	1779	1/1	0.88	0.52	74,74,74,74	0
56	MG	DA	3590	1/1	0.88	0.45	74,74,74,74	0
56	MG	DA	3474	1/1	0.88	0.26	55,55,55,55	0
56	MG	DA	3296	1/1	0.88	0.14	69,69,69,69	0
56	MG	DA	3335	1/1	0.88	0.29	38,38,38,38	0
56	MG	AA	1690	1/1	0.88	0.57	174,174,174,174	0
56	MG	AA	1614	1/1	0.88	0.33	51,51,51,51	0
56	MG	AA	1620	1/1	0.88	0.31	76,76,76,76	0
56	MG	AA	1908	1/1	0.88	0.47	56,56,56,56	0
56	MG	BA	3603	1/1	0.88	0.12	88,88,88,88	0
56	MG	DA	3076	1/1	0.88	0.26	88,88,88,88	0
56	MG	DA	3523	1/1	0.88	0.96	76,76,76,76	0
56	MG	DA	3262	1/1	0.88	0.42	65,65,65,65	0
56	MG	CA	1620	1/1	0.88	0.23	74,74,74,74	0
56	MG	BA	2986	1/1	0.88	0.40	45,45,45,45	0
56	MG	DA	3460	1/1	0.88	0.16	67,67,67,67	0
56	MG	CA	1768	1/1	0.88	0.24	55,55,55,55	0
56	MG	BA	3598	1/1	0.88	0.29	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3431	1/1	0.88	0.28	67,67,67,67	0
56	MG	CA	1664	1/1	0.88	0.25	78,78,78,78	0
56	MG	DA	3473	1/1	0.88	0.17	51,51,51,51	0
56	MG	DA	3393	1/1	0.88	0.74	95,95,95,95	0
56	MG	AA	1624	1/1	0.88	0.42	45,45,45,45	0
56	MG	CA	1648	1/1	0.88	0.47	155,155,155,155	0
56	MG	DB	202	1/1	0.88	0.12	51,51,51,51	0
56	MG	BA	3511	1/1	0.88	0.34	91,91,91,91	0
56	MG	DA	3139	1/1	0.88	0.20	33,33,33,33	0
56	MG	BA	3052	1/1	0.88	0.41	118,118,118,118	0
56	MG	DA	3358	1/1	0.89	0.18	141,141,141,141	0
56	MG	CA	1673	1/1	0.89	0.33	73,73,73,73	0
56	MG	DA	3174	1/1	0.89	0.29	49,49,49,49	0
56	MG	AA	1922	1/1	0.89	0.33	86,86,86,86	0
56	MG	DA	3093	1/1	0.89	0.53	76,76,76,76	0
56	MG	BP	201	1/1	0.89	0.31	54,54,54,54	0
56	MG	AA	1661	1/1	0.89	0.16	58,58,58,58	0
56	MG	BA	3476	1/1	0.89	0.69	52,52,52,52	0
56	MG	DA	3366	1/1	0.89	0.29	84,84,84,84	0
56	MG	AA	1803	1/1	0.89	0.37	77,77,77,77	0
56	MG	DQ	203	1/1	0.89	0.17	67,67,67,67	0
56	MG	BA	3594	1/1	0.89	0.34	88,88,88,88	0
56	MG	AA	1682	1/1	0.89	0.81	124,124,124,124	0
56	MG	BA	3647	1/1	0.89	0.30	88,88,88,88	0
56	MG	DA	3125	1/1	0.89	0.72	161,161,161,161	0
56	MG	BA	3704	1/1	0.89	0.22	43,43,43,43	0
56	MG	BA	3710	1/1	0.89	0.27	81,81,81,81	0
56	MG	AA	1972	1/1	0.89	0.41	56,56,56,56	0
56	MG	DA	3031	1/1	0.89	0.25	77,77,77,77	0
56	MG	AA	1857	1/1	0.89	0.59	45,45,45,45	0
56	MG	BA	2947	1/1	0.89	0.44	52,52,52,52	0
56	MG	BA	3026	1/1	0.89	0.60	114,114,114,114	0
56	MG	AA	1627	1/1	0.89	0.52	64,64,64,64	0
56	MG	DA	3383	1/1	0.89	0.38	51,51,51,51	0
56	MG	DA	3451	1/1	0.89	0.52	56,56,56,56	0
56	MG	DA	3000	1/1	0.89	0.22	68,68,68,68	0
56	MG	DA	3570	1/1	0.89	0.37	72,72,72,72	0
56	MG	DA	2982	1/1	0.89	0.25	44,44,44,44	0
56	MG	BA	3289	1/1	0.89	0.23	83,83,83,83	0
56	MG	BA	3034	1/1	0.89	0.23	36,36,36,36	0
56	MG	BA	3169	1/1	0.89	0.08	64,64,64,64	0
56	MG	BA	2979	1/1	0.89	1.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1629	1/1	0.89	0.24	93,93,93,93	0
56	MG	DA	2960	1/1	0.89	0.50	68,68,68,68	0
56	MG	DA	2994	1/1	0.89	0.33	62,62,62,62	0
56	MG	BA	3456	1/1	0.89	0.11	65,65,65,65	0
56	MG	DA	3333	1/1	0.89	0.11	47,47,47,47	0
56	MG	AA	1837	1/1	0.89	0.17	64,64,64,64	0
56	MG	BA	3198	1/1	0.89	0.41	66,66,66,66	0
56	MG	B1	101	1/1	0.89	0.44	75,75,75,75	0
56	MG	DA	3233	1/1	0.89	0.33	62,62,62,62	0
56	MG	DB	203	1/1	0.89	0.14	66,66,66,66	0
56	MG	DA	2965	1/1	0.89	0.33	74,74,74,74	0
56	MG	BA	3515	1/1	0.89	0.42	58,58,58,58	0
56	MG	BA	3499	1/1	0.89	0.20	40,40,40,40	0
56	MG	CA	1765	1/1	0.89	0.25	38,38,38,38	0
56	MG	D7	102	1/1	0.89	0.21	32,32,32,32	0
56	MG	DA	3340	1/1	0.89	0.37	67,67,67,67	0
56	MG	DA	3301	1/1	0.89	0.33	52,52,52,52	0
56	MG	CA	1723	1/1	0.89	0.15	76,76,76,76	0
56	MG	DA	2918	1/1	0.89	0.12	49,49,49,49	0
56	MG	DA	3219	1/1	0.89	0.30	42,42,42,42	0
56	MG	DA	2998	1/1	0.89	0.62	62,62,62,62	0
56	MG	DA	3061	1/1	0.89	0.12	62,62,62,62	0
56	MG	BT	201	1/1	0.89	0.27	63,63,63,63	0
56	MG	DA	3006	1/1	0.89	0.43	66,66,66,66	0
56	MG	BA	3313	1/1	0.89	0.31	63,63,63,63	0
56	MG	BA	3323	1/1	0.89	0.25	47,47,47,47	0
56	MG	BA	3171	1/1	0.89	0.20	43,43,43,43	0
56	MG	BA	3688	1/1	0.89	0.19	59,59,59,59	0
56	MG	BA	3645	1/1	0.89	0.33	48,48,48,48	0
56	MG	CA	1742	1/1	0.89	0.56	61,61,61,61	0
56	MG	BA	3449	1/1	0.89	0.33	49,49,49,49	0
56	MG	DA	3355	1/1	0.89	0.19	102,102,102,102	0
56	MG	DA	3127	1/1	0.89	0.52	88,88,88,88	0
56	MG	BA	3129	1/1	0.89	0.31	72,72,72,72	0
56	MG	DA	3039	1/1	0.89	0.81	72,72,72,72	0
56	MG	AA	1932	1/1	0.89	0.47	159,159,159,159	0
56	MG	BA	2931	1/1	0.89	0.47	98,98,98,98	0
56	MG	DA	3258	1/1	0.89	0.49	58,58,58,58	0
56	MG	AA	1630	1/1	0.89	0.58	55,55,55,55	0
56	MG	BA	3412	1/1	0.89	0.82	58,58,58,58	0
56	MG	BA	2953	1/1	0.89	0.18	56,56,56,56	0
56	MG	DA	3241	1/1	0.89	0.19	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3382	1/1	0.89	0.67	51,51,51,51	0
56	MG	DA	3337	1/1	0.89	0.28	51,51,51,51	0
56	MG	DA	3198	1/1	0.89	0.44	41,41,41,41	0
56	MG	CA	1651	1/1	0.89	0.38	95,95,95,95	0
56	MG	DA	3533	1/1	0.89	0.26	71,71,71,71	0
56	MG	BA	3099	1/1	0.89	0.54	141,141,141,141	0
56	MG	DA	3315	1/1	0.89	0.65	60,60,60,60	0
56	MG	DA	2954	1/1	0.89	0.50	90,90,90,90	0
56	MG	BA	3392	1/1	0.89	0.47	63,63,63,63	0
56	MG	BA	3621	1/1	0.89	0.38	106,106,106,106	0
56	MG	AA	1710	1/1	0.89	0.22	79,79,79,79	0
56	MG	BA	3126	1/1	0.89	0.80	235,235,235,235	0
56	MG	BA	3620	1/1	0.89	0.23	73,73,73,73	0
56	MG	DA	3505	1/1	0.89	0.18	63,63,63,63	0
56	MG	DA	3113	1/1	0.89	0.22	110,110,110,110	0
56	MG	BA	3177	1/1	0.89	0.15	78,78,78,78	0
56	MG	DA	3625	1/1	0.89	0.14	82,82,82,82	0
56	MG	BA	3286	1/1	0.89	0.55	63,63,63,63	0
56	MG	AA	1895	1/1	0.89	0.24	33,33,33,33	0
56	MG	DA	3103	1/1	0.89	0.15	65,65,65,65	0
56	MG	AA	1807	1/1	0.89	0.27	45,45,45,45	0
56	MG	AQ	201	1/1	0.89	0.17	68,68,68,68	0
56	MG	BA	3683	1/1	0.89	0.72	55,55,55,55	0
56	MG	DA	3041	1/1	0.89	0.18	59,59,59,59	0
56	MG	BB	212	1/1	0.89	0.35	99,99,99,99	0
56	MG	AA	1896	1/1	0.89	0.77	77,77,77,77	0
56	MG	CA	1785	1/1	0.89	0.37	63,63,63,63	0
56	MG	DA	3623	1/1	0.89	0.29	52,52,52,52	0
56	MG	AA	1691	1/1	0.89	0.11	84,84,84,84	0
56	MG	BA	3438	1/1	0.89	0.66	49,49,49,49	0
56	MG	AA	1692	1/1	0.89	0.55	134,134,134,134	0
56	MG	DA	3458	1/1	0.89	0.17	64,64,64,64	0
56	MG	DA	3602	1/1	0.89	0.25	22,22,22,22	0
56	MG	BA	3434	1/1	0.89	0.55	55,55,55,55	0
56	MG	CA	1624	1/1	0.89	0.36	98,98,98,98	0
56	MG	DA	3224	1/1	0.89	0.18	40,40,40,40	0
56	MG	DA	3600	1/1	0.89	0.22	23,23,23,23	0
56	MG	AA	1933	1/1	0.89	0.54	63,63,63,63	0
56	MG	CA	1786	1/1	0.89	0.41	84,84,84,84	0
56	MG	BA	3251	1/1	0.89	0.26	55,55,55,55	0
56	MG	AA	1656	1/1	0.89	0.26	61,61,61,61	0
56	MG	AA	1718	1/1	0.89	0.16	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	2990	1/1	0.89	0.29	61,61,61,61	0
56	MG	DA	3259	1/1	0.90	0.30	49,49,49,49	0
56	MG	CA	1773	1/1	0.90	0.14	62,62,62,62	0
56	MG	BA	2977	1/1	0.90	0.41	72,72,72,72	0
56	MG	DB	215	1/1	0.90	0.14	79,79,79,79	0
56	MG	DA	3269	1/1	0.90	0.25	42,42,42,42	0
56	MG	BA	3527	1/1	0.90	0.42	31,31,31,31	0
56	MG	BA	3634	1/1	0.90	0.37	11,11,11,11	0
56	MG	CA	1608	1/1	0.90	0.05	86,86,86,86	0
56	MG	BA	3296	1/1	0.90	0.58	59,59,59,59	0
56	MG	BA	2902	1/1	0.90	0.19	86,86,86,86	0
56	MG	DA	2957	1/1	0.90	0.23	64,64,64,64	0
56	MG	BA	3155	1/1	0.90	0.61	93,93,93,93	0
56	MG	CA	1883	1/1	0.90	0.28	78,78,78,78	0
56	MG	BA	3687	1/1	0.90	0.23	56,56,56,56	0
56	MG	AA	1958	1/1	0.90	0.29	72,72,72,72	0
56	MG	BA	3509	1/1	0.90	0.30	75,75,75,75	0
56	MG	BA	3063	1/1	0.90	0.48	75,75,75,75	0
56	MG	BA	3321	1/1	0.90	0.21	50,50,50,50	0
56	MG	BA	3552	1/1	0.90	0.23	29,29,29,29	0
56	MG	CA	1906	1/1	0.90	0.11	114,114,114,114	0
56	MG	BA	3000	1/1	0.90	0.11	64,64,64,64	0
56	MG	DA	3332	1/1	0.90	0.33	45,45,45,45	0
56	MG	DA	3305	1/1	0.90	0.38	46,46,46,46	0
56	MG	BA	3142	1/1	0.90	0.48	67,67,67,67	0
56	MG	DA	3011	1/1	0.90	0.40	47,47,47,47	0
56	MG	BA	3459	1/1	0.90	0.26	80,80,80,80	0
56	MG	BA	3430	1/1	0.90	0.26	47,47,47,47	0
56	MG	CA	1799	1/1	0.90	0.38	51,51,51,51	0
56	MG	DA	3422	1/1	0.90	0.26	77,77,77,77	0
56	MG	AA	1802	1/1	0.90	0.40	55,55,55,55	0
56	MG	DA	3420	1/1	0.90	0.24	86,86,86,86	0
56	MG	CA	1803	1/1	0.90	0.25	146,146,146,146	0
56	MG	DA	3114	1/1	0.90	0.19	81,81,81,81	0
56	MG	BA	3294	1/1	0.90	0.53	75,75,75,75	0
56	MG	BA	3127	1/1	0.90	0.47	102,102,102,102	0
56	MG	DB	220	1/1	0.90	0.30	40,40,40,40	0
56	MG	DA	3493	1/1	0.90	0.18	57,57,57,57	0
56	MG	D5	102	1/1	0.90	0.10	68,68,68,68	0
56	MG	BA	3679	1/1	0.90	0.26	27,27,27,27	0
56	MG	BA	3689	1/1	0.90	0.32	67,67,67,67	0
56	MG	BA	3646	1/1	0.90	0.21	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1888	1/1	0.90	0.41	49,49,49,49	0
56	MG	CA	1910	1/1	0.90	0.34	77,77,77,77	0
56	MG	AA	1955	1/1	0.90	0.33	87,87,87,87	0
56	MG	BA	3724	1/1	0.90	0.75	119,119,119,119	0
56	MG	BA	2969	1/1	0.90	0.27	79,79,79,79	0
56	MG	DA	3200	1/1	0.90	0.47	52,52,52,52	0
56	MG	BA	3066	1/1	0.90	0.16	61,61,61,61	0
56	MG	AA	1769	1/1	0.90	0.35	79,79,79,79	0
56	MG	BA	3041	1/1	0.90	0.25	68,68,68,68	0
56	MG	DA	3203	1/1	0.90	0.22	51,51,51,51	0
56	MG	BA	3038	1/1	0.90	0.15	58,58,58,58	0
56	MG	AA	1899	1/1	0.90	0.15	89,89,89,89	0
56	MG	AW	103	1/1	0.90	0.22	70,70,70,70	0
56	MG	AA	1648	1/1	0.90	0.24	61,61,61,61	0
56	MG	DA	2985	1/1	0.90	0.18	107,107,107,107	0
56	MG	BA	3027	1/1	0.90	0.24	85,85,85,85	0
56	MG	CA	1913	1/1	0.90	0.47	69,69,69,69	0
56	MG	CA	1875	1/1	0.90	1.09	267,267,267,267	0
56	MG	DA	2941	1/1	0.90	0.20	93,93,93,93	0
56	MG	DA	3526	1/1	0.90	0.29	61,61,61,61	0
56	MG	AA	1883	1/1	0.90	0.38	50,50,50,50	0
56	MG	DB	217	1/1	0.90	0.16	121,121,121,121	0
56	MG	AA	1940	1/1	0.90	0.17	82,82,82,82	0
56	MG	DA	3246	1/1	0.90	0.64	51,51,51,51	0
56	MG	DA	2981	1/1	0.90	0.41	105,105,105,105	0
56	MG	DA	3065	1/1	0.90	0.30	88,88,88,88	0
56	MG	DW	202	1/1	0.90	0.25	50,50,50,50	0
56	MG	CA	1864	1/1	0.90	0.39	157,157,157,157	0
56	MG	DA	2947	1/1	0.90	0.38	192,192,192,192	0
56	MG	BA	3014	1/1	0.90	0.20	44,44,44,44	0
56	MG	BA	3262	1/1	0.90	0.16	75,75,75,75	0
56	MG	DA	3391	1/1	0.90	0.19	57,57,57,57	0
56	MG	AA	1965	1/1	0.90	0.13	37,37,37,37	0
56	MG	AW	118	1/1	0.90	0.61	69,69,69,69	0
56	MG	DA	2929	1/1	0.90	0.24	77,77,77,77	0
56	MG	BA	3504	1/1	0.90	0.16	39,39,39,39	0
56	MG	AA	1669	1/1	0.90	0.60	68,68,68,68	0
56	MG	AA	1701	1/1	0.90	0.12	79,79,79,79	0
56	MG	DA	3283	1/1	0.90	0.32	26,26,26,26	0
56	MG	CA	1791	1/1	0.90	0.64	91,91,91,91	0
56	MG	DA	3413	1/1	0.90	0.71	79,79,79,79	0
56	MG	DA	3306	1/1	0.90	0.55	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3512	1/1	0.90	0.48	33,33,33,33	0
56	MG	DA	3475	1/1	0.90	0.13	54,54,54,54	0
56	MG	BA	3470	1/1	0.90	0.50	65,65,65,65	0
56	MG	BA	3394	1/1	0.90	0.49	56,56,56,56	0
56	MG	DA	3048	1/1	0.90	0.64	49,49,49,49	0
56	MG	AA	1841	1/1	0.90	0.31	113,113,113,113	0
56	MG	DA	3440	1/1	0.90	0.48	58,58,58,58	0
56	MG	DA	3268	1/1	0.90	0.34	52,52,52,52	0
56	MG	AA	1820	1/1	0.90	0.32	166,166,166,166	0
56	MG	DA	2973	1/1	0.90	0.23	57,57,57,57	0
56	MG	AA	1654	1/1	0.90	0.41	61,61,61,61	0
56	MG	BA	3254	1/1	0.90	0.24	93,93,93,93	0
56	MG	DA	2987	1/1	0.90	0.18	63,63,63,63	0
56	MG	AA	1901	1/1	0.90	0.27	71,71,71,71	0
56	MG	DA	3341	1/1	0.90	0.52	55,55,55,55	0
56	MG	BA	3466	1/1	0.90	0.40	39,39,39,39	0
56	MG	DA	3382	1/1	0.90	0.40	49,49,49,49	0
56	MG	BA	3671	1/1	0.90	0.24	84,84,84,84	0
56	MG	DA	3437	1/1	0.90	0.10	59,59,59,59	0
56	MG	DA	3435	1/1	0.90	0.73	68,68,68,68	0
56	MG	BA	3301	1/1	0.90	0.15	64,64,64,64	0
56	MG	BA	3376	1/1	0.90	0.16	59,59,59,59	0
56	MG	DA	2969	1/1	0.90	0.14	68,68,68,68	0
56	MG	AA	1962	1/1	0.90	0.30	55,55,55,55	0
56	MG	BA	3133	1/1	0.90	0.26	48,48,48,48	0
56	MG	DA	2906	1/1	0.90	0.26	70,70,70,70	0
56	MG	CA	1827	1/1	0.90	0.13	45,45,45,45	0
56	MG	BA	3353	1/1	0.90	0.35	54,54,54,54	0
56	MG	DA	3357	1/1	0.90	0.51	78,78,78,78	0
56	MG	BA	3446	1/1	0.91	0.22	93,93,93,93	0
56	MG	DA	3293	1/1	0.91	0.28	58,58,58,58	0
56	MG	BA	3145	1/1	0.91	0.38	53,53,53,53	0
56	MG	CA	1797	1/1	0.91	0.91	61,61,61,61	0
56	MG	DA	3624	1/1	0.91	0.25	35,35,35,35	0
56	MG	DA	3108	1/1	0.91	0.41	74,74,74,74	0
56	MG	AA	1737	1/1	0.91	0.30	72,72,72,72	0
56	MG	DA	3242	1/1	0.91	0.48	40,40,40,40	0
56	MG	CA	1771	1/1	0.91	0.20	70,70,70,70	0
56	MG	AA	1736	1/1	0.91	0.47	83,83,83,83	0
56	MG	AA	1743	1/1	0.91	0.41	81,81,81,81	0
56	MG	BA	3102	1/1	0.91	0.18	61,61,61,61	0
56	MG	CA	1925	1/1	0.91	0.33	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3281	1/1	0.91	0.15	48,48,48,48	0
56	MG	DA	3226	1/1	0.91	0.31	20,20,20,20	0
56	MG	BA	3324	1/1	0.91	0.34	15,15,15,15	0
56	MG	AA	1755	1/1	0.91	0.13	123,123,123,123	0
56	MG	BA	3669	1/1	0.91	0.65	53,53,53,53	0
56	MG	BA	3576	1/1	0.91	0.41	97,97,97,97	0
56	MG	DA	3085	1/1	0.91	0.22	49,49,49,49	0
56	MG	AW	108	1/1	0.91	0.39	72,72,72,72	0
56	MG	CA	1853	1/1	0.91	0.13	52,52,52,52	0
56	MG	BA	3624	1/1	0.91	0.27	83,83,83,83	0
56	MG	DA	3213	1/1	0.91	0.26	60,60,60,60	0
56	MG	BA	3495	1/1	0.91	0.08	51,51,51,51	0
56	MG	CA	1821	1/1	0.91	0.21	56,56,56,56	0
56	MG	DA	3156	1/1	0.91	0.35	33,33,33,33	0
56	MG	DA	3282	1/1	0.91	0.41	42,42,42,42	0
56	MG	BA	3413	1/1	0.91	0.13	21,21,21,21	0
56	MG	BA	3401	1/1	0.91	0.42	28,28,28,28	0
56	MG	DA	3050	1/1	0.91	0.55	56,56,56,56	0
56	MG	BA	3719	1/1	0.91	0.09	125,125,125,125	0
56	MG	BA	3272	1/1	0.91	0.40	49,49,49,49	0
56	MG	AW	114	1/1	0.91	0.19	82,82,82,82	0
56	MG	BB	220	1/1	0.91	0.13	123,123,123,123	0
56	MG	DA	3071	1/1	0.91	0.12	92,92,92,92	0
56	MG	DA	3529	1/1	0.91	0.29	70,70,70,70	0
56	MG	CA	1924	1/1	0.91	0.54	73,73,73,73	0
56	MG	BA	3535	1/1	0.91	0.33	68,68,68,68	0
56	MG	AA	1853	1/1	0.91	0.24	69,69,69,69	0
56	MG	AA	1677	1/1	0.91	0.18	65,65,65,65	0
56	MG	DA	2932	1/1	0.91	0.14	59,59,59,59	0
56	MG	DA	3520	1/1	0.91	0.63	93,93,93,93	0
56	MG	CA	1824	1/1	0.91	0.55	118,118,118,118	0
56	MG	DA	3207	1/1	0.91	0.47	41,41,41,41	0
56	MG	AA	1816	1/1	0.91	0.25	69,69,69,69	0
56	MG	DA	3255	1/1	0.91	0.30	44,44,44,44	0
56	MG	BA	3643	1/1	0.91	0.49	57,57,57,57	0
56	MG	BA	3172	1/1	0.91	0.29	62,62,62,62	0
56	MG	DA	3303	1/1	0.91	0.68	53,53,53,53	0
56	MG	CA	1848	1/1	0.91	0.32	113,113,113,113	0
56	MG	BA	3269	1/1	0.91	0.27	66,66,66,66	0
56	MG	AA	1771	1/1	0.91	0.14	55,55,55,55	0
56	MG	DA	3492	1/1	0.91	0.20	61,61,61,61	0
56	MG	DP	202	1/1	0.91	0.40	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3406	1/1	0.91	0.16	62,62,62,62	0
56	MG	DA	3110	1/1	0.91	0.20	63,63,63,63	0
56	MG	BA	3513	1/1	0.91	0.26	40,40,40,40	0
56	MG	DA	3565	1/1	0.91	0.18	51,51,51,51	0
56	MG	AA	1924	1/1	0.91	0.47	55,55,55,55	0
56	MG	BA	3572	1/1	0.91	0.20	62,62,62,62	0
56	MG	AA	1715	1/1	0.91	0.15	86,86,86,86	0
56	MG	BA	3521	1/1	0.91	0.23	53,53,53,53	0
56	MG	BA	3344	1/1	0.91	0.53	39,39,39,39	0
56	MG	AA	1833	1/1	0.91	0.26	72,72,72,72	0
56	MG	BB	210	1/1	0.91	0.11	88,88,88,88	0
56	MG	BA	3271	1/1	0.91	0.27	68,68,68,68	0
56	MG	BA	3437	1/1	0.91	0.72	82,82,82,82	0
56	MG	BB	217	1/1	0.91	0.19	99,99,99,99	0
56	MG	DA	3631	1/1	0.91	0.23	85,85,85,85	0
56	MG	AA	1707	1/1	0.91	0.11	67,67,67,67	0
56	MG	DA	3445	1/1	0.91	0.27	46,46,46,46	0
56	MG	BA	3125	1/1	0.91	0.36	106,106,106,106	0
56	MG	BA	3703	1/1	0.91	0.97	70,70,70,70	0
56	MG	AA	1991	1/1	0.91	0.09	96,96,96,96	0
56	MG	DA	3419	1/1	0.91	0.24	54,54,54,54	0
56	MG	BA	2945	1/1	0.91	0.40	76,76,76,76	0
56	MG	BA	2963	1/1	0.91	0.38	63,63,63,63	0
56	MG	AA	1674	1/1	0.91	0.27	126,126,126,126	0
56	MG	BA	3657	1/1	0.91	0.27	55,55,55,55	0
56	MG	DA	3102	1/1	0.91	0.53	126,126,126,126	0
56	MG	AA	1847	1/1	0.91	0.32	209,209,209,209	0
56	MG	CA	1733	1/1	0.91	0.23	197,197,197,197	0
56	MG	DA	3020	1/1	0.91	0.17	74,74,74,74	0
56	MG	DA	3615	1/1	0.91	0.27	57,57,57,57	0
56	MG	AA	1930	1/1	0.91	0.45	198,198,198,198	0
56	MG	CA	1641	1/1	0.91	0.13	135,135,135,135	0
56	MG	BA	3474	1/1	0.91	0.40	44,44,44,44	0
56	MG	DA	3212	1/1	0.91	0.53	42,42,42,42	0
56	MG	CA	1652	1/1	0.91	0.91	193,193,193,193	0
56	MG	DA	3514	1/1	0.91	0.21	48,48,48,48	0
56	MG	DA	3359	1/1	0.91	0.35	57,57,57,57	0
56	MG	DA	2920	1/1	0.91	0.21	83,83,83,83	0
56	MG	DA	3286	1/1	0.91	0.29	42,42,42,42	0
56	MG	AA	1926	1/1	0.91	0.39	37,37,37,37	0
56	MG	DA	3310	1/1	0.91	0.49	52,52,52,52	0
56	MG	AA	1834	1/1	0.91	0.25	178,178,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3525	1/1	0.91	0.44	40,40,40,40	0
56	MG	CA	1845	1/1	0.91	0.22	60,60,60,60	0
56	MG	BA	3439	1/1	0.91	0.37	59,59,59,59	0
56	MG	BA	2911	1/1	0.91	0.54	91,91,91,91	0
56	MG	DA	3619	1/1	0.91	0.49	53,53,53,53	0
56	MG	BA	3512	1/1	0.91	0.20	42,42,42,42	0
56	MG	BA	3441	1/1	0.91	0.27	56,56,56,56	0
56	MG	DA	3298	1/1	0.91	0.35	46,46,46,46	0
56	MG	AA	1766	1/1	0.91	0.34	77,77,77,77	0
56	MG	CA	1760	1/1	0.91	0.18	67,67,67,67	0
56	MG	DA	3417	1/1	0.91	0.29	145,145,145,145	0
56	MG	BA	3547	1/1	0.91	0.17	43,43,43,43	0
56	MG	DA	2919	1/1	0.91	0.62	50,50,50,50	0
56	MG	BA	3691	1/1	0.91	0.28	45,45,45,45	0
56	MG	BA	3006	1/1	0.91	0.21	107,107,107,107	0
56	MG	CA	1627	1/1	0.91	0.56	85,85,85,85	0
56	MG	DA	3462	1/1	0.91	0.66	55,55,55,55	0
56	MG	BA	2948	1/1	0.91	0.59	56,56,56,56	0
56	MG	CA	1744	1/1	0.91	0.21	95,95,95,95	0
56	MG	AA	1949	1/1	0.91	0.15	60,60,60,60	0
56	MG	DA	2977	1/1	0.91	0.68	84,84,84,84	0
56	MG	BA	3061	1/1	0.91	0.61	61,61,61,61	0
56	MG	BA	3681	1/1	0.91	0.19	42,42,42,42	0
56	MG	BA	3341	1/1	0.91	0.29	69,69,69,69	0
56	MG	DA	3036	1/1	0.91	0.10	80,80,80,80	0
56	MG	BA	3443	1/1	0.91	0.38	18,18,18,18	0
56	MG	BA	3174	1/1	0.91	0.15	69,69,69,69	0
56	MG	BA	3036	1/1	0.91	0.34	131,131,131,131	0
56	MG	DA	3547	1/1	0.91	0.38	70,70,70,70	0
56	MG	BA	3549	1/1	0.91	0.12	66,66,66,66	0
56	MG	DA	3415	1/1	0.91	0.37	46,46,46,46	0
56	MG	BA	3619	1/1	0.91	0.28	53,53,53,53	0
56	MG	BA	2909	1/1	0.91	0.34	114,114,114,114	0
56	MG	DA	3210	1/1	0.91	0.32	38,38,38,38	0
56	MG	BA	3195	1/1	0.91	0.18	97,97,97,97	0
56	MG	BA	3356	1/1	0.91	0.26	43,43,43,43	0
56	MG	BA	3056	1/1	0.91	0.47	117,117,117,117	0
56	MG	BA	3288	1/1	0.91	0.27	71,71,71,71	0
56	MG	DA	2924	1/1	0.91	0.56	43,43,43,43	0
56	MG	DA	3273	1/1	0.91	0.54	30,30,30,30	0
56	MG	BA	3675	1/1	0.91	0.26	145,145,145,145	0
56	MG	CA	1838	1/1	0.91	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1800	1/1	0.91	0.42	87,87,87,87	0
56	MG	BA	3226	1/1	0.91	0.25	58,58,58,58	0
56	MG	CA	1899	1/1	0.91	0.44	41,41,41,41	0
56	MG	DA	3101	1/1	0.91	0.31	101,101,101,101	0
56	MG	AA	1862	1/1	0.91	0.79	212,212,212,212	0
56	MG	DA	3276	1/1	0.91	0.18	26,26,26,26	0
56	MG	DA	3557	1/1	0.91	0.19	16,16,16,16	0
56	MG	BA	3398	1/1	0.92	0.61	64,64,64,64	0
56	MG	BA	3007	1/1	0.92	0.46	170,170,170,170	0
56	MG	BA	3656	1/1	0.92	0.20	31,31,31,31	0
56	MG	BA	3116	1/1	0.92	0.16	87,87,87,87	0
56	MG	BB	218	1/1	0.92	0.45	50,50,50,50	0
56	MG	DA	3051	1/1	0.92	0.17	64,64,64,64	0
56	MG	AA	1871	1/1	0.92	0.18	29,29,29,29	0
56	MG	CA	1666	1/1	0.92	0.31	73,73,73,73	0
56	MG	BA	2906	1/1	0.92	0.27	84,84,84,84	0
56	MG	CA	1715	1/1	0.92	0.32	79,79,79,79	0
56	MG	BA	3506	1/1	0.92	0.42	53,53,53,53	0
56	MG	AA	1959	1/1	0.92	0.23	63,63,63,63	0
56	MG	BA	3103	1/1	0.92	0.36	89,89,89,89	0
56	MG	DA	3363	1/1	0.92	0.18	42,42,42,42	0
56	MG	AA	1611	1/1	0.92	0.18	109,109,109,109	0
56	MG	AA	1754	1/1	0.92	0.58	72,72,72,72	0
56	MG	AA	1670	1/1	0.92	0.35	77,77,77,77	0
56	MG	BA	3219	1/1	0.92	0.62	78,78,78,78	0
56	MG	DA	3105	1/1	0.92	0.42	94,94,94,94	0
56	MG	DA	3388	1/1	0.92	0.14	63,63,63,63	0
56	MG	DA	3477	1/1	0.92	0.66	56,56,56,56	0
56	MG	BA	3018	1/1	0.92	0.18	59,59,59,59	0
56	MG	DA	3124	1/1	0.92	0.29	32,32,32,32	0
56	MG	AA	1832	1/1	0.92	0.15	67,67,67,67	0
56	MG	BA	3707	1/1	0.92	0.05	84,84,84,84	0
56	MG	BA	2933	1/1	0.92	0.22	69,69,69,69	0
56	MG	DA	3503	1/1	0.92	0.13	92,92,92,92	0
56	MG	AA	1865	1/1	0.92	0.42	98,98,98,98	0
56	MG	BA	3699	1/1	0.92	0.31	70,70,70,70	0
56	MG	BA	3426	1/1	0.92	0.29	28,28,28,28	0
56	MG	DA	3566	1/1	0.92	0.21	43,43,43,43	0
56	MG	AA	1821	1/1	0.92	0.13	70,70,70,70	0
56	MG	DA	3622	1/1	0.92	0.22	50,50,50,50	0
56	MG	BA	3293	1/1	0.92	0.19	62,62,62,62	0
56	MG	BA	3378	1/1	0.92	0.39	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3627	1/1	0.92	0.28	100,100,100,100	0
56	MG	AA	1983	1/1	0.92	1.07	76,76,76,76	0
56	MG	BA	2955	1/1	0.92	0.21	45,45,45,45	0
56	MG	DA	3211	1/1	0.92	0.32	33,33,33,33	0
56	MG	AA	1859	1/1	0.92	0.33	177,177,177,177	0
56	MG	DA	3252	1/1	0.92	0.28	42,42,42,42	0
56	MG	BA	3203	1/1	0.92	0.49	98,98,98,98	0
56	MG	DA	3263	1/1	0.92	0.35	61,61,61,61	0
56	MG	BA	3220	1/1	0.92	0.24	58,58,58,58	0
56	MG	BA	3187	1/1	0.92	0.24	56,56,56,56	0
56	MG	BA	3579	1/1	0.92	0.46	65,65,65,65	0
56	MG	CW	103	1/1	0.92	0.08	57,57,57,57	0
56	MG	DA	3396	1/1	0.92	0.24	18,18,18,18	0
56	MG	DA	3524	1/1	0.92	0.18	67,67,67,67	0
56	MG	CA	1826	1/1	0.92	0.36	73,73,73,73	0
56	MG	DA	3507	1/1	0.92	0.43	70,70,70,70	0
56	MG	BA	3235	1/1	0.92	0.07	63,63,63,63	0
56	MG	CA	1716	1/1	0.92	0.21	86,86,86,86	0
56	MG	CA	1852	1/1	0.92	0.25	93,93,93,93	0
56	MG	BA	3373	1/1	0.92	0.49	39,39,39,39	0
56	MG	BA	3362	1/1	0.92	0.26	26,26,26,26	0
56	MG	DA	3487	1/1	0.92	0.61	108,108,108,108	0
56	MG	BA	3510	1/1	0.92	0.34	86,86,86,86	0
56	MG	BA	3429	1/1	0.92	0.61	43,43,43,43	0
56	MG	BA	2937	1/1	0.92	0.23	71,71,71,71	0
56	MG	CA	1628	1/1	0.92	0.16	86,86,86,86	0
56	MG	DA	3208	1/1	0.92	0.59	29,29,29,29	0
56	MG	DA	3005	1/1	0.92	0.47	89,89,89,89	0
56	MG	BA	3134	1/1	0.92	0.85	122,122,122,122	0
56	MG	AA	1954	1/1	0.92	0.29	142,142,142,142	0
56	MG	AA	1761	1/1	0.92	0.30	118,118,118,118	0
56	MG	DA	3344	1/1	0.92	0.33	29,29,29,29	0
56	MG	BA	3658	1/1	0.92	0.43	71,71,71,71	0
56	MG	DA	3278	1/1	0.92	0.30	83,83,83,83	0
56	MG	DA	3312	1/1	0.92	0.17	61,61,61,61	0
56	MG	AA	1961	1/1	0.92	0.18	53,53,53,53	0
56	MG	BA	2984	1/1	0.92	0.48	40,40,40,40	0
56	MG	BA	3471	1/1	0.92	0.11	45,45,45,45	0
56	MG	CA	1834	1/1	0.92	0.33	108,108,108,108	0
56	MG	BB	204	1/1	0.92	0.13	53,53,53,53	0
56	MG	DA	3537	1/1	0.92	0.33	62,62,62,62	0
56	MG	BA	2961	1/1	0.92	0.24	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1984	1/1	0.92	0.23	42,42,42,42	0
56	MG	AA	1663	1/1	0.92	0.25	44,44,44,44	0
56	MG	BA	2982	1/1	0.92	0.31	86,86,86,86	0
56	MG	AA	1845	1/1	0.92	0.49	67,67,67,67	0
56	MG	BA	3238	1/1	0.92	0.37	61,61,61,61	0
56	MG	BA	3051	1/1	0.92	0.31	32,32,32,32	0
56	MG	BA	3144	1/1	0.92	0.15	53,53,53,53	0
56	MG	BA	3530	1/1	0.92	0.38	57,57,57,57	0
56	MG	BA	3266	1/1	0.92	0.33	73,73,73,73	0
56	MG	BA	3091	1/1	0.92	0.20	125,125,125,125	0
56	MG	CA	1726	1/1	0.92	0.26	80,80,80,80	0
56	MG	DA	3495	1/1	0.92	0.12	63,63,63,63	0
56	MG	AA	1886	1/1	0.92	0.40	65,65,65,65	0
56	MG	DI	201	1/1	0.92	0.21	49,49,49,49	0
56	MG	DB	211	1/1	0.92	0.31	35,35,35,35	0
56	MG	BA	3216	1/1	0.92	0.24	48,48,48,48	0
56	MG	AA	1618	1/1	0.92	0.41	104,104,104,104	0
56	MG	AA	1880	1/1	0.92	0.32	43,43,43,43	0
56	MG	AA	1812	1/1	0.92	0.39	273,273,273,273	0
56	MG	DA	2942	1/1	0.92	0.19	69,69,69,69	0
56	MG	AA	1703	1/1	0.92	0.40	64,64,64,64	0
56	MG	AA	1747	1/1	0.92	0.29	109,109,109,109	0
56	MG	DI	202	1/1	0.92	0.14	54,54,54,54	0
56	MG	DA	3433	1/1	0.92	0.17	27,27,27,27	0
56	MG	BA	3489	1/1	0.92	0.22	54,54,54,54	0
56	MG	AA	1843	1/1	0.92	0.24	124,124,124,124	0
56	MG	DA	3190	1/1	0.92	0.15	25,25,25,25	0
56	MG	BA	3336	1/1	0.92	0.34	31,31,31,31	0
56	MG	BA	2912	1/1	0.92	0.37	67,67,67,67	0
56	MG	BA	3160	1/1	0.92	0.34	51,51,51,51	0
56	MG	DA	3251	1/1	0.92	0.29	32,32,32,32	0
56	MG	CA	1858	1/1	0.92	0.22	97,97,97,97	0
56	MG	DA	3466	1/1	0.92	0.26	90,90,90,90	0
56	MG	BA	3183	1/1	0.92	0.20	79,79,79,79	0
56	MG	AA	1944	1/1	0.92	0.42	67,67,67,67	0
56	MG	CA	1880	1/1	0.92	0.82	118,118,118,118	0
56	MG	BA	3580	1/1	0.92	0.54	60,60,60,60	0
56	MG	BA	3249	1/1	0.92	0.24	84,84,84,84	0
56	MG	BA	3505	1/1	0.92	1.25	101,101,101,101	0
56	MG	CA	1694	1/1	0.92	0.64	69,69,69,69	0
56	MG	DA	2992	1/1	0.92	0.28	63,63,63,63	0
56	MG	DA	3220	1/1	0.92	0.29	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1775	1/1	0.92	0.20	47,47,47,47	0
56	MG	AA	1948	1/1	0.92	0.95	103,103,103,103	0
56	MG	AA	1730	1/1	0.92	0.20	78,78,78,78	0
56	MG	BA	3136	1/1	0.92	0.64	205,205,205,205	0
56	MG	BA	3534	1/1	0.92	0.13	32,32,32,32	0
56	MG	DA	2958	1/1	0.92	0.85	95,95,95,95	0
56	MG	DA	3485	1/1	0.92	0.79	120,120,120,120	0
56	MG	BA	3716	1/1	0.92	0.07	80,80,80,80	0
56	MG	BA	3399	1/1	0.92	0.55	38,38,38,38	0
56	MG	BA	3425	1/1	0.92	0.33	202,202,202,202	0
56	MG	DA	3227	1/1	0.92	0.20	45,45,45,45	0
56	MG	CV	101	1/1	0.92	0.28	87,87,87,87	0
56	MG	BA	3454	1/1	0.92	0.24	60,60,60,60	0
56	MG	B5	101	1/1	0.92	0.21	34,34,34,34	0
56	MG	DA	3024	1/1	0.92	0.27	65,65,65,65	0
56	MG	BA	3526	1/1	0.92	0.36	65,65,65,65	0
56	MG	BA	3695	1/1	0.92	0.10	95,95,95,95	0
56	MG	DA	3279	1/1	0.93	0.27	29,29,29,29	0
56	MG	BA	3670	1/1	0.93	0.30	79,79,79,79	0
56	MG	DA	3563	1/1	0.93	0.48	62,62,62,62	0
56	MG	AA	1706	1/1	0.93	0.43	186,186,186,186	0
56	MG	DA	3372	1/1	0.93	0.19	40,40,40,40	0
56	MG	DA	3334	1/1	0.93	0.36	72,72,72,72	0
56	MG	BA	3609	1/1	0.93	0.57	149,149,149,149	0
56	MG	BA	3555	1/1	0.93	0.18	94,94,94,94	0
56	MG	AA	1711	1/1	0.93	0.21	83,83,83,83	0
56	MG	BA	3411	1/1	0.93	0.36	31,31,31,31	0
56	MG	BA	3440	1/1	0.93	0.40	37,37,37,37	0
56	MG	CA	1891	1/1	0.93	0.22	63,63,63,63	0
56	MG	AA	1863	1/1	0.93	0.34	53,53,53,53	0
56	MG	DA	2908	1/1	0.93	0.28	60,60,60,60	0
56	MG	AA	1741	1/1	0.93	0.29	91,91,91,91	0
56	MG	DA	3175	1/1	0.93	0.33	38,38,38,38	0
56	MG	AA	1936	1/1	0.93	0.77	94,94,94,94	0
56	MG	CA	1763	1/1	0.93	0.19	46,46,46,46	0
56	MG	BA	3648	1/1	0.93	0.29	54,54,54,54	0
56	MG	AA	1781	1/1	0.93	0.34	42,42,42,42	0
56	MG	BA	3652	1/1	0.93	0.19	63,63,63,63	0
56	MG	DA	3525	1/1	0.93	0.13	58,58,58,58	0
56	MG	DA	3543	1/1	0.93	0.17	88,88,88,88	0
56	MG	AA	1671	1/1	0.93	0.30	87,87,87,87	0
56	MG	DA	3230	1/1	0.93	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3237	1/1	0.93	0.47	42,42,42,42	0
56	MG	DA	3538	1/1	0.93	0.11	70,70,70,70	0
56	MG	AA	1910	1/1	0.93	0.56	68,68,68,68	0
56	MG	AO	101	1/1	0.93	0.33	110,110,110,110	0
56	MG	CA	1888	1/1	0.93	0.17	67,67,67,67	0
56	MG	DA	3221	1/1	0.93	0.25	38,38,38,38	0
56	MG	AA	1636	1/1	0.93	0.20	97,97,97,97	0
56	MG	DA	3518	1/1	0.93	0.44	63,63,63,63	0
56	MG	CA	1862	1/1	0.93	0.31	117,117,117,117	0
56	MG	BA	3660	1/1	0.93	0.36	45,45,45,45	0
56	MG	DA	3272	1/1	0.93	0.25	53,53,53,53	0
56	MG	DA	3361	1/1	0.93	0.29	73,73,73,73	0
56	MG	DA	2901	1/1	0.93	0.27	47,47,47,47	0
56	MG	BA	3372	1/1	0.93	0.27	27,27,27,27	0
56	MG	AA	1756	1/1	0.93	0.14	87,87,87,87	0
56	MG	AA	1785	1/1	0.93	0.32	62,62,62,62	0
56	MG	BA	3045	1/1	0.93	1.47	103,103,103,103	0
56	MG	DA	3448	1/1	0.93	0.21	43,43,43,43	0
56	MG	DA	3291	1/1	0.93	0.41	44,44,44,44	0
56	MG	BA	3046	1/1	0.93	0.45	126,126,126,126	0
56	MG	AA	1875	1/1	0.93	0.14	37,37,37,37	0
56	MG	BA	3001	1/1	0.93	0.08	86,86,86,86	0
56	MG	DA	3159	1/1	0.93	0.32	62,62,62,62	0
56	MG	AA	1776	1/1	0.93	0.56	146,146,146,146	0
56	MG	AA	1712	1/1	0.93	0.31	166,166,166,166	0
56	MG	CA	1701	1/1	0.93	0.21	88,88,88,88	0
56	MG	CA	1635	1/1	0.93	0.18	119,119,119,119	0
56	MG	AA	1918	1/1	0.93	0.21	51,51,51,51	0
56	MG	BA	3057	1/1	0.93	0.34	65,65,65,65	0
56	MG	DA	3443	1/1	0.93	0.22	45,45,45,45	0
56	MG	CA	1749	1/1	0.93	0.18	64,64,64,64	0
56	MG	DA	3469	1/1	0.93	0.20	55,55,55,55	0
56	MG	BA	3408	1/1	0.93	0.28	50,50,50,50	0
56	MG	BA	3586	1/1	0.93	0.26	17,17,17,17	0
56	MG	BA	3228	1/1	0.93	0.13	83,83,83,83	0
56	MG	BA	3630	1/1	0.93	0.36	19,19,19,19	0
56	MG	DP	201	1/1	0.93	0.26	43,43,43,43	0
56	MG	BA	3201	1/1	0.93	0.29	71,71,71,71	0
56	MG	BA	2989	1/1	0.93	0.33	84,84,84,84	0
56	MG	DA	3087	1/1	0.93	0.74	52,52,52,52	0
56	MG	BY	201	1/1	0.93	0.21	30,30,30,30	0
56	MG	DA	3387	1/1	0.93	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3267	1/1	0.93	0.16	32,32,32,32	0
56	MG	BA	3113	1/1	0.93	0.48	109,109,109,109	0
56	MG	BA	3233	1/1	0.93	0.30	55,55,55,55	0
56	MG	DA	3567	1/1	0.93	0.20	74,74,74,74	0
56	MG	DA	3256	1/1	0.93	0.18	41,41,41,41	0
56	MG	DA	3034	1/1	0.93	0.60	49,49,49,49	0
56	MG	BA	3042	1/1	0.93	0.30	67,67,67,67	0
56	MG	BA	3161	1/1	0.93	0.45	73,73,73,73	0
56	MG	DA	2922	1/1	0.93	0.15	47,47,47,47	0
56	MG	BA	3231	1/1	0.93	0.20	39,39,39,39	0
56	MG	DA	3299	1/1	0.93	0.41	38,38,38,38	0
56	MG	BA	3635	1/1	0.93	0.43	37,37,37,37	0
56	MG	CA	1697	1/1	0.93	0.74	50,50,50,50	0
56	MG	DA	3164	1/1	0.93	0.17	30,30,30,30	0
56	MG	DA	3280	1/1	0.93	0.49	59,59,59,59	0
56	MG	DA	3584	1/1	0.93	0.34	49,49,49,49	0
56	MG	DA	3444	1/1	0.93	0.25	55,55,55,55	0
56	MG	DA	3457	1/1	0.93	0.44	64,64,64,64	0
56	MG	AA	1985	1/1	0.93	0.32	108,108,108,108	0
56	MG	CA	1774	1/1	0.93	0.26	59,59,59,59	0
56	MG	AA	1889	1/1	0.93	0.20	81,81,81,81	0
56	MG	CA	1769	1/1	0.93	0.17	58,58,58,58	0
56	MG	CA	1707	1/1	0.93	0.18	50,50,50,50	0
56	MG	DA	2968	1/1	0.93	0.15	54,54,54,54	0
56	MG	BA	2901	1/1	0.93	0.93	123,123,123,123	0
56	MG	DA	3412	1/1	0.93	0.26	60,60,60,60	0
56	MG	BA	3280	1/1	0.93	0.16	84,84,84,84	0
56	MG	AA	1789	1/1	0.93	0.18	63,63,63,63	0
56	MG	BA	3464	1/1	0.93	0.33	84,84,84,84	0
56	MG	DA	3414	1/1	0.93	0.15	48,48,48,48	0
56	MG	BA	3385	1/1	0.93	0.35	50,50,50,50	0
56	MG	DA	3562	1/1	0.93	0.20	45,45,45,45	0
56	MG	AA	1623	1/1	0.93	0.10	84,84,84,84	0
56	MG	AA	1969	1/1	0.93	0.55	63,63,63,63	0
56	MG	CA	1818	1/1	0.93	0.26	71,71,71,71	0
56	MG	CA	1784	1/1	0.93	0.50	96,96,96,96	0
56	MG	CA	1903	1/1	0.93	0.26	73,73,73,73	0
56	MG	B8	102	1/1	0.93	0.27	39,39,39,39	0
56	MG	AA	1603	1/1	0.93	0.22	64,64,64,64	0
56	MG	DA	3573	1/1	0.93	0.14	34,34,34,34	0
56	MG	AA	1795	1/1	0.94	0.08	65,65,65,65	0
56	MG	DA	2943	1/1	0.94	0.15	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CY	402	1/1	0.94	0.26	44,44,44,44	0
56	MG	AW	111	1/1	0.94	0.12	91,91,91,91	0
56	MG	BA	3383	1/1	0.94	0.34	39,39,39,39	0
56	MG	CA	1846	1/1	0.94	0.39	101,101,101,101	0
56	MG	DA	3176	1/1	0.94	0.41	13,13,13,13	0
56	MG	DA	3446	1/1	0.94	0.16	59,59,59,59	0
56	MG	AA	1719	1/1	0.94	0.13	92,92,92,92	0
56	MG	CA	1745	1/1	0.94	0.20	115,115,115,115	0
56	MG	AA	1696	1/1	0.94	0.22	96,96,96,96	0
56	MG	AA	1720	1/1	0.94	0.36	86,86,86,86	0
56	MG	BB	201	1/1	0.94	0.14	59,59,59,59	0
56	MG	CA	1873	1/1	0.94	0.21	207,207,207,207	0
56	MG	AA	1784	1/1	0.94	0.07	72,72,72,72	0
56	MG	CA	1612	1/1	0.94	0.30	82,82,82,82	0
56	MG	AA	1685	1/1	0.94	0.15	199,199,199,199	0
56	MG	BA	3615	1/1	0.94	0.22	73,73,73,73	0
56	MG	CW	114	1/1	0.94	0.20	61,61,61,61	0
56	MG	BA	3690	1/1	0.94	0.12	66,66,66,66	0
56	MG	CA	1894	1/1	0.94	0.07	89,89,89,89	0
56	MG	BA	3447	1/1	0.94	0.20	64,64,64,64	0
56	MG	CA	1805	1/1	0.94	0.25	63,63,63,63	0
56	MG	AA	1887	1/1	0.94	0.09	70,70,70,70	0
56	MG	DA	3431	1/1	0.94	0.27	74,74,74,74	0
56	MG	BA	3268	1/1	0.94	0.50	102,102,102,102	0
56	MG	DA	2933	1/1	0.94	0.34	35,35,35,35	0
56	MG	D5	101	1/1	0.94	0.28	71,71,71,71	0
56	MG	BA	3400	1/1	0.94	0.19	37,37,37,37	0
56	MG	DA	3141	1/1	0.94	0.44	15,15,15,15	0
56	MG	AA	1851	1/1	0.94	0.28	111,111,111,111	0
56	MG	CA	1781	1/1	0.94	0.50	59,59,59,59	0
56	MG	DA	3316	1/1	0.94	0.23	49,49,49,49	0
56	MG	AA	1628	1/1	0.94	0.64	213,213,213,213	0
56	MG	AW	106	1/1	0.94	0.20	87,87,87,87	0
56	MG	AA	1840	1/1	0.94	1.44	79,79,79,79	0
56	MG	AA	1793	1/1	0.94	0.36	127,127,127,127	0
56	MG	DA	3264	1/1	0.94	0.23	44,44,44,44	0
56	MG	BA	3556	1/1	0.94	0.63	54,54,54,54	0
56	MG	AA	1964	1/1	0.94	0.16	84,84,84,84	0
56	MG	AA	1885	1/1	0.94	0.15	61,61,61,61	0
56	MG	DA	3515	1/1	0.94	0.09	76,76,76,76	0
56	MG	BA	3395	1/1	0.94	0.75	107,107,107,107	0
56	MG	AA	1856	1/1	0.94	0.46	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CW	106	1/1	0.94	0.20	59,59,59,59	0
56	MG	BA	3283	1/1	0.94	0.21	67,67,67,67	0
56	MG	BA	3109	1/1	0.94	0.23	63,63,63,63	0
56	MG	BA	2998	1/1	0.94	0.31	65,65,65,65	0
56	MG	BA	3354	1/1	0.94	0.32	38,38,38,38	0
56	MG	AW	101	1/1	0.94	0.33	105,105,105,105	0
56	MG	BA	2942	1/1	0.94	0.51	37,37,37,37	0
56	MG	AA	1799	1/1	0.94	0.78	85,85,85,85	0
56	MG	DA	3377	1/1	0.94	0.32	58,58,58,58	0
56	MG	DA	3129	1/1	0.94	0.35	104,104,104,104	0
56	MG	BA	3207	1/1	0.94	0.19	65,65,65,65	0
56	MG	DA	3581	1/1	0.94	0.32	69,69,69,69	0
56	MG	AA	1927	1/1	0.94	0.17	48,48,48,48	0
56	MG	DA	3084	1/1	0.94	0.35	83,83,83,83	0
56	MG	BA	3384	1/1	0.94	0.09	71,71,71,71	0
56	MG	AA	1708	1/1	0.94	0.23	103,103,103,103	0
56	MG	DE	301	1/1	0.94	0.29	29,29,29,29	0
56	MG	BA	2970	1/1	0.94	0.25	93,93,93,93	0
56	MG	DA	3614	1/1	0.94	0.29	50,50,50,50	0
56	MG	DA	3025	1/1	0.94	0.14	30,30,30,30	0
56	MG	DA	3452	1/1	0.94	0.28	73,73,73,73	0
56	MG	AA	1893	1/1	0.94	0.52	48,48,48,48	0
56	MG	BA	3311	1/1	0.94	0.40	17,17,17,17	0
56	MG	BA	3562	1/1	0.94	0.34	45,45,45,45	0
56	MG	BA	3551	1/1	0.94	0.26	52,52,52,52	0
56	MG	AA	1709	1/1	0.94	0.23	71,71,71,71	0
56	MG	DA	3167	1/1	0.94	0.18	13,13,13,13	0
56	MG	BA	2956	1/1	0.94	0.16	42,42,42,42	0
56	MG	CA	1625	1/1	0.94	0.36	125,125,125,125	0
56	MG	AA	1731	1/1	0.94	0.14	57,57,57,57	0
56	MG	DA	3323	1/1	0.94	0.14	42,42,42,42	0
56	MG	AA	1861	1/1	0.94	0.52	42,42,42,42	0
56	MG	DA	3465	1/1	0.94	0.20	60,60,60,60	0
56	MG	BA	3396	1/1	0.94	0.34	43,43,43,43	0
56	MG	BA	3483	1/1	0.94	0.13	23,23,23,23	0
56	MG	DA	3204	1/1	0.94	0.17	35,35,35,35	0
56	MG	BA	3493	1/1	0.94	0.23	61,61,61,61	0
56	MG	AA	1963	1/1	0.94	0.21	80,80,80,80	0
56	MG	BA	3714	1/1	0.94	0.12	94,94,94,94	0
56	MG	BA	3019	1/1	0.94	0.20	109,109,109,109	0
56	MG	BA	3363	1/1	0.94	0.44	19,19,19,19	0
56	MG	DA	3218	1/1	0.94	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	2913	1/1	0.94	0.73	70,70,70,70	0
56	MG	BA	3210	1/1	0.94	0.10	76,76,76,76	0
56	MG	DA	3330	1/1	0.94	0.40	36,36,36,36	0
56	MG	CA	1692	1/1	0.94	0.27	62,62,62,62	0
56	MG	BA	2916	1/1	0.94	0.32	37,37,37,37	0
56	MG	AA	1987	1/1	0.94	0.58	121,121,121,121	0
56	MG	BA	3277	1/1	0.94	0.27	51,51,51,51	0
56	MG	DA	3546	1/1	0.94	0.34	62,62,62,62	0
56	MG	AA	1655	1/1	0.94	0.52	80,80,80,80	0
56	MG	AA	1649	1/1	0.94	0.90	110,110,110,110	0
56	MG	DA	3370	1/1	0.94	0.42	66,66,66,66	0
56	MG	DA	2978	1/1	0.94	0.46	64,64,64,64	0
56	MG	DA	3209	1/1	0.94	0.21	17,17,17,17	0
56	MG	BA	3625	1/1	0.94	0.38	117,117,117,117	0
56	MG	AA	1683	1/1	0.94	0.15	249,249,249,249	0
56	MG	BA	3565	1/1	0.94	0.30	63,63,63,63	0
56	MG	BA	3295	1/1	0.94	0.65	97,97,97,97	0
56	MG	DA	3468	1/1	0.94	0.38	33,33,33,33	0
56	MG	DA	3480	1/1	0.94	0.28	42,42,42,42	0
56	MG	BA	3558	1/1	0.94	0.23	71,71,71,71	0
56	MG	CA	1656	1/1	0.94	0.48	52,52,52,52	0
56	MG	BA	3457	1/1	0.94	0.24	68,68,68,68	0
56	MG	DA	3345	1/1	0.94	0.24	68,68,68,68	0
56	MG	DA	2959	1/1	0.94	0.51	48,48,48,48	0
56	MG	DA	3389	1/1	0.94	0.21	68,68,68,68	0
56	MG	AA	1980	1/1	0.94	0.66	76,76,76,76	0
56	MG	AA	1876	1/1	0.94	0.50	123,123,123,123	0
56	MG	CA	1778	1/1	0.94	0.45	36,36,36,36	0
56	MG	BA	3232	1/1	0.94	0.22	65,65,65,65	0
56	MG	BA	3340	1/1	0.94	0.33	31,31,31,31	0
56	MG	DA	3096	1/1	0.94	0.31	82,82,82,82	0
56	MG	CA	1804	1/1	0.94	0.37	78,78,78,78	0
56	MG	AA	1673	1/1	0.94	0.20	104,104,104,104	0
56	MG	CA	1679	1/1	0.94	0.19	81,81,81,81	0
56	MG	DA	3228	1/1	0.94	0.39	31,31,31,31	0
56	MG	BA	3575	1/1	0.94	0.21	63,63,63,63	0
56	MG	AA	1602	1/1	0.94	0.24	163,163,163,163	0
56	MG	BA	3106	1/1	0.94	0.22	57,57,57,57	0
56	MG	AA	1791	1/1	0.94	0.37	59,59,59,59	0
56	MG	DA	3239	1/1	0.94	0.44	43,43,43,43	0
56	MG	BA	3677	1/1	0.94	0.40	18,18,18,18	0
56	MG	BA	3427	1/1	0.94	0.38	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3649	1/1	0.94	0.27	104,104,104,104	0
56	MG	CW	108	1/1	0.94	0.37	26,26,26,26	0
56	MG	CA	1758	1/1	0.94	0.20	40,40,40,40	0
56	MG	BA	3342	1/1	0.95	0.20	25,25,25,25	0
56	MG	BA	2905	1/1	0.95	0.35	54,54,54,54	0
56	MG	BA	3090	1/1	0.95	0.43	60,60,60,60	0
56	MG	CA	1654	1/1	0.95	0.27	106,106,106,106	0
56	MG	DA	3193	1/1	0.95	0.08	34,34,34,34	0
56	MG	DA	3099	1/1	0.95	0.07	79,79,79,79	0
56	MG	DA	3397	1/1	0.95	0.36	54,54,54,54	0
56	MG	DA	3022	1/1	0.95	0.21	80,80,80,80	0
56	MG	BA	3337	1/1	0.95	0.52	20,20,20,20	0
56	MG	AA	1915	1/1	0.95	0.14	50,50,50,50	0
56	MG	BA	3544	1/1	0.95	0.17	55,55,55,55	0
56	MG	CA	1713	1/1	0.95	0.19	88,88,88,88	0
56	MG	DA	3194	1/1	0.95	0.10	28,28,28,28	0
56	MG	BB	221	1/1	0.95	0.10	65,65,65,65	0
56	MG	BA	3637	1/1	0.95	0.15	20,20,20,20	0
56	MG	DA	3123	1/1	0.95	0.63	72,72,72,72	0
56	MG	DA	3408	1/1	0.95	0.20	51,51,51,51	0
56	MG	BA	3260	1/1	0.95	0.25	109,109,109,109	0
56	MG	DA	2939	1/1	0.95	0.63	66,66,66,66	0
56	MG	AA	1813	1/1	0.95	0.29	134,134,134,134	0
56	MG	BA	3120	1/1	0.95	0.51	62,62,62,62	0
56	MG	BA	3327	1/1	0.95	0.33	28,28,28,28	0
56	MG	BA	3029	1/1	0.95	0.27	44,44,44,44	0
56	MG	CA	1855	1/1	0.95	0.27	197,197,197,197	0
56	MG	DA	3483	1/1	0.95	0.33	96,96,96,96	0
56	MG	BA	3338	1/1	0.95	0.21	28,28,28,28	0
56	MG	BA	3633	1/1	0.95	0.48	12,12,12,12	0
56	MG	BA	3386	1/1	0.95	0.16	39,39,39,39	0
56	MG	BA	3335	1/1	0.95	0.73	49,49,49,49	0
56	MG	AA	1768	1/1	0.95	0.19	183,183,183,183	0
56	MG	BA	3461	1/1	0.95	0.50	23,23,23,23	0
56	MG	CA	1639	1/1	0.95	0.09	100,100,100,100	0
56	MG	DA	3132	1/1	0.95	0.46	13,13,13,13	0
56	MG	CA	1787	1/1	0.95	0.28	77,77,77,77	0
56	MG	BA	3108	1/1	0.95	0.38	61,61,61,61	0
56	MG	AA	1878	1/1	0.95	0.28	56,56,56,56	0
56	MG	AA	1608	1/1	0.95	0.76	108,108,108,108	0
56	MG	BA	3680	1/1	0.95	0.14	35,35,35,35	0
56	MG	DA	3249	1/1	0.95	0.48	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3056	1/1	0.95	0.21	77,77,77,77	0
56	MG	AA	1842	1/1	0.95	0.20	98,98,98,98	0
56	MG	BA	3528	1/1	0.95	0.54	53,53,53,53	0
56	MG	BA	3659	1/1	0.95	0.15	46,46,46,46	0
56	MG	DA	3131	1/1	0.95	0.55	40,40,40,40	0
56	MG	DA	3115	1/1	0.95	0.16	60,60,60,60	0
56	MG	AA	1911	1/1	0.95	0.11	38,38,38,38	0
56	MG	DA	3295	1/1	0.95	0.33	48,48,48,48	0
56	MG	BA	2944	1/1	0.95	0.19	62,62,62,62	0
56	MG	DA	3374	1/1	0.95	0.29	54,54,54,54	0
56	MG	BA	3365	1/1	0.95	0.34	14,14,14,14	0
56	MG	DA	3199	1/1	0.95	0.53	36,36,36,36	0
56	MG	AA	1982	1/1	0.95	0.14	73,73,73,73	0
56	MG	AY	402	1/1	0.95	0.16	40,40,40,40	0
56	MG	BA	3028	1/1	0.95	0.48	70,70,70,70	0
56	MG	DA	3554	1/1	0.95	0.44	13,13,13,13	0
56	MG	CA	1923	1/1	0.95	0.14	77,77,77,77	0
56	MG	CA	1685	1/1	0.95	0.18	104,104,104,104	0
56	MG	DA	3378	1/1	0.95	0.37	54,54,54,54	0
56	MG	DA	3536	1/1	0.95	0.55	50,50,50,50	0
56	MG	DA	3247	1/1	0.95	0.19	55,55,55,55	0
56	MG	BA	3706	1/1	0.95	0.46	102,102,102,102	0
56	MG	AA	1749	1/1	0.95	0.29	114,114,114,114	0
56	MG	CA	1661	1/1	0.95	0.20	68,68,68,68	0
56	MG	DA	2961	1/1	0.95	0.37	143,143,143,143	0
56	MG	DA	3134	1/1	0.95	0.44	18,18,18,18	0
56	MG	DA	3018	1/1	0.95	0.08	83,83,83,83	0
56	MG	BA	3379	1/1	0.95	0.39	23,23,23,23	0
56	MG	BA	3330	1/1	0.95	0.31	27,27,27,27	0
56	MG	AA	1904	1/1	0.95	0.42	43,43,43,43	0
56	MG	AA	1704	1/1	0.95	0.45	186,186,186,186	0
56	MG	AA	1665	1/1	0.95	0.15	59,59,59,59	0
56	MG	BA	3253	1/1	0.95	0.13	73,73,73,73	0
56	MG	DA	3404	1/1	0.95	0.54	61,61,61,61	0
56	MG	DA	3360	1/1	0.95	0.16	64,64,64,64	0
56	MG	BA	3417	1/1	0.95	0.25	56,56,56,56	0
56	MG	DA	3148	1/1	0.95	0.53	34,34,34,34	0
56	MG	BA	3047	1/1	0.95	0.30	50,50,50,50	0
56	MG	DA	3012	1/1	0.95	0.34	102,102,102,102	0
56	MG	DA	3215	1/1	0.95	0.54	46,46,46,46	0
56	MG	AA	1662	1/1	0.95	0.27	108,108,108,108	0
56	MG	DA	3605	1/1	0.95	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	1762	1/1	0.95	0.14	28,28,28,28	0
56	MG	DA	3078	1/1	0.95	0.19	75,75,75,75	0
56	MG	CA	1915	1/1	0.95	0.70	67,67,67,67	0
56	MG	CA	1814	1/1	0.95	0.25	156,156,156,156	0
56	MG	DA	3399	1/1	0.95	0.09	85,85,85,85	0
56	MG	DA	3354	1/1	0.95	0.47	33,33,33,33	0
56	MG	BA	3388	1/1	0.95	0.59	22,22,22,22	0
56	MG	DA	3245	1/1	0.95	0.48	45,45,45,45	0
56	MG	BA	3458	1/1	0.95	0.20	52,52,52,52	0
56	MG	DA	3613	1/1	0.95	0.11	49,49,49,49	0
56	MG	BA	3009	1/1	0.95	0.18	86,86,86,86	0
56	MG	BA	3005	1/1	0.95	0.23	45,45,45,45	0
56	MG	DA	3183	1/1	0.95	0.38	16,16,16,16	0
56	MG	DA	3206	1/1	0.95	0.42	23,23,23,23	0
56	MG	AA	1838	1/1	0.95	0.19	56,56,56,56	0
56	MG	BA	3484	1/1	0.95	0.34	104,104,104,104	0
56	MG	DA	3593	1/1	0.95	0.15	70,70,70,70	0
56	MG	DA	3150	1/1	0.95	0.44	17,17,17,17	0
56	MG	AA	1884	1/1	0.95	0.39	47,47,47,47	0
56	MG	DA	2962	1/1	0.95	0.14	59,59,59,59	0
56	MG	AA	1869	1/1	0.95	0.56	34,34,34,34	0
56	MG	BA	3595	1/1	0.95	0.27	39,39,39,39	0
56	MG	BA	3101	1/1	0.95	0.16	106,106,106,106	0
56	MG	DA	2946	1/1	0.95	0.58	55,55,55,55	0
56	MG	CA	1638	1/1	0.95	0.17	118,118,118,118	0
56	MG	DA	3146	1/1	0.95	0.74	50,50,50,50	0
56	MG	DA	3135	1/1	0.95	0.49	17,17,17,17	0
56	MG	AA	1773	1/1	0.95	0.49	281,281,281,281	0
56	MG	CA	1829	1/1	0.95	0.68	49,49,49,49	0
56	MG	AA	1814	1/1	0.95	0.48	58,58,58,58	0
56	MG	AA	1657	1/1	0.95	0.28	112,112,112,112	0
56	MG	DA	3418	1/1	0.95	0.20	11,11,11,11	0
56	MG	BA	3037	1/1	0.95	0.18	101,101,101,101	0
56	MG	DA	3181	1/1	0.95	0.36	13,13,13,13	0
56	MG	BA	3686	1/1	0.95	0.43	28,28,28,28	0
56	MG	BA	3118	1/1	0.95	0.44	132,132,132,132	0
56	MG	BA	3375	1/1	0.95	0.32	30,30,30,30	0
56	MG	AA	1659	1/1	0.95	0.23	88,88,88,88	0
56	MG	DA	3166	1/1	0.96	0.25	25,25,25,25	0
56	MG	AA	1805	1/1	0.96	0.24	71,71,71,71	0
56	MG	DA	3147	1/1	0.96	0.23	20,20,20,20	0
56	MG	BA	3058	1/1	0.96	0.38	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	2925	1/1	0.96	0.55	80,80,80,80	0
56	MG	DA	3253	1/1	0.96	0.36	30,30,30,30	0
56	MG	DA	3587	1/1	0.96	0.10	90,90,90,90	0
56	MG	DA	3606	1/1	0.96	0.17	54,54,54,54	0
56	MG	BA	3351	1/1	0.96	0.54	29,29,29,29	0
56	MG	DA	2902	1/1	0.96	0.25	65,65,65,65	0
56	MG	DB	216	1/1	0.96	0.09	51,51,51,51	0
56	MG	AA	1818	1/1	0.96	0.16	44,44,44,44	0
56	MG	DA	2927	1/1	0.96	0.30	91,91,91,91	0
56	MG	DA	3506	1/1	0.96	0.20	53,53,53,53	0
56	MG	DA	3192	1/1	0.96	0.25	38,38,38,38	0
56	MG	AW	117	1/1	0.96	0.14	68,68,68,68	0
56	MG	DA	3254	1/1	0.96	0.31	50,50,50,50	0
56	MG	BA	3274	1/1	0.96	0.12	105,105,105,105	0
56	MG	BA	3490	1/1	0.96	0.22	45,45,45,45	0
56	MG	BA	3452	1/1	0.96	0.67	53,53,53,53	0
56	MG	DA	3311	1/1	0.96	0.30	54,54,54,54	0
56	MG	BA	3463	1/1	0.96	0.30	106,106,106,106	0
56	MG	DA	3040	1/1	0.96	0.32	102,102,102,102	0
56	MG	DN	201	1/1	0.96	0.14	56,56,56,56	0
56	MG	CA	1859	1/1	0.96	0.60	132,132,132,132	0
56	MG	DA	3324	1/1	0.96	0.48	13,13,13,13	0
56	MG	BA	3159	1/1	0.96	0.20	151,151,151,151	0
56	MG	BA	3347	1/1	0.96	0.23	27,27,27,27	0
56	MG	DA	3555	1/1	0.96	0.28	14,14,14,14	0
56	MG	DA	2984	1/1	0.96	0.26	34,34,34,34	0
56	MG	DA	3173	1/1	0.96	0.60	46,46,46,46	0
56	MG	CA	1601	1/1	0.96	0.17	34,34,34,34	0
56	MG	DA	3409	1/1	0.96	0.32	102,102,102,102	0
56	MG	AA	1968	1/1	0.96	0.89	86,86,86,86	0
56	MG	DA	2923	1/1	0.96	0.15	28,28,28,28	0
56	MG	AA	1974	1/1	0.96	0.20	48,48,48,48	0
56	MG	BA	3694	1/1	0.96	0.15	35,35,35,35	0
56	MG	DA	3100	1/1	0.96	0.42	97,97,97,97	0
56	MG	AA	1905	1/1	0.96	0.19	59,59,59,59	0
56	MG	BA	3355	1/1	0.96	0.26	18,18,18,18	0
56	MG	BA	3428	1/1	0.96	0.26	51,51,51,51	0
56	MG	AA	1626	1/1	0.96	0.09	91,91,91,91	0
56	MG	CA	1832	1/1	0.96	0.19	65,65,65,65	0
56	MG	BA	3349	1/1	0.96	0.39	43,43,43,43	0
56	MG	DA	3556	1/1	0.96	0.23	19,19,19,19	0
56	MG	DA	3558	1/1	0.96	0.34	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3673	1/1	0.96	0.24	133,133,133,133	0
56	MG	DA	3540	1/1	0.96	0.20	85,85,85,85	0
56	MG	BA	3418	1/1	0.96	0.20	27,27,27,27	0
56	MG	DA	3133	1/1	0.96	0.36	20,20,20,20	0
56	MG	DA	2974	1/1	0.96	0.18	90,90,90,90	0
56	MG	DA	3165	1/1	0.96	0.47	25,25,25,25	0
57	ZN	CN	101	1/1	0.96	0.15	111,111,111,111	0
56	MG	BA	3481	1/1	0.96	0.16	59,59,59,59	0
56	MG	BA	3285	1/1	0.96	0.24	66,66,66,66	0
56	MG	DA	3488	1/1	0.96	0.07	70,70,70,70	0
56	MG	AA	1633	1/1	0.96	0.16	45,45,45,45	0
56	MG	AA	1693	1/1	0.96	0.33	74,74,74,74	0
56	MG	DA	3152	1/1	0.96	0.39	23,23,23,23	0
56	MG	DA	3617	1/1	0.96	0.18	46,46,46,46	0
56	MG	DA	3438	1/1	0.96	0.28	73,73,73,73	0
56	MG	BA	3516	1/1	0.96	0.16	29,29,29,29	0
56	MG	DA	3235	1/1	0.96	0.59	41,41,41,41	0
56	MG	BA	3023	1/1	0.96	0.54	58,58,58,58	0
56	MG	CA	1609	1/1	0.96	0.19	100,100,100,100	0
56	MG	AA	1610	1/1	0.96	0.19	65,65,65,65	0
56	MG	DA	3314	1/1	0.96	0.36	65,65,65,65	0
56	MG	CA	1889	1/1	0.96	0.06	92,92,92,92	0
56	MG	BA	3467	1/1	0.96	0.16	103,103,103,103	0
56	MG	DA	3140	1/1	0.96	0.41	11,11,11,11	0
56	MG	BA	2914	1/1	0.96	0.32	122,122,122,122	0
56	MG	DA	3394	1/1	0.96	0.28	49,49,49,49	0
56	MG	DA	3137	1/1	0.96	0.29	23,23,23,23	0
56	MG	DA	3229	1/1	0.96	0.28	37,37,37,37	0
56	MG	CA	1751	1/1	0.96	0.58	163,163,163,163	0
56	MG	DA	3153	1/1	0.96	0.48	22,22,22,22	0
56	MG	DA	3442	1/1	0.96	0.40	64,64,64,64	0
56	MG	BA	3317	1/1	0.96	0.39	16,16,16,16	0
56	MG	AA	1844	1/1	0.96	0.26	78,78,78,78	0
56	MG	DA	3191	1/1	0.96	0.37	28,28,28,28	0
56	MG	BA	3445	1/1	0.96	0.16	19,19,19,19	0
56	MG	AA	1788	1/1	0.96	0.28	175,175,175,175	0
56	MG	CA	1759	1/1	0.96	0.41	65,65,65,65	0
56	MG	BA	3498	1/1	0.96	0.07	67,67,67,67	0
56	MG	DA	3607	1/1	0.96	0.19	30,30,30,30	0
56	MG	BA	3402	1/1	0.96	0.33	37,37,37,37	0
56	MG	BA	3094	1/1	0.96	0.43	38,38,38,38	0
56	MG	DA	3179	1/1	0.96	0.21	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	3475	1/1	0.96	0.61	55,55,55,55	0
56	MG	BA	3360	1/1	0.96	0.54	24,24,24,24	0
56	MG	DA	3225	1/1	0.96	0.39	59,59,59,59	0
56	MG	DA	3347	1/1	0.96	0.21	23,23,23,23	0
56	MG	CW	109	1/1	0.96	0.08	49,49,49,49	0
56	MG	BA	3374	1/1	0.96	0.24	30,30,30,30	0
56	MG	BA	3325	1/1	0.96	0.55	39,39,39,39	0
56	MG	DA	3126	1/1	0.96	0.71	65,65,65,65	0
56	MG	DA	3232	1/1	0.96	0.61	48,48,48,48	0
56	MG	DA	3111	1/1	0.96	0.28	84,84,84,84	0
56	MG	BA	3072	1/1	0.96	0.17	88,88,88,88	0
56	MG	BA	2938	1/1	0.96	0.21	81,81,81,81	0
56	MG	BA	3030	1/1	0.96	0.45	64,64,64,64	0
56	MG	BA	3334	1/1	0.96	0.35	65,65,65,65	0
56	MG	BA	3044	1/1	0.96	0.35	53,53,53,53	0
56	MG	DA	3410	1/1	0.97	0.15	22,22,22,22	0
56	MG	BA	3421	1/1	0.97	0.21	79,79,79,79	0
56	MG	BA	3578	1/1	0.97	0.27	32,32,32,32	0
56	MG	DA	3157	1/1	0.97	0.21	23,23,23,23	0
56	MG	DA	3572	1/1	0.97	0.12	51,51,51,51	0
56	MG	AA	1870	1/1	0.97	0.42	73,73,73,73	0
56	MG	DA	3597	1/1	0.97	0.41	22,22,22,22	0
56	MG	BA	3314	1/1	0.97	0.49	13,13,13,13	0
56	MG	AA	1919	1/1	0.97	0.56	47,47,47,47	0
56	MG	DA	3214	1/1	0.97	0.39	22,22,22,22	0
56	MG	AA	1877	1/1	0.97	0.49	37,37,37,37	0
56	MG	CA	1623	1/1	0.97	0.17	43,43,43,43	0
56	MG	DA	3534	1/1	0.97	0.52	70,70,70,70	0
56	MG	DA	3277	1/1	0.97	0.38	45,45,45,45	0
56	MG	BA	3420	1/1	0.97	0.39	34,34,34,34	0
56	MG	BA	3100	1/1	0.97	0.22	70,70,70,70	0
56	MG	AA	1735	1/1	0.97	0.36	52,52,52,52	0
56	MG	CA	1632	1/1	0.97	0.17	84,84,84,84	0
56	MG	DA	3177	1/1	0.97	0.31	21,21,21,21	0
56	MG	DA	3234	1/1	0.97	0.13	31,31,31,31	0
56	MG	BA	3631	1/1	0.97	0.34	8,8,8,8	0
56	MG	DA	3479	1/1	0.97	0.12	55,55,55,55	0
56	MG	BA	3021	1/1	0.97	0.13	111,111,111,111	0
56	MG	BA	2980	1/1	0.97	0.25	74,74,74,74	0
56	MG	DA	3464	1/1	0.97	0.60	42,42,42,42	0
56	MG	BX	101	1/1	0.97	0.12	55,55,55,55	0
56	MG	DA	3021	1/1	0.97	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1960	1/1	0.97	0.24	48,48,48,48	0
56	MG	DA	3608	1/1	0.97	0.57	50,50,50,50	0
56	MG	BA	3692	1/1	0.97	0.36	56,56,56,56	0
56	MG	BA	3632	1/1	0.97	0.39	15,15,15,15	0
56	MG	AA	1694	1/1	0.97	0.28	165,165,165,165	0
56	MG	DA	3545	1/1	0.97	0.19	91,91,91,91	0
56	MG	DA	2928	1/1	0.97	0.20	55,55,55,55	0
56	MG	BD	301	1/1	0.97	0.23	15,15,15,15	0
56	MG	DA	2935	1/1	0.97	0.14	89,89,89,89	0
56	MG	AA	1849	1/1	0.97	0.12	95,95,95,95	0
56	MG	AA	1664	1/1	0.97	0.30	64,64,64,64	0
56	MG	AA	1902	1/1	0.97	0.22	33,33,33,33	0
56	MG	BA	3642	1/1	0.97	0.35	34,34,34,34	0
56	MG	DA	3236	1/1	0.97	0.64	30,30,30,30	0
56	MG	BA	3352	1/1	0.97	0.25	17,17,17,17	0
56	MG	BA	3339	1/1	0.97	0.28	26,26,26,26	0
56	MG	BA	2978	1/1	0.97	0.67	72,72,72,72	0
56	MG	BA	3214	1/1	0.97	0.23	85,85,85,85	0
56	MG	DA	3231	1/1	0.97	0.42	32,32,32,32	0
56	MG	DA	3217	1/1	0.97	0.40	24,24,24,24	0
56	MG	AA	1601	1/1	0.97	0.36	92,92,92,92	0
56	MG	BB	219	1/1	0.97	0.30	33,33,33,33	0
56	MG	DA	3197	1/1	0.97	0.22	21,21,21,21	0
56	MG	BA	3705	1/1	0.97	0.12	62,62,62,62	0
56	MG	BA	3453	1/1	0.97	0.47	40,40,40,40	0
56	MG	DA	3553	1/1	0.97	0.45	21,21,21,21	0
56	MG	DA	3550	1/1	0.97	0.39	18,18,18,18	0
56	MG	AA	1943	1/1	0.97	0.13	45,45,45,45	0
56	MG	DA	3180	1/1	0.97	0.45	37,37,37,37	0
56	MG	BA	3416	1/1	0.97	0.42	42,42,42,42	0
56	MG	DA	3240	1/1	0.97	0.14	35,35,35,35	0
56	MG	CA	1721	1/1	0.97	0.12	74,74,74,74	0
56	MG	BA	3566	1/1	0.97	0.14	63,63,63,63	0
56	MG	AA	1798	1/1	0.97	0.17	47,47,47,47	0
56	MG	DA	3154	1/1	0.97	0.28	12,12,12,12	0
56	MG	DA	3136	1/1	0.97	0.45	12,12,12,12	0
56	MG	DA	3202	1/1	0.97	0.40	25,25,25,25	0
56	MG	DA	3476	1/1	0.97	0.31	73,73,73,73	0
56	MG	DA	3328	1/1	0.97	0.52	48,48,48,48	0
56	MG	DA	3580	1/1	0.97	0.49	79,79,79,79	0
56	MG	BA	3025	1/1	0.97	0.30	66,66,66,66	0
56	MG	AA	1976	1/1	0.97	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3168	1/1	0.97	0.40	33,33,33,33	0
56	MG	DA	3182	1/1	0.97	0.50	24,24,24,24	0
56	MG	DA	3603	1/1	0.97	0.09	17,17,17,17	0
56	MG	DA	3069	1/1	0.97	0.23	32,32,32,32	0
56	MG	CA	1830	1/1	0.97	0.15	80,80,80,80	0
56	MG	AA	1978	1/1	0.97	0.30	129,129,129,129	0
56	MG	BA	3518	1/1	0.97	0.25	27,27,27,27	0
56	MG	BA	3184	1/1	0.97	0.29	37,37,37,37	0
56	MG	BA	3328	1/1	0.97	0.57	35,35,35,35	0
56	MG	BA	3636	1/1	0.97	0.47	28,28,28,28	0
56	MG	BA	3312	1/1	0.97	0.52	20,20,20,20	0
56	MG	BA	3015	1/1	0.97	0.33	71,71,71,71	0
56	MG	BA	3424	1/1	0.97	0.13	32,32,32,32	0
56	MG	DA	2904	1/1	0.97	0.60	71,71,71,71	0
56	MG	DA	3172	1/1	0.97	0.58	24,24,24,24	0
56	MG	DA	3561	1/1	0.97	0.18	16,16,16,16	0
56	MG	DA	3163	1/1	0.98	0.29	31,31,31,31	0
56	MG	DA	3186	1/1	0.98	0.18	51,51,51,51	0
57	ZN	CD	301	1/1	0.98	0.34	109,109,109,109	0
56	MG	DA	3552	1/1	0.98	0.50	19,19,19,19	0
56	MG	BA	3350	1/1	0.98	0.38	28,28,28,28	0
56	MG	BA	3410	1/1	0.98	0.10	25,25,25,25	0
56	MG	DA	3184	1/1	0.98	0.38	14,14,14,14	0
56	MG	DA	3274	1/1	0.98	0.36	45,45,45,45	0
56	MG	DA	3450	1/1	0.98	0.15	64,64,64,64	0
56	MG	DA	3205	1/1	0.98	0.24	36,36,36,36	0
56	MG	DA	3513	1/1	0.98	0.20	34,34,34,34	0
56	MG	DA	3144	1/1	0.98	0.41	14,14,14,14	0
56	MG	DA	3187	1/1	0.98	0.27	32,32,32,32	0
56	MG	CA	1878	1/1	0.98	0.35	66,66,66,66	0
56	MG	DA	3053	1/1	0.98	0.12	61,61,61,61	0
56	MG	DA	3138	1/1	0.98	0.36	12,12,12,12	0
56	MG	DA	3549	1/1	0.98	0.34	16,16,16,16	0
56	MG	BA	3320	1/1	0.98	0.39	23,23,23,23	0
56	MG	BA	3033	1/1	0.98	0.24	78,78,78,78	0
56	MG	DA	3628	1/1	0.98	0.21	295,295,295,295	0
56	MG	BA	3104	1/1	0.98	0.15	120,120,120,120	0
56	MG	DA	3509	1/1	0.98	0.22	142,142,142,142	0
56	MG	DA	3149	1/1	0.98	0.41	22,22,22,22	0
56	MG	BA	3316	1/1	0.98	0.15	26,26,26,26	0
56	MG	BA	3678	1/1	0.98	0.30	20,20,20,20	0
56	MG	DA	3596	1/1	0.98	0.43	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3620	1/1	0.98	0.48	50,50,50,50	0
56	MG	DA	3171	1/1	0.98	0.23	25,25,25,25	0
56	MG	BB	207	1/1	0.98	0.14	84,84,84,84	0
56	MG	DA	3155	1/1	0.98	0.39	18,18,18,18	0
56	MG	D5	103	1/1	0.98	0.33	61,61,61,61	0
56	MG	BA	3545	1/1	0.98	0.51	245,245,245,245	0
56	MG	DA	2971	1/1	0.98	0.15	132,132,132,132	0
56	MG	DA	3170	1/1	0.98	0.11	12,12,12,12	0
56	MG	DA	3195	1/1	0.98	0.17	20,20,20,20	0
56	MG	B3	101	1/1	0.98	0.43	26,26,26,26	0
56	MG	DA	3599	1/1	0.98	0.31	14,14,14,14	0
56	MG	AA	1906	1/1	0.98	0.70	38,38,38,38	0
56	MG	BA	3345	1/1	0.98	0.29	20,20,20,20	0
56	MG	DA	3143	1/1	0.98	0.48	19,19,19,19	0
56	MG	BA	3357	1/1	0.98	0.17	64,64,64,64	0
56	MG	BA	3684	1/1	0.98	0.29	47,47,47,47	0
56	MG	DA	3551	1/1	0.98	0.38	13,13,13,13	0
56	MG	DA	3598	1/1	0.98	0.36	12,12,12,12	0
56	MG	DA	3265	1/1	0.98	0.15	40,40,40,40	0
56	MG	DA	3313	1/1	0.98	0.39	12,12,12,12	0
56	MG	DA	3588	1/1	0.98	0.26	24,24,24,24	0
56	MG	BA	3368	1/1	0.98	0.28	25,25,25,25	0
56	MG	BA	3319	1/1	0.98	0.41	19,19,19,19	0
56	MG	BA	3315	1/1	0.98	0.19	17,17,17,17	0
56	MG	BA	3243	1/1	0.98	0.25	149,149,149,149	0
56	MG	DA	3185	1/1	0.98	0.17	12,12,12,12	0
56	MG	BA	3381	1/1	0.98	0.34	17,17,17,17	0
56	MG	AA	1647	1/1	0.98	0.21	34,34,34,34	0
56	MG	BA	2990	1/1	0.98	0.12	47,47,47,47	0
56	MG	BA	3667	1/1	0.98	0.37	52,52,52,52	0
56	MG	AA	1810	1/1	0.98	0.06	87,87,87,87	0
56	MG	CA	1757	1/1	0.99	0.45	43,43,43,43	0
57	ZN	AN	101	1/1	0.99	0.17	115,115,115,115	0
56	MG	DA	3222	1/1	0.99	0.35	17,17,17,17	0
56	MG	BA	3502	1/1	0.99	0.23	26,26,26,26	0
56	MG	BA	3348	1/1	0.99	0.43	25,25,25,25	0
56	MG	BA	3250	1/1	0.99	0.17	269,269,269,269	0
56	MG	BA	3329	1/1	0.99	0.46	19,19,19,19	0
56	MG	DA	3169	1/1	0.99	0.31	33,33,33,33	0
56	MG	DA	3575	1/1	0.99	0.10	49,49,49,49	0
56	MG	DA	3142	1/1	0.99	0.42	30,30,30,30	0
56	MG	DA	3151	1/1	0.99	0.22	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1928	1/1	0.99	0.08	67,67,67,67	0
57	ZN	AD	301	1/1	0.99	0.29	71,71,71,71	0
56	MG	BA	3333	1/1	0.99	0.42	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.