wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:18 PM GMT

PDB ID	:	4V83
Title	:	Crystal structure of a complex containing domain 3 from the PSIV IGR IRES RNA bound to the 70S ribosome.
Authors	:	Zhu, J.; Korostelev, A.; Costantino, D.; Noller, H.F.; Kieft, J.S.
Deposited on	:	2010-12-13
Resolution	:	3.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

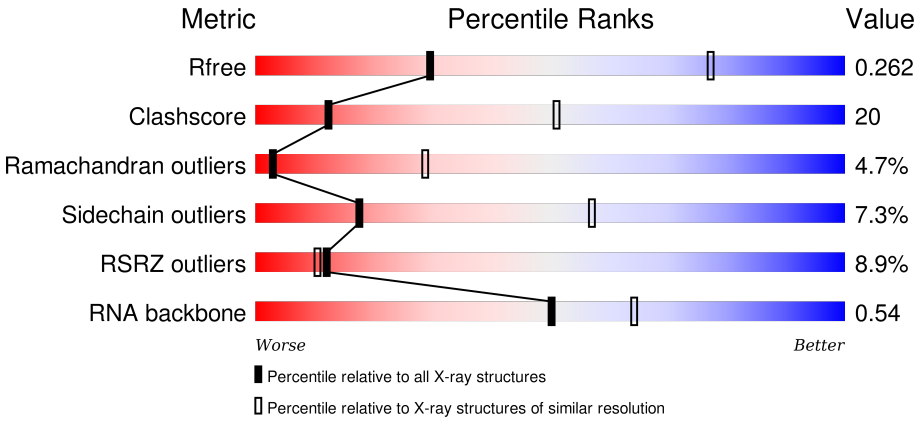
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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. 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 <=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	1506	4% 47% 44% 7% •
1	CA	1506	7% 47% 44% 7% •
2	AB	234	34% 50% 45% 5%
2	CB	234	31% 51% 44% •

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Mol	Chain	Length	Quality of chain
3	AC	206	11% 47% 48% 5%
3	CC	206	16% 50% 46% 5%
4	AD	208	2% 46% 48% 6%
4	CD	208	10% 49% 46% 6%
5	AE	151	2% 52% 44% 5%
5	CE	151	4% 52% 44% 5%
6	AF	101	19% 45% 53%
6	CF	101	5% 44% 54%
7	AG	155	19% 57% 42%
7	CG	155	22% 57% 43%
8	AH	138	11% 50% 48%
8	CH	138	14% 51% 47%
9	AI	127	39% 48% 48%
9	CI	127	31% 49% 47%
10	AJ	98	47% 50% 37% 12%
10	CJ	98	41% 52% 34% 13%
11	AK	119	8% 49% 49%
11	CK	119	7% 50% 47%
12	AL	124	7% 52% 39% 10%
12	CL	124	10% 52% 37% 10%
13	AM	116	22% 41% 53% 5%
13	CM	116	44% 38% 57%
14	AN	60	28% 52% 42% 7%
14	CN	60	42% 58% 37% 5%
15	AO	88	61% 38%

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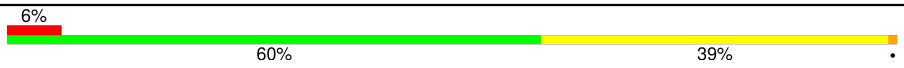
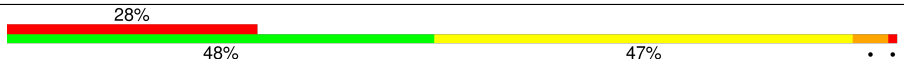
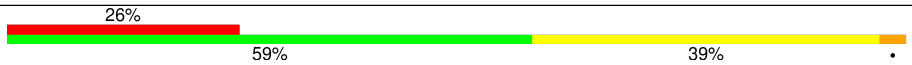
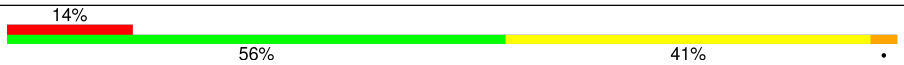
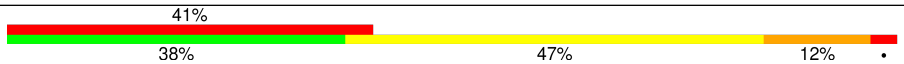
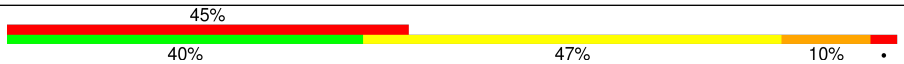
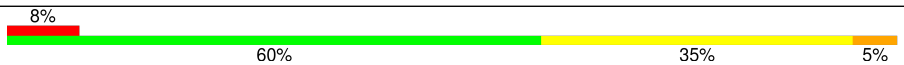
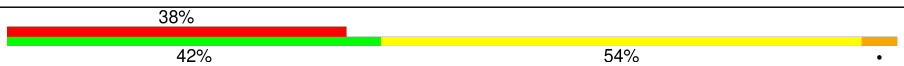
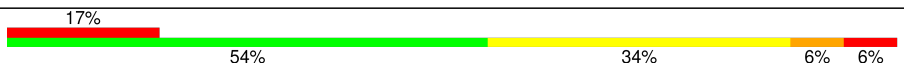
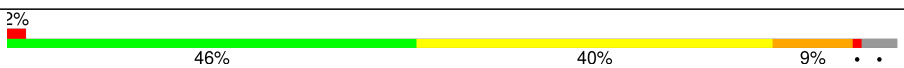
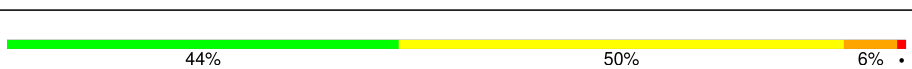
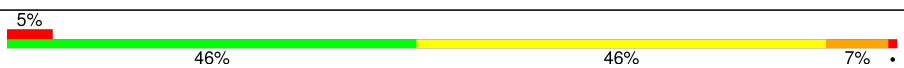
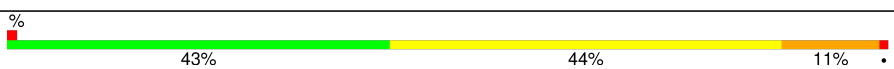
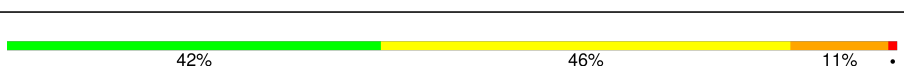
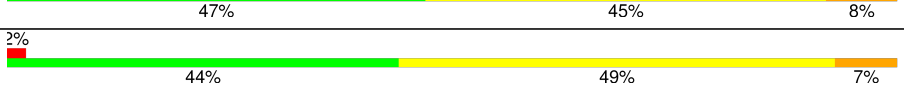
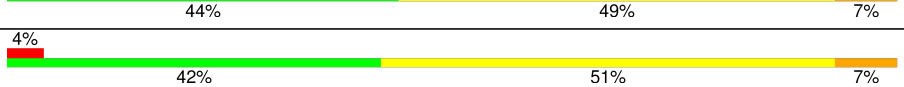
Mol	Chain	Length	Quality of chain
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	35	
22	CV	35	
23	BA	2879	
23	DA	2879	
24	BB	119	
24	DB	119	
25	BC	271	
25	DC	271	
26	BD	204	
26	DD	204	
27	BE	202	
27	DE	202	

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Mol	Chain	Length	Quality of chain
28	BF	181	10% 40% 53% 6%
28	DF	181	11% 40% 52% 7%
29	BG	159	30% 55% 38% 7%
29	DG	159	6% 53% 40% 7%
30	BH	145	29% 48% 45% 8%
30	DH	145	34% 49% 43% 8%
31	BI	65	48% 37% 12% 51%
31	DI	65	32% 37% 12% 51%
32	BJ	137	2% 36% 50% 14%
32	DJ	137	% 39% 47% 14%
33	BK	122	54% 39% 7%
33	DK	122	55% 38% 7%
34	BL	146	7% 32% 46% 19%
34	DL	146	8% 32% 46% 19%
35	BM	136	3% 41% 46% 13%
35	DM	136	6% 39% 49% 13%
36	BN	117	2% 46% 47% 6%
36	DN	117	2% 47% 47% 5%
37	BO	98	47% 34% 52% 11%
37	DO	98	18% 33% 54% 10%
38	BP	137	4% 45% 47% 7%
38	DP	137	8% 44% 49% 7%
39	BQ	116	2% 53% 43%
39	DQ	116	53% 43%
40	BR	101	42% 50% 8%

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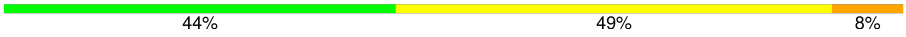
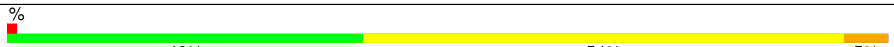
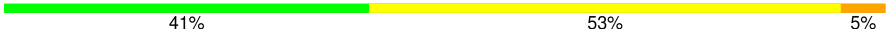
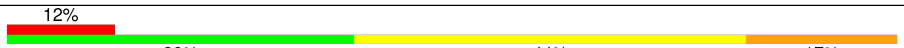
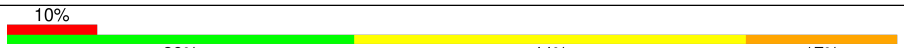
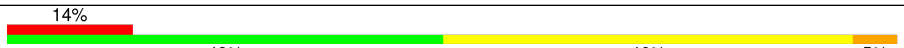
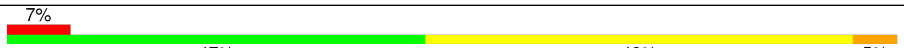
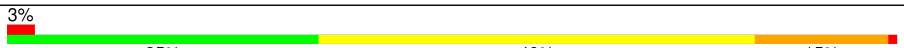
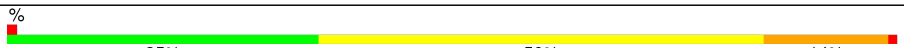
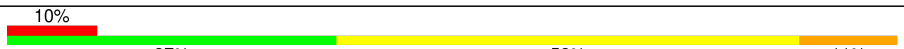
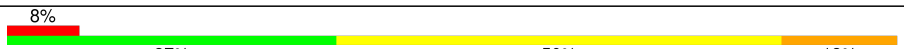
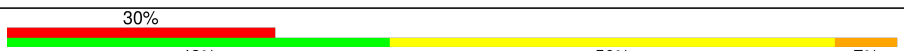
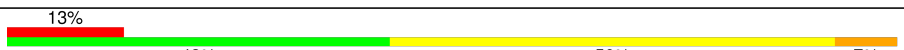
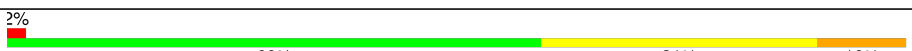
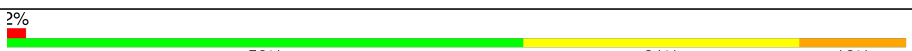
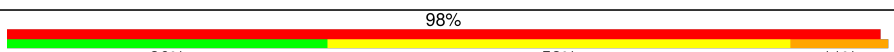
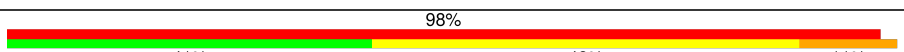
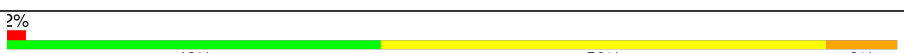
Mol	Chain	Length	Quality of chain
40	DR	101	
41	BS	112	
41	DS	112	
42	BT	92	
42	DT	92	
43	BU	100	
43	DU	100	
44	BV	188	
44	DV	188	
45	BW	76	
45	DW	76	
46	BX	88	
46	DX	88	
47	BY	62	
47	DY	62	
48	BZ	59	
48	DZ	59	
49	B1	30	
49	D1	30	
50	B2	52	
50	D2	52	
51	B3	44	
51	D3	44	
52	B4	48	
52	D4	48	

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Mol	Chain	Length	Quality of chain
53	B5	63	2% 37% 57% 6%
53	D5	63	38% 57% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1603	-	-	-	X
54	MG	AA	1606	-	-	-	X
54	MG	AA	1609	-	-	-	X
54	MG	AA	1610	-	-	-	X
54	MG	AA	1613	-	-	-	X
54	MG	AA	1615	-	-	-	X
54	MG	AA	1620	-	-	-	X
54	MG	AA	1625	-	-	-	X
54	MG	AA	1626	-	-	-	X
54	MG	AA	1628	-	-	-	X
54	MG	AA	1630	-	-	-	X
54	MG	AA	1631	-	-	-	X
54	MG	AA	1632	-	-	-	X
54	MG	AA	1635	-	-	-	X
54	MG	AA	1641	-	-	-	X
54	MG	AA	1647	-	-	-	X
54	MG	AA	1651	-	-	-	X
54	MG	AA	1664	-	-	-	X
54	MG	AA	1665	-	-	-	X
54	MG	AA	1667	-	-	-	X
54	MG	AA	1681	-	-	-	X
54	MG	AA	1685	-	-	-	X
54	MG	AA	1711	-	-	-	X
54	MG	AA	1720	-	-	-	X
54	MG	AA	1724	-	-	-	X
54	MG	AA	1729	-	-	-	X
54	MG	AA	1760	-	-	-	X
54	MG	AA	1778	-	-	-	X
54	MG	AA	1784	-	-	-	X
54	MG	AA	1800	-	-	-	X
54	MG	AA	1820	-	-	-	X
54	MG	AA	1828	-	-	-	X
54	MG	AA	1846	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	AA	1860	-	-	-	X
54	MG	AA	1870	-	-	-	X
54	MG	AD	303	-	-	-	X
54	MG	AT	202	-	-	-	X
54	MG	B5	101	-	-	-	X
54	MG	BA	2902	-	-	-	X
54	MG	BA	2903	-	-	-	X
54	MG	BA	2906	-	-	-	X
54	MG	BA	2907	-	-	-	X
54	MG	BA	2909	-	-	-	X
54	MG	BA	2911	-	-	-	X
54	MG	BA	2912	-	-	-	X
54	MG	BA	2913	-	-	-	X
54	MG	BA	2914	-	-	-	X
54	MG	BA	2916	-	-	-	X
54	MG	BA	2919	-	-	-	X
54	MG	BA	2920	-	-	-	X
54	MG	BA	2922	-	-	-	X
54	MG	BA	2923	-	-	-	X
54	MG	BA	2924	-	-	-	X
54	MG	BA	2926	-	-	-	X
54	MG	BA	2929	-	-	-	X
54	MG	BA	2931	-	-	-	X
54	MG	BA	2934	-	-	-	X
54	MG	BA	2939	-	-	-	X
54	MG	BA	2943	-	-	-	X
54	MG	BA	2945	-	-	-	X
54	MG	BA	2954	-	-	-	X
54	MG	BA	2955	-	-	-	X
54	MG	BA	2957	-	-	-	X
54	MG	BA	2960	-	-	-	X
54	MG	BA	2963	-	-	-	X
54	MG	BA	2968	-	-	-	X
54	MG	BA	2975	-	-	-	X
54	MG	BA	2981	-	-	-	X
54	MG	BA	2990	-	-	-	X
54	MG	BA	2991	-	-	-	X
54	MG	BA	3003	-	-	-	X
54	MG	BA	3004	-	-	-	X
54	MG	BA	3008	-	-	-	X
54	MG	BA	3013	-	-	-	X
54	MG	BA	3019	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3020	-	-	-	X
54	MG	BA	3021	-	-	-	X
54	MG	BA	3022	-	-	-	X
54	MG	BA	3023	-	-	-	X
54	MG	BA	3038	-	-	-	X
54	MG	BA	3040	-	-	-	X
54	MG	BA	3047	-	-	-	X
54	MG	BA	3048	-	-	-	X
54	MG	BA	3049	-	-	-	X
54	MG	BA	3051	-	-	-	X
54	MG	BA	3058	-	-	-	X
54	MG	BA	3060	-	-	-	X
54	MG	BA	3064	-	-	-	X
54	MG	BA	3068	-	-	-	X
54	MG	BA	3070	-	-	-	X
54	MG	BA	3072	-	-	-	X
54	MG	BA	3073	-	-	-	X
54	MG	BA	3088	-	-	-	X
54	MG	BA	3098	-	-	-	X
54	MG	BA	3110	-	-	-	X
54	MG	BA	3114	-	-	-	X
54	MG	BA	3122	-	-	-	X
54	MG	BA	3126	-	-	-	X
54	MG	BA	3136	-	-	-	X
54	MG	BA	3150	-	-	-	X
54	MG	BA	3159	-	-	-	X
54	MG	BA	3164	-	-	-	X
54	MG	BA	3169	-	-	-	X
54	MG	BA	3172	-	-	-	X
54	MG	BA	3175	-	-	-	X
54	MG	BA	3178	-	-	-	X
54	MG	BA	3187	-	-	-	X
54	MG	BA	3196	-	-	-	X
54	MG	BA	3227	-	-	-	X
54	MG	BA	3238	-	-	-	X
54	MG	BA	3239	-	-	-	X
54	MG	BA	3243	-	-	-	X
54	MG	BA	3289	-	-	-	X
54	MG	BA	3301	-	-	-	X
54	MG	BA	3327	-	-	-	X
54	MG	BA	3334	-	-	-	X
54	MG	BA	3340	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3411	-	-	-	X
54	MG	BA	3425	-	-	-	X
54	MG	BA	3432	-	-	-	X
54	MG	BA	3434	-	-	-	X
54	MG	BA	3438	-	-	-	X
54	MG	BA	3442	-	-	-	X
54	MG	BA	3443	-	-	-	X
54	MG	BA	3451	-	-	-	X
54	MG	BA	3455	-	-	-	X
54	MG	BA	3459	-	-	-	X
54	MG	BA	3461	-	-	-	X
54	MG	BA	3467	-	-	-	X
54	MG	BA	3469	-	-	-	X
54	MG	BA	3471	-	-	-	X
54	MG	BA	3556	-	-	-	X
54	MG	BA	3570	-	-	-	X
54	MG	BA	3575	-	-	-	X
54	MG	BA	3597	-	-	-	X
54	MG	BA	3626	-	-	-	X
54	MG	BA	3634	-	-	-	X
54	MG	BA	3643	-	-	-	X
54	MG	BA	3673	-	-	-	X
54	MG	BB	218	-	-	-	X
54	MG	BC	303	-	-	-	X
54	MG	BE	302	-	-	-	X
54	MG	BM	203	-	-	-	X
54	MG	BX	102	-	-	-	X
54	MG	CA	1601	-	-	-	X
54	MG	CA	1602	-	-	-	X
54	MG	CA	1606	-	-	-	X
54	MG	CA	1619	-	-	-	X
54	MG	CA	1651	-	-	-	X
54	MG	CA	1659	-	-	-	X
54	MG	CA	1665	-	-	-	X
54	MG	CA	1676	-	-	-	X
54	MG	CA	1680	-	-	-	X
54	MG	CA	1688	-	-	-	X
54	MG	CA	1733	-	-	-	X
54	MG	CA	1737	-	-	-	X
54	MG	CA	1760	-	-	-	X
54	MG	CA	1788	-	-	-	X
54	MG	CA	1862	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	CA	1875	-	-	-	X
54	MG	CA	1881	-	-	-	X
54	MG	CA	1891	-	-	-	X
54	MG	CA	1915	-	-	-	X
54	MG	CA	1943	-	-	-	X
54	MG	CD	304	-	-	-	X
54	MG	CM	201	-	-	-	X
54	MG	CN	102	-	-	-	X
54	MG	DA	2901	-	-	-	X
54	MG	DA	2902	-	-	-	X
54	MG	DA	2904	-	-	-	X
54	MG	DA	2906	-	-	-	X
54	MG	DA	2907	-	-	-	X
54	MG	DA	2908	-	-	-	X
54	MG	DA	2913	-	-	-	X
54	MG	DA	2918	-	-	-	X
54	MG	DA	2923	-	-	-	X
54	MG	DA	2925	-	-	-	X
54	MG	DA	2926	-	-	-	X
54	MG	DA	2927	-	-	-	X
54	MG	DA	2928	-	-	-	X
54	MG	DA	2932	-	-	-	X
54	MG	DA	2934	-	-	-	X
54	MG	DA	2938	-	-	-	X
54	MG	DA	2943	-	-	-	X
54	MG	DA	2947	-	-	-	X
54	MG	DA	2953	-	-	-	X
54	MG	DA	2954	-	-	-	X
54	MG	DA	2957	-	-	-	X
54	MG	DA	2971	-	-	-	X
54	MG	DA	2973	-	-	-	X
54	MG	DA	2975	-	-	-	X
54	MG	DA	2980	-	-	-	X
54	MG	DA	2982	-	-	-	X
54	MG	DA	2985	-	-	-	X
54	MG	DA	2986	-	-	-	X
54	MG	DA	2997	-	-	-	X
54	MG	DA	3005	-	-	-	X
54	MG	DA	3010	-	-	-	X
54	MG	DA	3013	-	-	-	X
54	MG	DA	3014	-	-	-	X
54	MG	DA	3015	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3018	-	-	-	X
54	MG	DA	3020	-	-	-	X
54	MG	DA	3024	-	-	-	X
54	MG	DA	3028	-	-	-	X
54	MG	DA	3035	-	-	-	X
54	MG	DA	3038	-	-	-	X
54	MG	DA	3045	-	-	-	X
54	MG	DA	3048	-	-	-	X
54	MG	DA	3052	-	-	-	X
54	MG	DA	3056	-	-	-	X
54	MG	DA	3057	-	-	-	X
54	MG	DA	3059	-	-	-	X
54	MG	DA	3063	-	-	-	X
54	MG	DA	3064	-	-	-	X
54	MG	DA	3065	-	-	-	X
54	MG	DA	3072	-	-	-	X
54	MG	DA	3074	-	-	-	X
54	MG	DA	3080	-	-	-	X
54	MG	DA	3082	-	-	-	X
54	MG	DA	3098	-	-	-	X
54	MG	DA	3103	-	-	-	X
54	MG	DA	3106	-	-	-	X
54	MG	DA	3108	-	-	-	X
54	MG	DA	3121	-	-	-	X
54	MG	DA	3126	-	-	-	X
54	MG	DA	3144	-	-	-	X
54	MG	DA	3152	-	-	-	X
54	MG	DA	3153	-	-	-	X
54	MG	DA	3154	-	-	-	X
54	MG	DA	3158	-	-	-	X
54	MG	DA	3160	-	-	-	X
54	MG	DA	3161	-	-	-	X
54	MG	DA	3172	-	-	-	X
54	MG	DA	3173	-	-	-	X
54	MG	DA	3177	-	-	-	X
54	MG	DA	3178	-	-	-	X
54	MG	DA	3180	-	-	-	X
54	MG	DA	3185	-	-	-	X
54	MG	DA	3186	-	-	-	X
54	MG	DA	3193	-	-	-	X
54	MG	DA	3197	-	-	-	X
54	MG	DA	3226	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3227	-	-	-	X
54	MG	DA	3258	-	-	-	X
54	MG	DA	3267	-	-	-	X
54	MG	DA	3268	-	-	-	X
54	MG	DA	3289	-	-	-	X
54	MG	DA	3310	-	-	-	X
54	MG	DA	3311	-	-	-	X
54	MG	DA	3320	-	-	-	X
54	MG	DA	3321	-	-	-	X
54	MG	DA	3329	-	-	-	X
54	MG	DA	3333	-	-	-	X
54	MG	DA	3343	-	-	-	X
54	MG	DA	3353	-	-	-	X
54	MG	DA	3357	-	-	-	X
54	MG	DA	3360	-	-	-	X
54	MG	DA	3412	-	-	-	X
54	MG	DA	3414	-	-	-	X
54	MG	DA	3415	-	-	-	X
54	MG	DA	3431	-	-	-	X
54	MG	DA	3455	-	-	-	X
54	MG	DA	3472	-	-	-	X
54	MG	DA	3506	-	-	-	X
54	MG	DA	3511	-	-	-	X
54	MG	DA	3529	-	-	-	X
54	MG	DA	3534	-	-	-	X
54	MG	DA	3563	-	-	-	X
54	MG	DA	3569	-	-	-	X
54	MG	DA	3590	-	-	-	X
54	MG	DA	3599	-	-	-	X
54	MG	DA	3603	-	-	-	X
54	MG	DA	3605	-	-	-	X
54	MG	DA	3606	-	-	-	X
54	MG	DA	3607	-	-	-	X
54	MG	DA	3622	-	-	-	X
54	MG	DA	3629	-	-	-	X
54	MG	DA	3633	-	-	-	X
54	MG	DA	3634	-	-	-	X
54	MG	DA	3637	-	-	-	X
54	MG	DA	3638	-	-	-	X
54	MG	DA	3646	-	-	-	X
54	MG	DA	3650	-	-	-	X
54	MG	DA	3655	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3658	-	-	-	X
54	MG	DA	3667	-	-	-	X
54	MG	DA	3672	-	-	-	X
54	MG	DA	3684	-	-	-	X
54	MG	DA	3689	-	-	-	X
54	MG	DA	3698	-	-	-	X
54	MG	DA	3733	-	-	-	X
54	MG	DA	3736	-	-	-	X
54	MG	DA	3742	-	-	-	X
54	MG	DA	3750	-	-	-	X
54	MG	DA	3771	-	-	-	X
54	MG	DA	3840	-	-	-	X
54	MG	DA	3851	-	-	-	X
54	MG	DA	3859	-	-	-	X
54	MG	DA	3863	-	-	-	X
54	MG	DB	204	-	-	-	X
54	MG	DB	207	-	-	-	X
54	MG	DB	216	-	-	-	X
54	MG	DC	302	-	-	-	X
54	MG	DD	301	-	-	-	X
54	MG	DD	305	-	-	-	X
54	MG	DJ	204	-	-	-	X
54	MG	DJ	205	-	-	-	X
54	MG	DW	101	-	-	-	X
54	MG	DX	101	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 283641 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 ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14409	5999	10459	1505			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			
13	CM	116	Total	C	N	O	S	0	0	0
			929	574	191	162	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

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

- Molecule 22 is a RNA chain called domain 3 of PSIC IGR IRES RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	35	Total	C	N	O	P	0	0	0
			736	332	128	243	33			
22	CV	35	Total	C	N	O	P	0	0	0
			736	332	128	243	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			
23	DA	2760	Total	C	N	O	P	0	0	0
			59442	26456	11114	19113	2759			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1142	U	C	SEE REMARK 999	GB AE017221.1
BA	2825	U	G	SEE REMARK 999	GB AE017221.1
DA	1142	U	C	SEE REMARK 999	GB AE017221.1
DA	2825	U	G	SEE REMARK 999	GB AE017221.1

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

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

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
26	DD	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			
27	DE	202	Total	C	N	O	S	0	0	0
			1587	1011	297	276	3			

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
28	DF	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
29	DG	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			
30	DH	145	Total	C	N	O	S	0	0	0
			1133	724	200	208	1			

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	BI	32	Total	C	N	O	0	0	0
			254	157	49	48			
31	DI	32	Total	C	N	O	0	0	0
			254	157	49	48			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			
32	DJ	137	Total	C	N	O	S	0	0	0
			1097	707	205	182	3			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			
33	DK	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DL	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
35	DM	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BN	117	Total 960	C 599	N 202	O 159	0	0	0
36	DN	117	Total 960	C 599	N 202	O 159	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BO	98	Total 771	C 486	N 154	O 131	0	0	0
37	DO	98	Total 771	C 486	N 154	O 131	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	137	Total 1144	C 713	N 234	O 196	S 1	0	0	0
38	DP	137	Total 1144	C 713	N 234	O 196	S 1	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	116	Total 953	C 601	N 201	O 150	S 1	0	0	0
39	DQ	116	Total 953	C 601	N 201	O 150	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	PHE	DELETION	UNP Q72L76
DQ	?	-	PHE	DELETION	UNP Q72L76

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	101	Total 779	C 501	N 142	O 135	S 1	0	0	0
40	DR	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			
41	DS	112	Total	C	N	O	S	0	0	0
			891	560	175	154	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O	0	0	0
			726	471	131	124			
42	DT	92	Total	C	N	O	0	0	0
			726	471	131	124			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
43	DU	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			
44	DV	188	Total	C	N	O	S	0	0	0
			1492	950	265	275	2			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
45	DW	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	88	Total 695	C 435	N 141	O 119	0	0	0
46	DX	88	Total 695	C 435	N 141	O 119	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	62	Total 521	C 325	N 102	O 92	S 2	0	0	0
47	DY	62	Total 521	C 325	N 102	O 92	S 2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	59	Total 468	C 298	N 90	O 79	S 1	0	0	0
48	DZ	59	Total 468	C 298	N 90	O 79	S 1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B1	30	Total 226	C 142	N 36	O 44	S 4	0	0	0
49	D1	30	Total 226	C 142	N 36	O 44	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B2	52	Total 405	C 255	N 79	O 66	S 5	0	0	0
50	D2	52	Total 405	C 255	N 79	O 66	S 5	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B3	44	Total 381	C 235	N 77	O 65	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	D3	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
52	D4	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
53	D5	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DC	3	Total	Mg	0	0
			3	3		
54	DX	3	Total	Mg	0	0
			3	3		
54	B4	1	Total	Mg	0	0
			1	1		
54	BA	781	Total	Mg	0	0
			781	781		
54	AK	2	Total	Mg	0	0
			2	2		
54	DQ	2	Total	Mg	0	0
			2	2		
54	AB	3	Total	Mg	0	0
			3	3		
54	DF	2	Total	Mg	0	0
			2	2		
54	CV	7	Total	Mg	0	0
			7	7		
54	DL	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	BE	2	Total Mg 2 2	0	0
54	DU	1	Total Mg 1 1	0	0
54	DY	2	Total Mg 2 2	0	0
54	AN	1	Total Mg 1 1	0	0
54	BP	2	Total Mg 2 2	0	0
54	CN	1	Total Mg 1 1	0	0
54	BI	1	Total Mg 1 1	0	0
54	AS	1	Total Mg 1 1	0	0
54	CA	372	Total Mg 372 372	0	0
54	B5	1	Total Mg 1 1	0	0
54	BB	27	Total Mg 27 27	0	0
54	BT	2	Total Mg 2 2	0	0
54	DO	1	Total Mg 1 1	0	0
54	AE	5	Total Mg 5 5	0	0
54	BM	3	Total Mg 3 3	0	0
54	CF	2	Total Mg 2 2	0	0
54	D3	1	Total Mg 1 1	0	0
54	BF	1	Total Mg 1 1	0	0
54	AV	8	Total Mg 8 8	0	0
54	BX	2	Total Mg 2 2	0	0
54	DA	964	Total Mg 964 964	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	B2	3	Total Mg 3 3	0	0
54	AA	279	Total Mg 279 279	0	0
54	CQ	2	Total Mg 2 2	0	0
54	BJ	3	Total Mg 3 3	0	0
54	DV	4	Total Mg 4 4	0	0
54	BC	3	Total Mg 3 3	0	0
54	AM	1	Total Mg 1 1	0	0
54	BU	2	Total Mg 2 2	0	0
54	CC	8	Total Mg 8 8	0	0
54	AD	3	Total Mg 3 3	0	0
54	BN	2	Total Mg 2 2	0	0
54	CM	2	Total Mg 2 2	0	0
54	DS	2	Total Mg 2 2	0	0
54	DM	1	Total Mg 1 1	0	0
54	AI	1	Total Mg 1 1	0	0
54	BY	3	Total Mg 3 3	0	0
54	DE	3	Total Mg 3 3	0	0
54	B3	1	Total Mg 1 1	0	0
54	DG	3	Total Mg 3 3	0	0
54	BR	1	Total Mg 1 1	0	0
54	DK	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	D4	4	Total Mg 4 4	0	0
54	BK	1	Total Mg 1 1	0	0
54	CE	5	Total Mg 5 5	0	0
54	DW	1	Total Mg 1 1	0	0
54	D5	3	Total Mg 3 3	0	0
54	DD	6	Total Mg 6 6	0	0
54	D2	3	Total Mg 3 3	0	0
54	AL	2	Total Mg 2 2	0	0
54	BV	3	Total Mg 3 3	0	0
54	AG	2	Total Mg 2 2	0	0
54	BO	1	Total Mg 1 1	0	0
54	AQ	3	Total Mg 3 3	0	0
54	D1	1	Total Mg 1 1	0	0
54	DI	1	Total Mg 1 1	0	0
54	AH	1	Total Mg 1 1	0	0
54	DJ	6	Total Mg 6 6	0	0
54	CO	4	Total Mg 4 4	0	0
54	AC	2	Total Mg 2 2	0	0
54	BS	1	Total Mg 1 1	0	0
54	DB	43	Total Mg 43 43	0	0
54	CB	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	CD	3	Total Mg 3 3	0	0
54	DN	1	Total Mg 1 1	0	0
54	AT	2	Total Mg 2 2	0	0
54	CL	6	Total Mg 6 6	0	0
54	DP	2	Total Mg 2 2	0	0
54	AO	3	Total Mg 3 3	0	0
54	BW	1	Total Mg 1 1	0	0
54	CG	3	Total Mg 3 3	0	0
54	CK	1	Total Mg 1 1	0	0
54	AF	1	Total Mg 1 1	0	0
54	BH	1	Total Mg 1 1	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

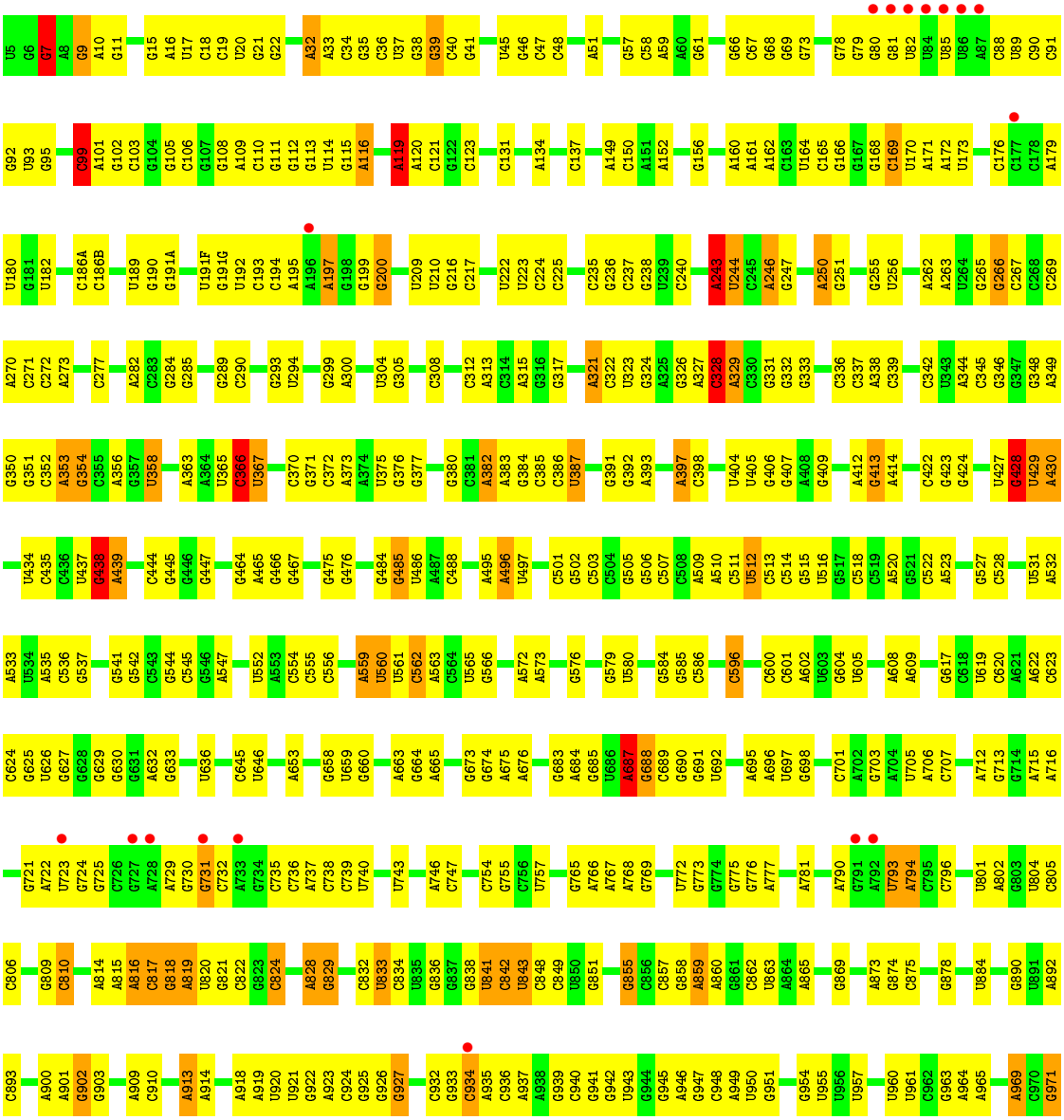
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	CN	1	Total Zn 1 1	0	0
55	AD	1	Total Zn 1 1	0	0
55	CD	1	Total Zn 1 1	0	0
55	AN	1	Total Zn 1 1	0	0

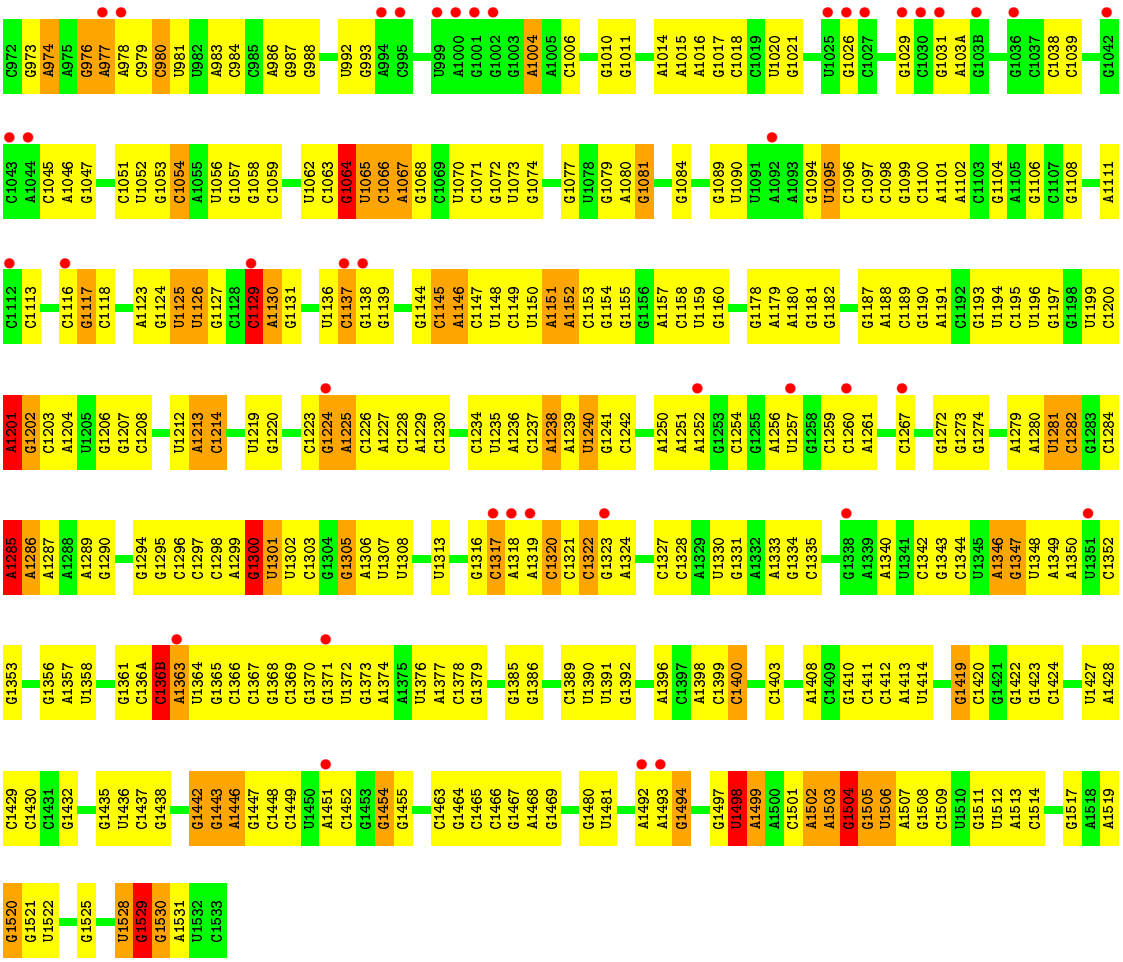
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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: ribosomal RNA 16S

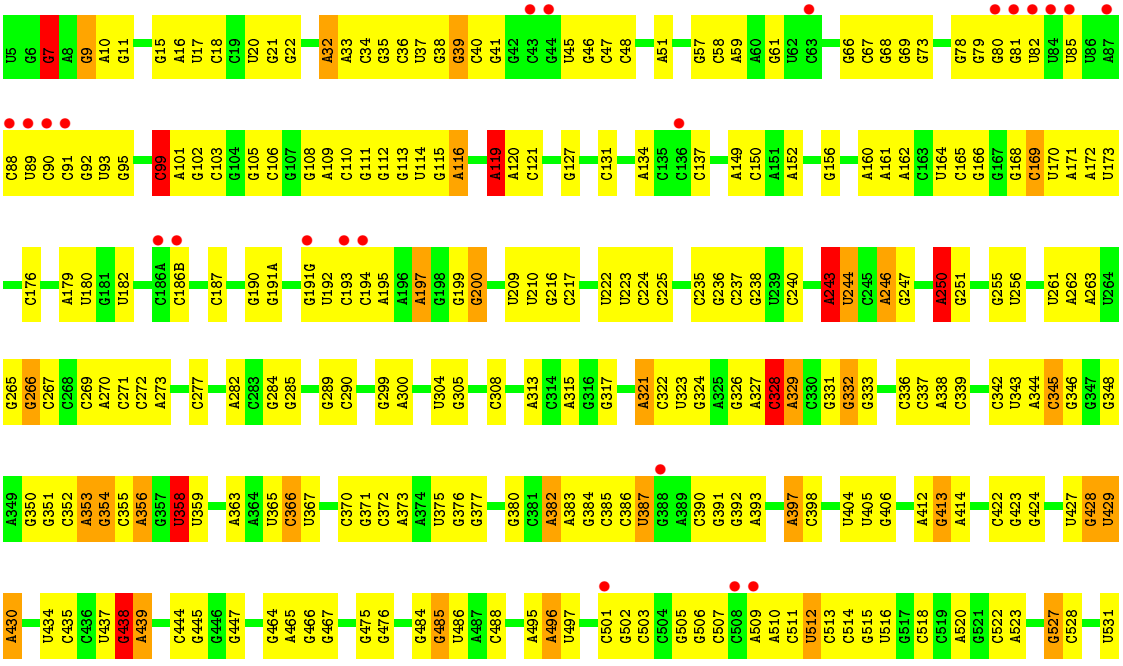
Chain AA: 

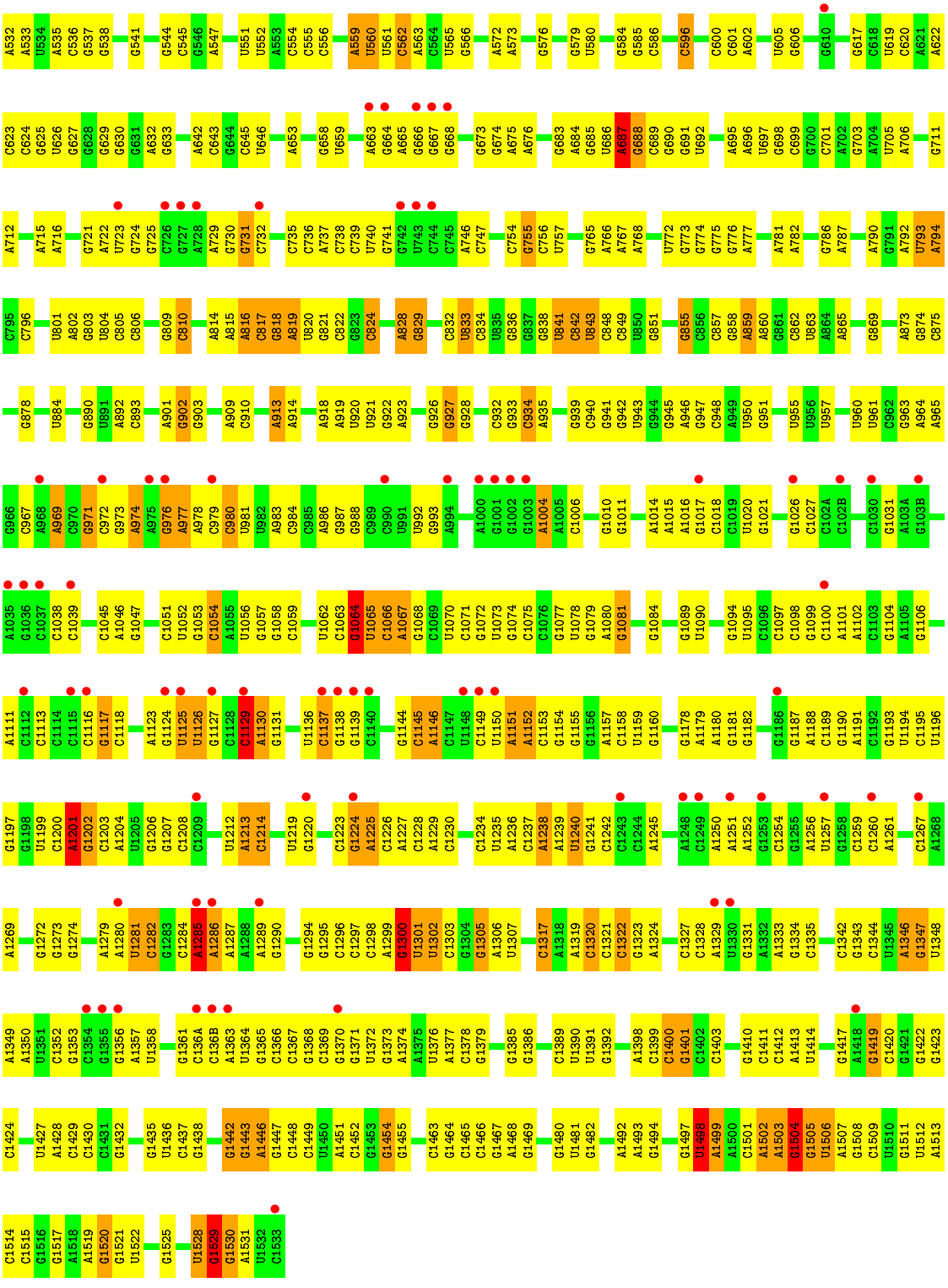




- Molecule 1: ribosomal RNA 16S

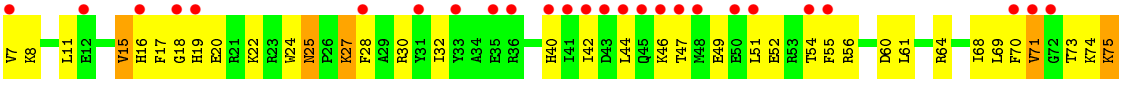
Chain CA:

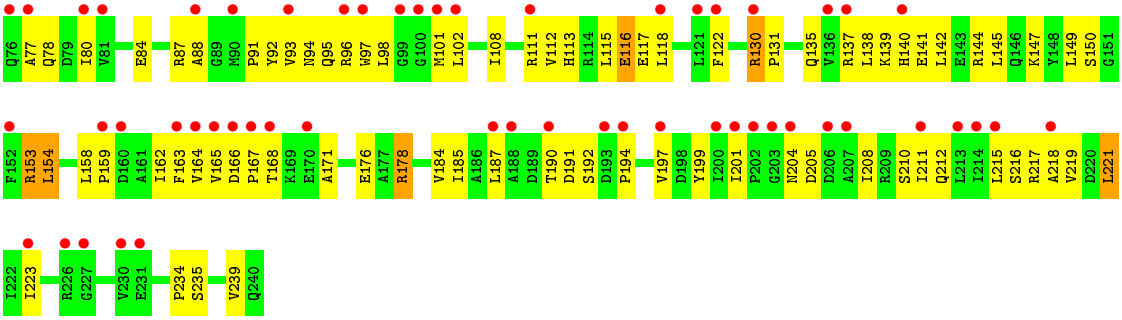




- Molecule 2: 30S ribosomal protein S2

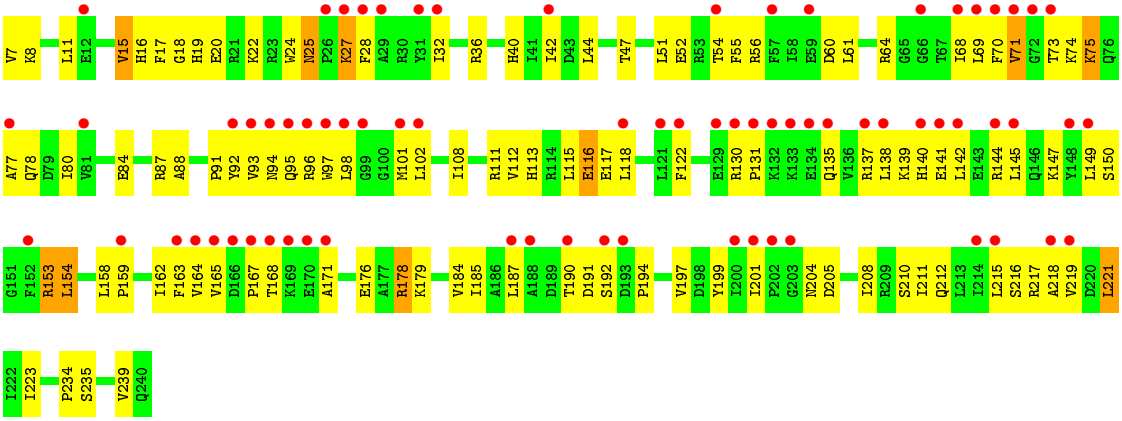
Chain AB:





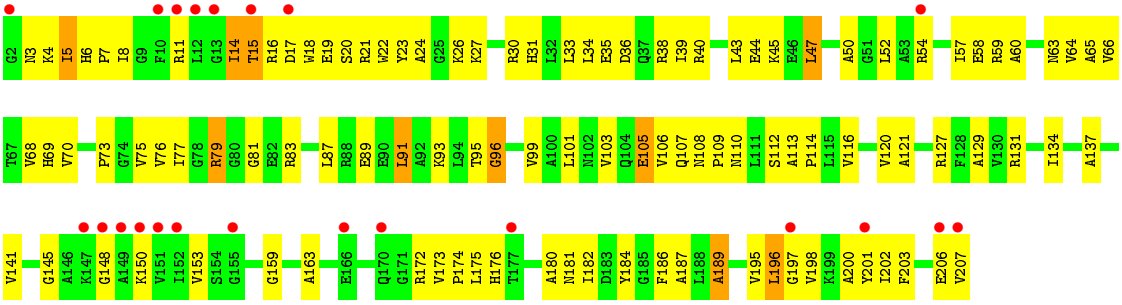
• Molecule 2: 30S ribosomal protein S2

Chain CB:



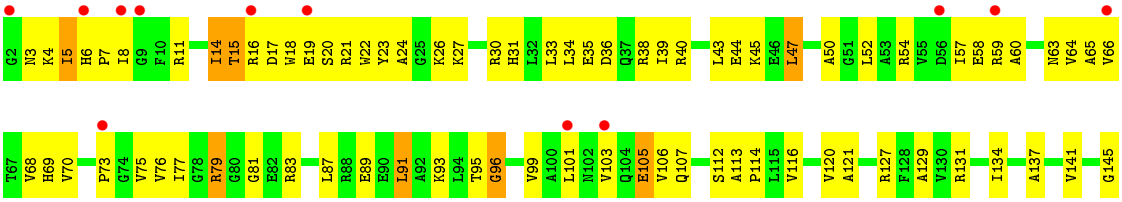
• Molecule 3: 30S ribosomal protein S3

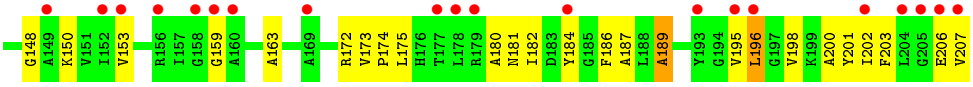
Chain AC:



• Molecule 3: 30S ribosomal protein S3

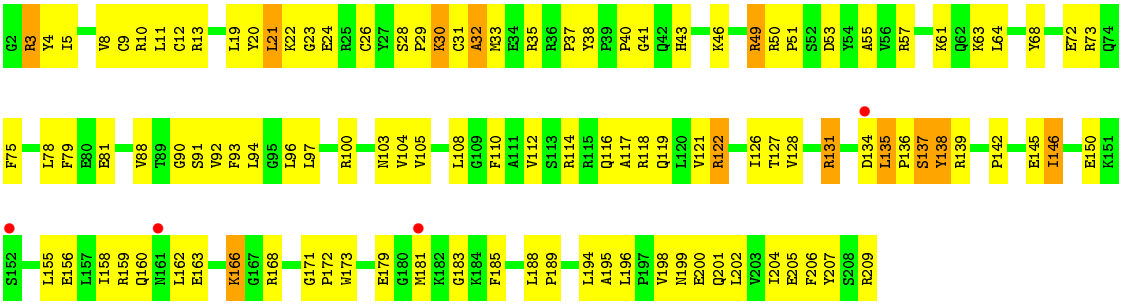
Chain CC:





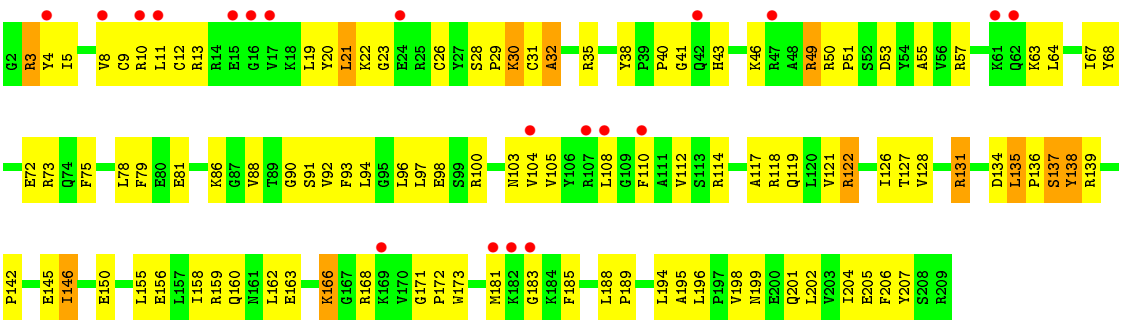
• Molecule 4: 30S ribosomal protein S4

Chain AD:



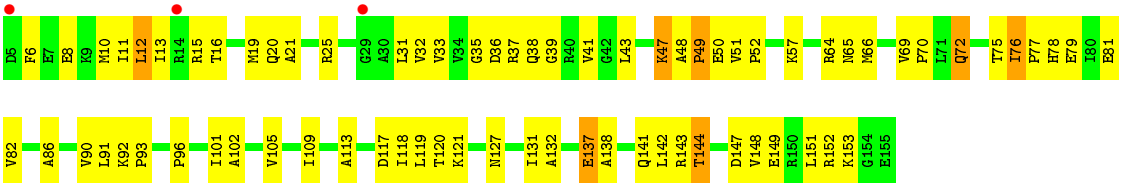
• Molecule 4: 30S ribosomal protein S4

Chain CD:



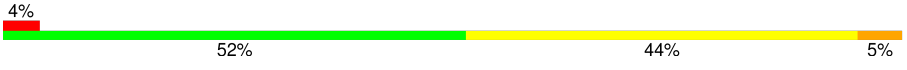
• Molecule 5: 30S ribosomal protein S5

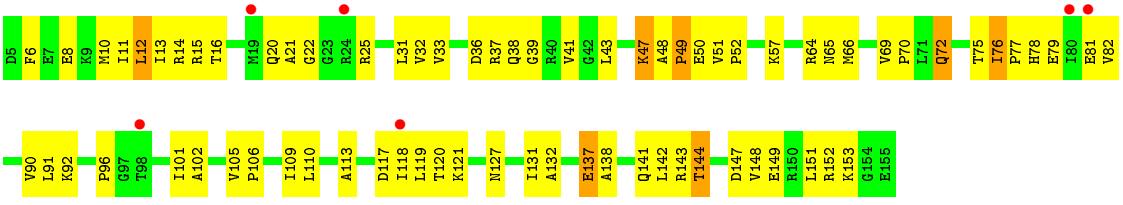
Chain AE:



• Molecule 5: 30S ribosomal protein S5

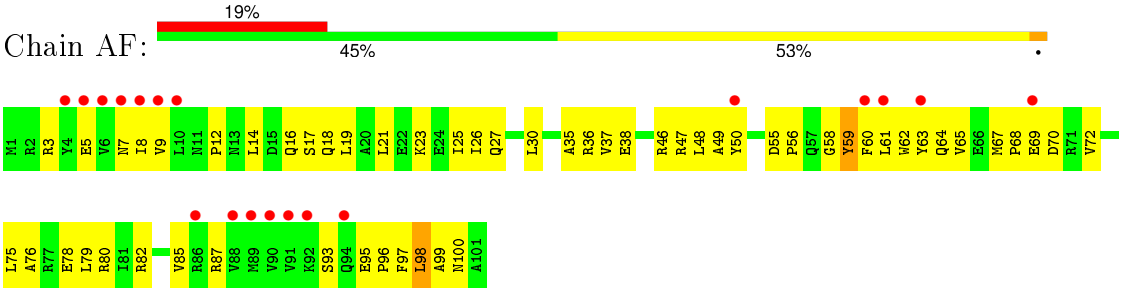
Chain CE:





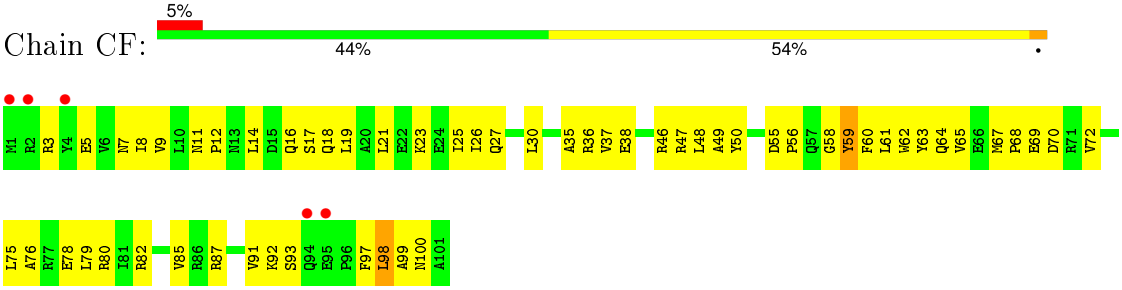
• Molecule 6: 30S ribosomal protein S6

Chain AF:



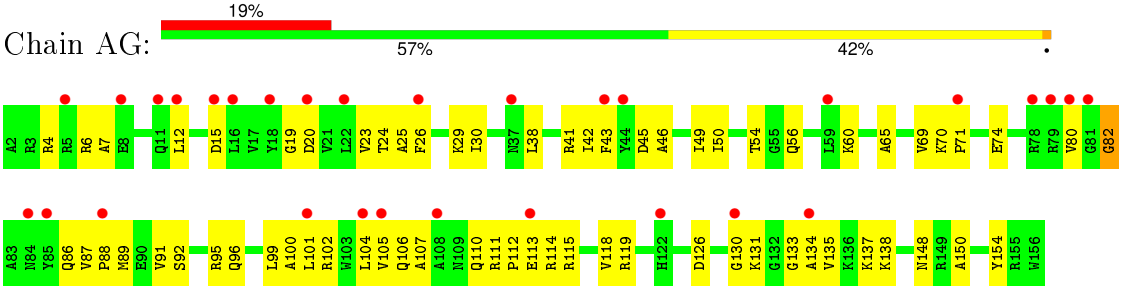
• Molecule 6: 30S ribosomal protein S6

Chain CF:



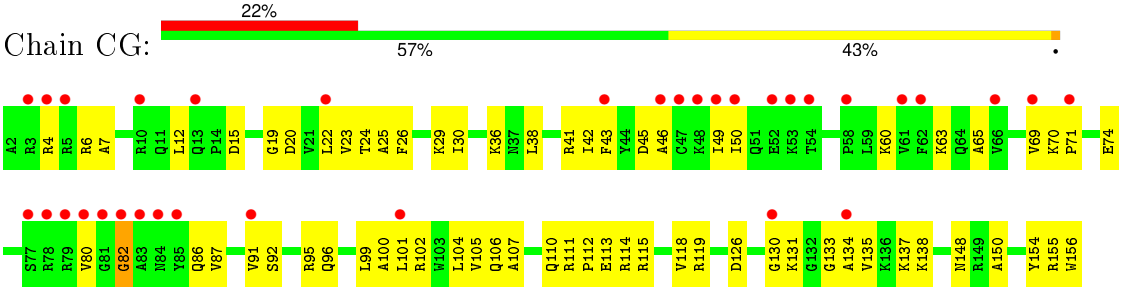
• Molecule 7: 30S ribosomal protein S7

Chain AG:



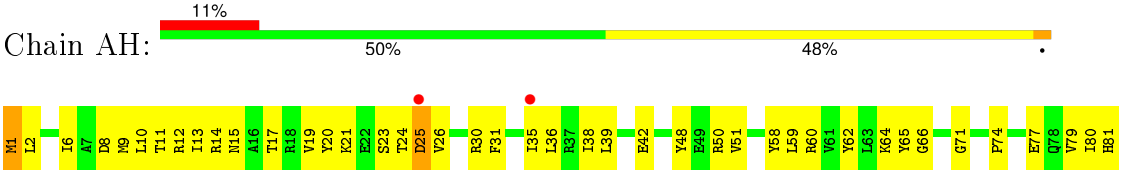
• Molecule 7: 30S ribosomal protein S7

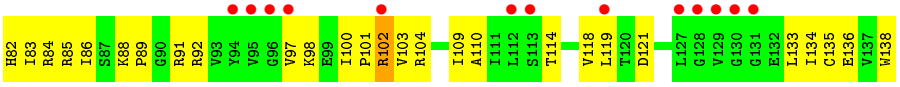
Chain CG:



• Molecule 8: 30S ribosomal protein S8

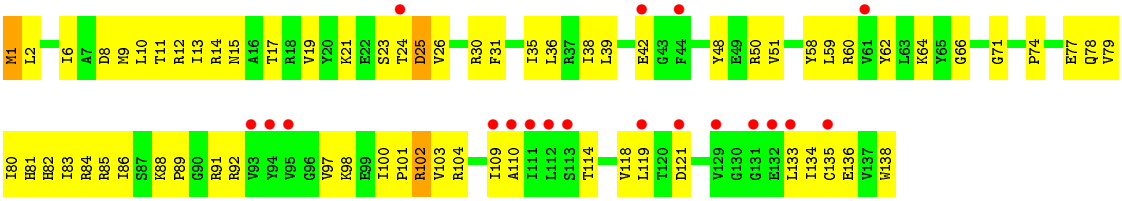
Chain AH:





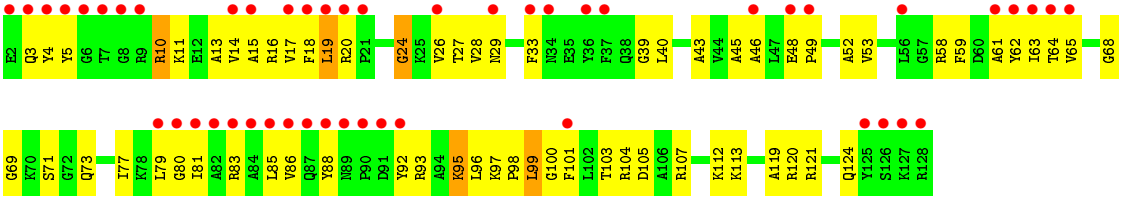
• Molecule 8: 30S ribosomal protein S8

Chain CH:



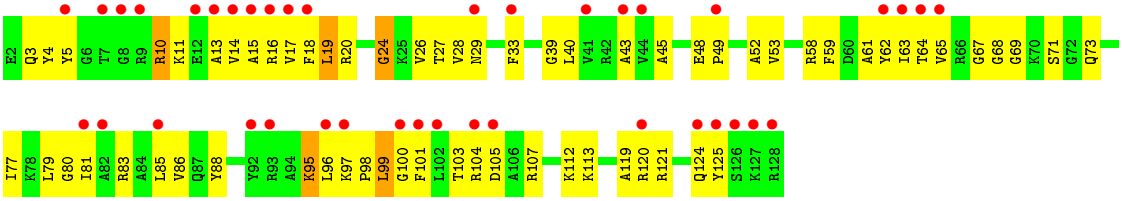
• Molecule 9: 30S ribosomal protein S9

Chain AI:



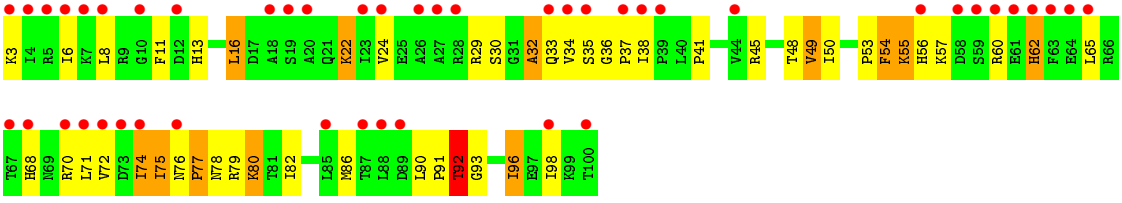
• Molecule 9: 30S ribosomal protein S9

Chain CI:



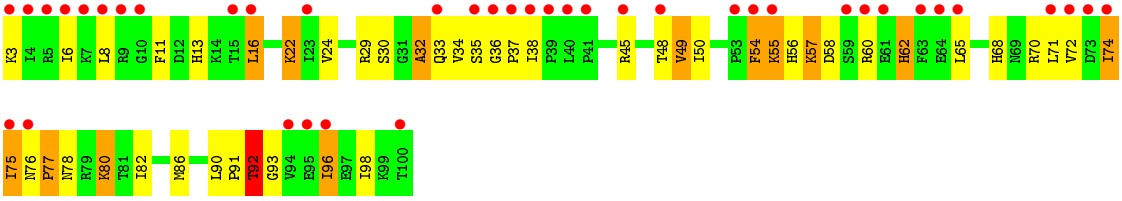
• Molecule 10: 30S ribosomal protein S10

Chain AJ:

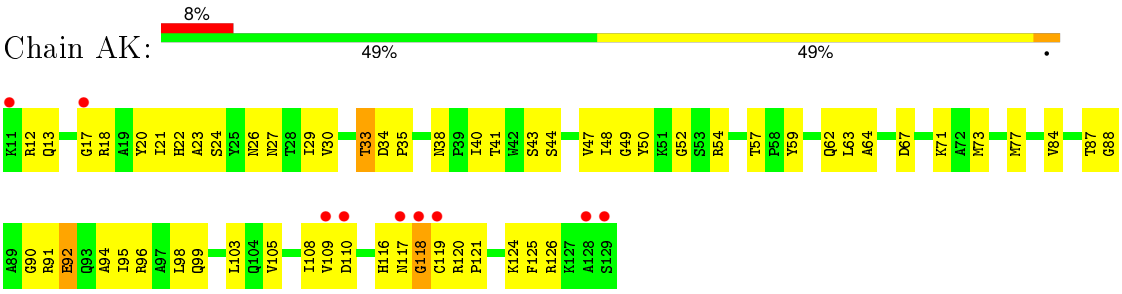


• Molecule 10: 30S ribosomal protein S10

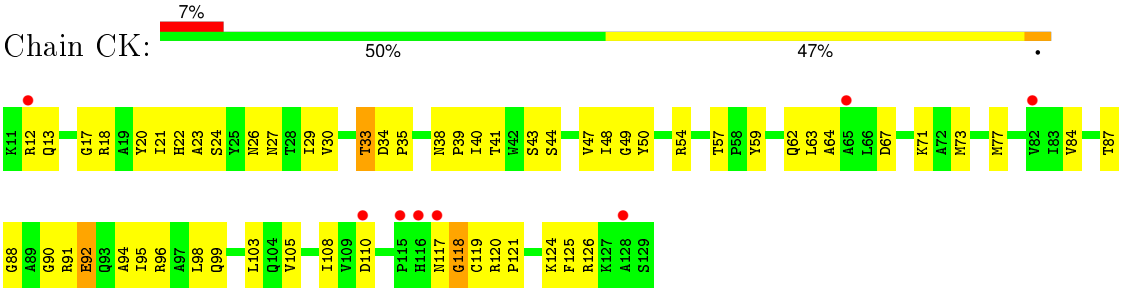
Chain CJ:



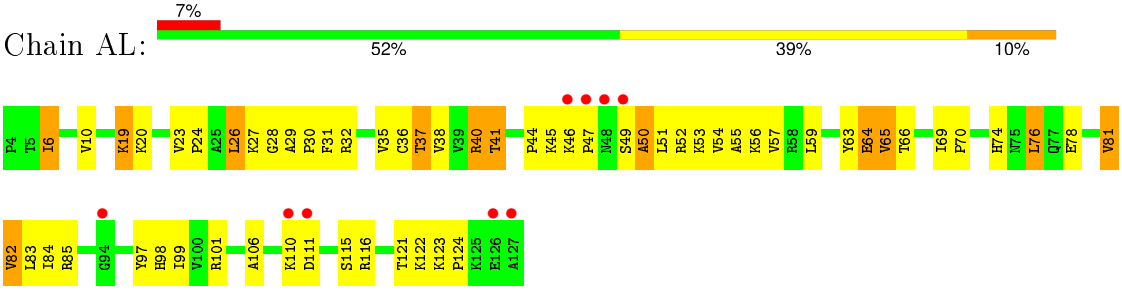
• Molecule 11: 30S ribosomal protein S11



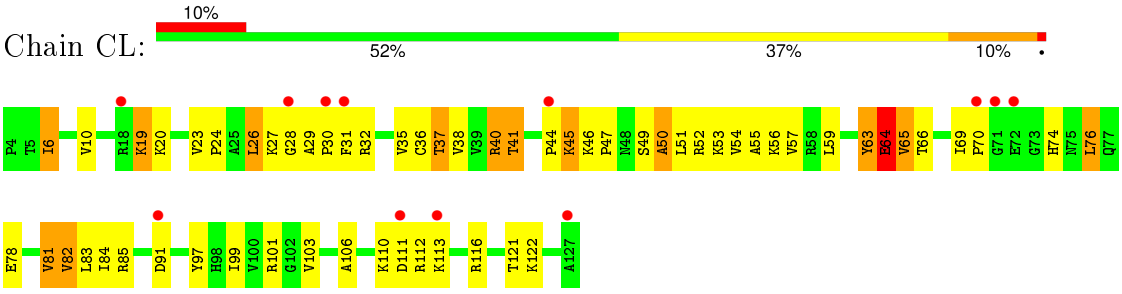
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

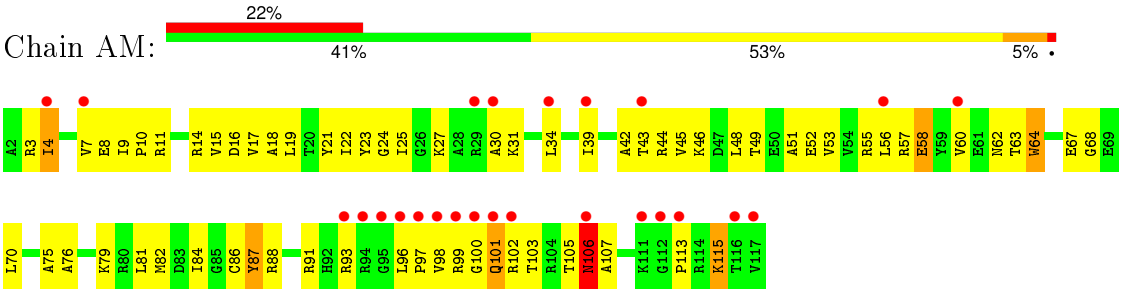


• Molecule 12: 30S ribosomal protein S12



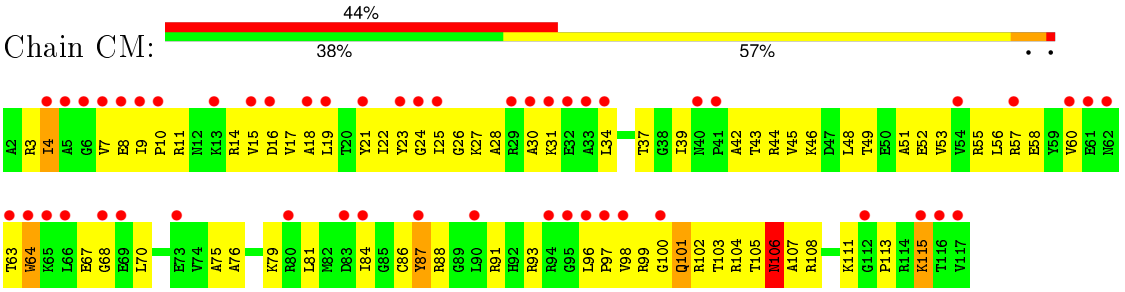
• Molecule 13: 30S ribosomal protein S13

Chain AM:



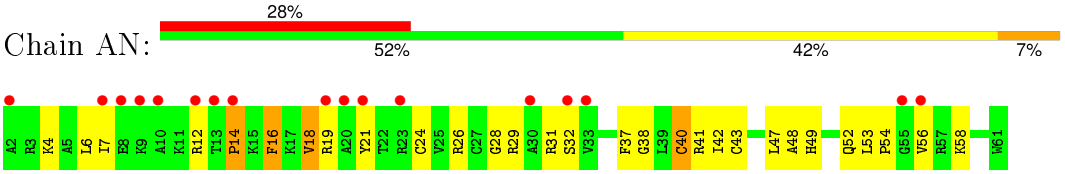
• Molecule 13: 30S ribosomal protein S13

Chain CM:



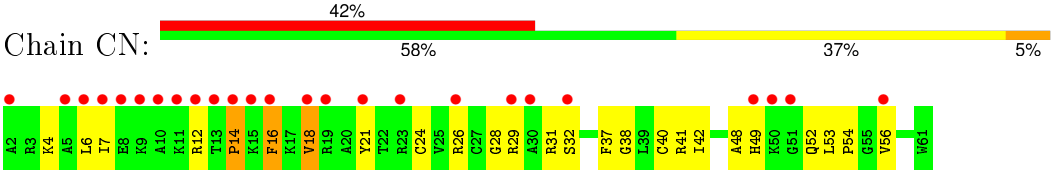
• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



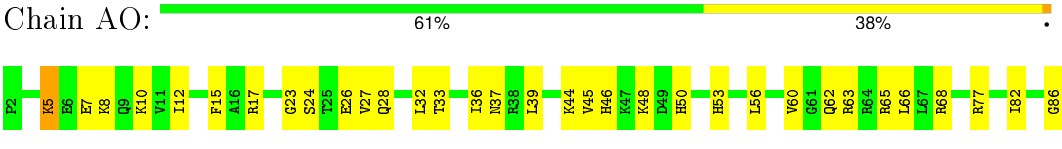
• Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



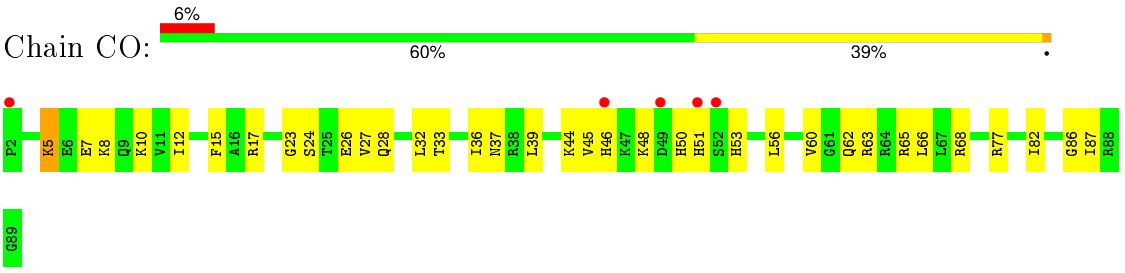
• Molecule 15: 30S ribosomal protein S15

Chain AO:



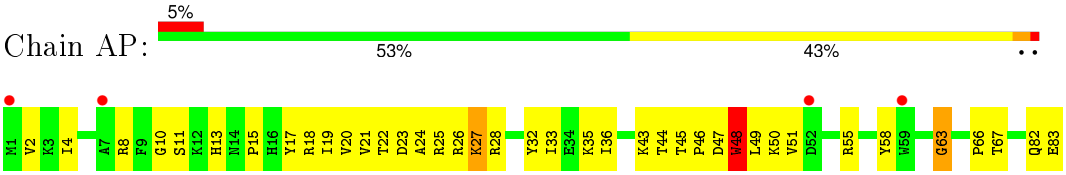
• Molecule 15: 30S ribosomal protein S15

Chain CO:



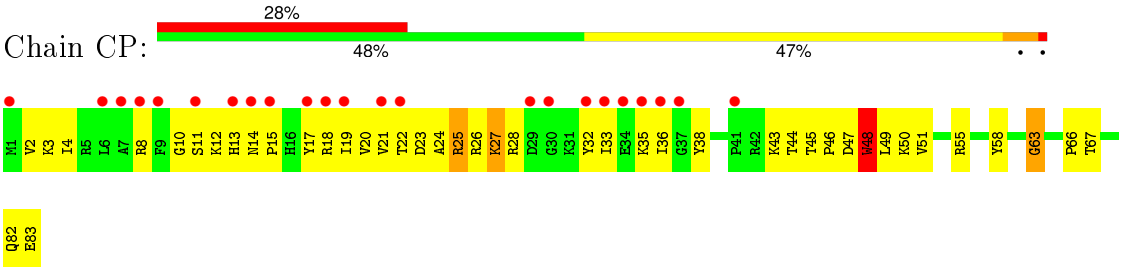
• Molecule 16: 30S ribosomal protein S16

Chain AP:



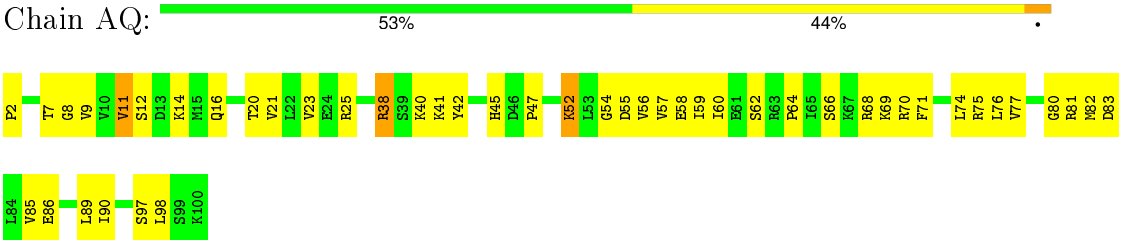
• Molecule 16: 30S ribosomal protein S16

Chain CP:



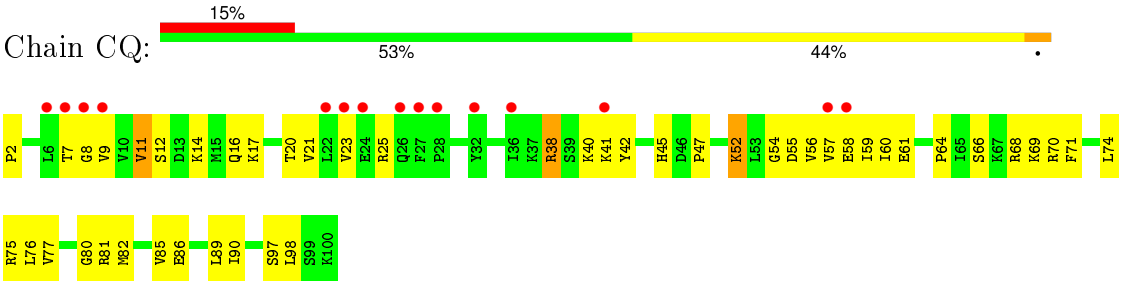
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



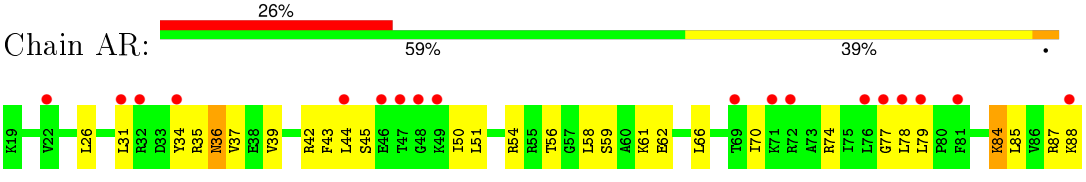
• Molecule 17: 30S ribosomal protein S17

Chain CQ:



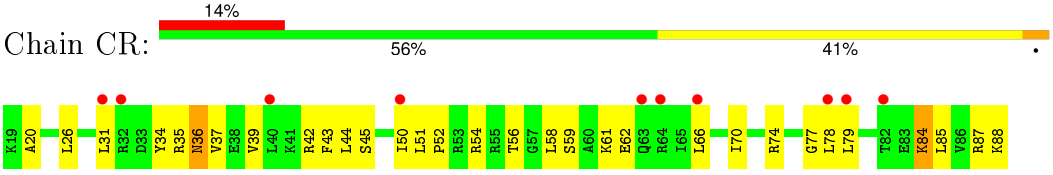
• Molecule 18: 30S ribosomal protein S18

Chain AR:



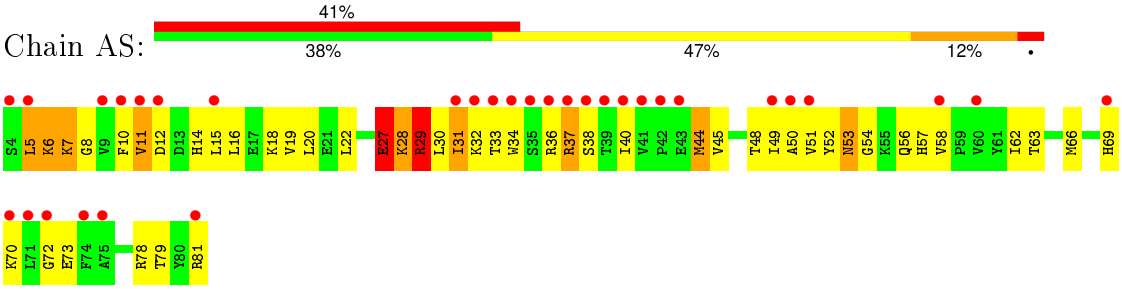
• Molecule 18: 30S ribosomal protein S18

Chain CR:



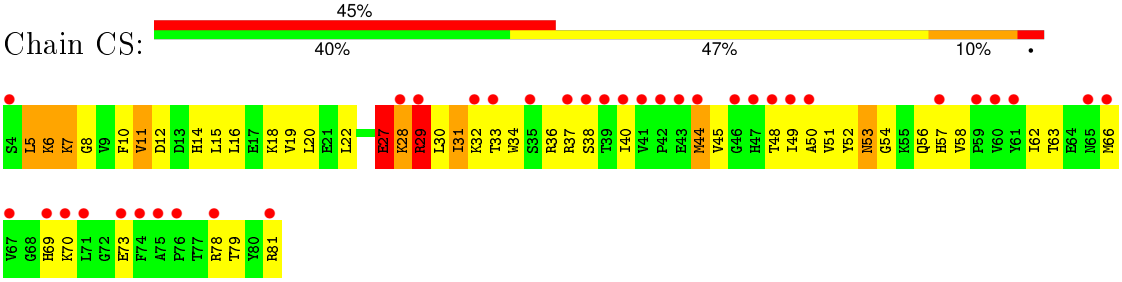
- Molecule 19: 30S ribosomal protein S19

Chain AS:



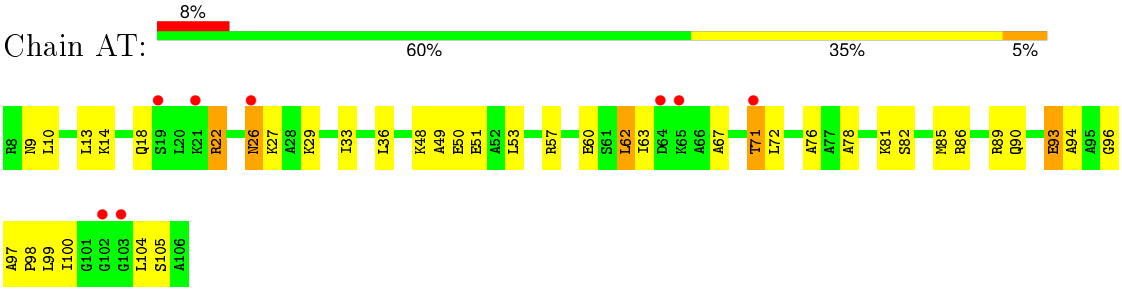
- Molecule 19: 30S ribosomal protein S19

Chain CS:



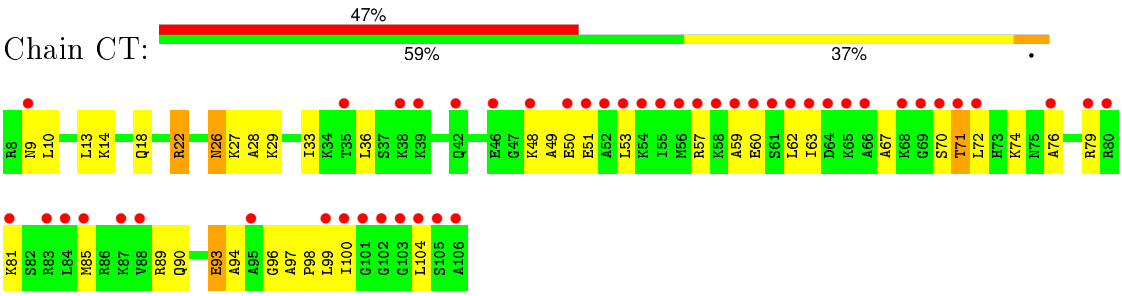
- Molecule 20: 30S ribosomal protein S20

Chain AT:



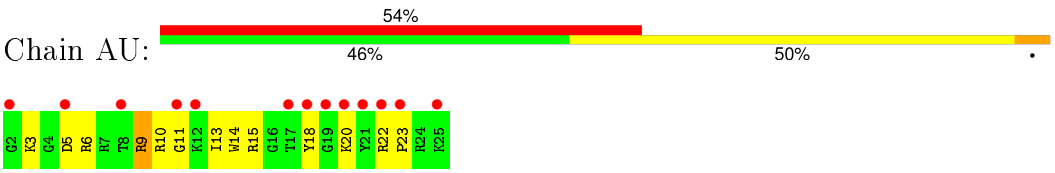
- Molecule 20: 30S ribosomal protein S20

Chain CT:



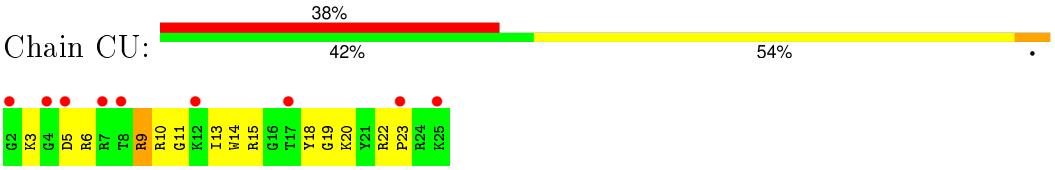
- Molecule 21: 30S ribosomal protein Thx

Chain AU:



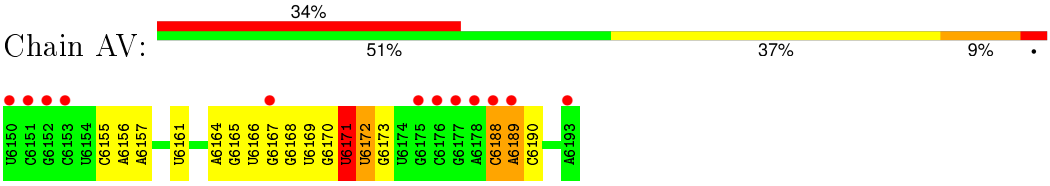
- Molecule 21: 30S ribosomal protein Thx

Chain CU:



• Molecule 22: domain 3 of PSIC IGR IRES RNA

Chain AV:

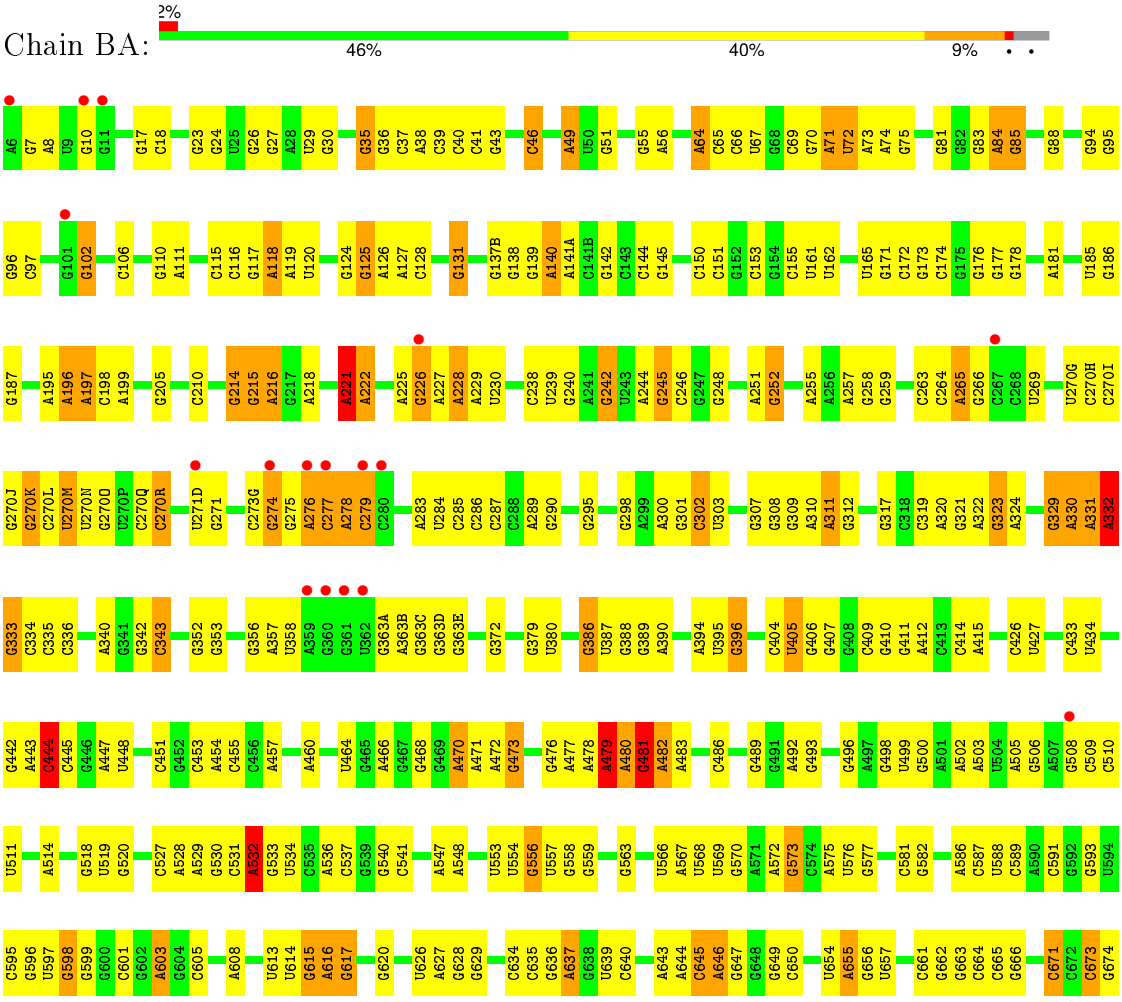


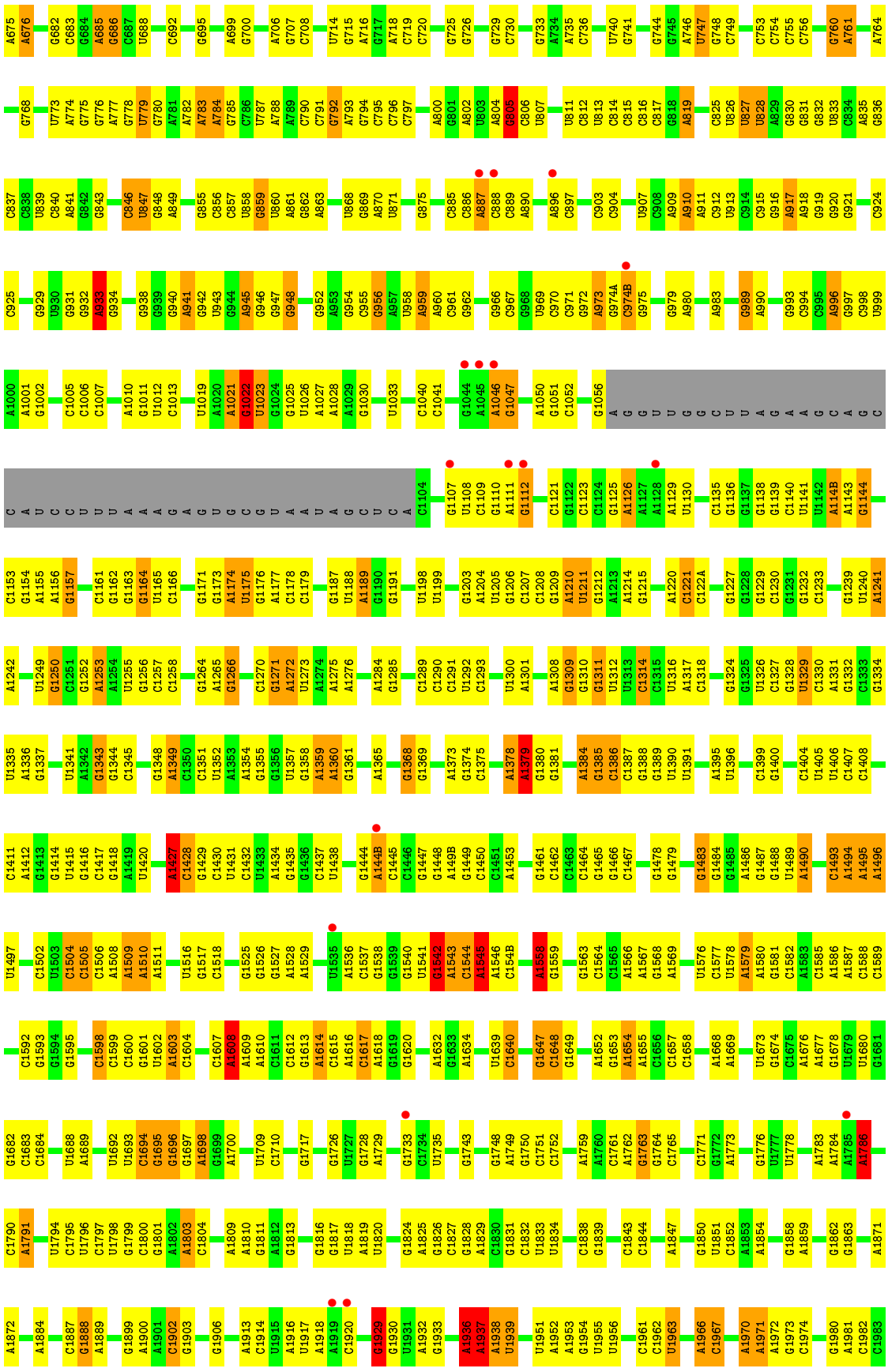
• Molecule 22: domain 3 of PSIC IGR IRES RNA

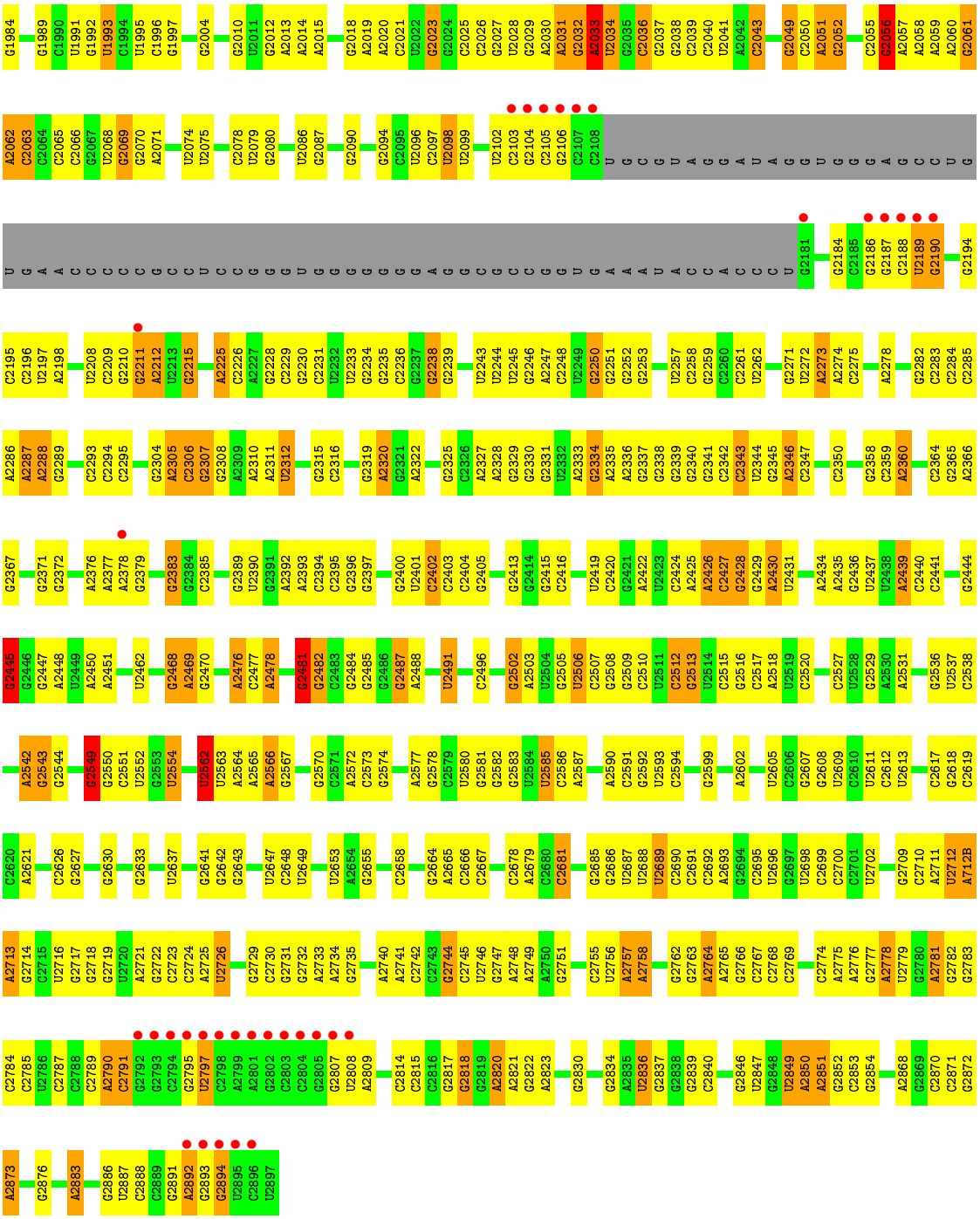
Chain CV:

• Molecule 23: 23S ribosomal RNA

Chain BA:

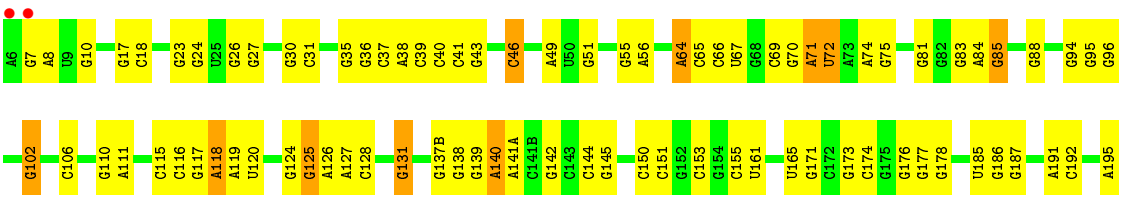


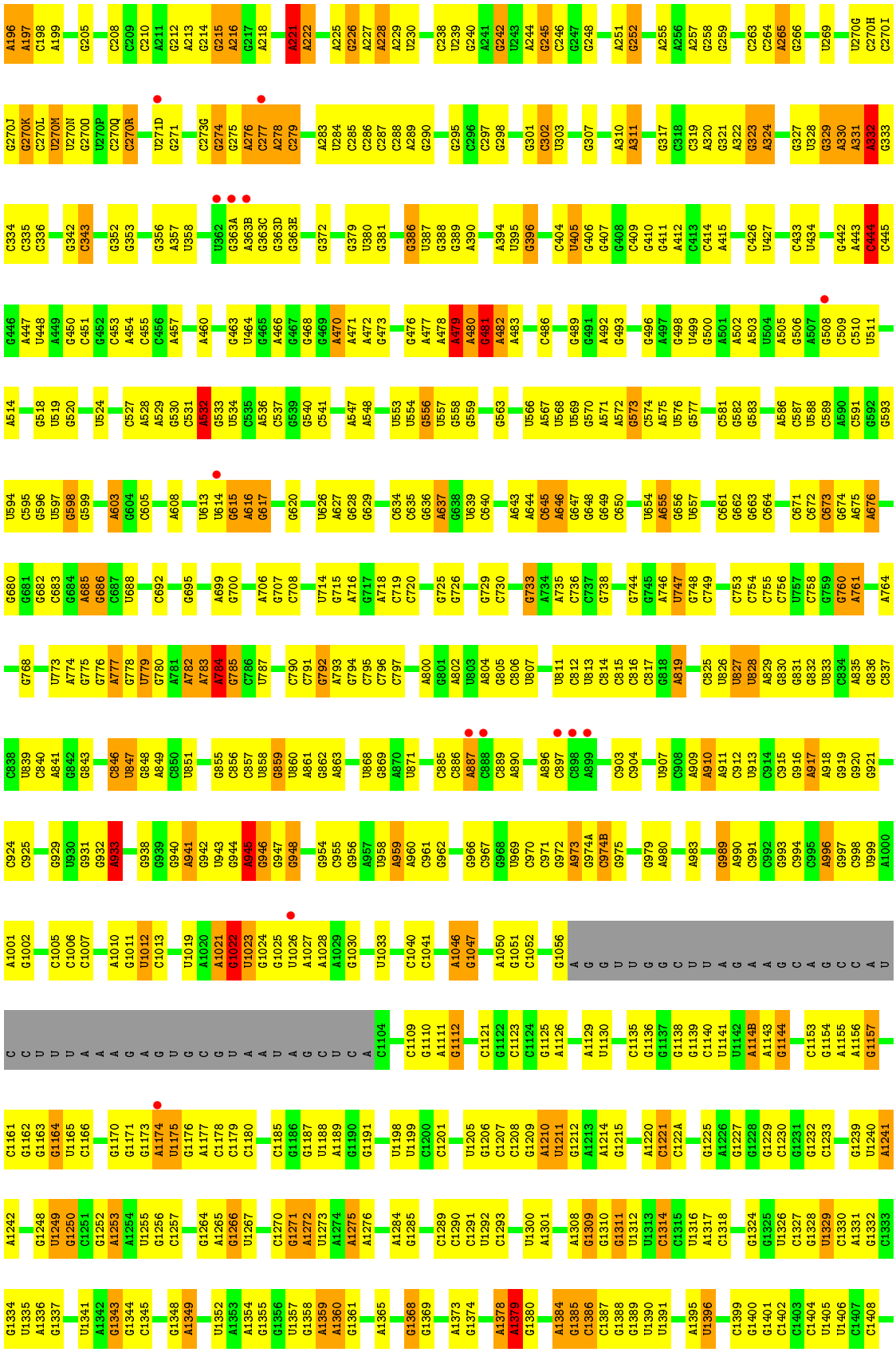




• Molecule 23: 23S ribosomal RNA

Chain DA:

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A514 G518 U519 G520 U524 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G539 G540 C541 A547 A548 U553 U554 G556 U557 G558 G559 G563 U566 A567 U568 U569 G570 A571 A572 G573 C574 A575 U576 G577 C581 G582 G583 A586 C587 U588 C589 A590 C591 G592 G593
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C C U U U A A A G A G U G C G U A A U A G C U C A 1104 C1109 G1110 A1111 G1112 C1121 G1122 C1123 C1124 G1125 A1126 A1129 U1130 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A114B A1143 G1144 C1153 G1154 A1155 A1156 G1157
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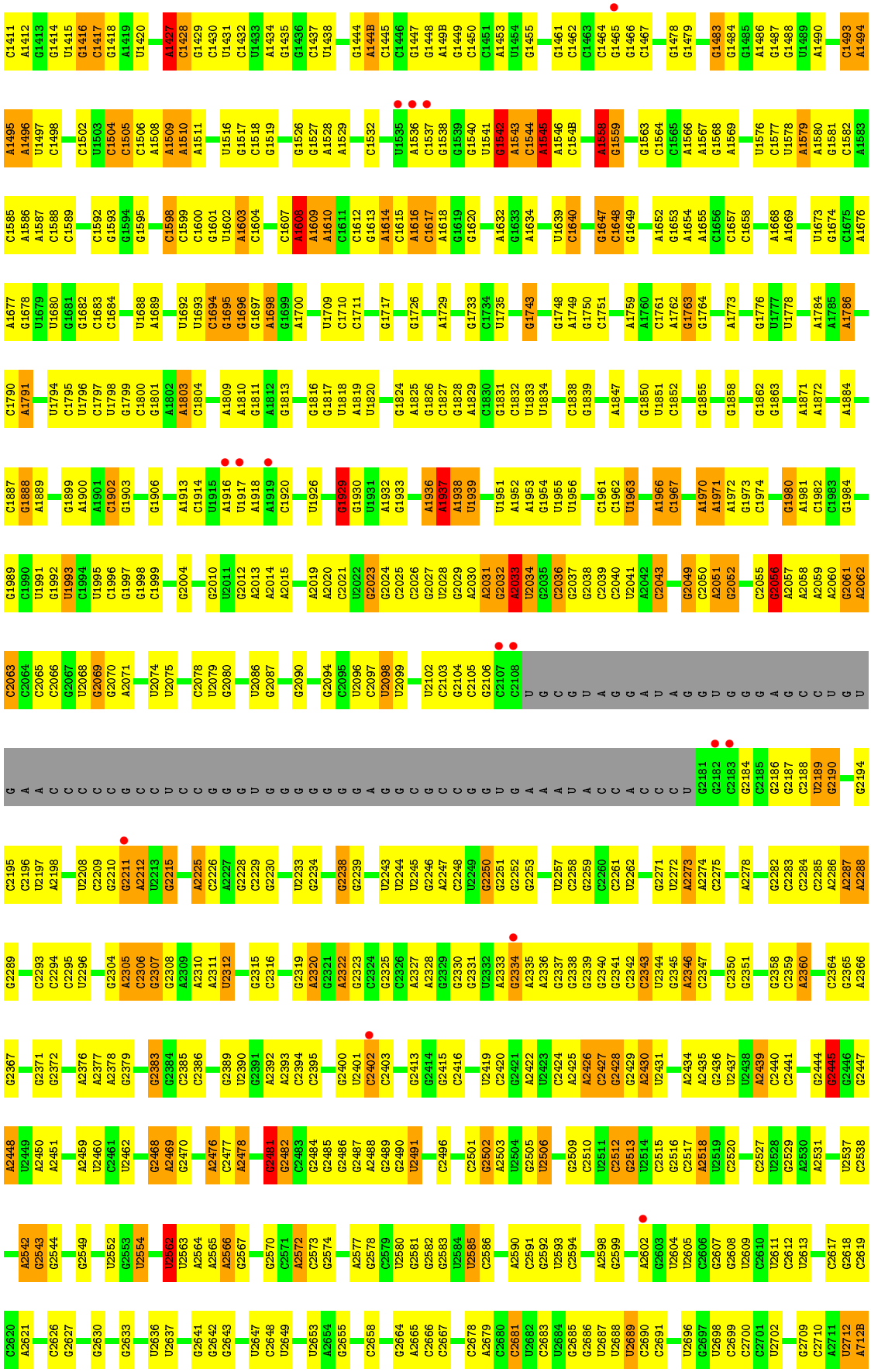
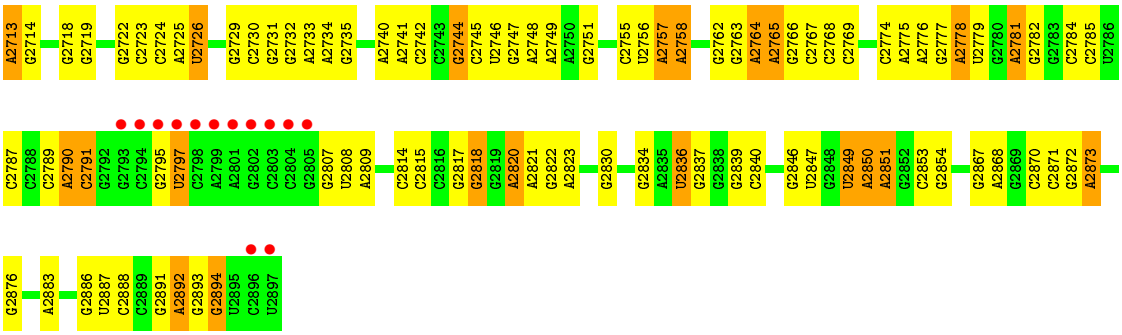
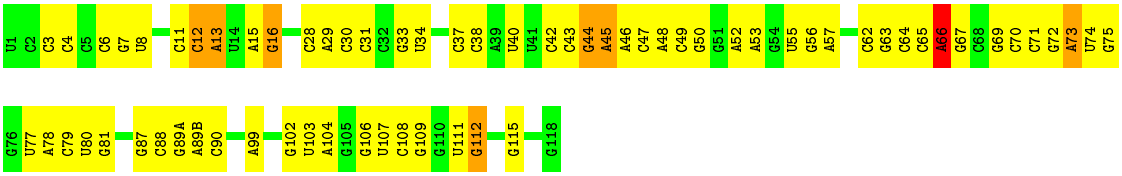




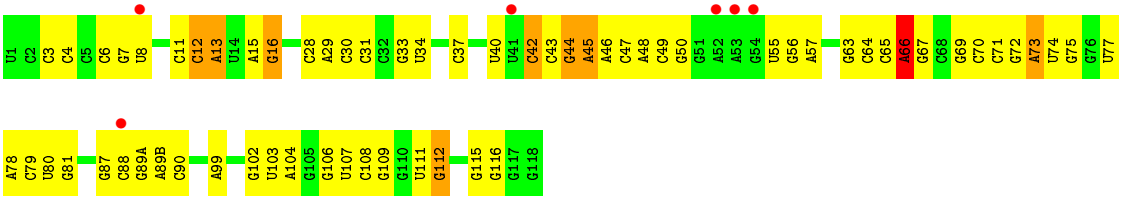
• Molecule 24: 5S ribosomal RNA

Chain BB:



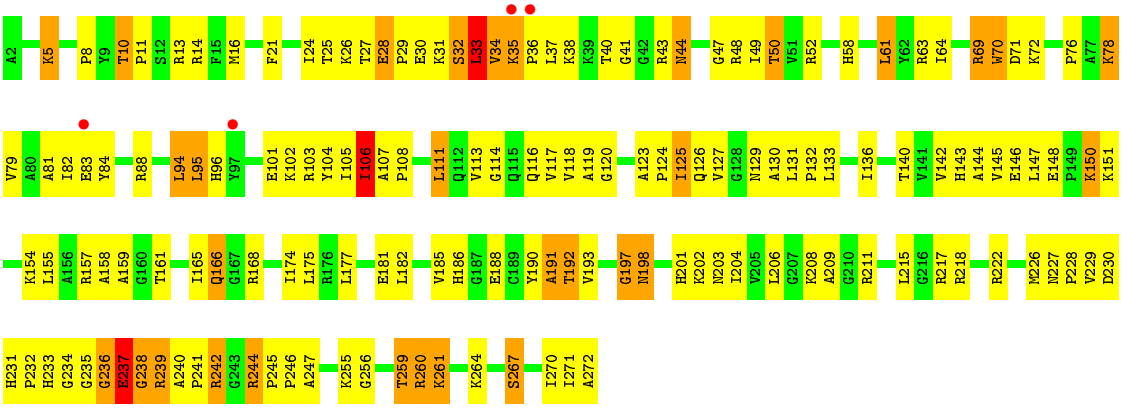
• Molecule 24: 5S ribosomal RNA

Chain DB:



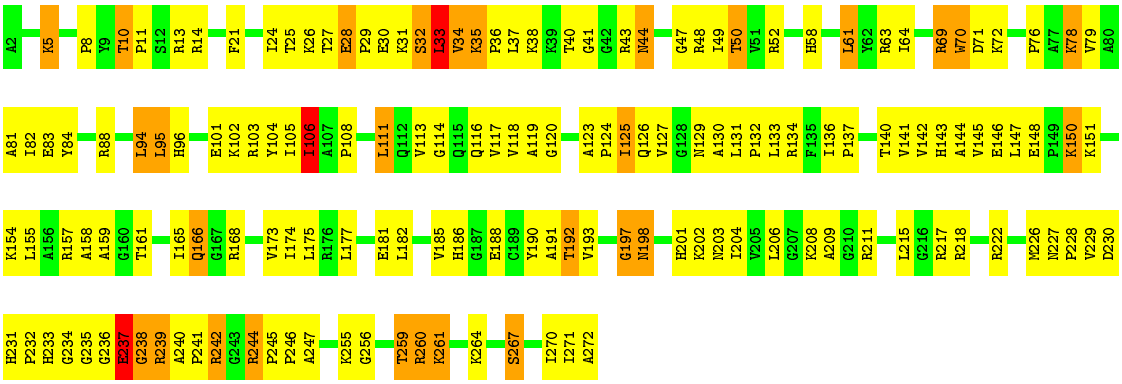
• Molecule 25: 50S ribosomal protein L2

Chain BC:



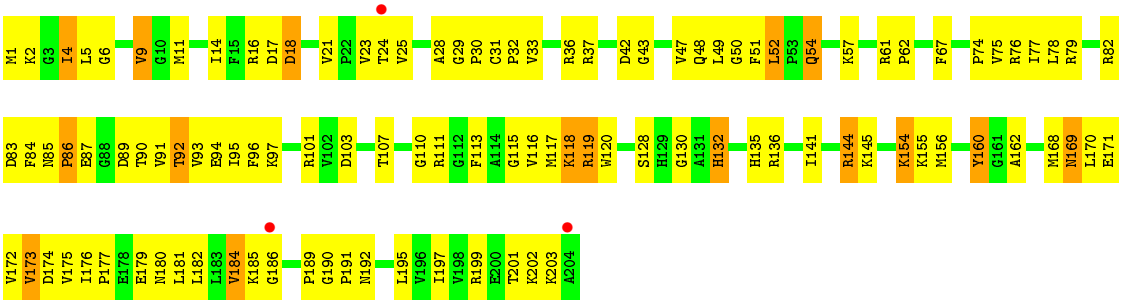
• Molecule 25: 50S ribosomal protein L2

Chain DC:



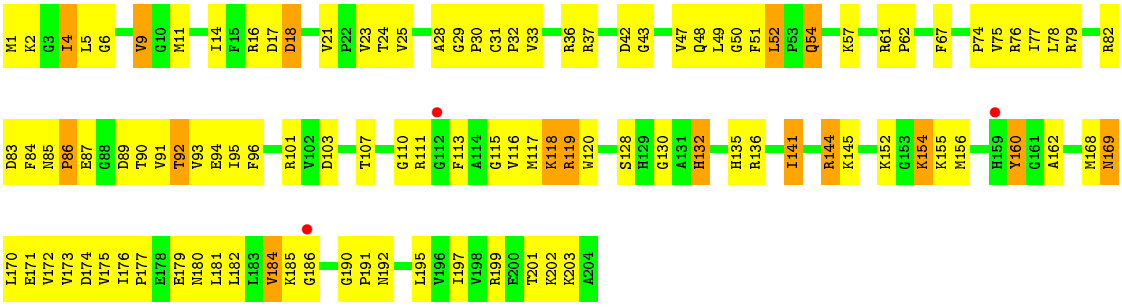
• Molecule 26: 50S ribosomal protein L3

Chain BD:



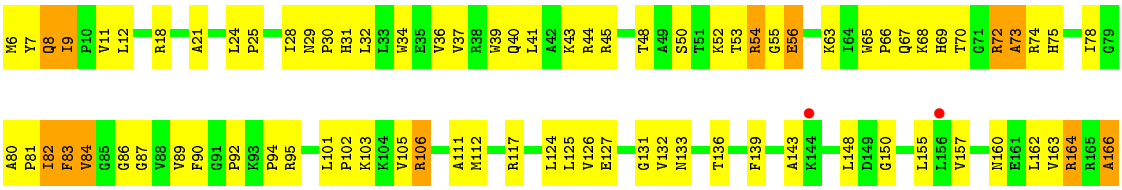
• Molecule 26: 50S ribosomal protein L3

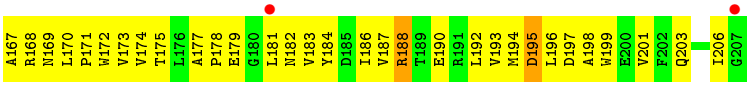
Chain DD:



• Molecule 27: 50S ribosomal protein L4

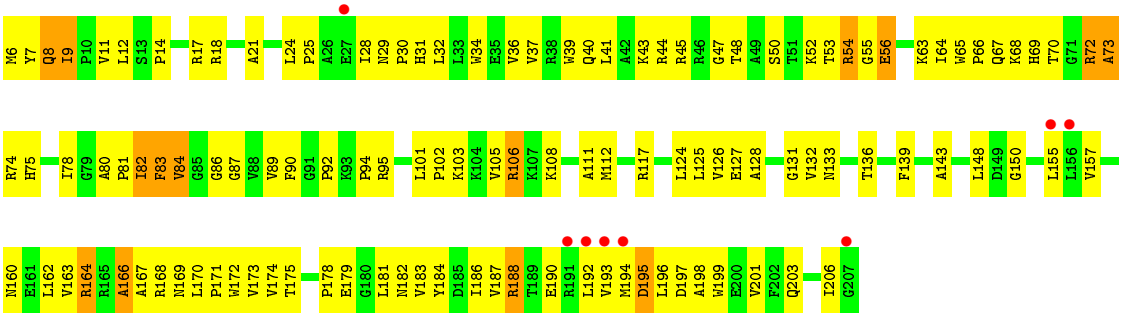
Chain BE:





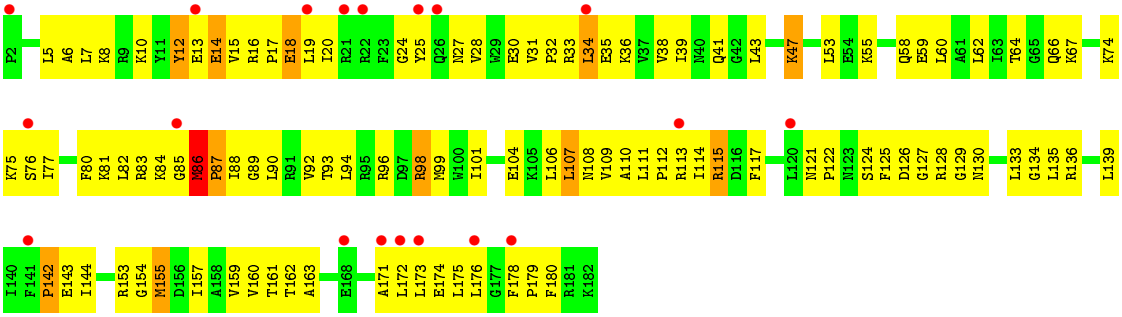
• Molecule 27: 50S ribosomal protein L4

Chain DE:



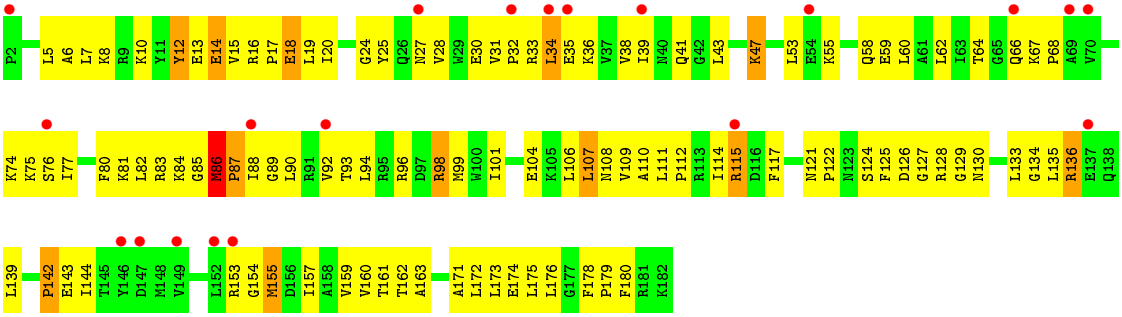
• Molecule 28: 50S ribosomal protein L5

Chain BF:



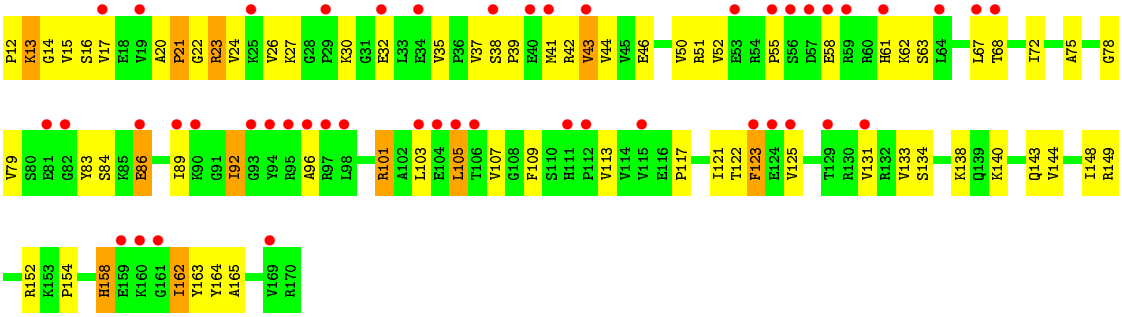
• Molecule 28: 50S ribosomal protein L5

Chain DF:



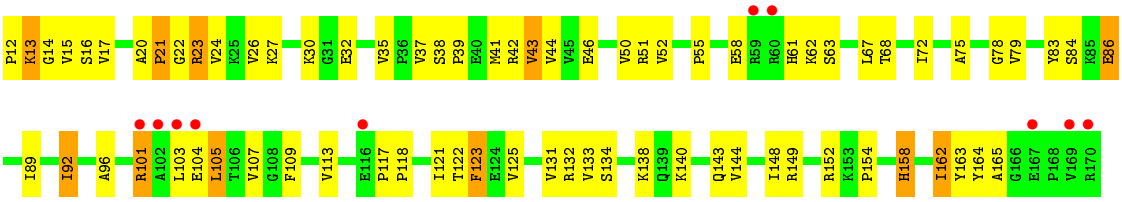
• Molecule 29: 50S ribosomal protein L6

Chain BG:



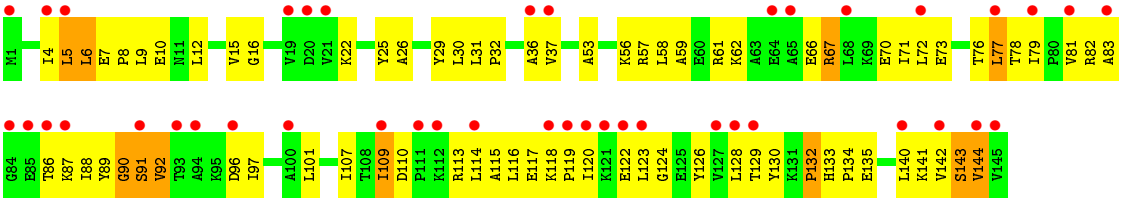
• Molecule 29: 50S ribosomal protein L6

Chain DG:



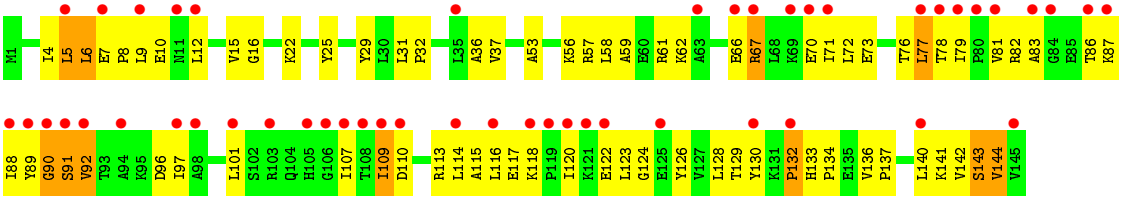
• Molecule 30: 50S ribosomal protein L9

Chain BH:



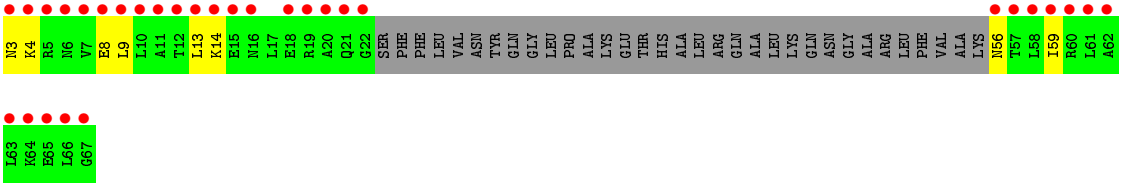
• Molecule 30: 50S ribosomal protein L9

Chain DH:



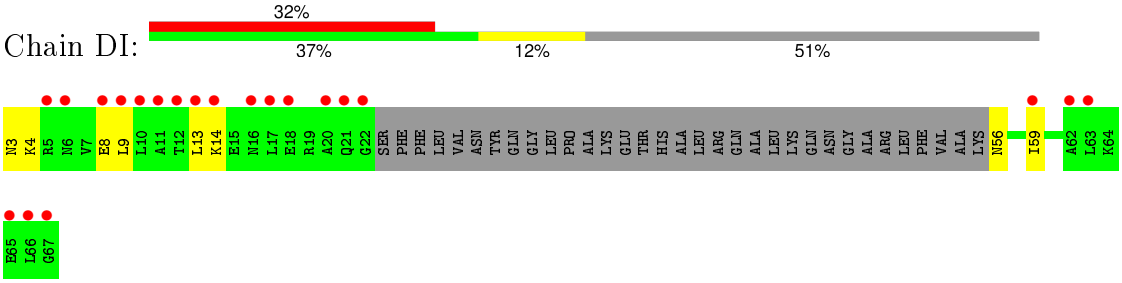
• Molecule 31: 50S ribosomal protein L10

Chain BI:



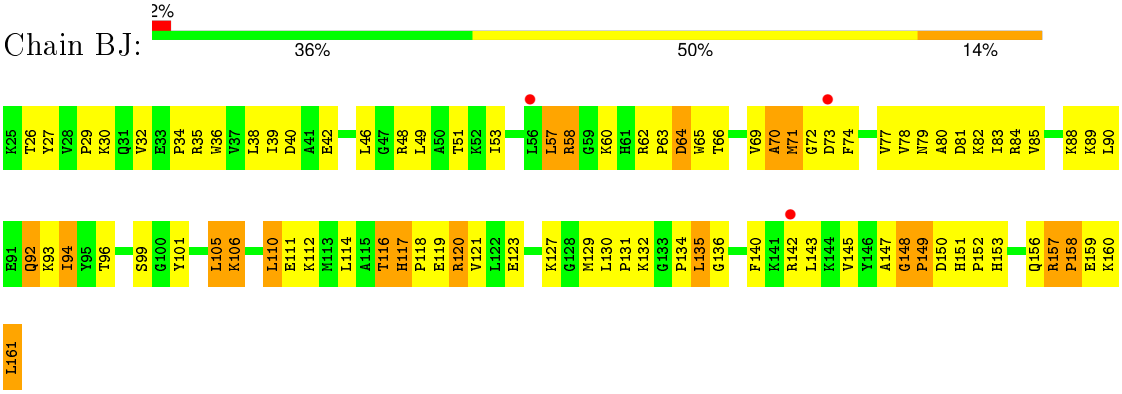
• Molecule 31: 50S ribosomal protein L10

Chain DI:



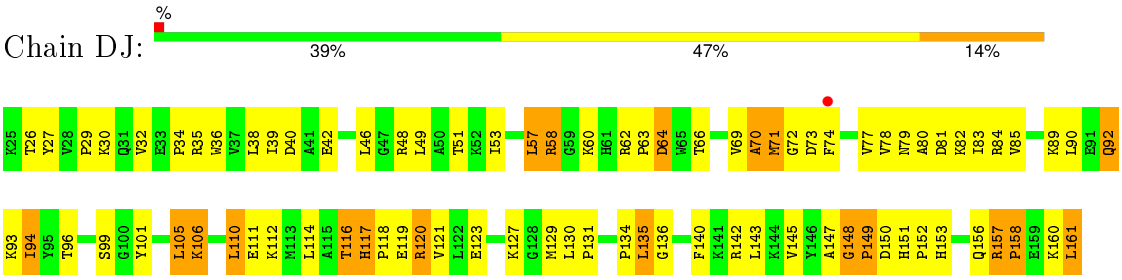
• Molecule 32: 50S ribosomal protein L13

Chain BJ:



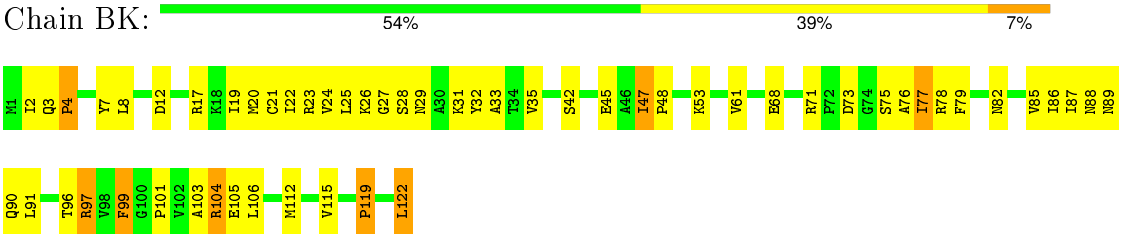
• Molecule 32: 50S ribosomal protein L13

Chain DJ:



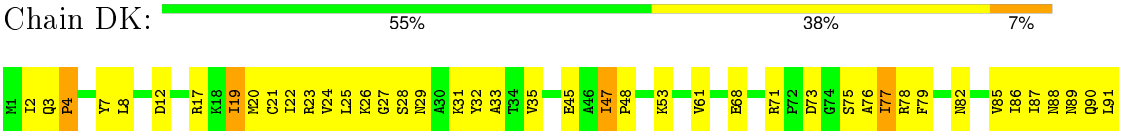
• Molecule 33: 50S ribosomal protein L14

Chain BK:

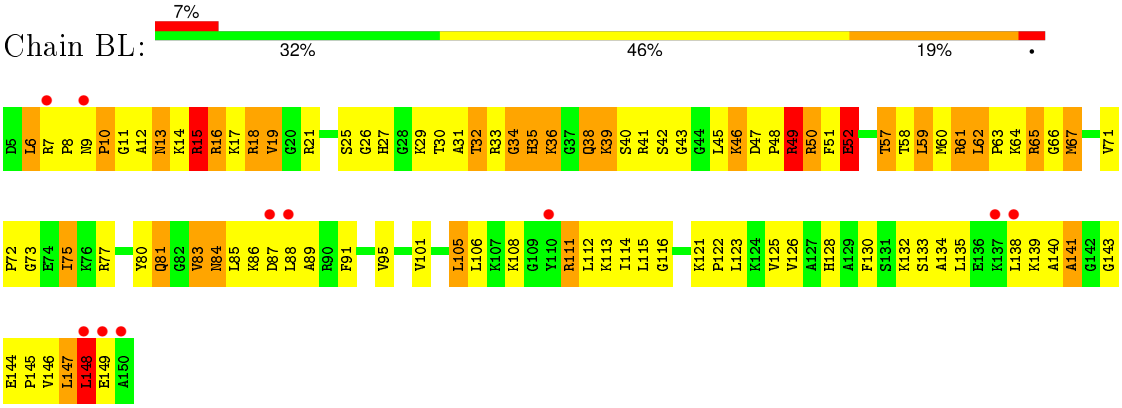


• Molecule 33: 50S ribosomal protein L14

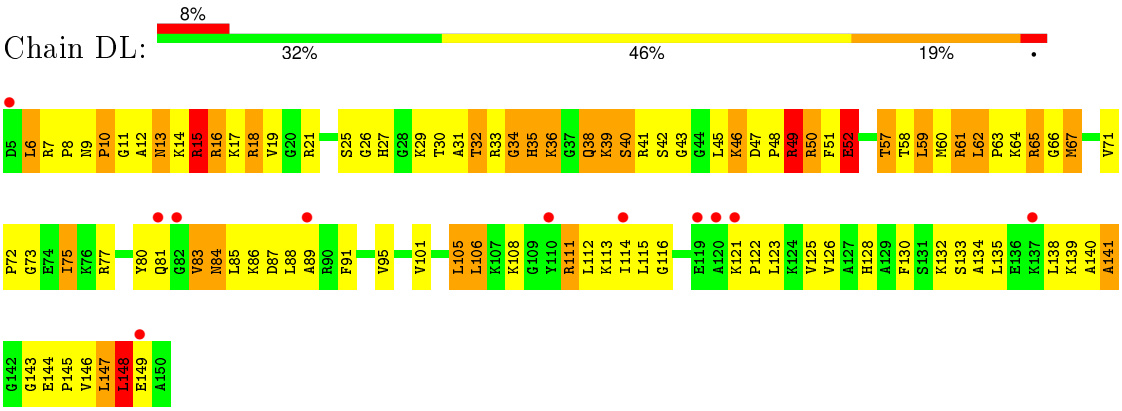
Chain DK:



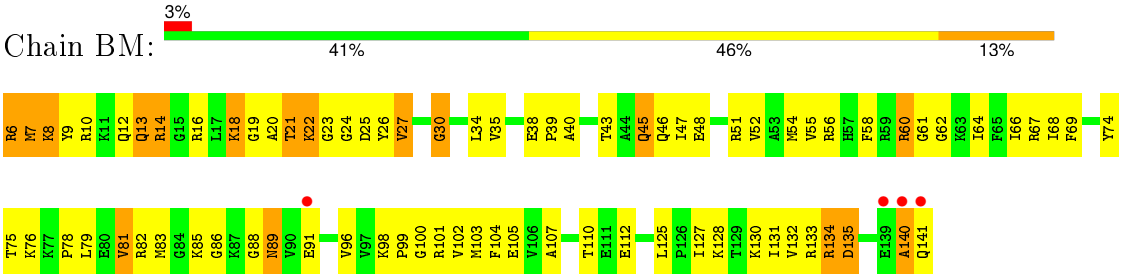
• Molecule 34: 50S ribosomal protein L15



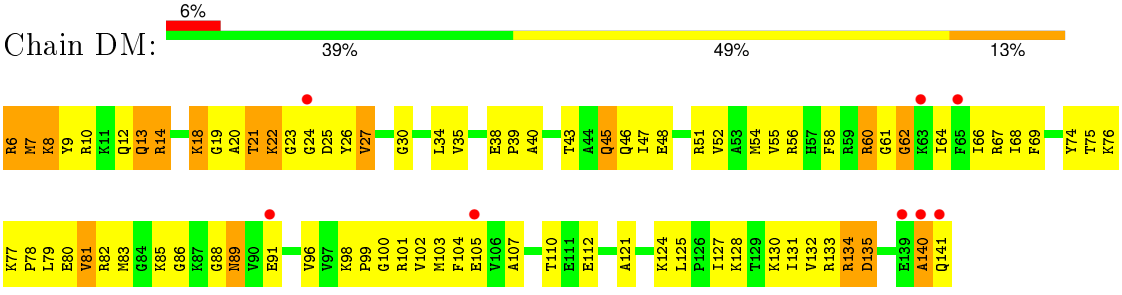
• Molecule 34: 50S ribosomal protein L15



• Molecule 35: 50S ribosomal protein L16

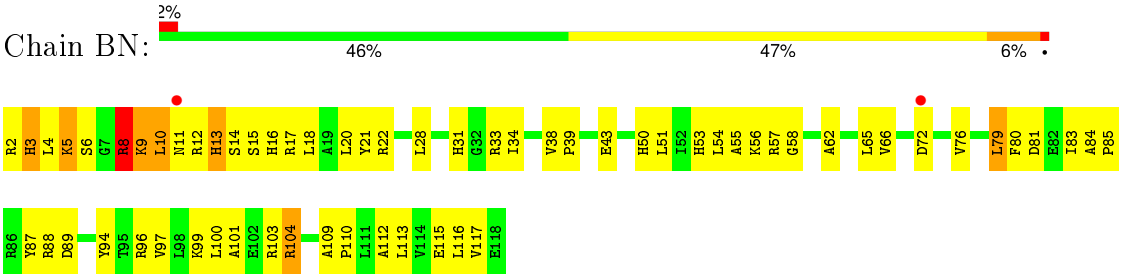


• Molecule 35: 50S ribosomal protein L16



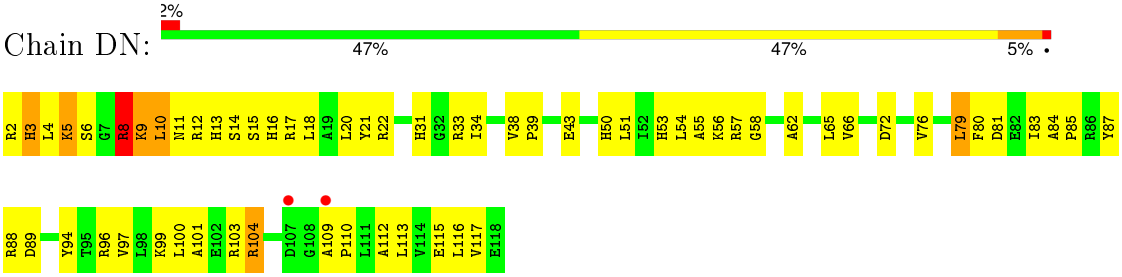
• Molecule 36: 50S ribosomal protein L17

Chain BN:



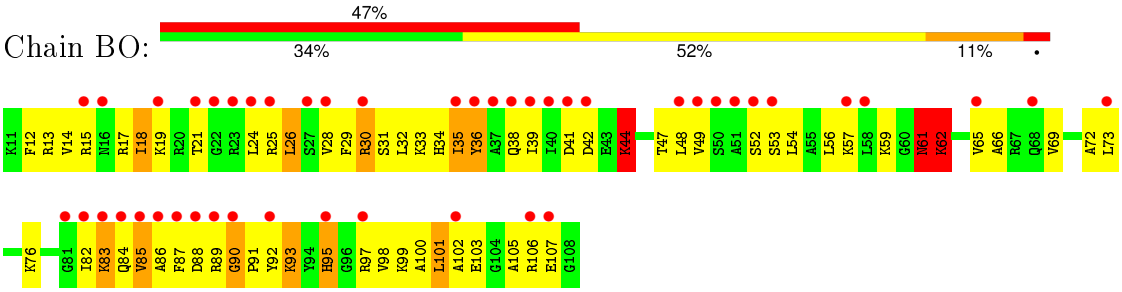
• Molecule 36: 50S ribosomal protein L17

Chain DN:



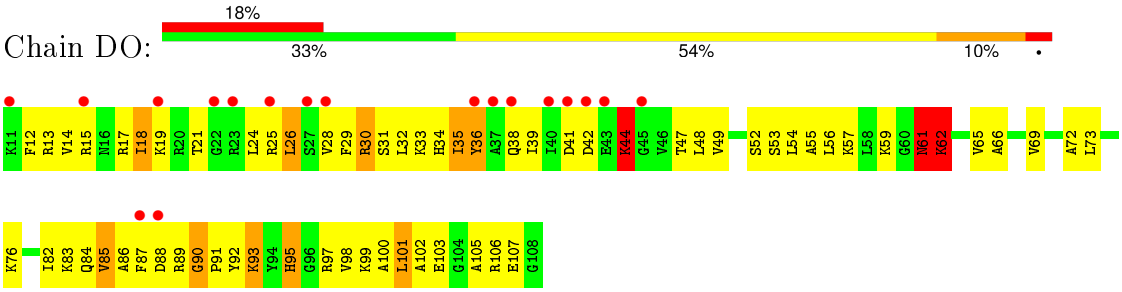
• Molecule 37: 50S ribosomal protein L18

Chain BO:



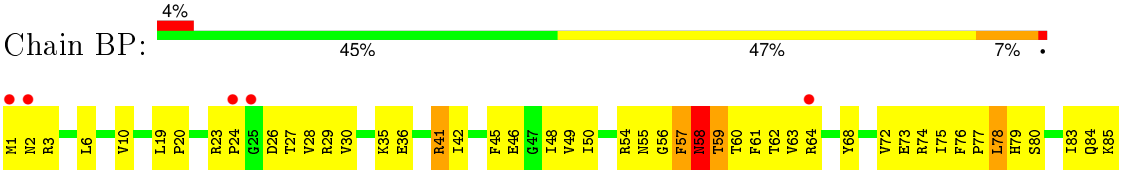
• Molecule 37: 50S ribosomal protein L18

Chain DO:



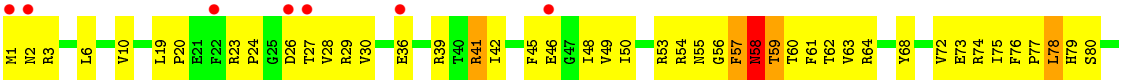
• Molecule 38: 50S ribosomal protein L19

Chain BP:



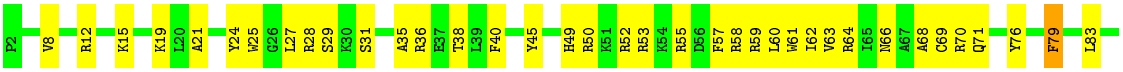
• Molecule 38: 50S ribosomal protein L19

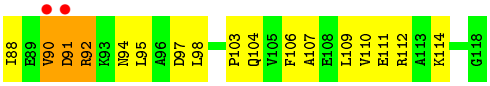
Chain DP:



• Molecule 39: 50S ribosomal protein L20

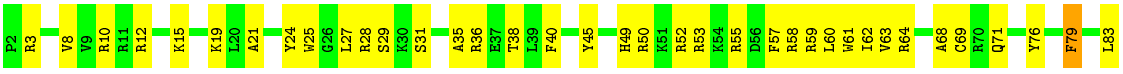
Chain BQ:

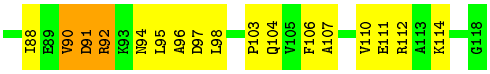




• Molecule 39: 50S ribosomal protein L20

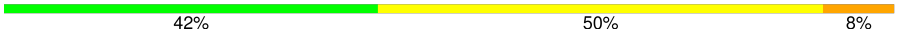
Chain DQ:

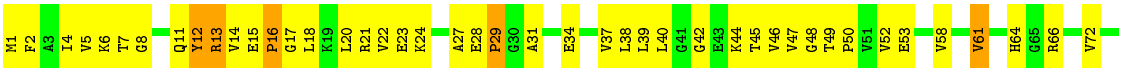


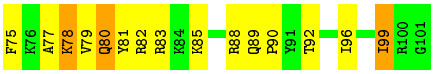


• Molecule 40: 50S ribosomal protein L21

Chain BR:

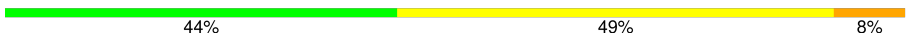


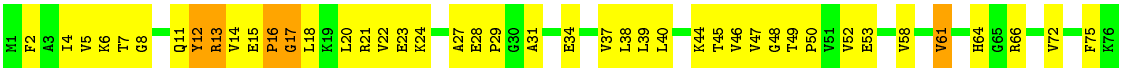


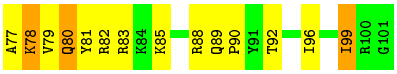


• Molecule 40: 50S ribosomal protein L21

Chain DR:

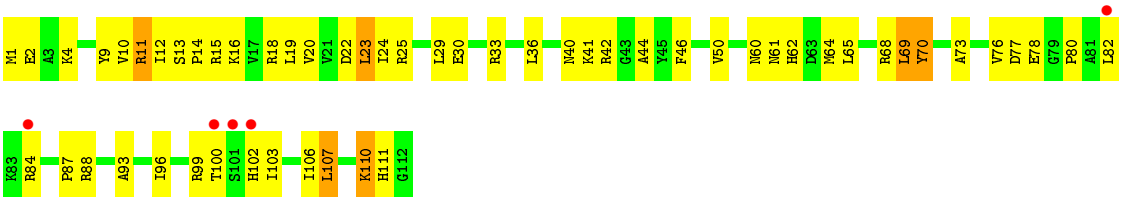






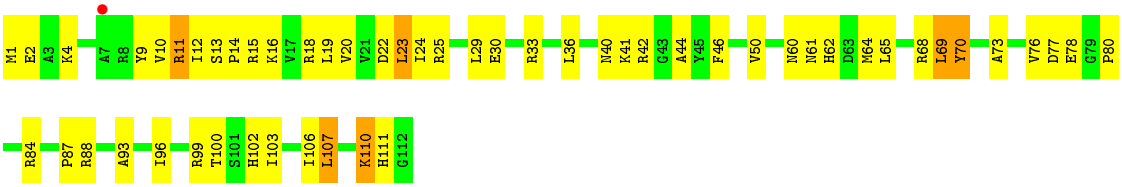
• Molecule 41: 50S ribosomal protein L22

Chain BS:



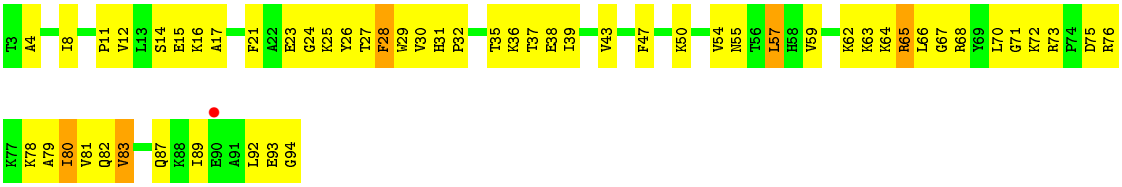
• Molecule 41: 50S ribosomal protein L22

Chain DS:



• Molecule 42: 50S ribosomal protein L23

Chain BT:

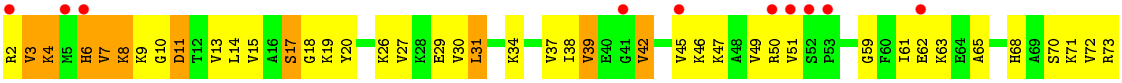


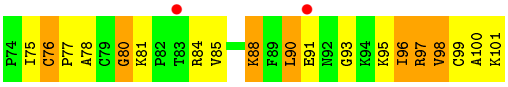
• Molecule 42: 50S ribosomal protein L23

Chain DT:

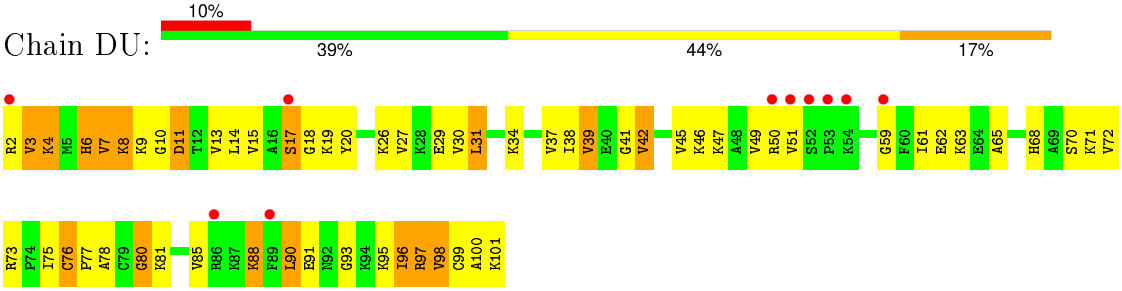
• Molecule 43: 50S ribosomal protein L24

Chain BU:

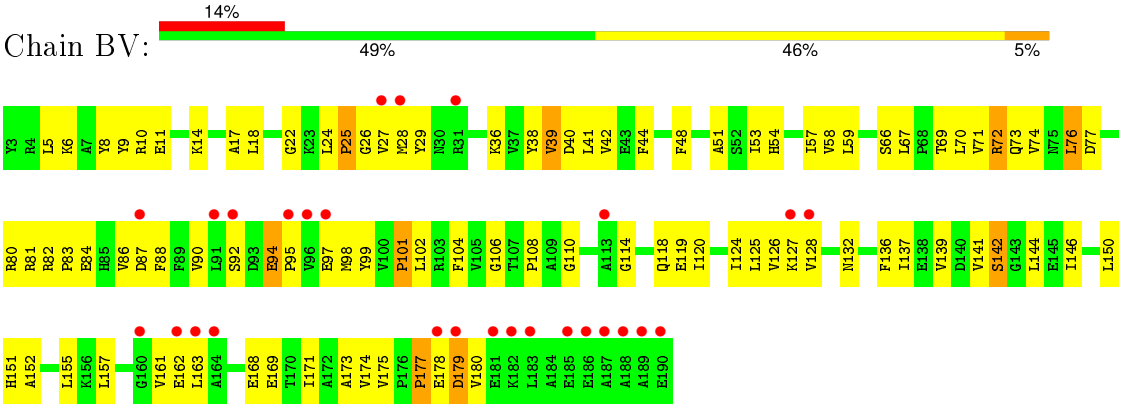




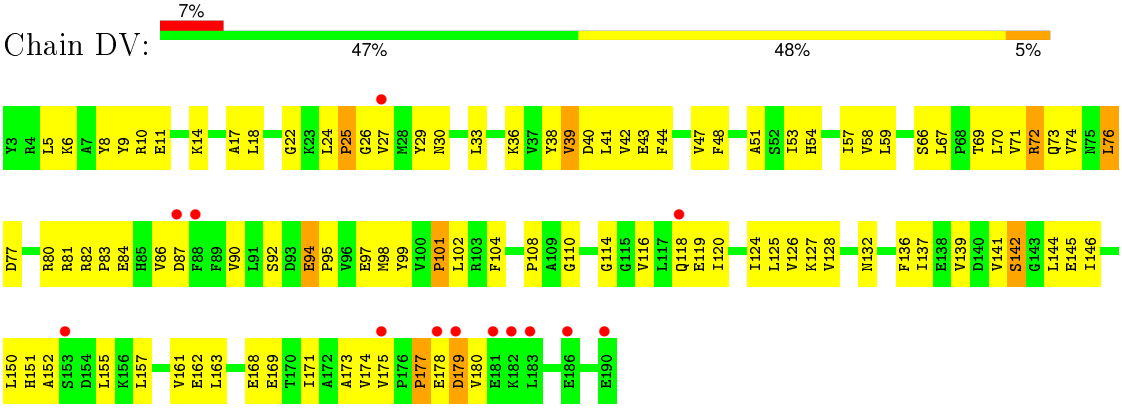
• Molecule 43: 50S ribosomal protein L24



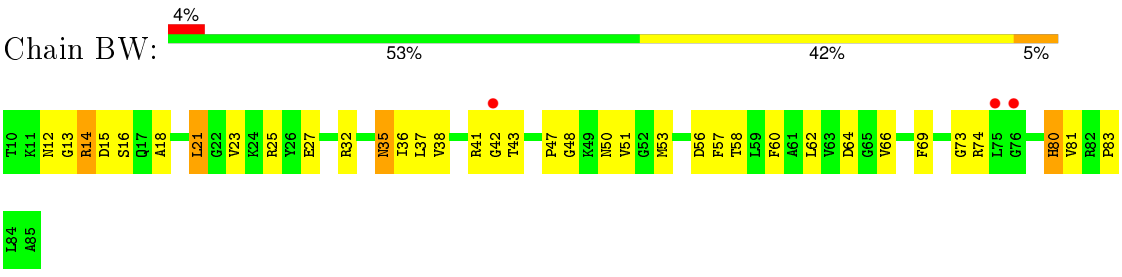
• Molecule 44: 50S ribosomal protein L25



• Molecule 44: 50S ribosomal protein L25

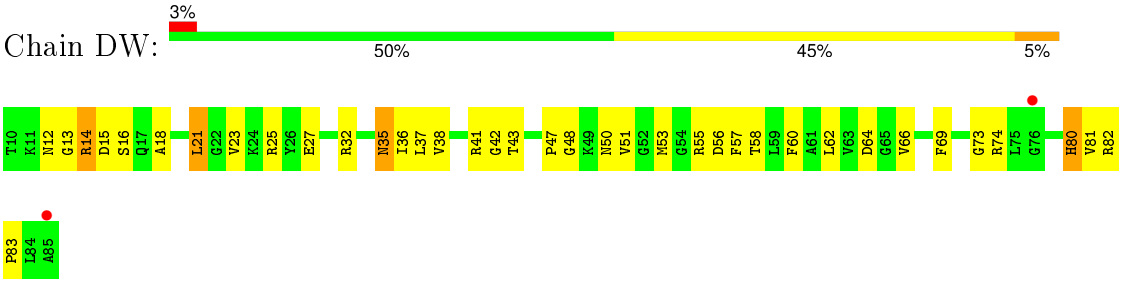


• Molecule 45: 50S ribosomal protein L27



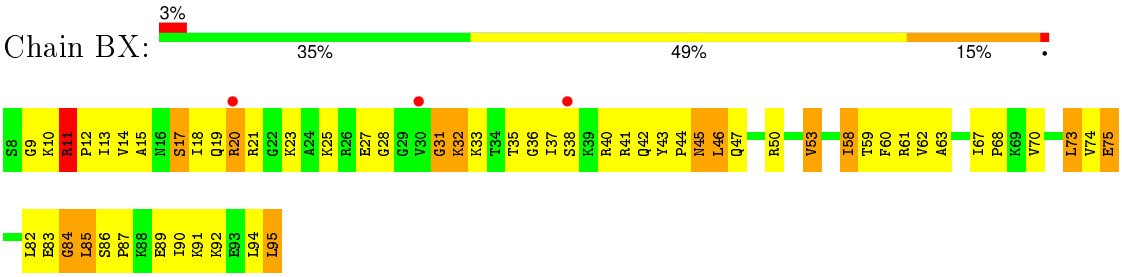
• Molecule 45: 50S ribosomal protein L27

Chain DW:



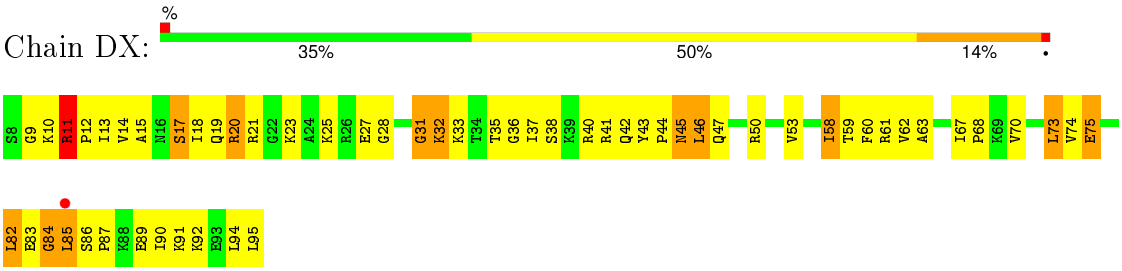
• Molecule 46: 50S ribosomal protein L28

Chain BX:



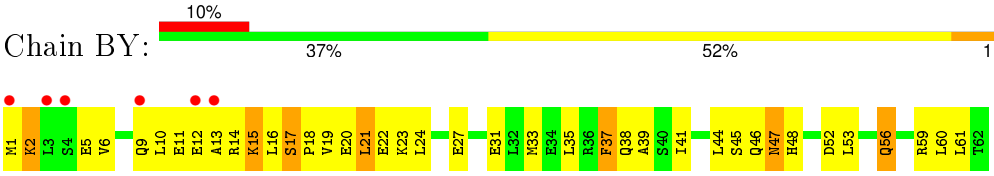
• Molecule 46: 50S ribosomal protein L28

Chain DX:



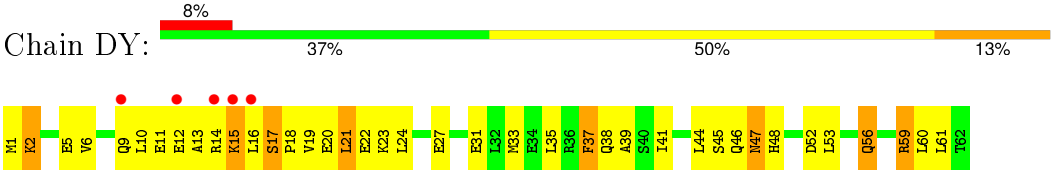
• Molecule 47: 50S ribosomal protein L29

Chain BY:



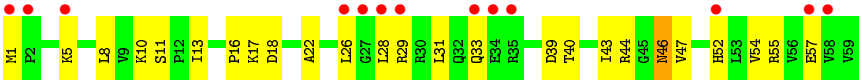
• Molecule 47: 50S ribosomal protein L29

Chain DY:



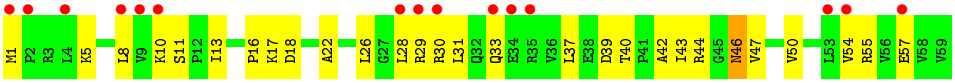
• Molecule 48: 50S ribosomal protein L30

Chain BZ:



• Molecule 48: 50S ribosomal protein L30

Chain DZ:

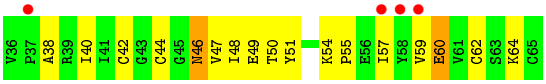


• Molecule 49: 50S ribosomal protein L31

Chain B1:

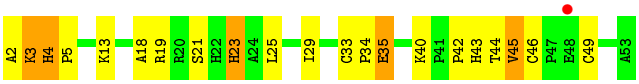
• Molecule 49: 50S ribosomal protein L31

Chain D1:



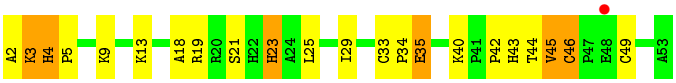
• Molecule 50: 50S ribosomal protein L32

Chain B2:



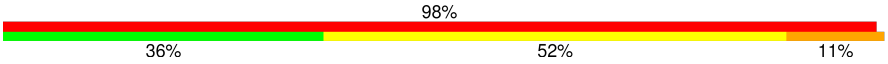
• Molecule 50: 50S ribosomal protein L32

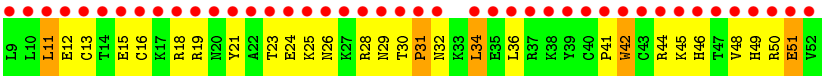
Chain D2:



• Molecule 51: 50S ribosomal protein L33

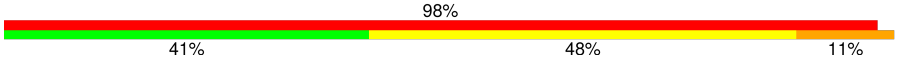
Chain B3:

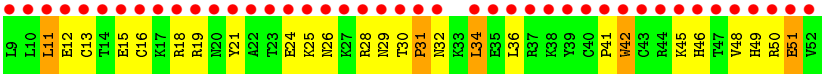




• Molecule 51: 50S ribosomal protein L33

Chain D3:



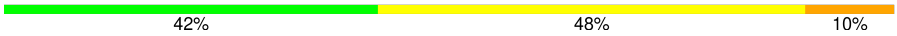


- Molecule 52: 50S ribosomal protein L34

Chain B4:

- Molecule 52: 50S ribosomal protein L34

Chain D4:

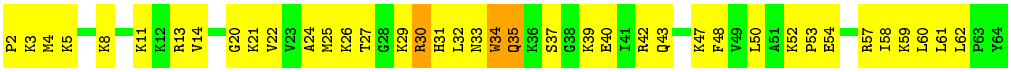


- Molecule 53: 50S ribosomal protein L35

Chain B5:

- Molecule 53: 50S ribosomal protein L35

Chain D5:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.94Å 455.59Å 618.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 60.01 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.6 (60.01-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.233 , 0.264 0.229 , 0.262	Depositor DCC
R_{free} test set	7363 reflections (0.99%)	DCC
Wilson B-factor (Å^2)	106.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 109.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	1 of 746568 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	283641	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.45	0/36238	0.90	34/56561 (0.1%)
1	CA	0.44	0/36238	0.90	34/56561 (0.1%)
2	AB	0.21	0/1936	0.38	0/2609
2	CB	0.21	0/1936	0.38	0/2609
3	AC	0.21	0/1637	0.37	0/2205
3	CC	0.21	0/1637	0.37	0/2205
4	AD	0.24	0/1733	0.40	0/2318
4	CD	0.23	0/1733	0.39	0/2318
5	AE	0.24	0/1172	0.41	0/1576
5	CE	0.23	0/1172	0.40	0/1576
6	AF	0.23	0/856	0.42	0/1154
6	CF	0.23	0/856	0.43	0/1154
7	AG	0.21	0/1276	0.36	0/1709
7	CG	0.22	0/1276	0.36	0/1709
8	AH	0.23	0/1136	0.41	0/1527
8	CH	0.22	0/1136	0.41	0/1527
9	AI	0.22	0/1029	0.38	0/1378
9	CI	0.22	0/1029	0.38	0/1378
10	AJ	0.21	0/808	0.39	0/1085
10	CJ	0.21	0/808	0.39	0/1085
11	AK	0.23	0/900	0.40	0/1213
11	CK	0.23	0/900	0.40	0/1213
12	AL	0.25	0/987	0.46	0/1320
12	CL	0.24	0/987	0.46	0/1320
13	AM	0.24	0/939	0.41	0/1258
13	CM	0.24	0/939	0.41	0/1258
14	AN	0.23	0/501	0.37	0/664
14	CN	0.22	0/501	0.37	0/664
15	AO	0.24	0/745	0.38	0/992
15	CO	0.24	0/745	0.38	0/992
16	AP	0.36	1/717 (0.1%)	0.44	0/963
16	CP	0.44	1/717 (0.1%)	0.45	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.24	0/837	0.41	0/1117
17	CQ	0.23	0/837	0.40	0/1117
18	AR	0.24	0/579	0.42	0/768
18	CR	0.23	0/579	0.42	0/768
19	AS	0.20	0/643	0.37	0/865
19	CS	0.21	0/643	0.37	0/865
20	AT	0.23	0/764	0.39	0/1006
20	CT	0.22	0/764	0.39	0/1006
21	AU	0.20	0/213	0.37	0/277
21	CU	0.19	0/213	0.37	0/277
22	AV	0.43	0/821	0.86	2/1275 (0.2%)
22	CV	0.44	0/821	0.86	2/1275 (0.2%)
23	BA	0.51	0/66575	1.03	115/103930 (0.1%)
23	DA	0.54	0/66575	1.04	119/103930 (0.1%)
24	BB	0.44	0/2853	0.92	1/4451 (0.0%)
24	DB	0.44	0/2853	0.93	2/4451 (0.0%)
25	BC	0.33	0/2155	0.51	0/2905
25	DC	0.34	0/2155	0.52	0/2905
26	BD	0.27	0/1597	0.48	0/2153
26	DD	0.27	0/1597	0.48	0/2153
27	BE	0.29	0/1622	0.46	0/2194
27	DE	0.31	0/1622	0.47	0/2194
28	BF	0.23	0/1500	0.42	0/2017
28	DF	0.23	0/1500	0.42	0/2017
29	BG	0.22	0/1246	0.42	0/1682
29	DG	0.24	0/1246	0.43	0/1682
30	BH	0.29	0/1148	0.46	0/1552
30	DH	0.31	0/1148	0.47	0/1552
31	BI	0.21	0/252	0.38	0/333
31	DI	0.22	0/252	0.38	0/333
32	BJ	0.26	0/1124	0.47	0/1515
32	DJ	0.27	0/1124	0.47	0/1515
33	BK	0.27	0/942	0.48	0/1268
33	DK	0.28	0/942	0.49	0/1268
34	BL	0.30	0/1131	0.56	0/1504
34	DL	0.32	0/1131	0.57	0/1504
35	BM	0.30	0/1099	0.49	0/1468
35	DM	0.30	0/1099	0.50	0/1468
36	BN	0.26	0/974	0.45	0/1302
36	DN	0.27	0/974	0.45	0/1302
37	BO	0.23	0/779	0.42	0/1036
37	DO	0.24	0/779	0.42	0/1036
38	BP	0.27	0/1158	0.44	0/1544

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	DP	0.27	0/1158	0.44	0/1544
39	BQ	0.29	0/970	0.46	0/1290
39	DQ	0.31	0/970	0.47	0/1290
40	BR	0.27	0/790	0.45	0/1057
40	DR	0.29	0/790	0.46	0/1057
41	BS	0.31	0/902	0.51	0/1209
41	DS	0.30	0/902	0.50	0/1209
42	BT	0.30	0/740	0.49	0/993
42	DT	0.33	0/740	0.50	0/993
43	BU	0.25	0/789	0.44	0/1051
43	DU	0.26	0/789	0.45	0/1051
44	BV	0.23	0/1524	0.44	0/2068
44	DV	0.23	0/1524	0.45	0/2068
45	BW	0.26	0/613	0.43	0/816
45	DW	0.27	0/613	0.43	0/816
46	BX	0.30	0/702	0.56	0/932
46	DX	0.31	0/702	0.57	0/932
47	BY	0.29	0/523	0.52	0/690
47	DY	0.31	0/523	0.54	0/690
48	BZ	0.23	0/473	0.41	0/634
48	DZ	0.24	0/473	0.41	0/634
49	B1	0.20	0/229	0.38	0/309
49	D1	0.20	0/229	0.38	0/309
50	B2	0.28	0/419	0.51	0/567
50	D2	0.28	0/419	0.51	0/567
51	B3	0.21	0/388	0.40	0/518
51	D3	0.21	0/388	0.40	0/518
52	B4	0.34	0/427	0.52	0/561
52	D4	0.38	0/427	0.53	0/561
53	B5	0.31	0/516	0.50	0/679
53	D5	0.32	0/516	0.51	0/679
All	All	0.44	2/305254 (0.0%)	0.87	309/456136 (0.1%)

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
28	BF	0	1
28	DF	0	1
34	BL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	DL	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	CP	48	TRP	CG-CD1	7.51	1.47	1.36
16	AP	48	TRP	CG-CD1	6.09	1.45	1.36

The worst 5 of 309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	BA	945	A	C1'-O4'-C4'	-10.48	101.52	109.90
23	BA	1786	A	C1'-O4'-C4'	-10.25	101.70	109.90
23	DA	676	A	C1'-O4'-C4'	-9.79	102.07	109.90
23	DA	1786	A	C1'-O4'-C4'	-9.78	102.07	109.90
23	DA	945	A	C1'-O4'-C4'	-9.73	102.11	109.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BF	75	LYS	Peptide
34	BL	52	GLU	Peptide
28	DF	75	LYS	Peptide
34	DL	52	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32372	0	16339	682	0
1	CA	32372	0	16339	694	0
2	AB	1901	0	1951	103	0
2	CB	1901	0	1951	103	0
3	AC	1613	0	1677	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	1613	0	1677	95	0
4	AD	1703	0	1764	100	0
4	CD	1703	0	1765	92	0
5	AE	1156	0	1213	68	0
5	CE	1156	0	1213	66	0
6	AF	843	0	857	46	0
6	CF	843	0	857	46	0
7	AG	1257	0	1296	60	0
7	CG	1257	0	1296	62	0
8	AH	1116	0	1177	57	0
8	CH	1116	0	1177	59	0
9	AI	1011	0	1043	62	0
9	CI	1011	0	1043	58	0
10	AJ	795	0	840	59	0
10	CJ	795	0	840	59	0
11	AK	885	0	904	56	0
11	CK	885	0	904	50	0
12	AL	971	0	1057	60	0
12	CL	971	0	1057	66	0
13	AM	929	0	987	66	0
13	CM	929	0	987	64	0
14	AN	492	0	529	29	0
14	CN	492	0	533	26	0
15	AO	734	0	771	26	0
15	CO	734	0	771	29	0
16	AP	701	0	720	30	0
16	CP	701	0	720	38	0
17	AQ	824	0	893	42	0
17	CQ	824	0	893	44	0
18	AR	574	0	644	30	0
18	CR	574	0	644	32	0
19	AS	630	0	652	59	0
19	CS	630	0	652	54	0
20	AT	762	0	859	32	0
20	CT	762	0	859	31	0
21	AU	209	0	221	13	0
21	CU	209	0	221	14	0
22	AV	736	0	378	19	0
22	CV	736	0	378	18	0
23	BA	59442	0	29966	1292	0
23	DA	59442	0	29966	1295	0
24	BB	2551	0	1295	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DB	2551	0	1295	53	0
25	BC	2105	0	2182	202	0
25	DC	2105	0	2182	214	0
26	BD	1564	0	1629	117	0
26	DD	1564	0	1629	112	0
27	BE	1587	0	1632	107	0
27	DE	1587	0	1632	106	0
28	BF	1475	0	1537	109	0
28	DF	1475	0	1537	109	0
29	BG	1223	0	1282	64	0
29	DG	1223	0	1282	66	0
30	BH	1133	0	1220	83	0
30	DH	1133	0	1220	80	0
31	BI	254	0	275	8	0
31	DI	254	0	275	8	0
32	BJ	1097	0	1168	82	0
32	DJ	1097	0	1168	83	0
33	BK	932	0	994	54	0
33	DK	932	0	994	56	0
34	BL	1114	0	1187	167	0
34	DL	1114	0	1187	169	0
35	BM	1079	0	1127	96	0
35	DM	1079	0	1127	99	0
36	BN	960	0	1021	73	0
36	DN	960	0	1021	71	0
37	BO	771	0	832	67	0
37	DO	771	0	832	70	0
38	BP	1144	0	1211	69	0
38	DP	1144	0	1211	74	0
39	BQ	953	0	1013	71	0
39	DQ	953	0	1013	71	0
40	BR	779	0	852	76	0
40	DR	779	0	852	73	0
41	BS	891	0	951	50	0
41	DS	891	0	951	52	0
42	BT	726	0	778	58	0
42	DT	726	0	778	59	0
43	BU	776	0	870	78	0
43	DU	776	0	870	76	0
44	BV	1492	0	1513	94	0
44	DV	1492	0	1513	92	0
45	BW	605	0	628	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	DW	605	0	628	38	0
46	BX	695	0	764	69	0
46	DX	695	0	764	68	0
47	BY	521	0	575	45	0
47	DY	521	0	575	45	0
48	BZ	468	0	523	20	0
48	DZ	468	0	523	24	0
49	B1	226	0	225	17	0
49	D1	226	0	225	17	0
50	B2	405	0	420	27	0
50	D2	405	0	420	29	0
51	B3	381	0	391	28	0
51	D3	381	0	391	26	0
52	B4	419	0	467	30	0
52	D4	419	0	467	32	0
53	B5	508	0	576	54	0
53	D5	508	0	576	55	0
54	AA	279	0	0	0	0
54	AB	3	0	0	0	0
54	AC	2	0	0	0	0
54	AD	3	0	0	0	0
54	AE	5	0	0	0	0
54	AF	1	0	0	0	0
54	AG	2	0	0	0	0
54	AH	1	0	0	0	0
54	AI	1	0	0	0	0
54	AK	2	0	0	0	0
54	AL	2	0	0	0	0
54	AM	1	0	0	0	0
54	AN	1	0	0	0	0
54	AO	3	0	0	0	0
54	AQ	3	0	0	0	0
54	AS	1	0	0	0	0
54	AT	2	0	0	0	0
54	AV	8	0	0	0	0
54	B2	3	0	0	0	0
54	B3	1	0	0	0	0
54	B4	1	0	0	0	0
54	B5	1	0	0	0	0
54	BA	781	0	0	0	0
54	BB	27	0	0	0	0
54	BC	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	BE	2	0	0	0	0
54	BF	1	0	0	0	0
54	BH	1	0	0	0	0
54	BI	1	0	0	0	0
54	BJ	3	0	0	0	0
54	BK	1	0	0	0	0
54	BM	3	0	0	0	0
54	BN	2	0	0	0	0
54	BO	1	0	0	0	0
54	BP	2	0	0	0	0
54	BR	1	0	0	0	0
54	BS	1	0	0	0	0
54	BT	2	0	0	0	0
54	BU	2	0	0	0	0
54	BV	3	0	0	0	0
54	BW	1	0	0	0	0
54	BX	2	0	0	0	0
54	BY	3	0	0	0	0
54	CA	372	0	0	0	0
54	CB	3	0	0	0	0
54	CC	8	0	0	0	0
54	CD	3	0	0	0	0
54	CE	5	0	0	0	0
54	CF	2	0	0	0	0
54	CG	3	0	0	0	0
54	CK	1	0	0	0	0
54	CL	6	0	0	0	0
54	CM	2	0	0	0	0
54	CN	1	0	0	0	0
54	CO	4	0	0	0	0
54	CQ	2	0	0	0	0
54	CV	7	0	0	0	0
54	D1	1	0	0	0	0
54	D2	3	0	0	0	0
54	D3	1	0	0	0	0
54	D4	4	0	0	0	0
54	D5	3	0	0	0	0
54	DA	964	0	0	0	0
54	DB	43	0	0	0	0
54	DC	3	0	0	0	0
54	DD	6	0	0	0	0
54	DE	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	DF	2	0	0	0	0
54	DG	3	0	0	0	0
54	DI	1	0	0	0	0
54	DJ	6	0	0	0	0
54	DK	3	0	0	0	0
54	DL	3	0	0	0	0
54	DM	1	0	0	0	0
54	DN	1	0	0	0	0
54	DO	1	0	0	0	0
54	DP	2	0	0	0	0
54	DQ	2	0	0	0	0
54	DS	2	0	0	0	0
54	DU	1	0	0	0	0
54	DV	4	0	0	0	0
54	DW	1	0	0	0	0
54	DX	3	0	0	0	0
54	DY	2	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
All	All	283641	0	191757	9280	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 20.

The worst 5 of 9280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1399:C:H4'	1:AA:1400:C:H5'	1.26	1.16
34:BL:33:ARG:HG3	34:BL:36:LYS:HD3	1.31	1.12
34:BL:128:HIS:HA	34:BL:147:LEU:HB3	1.30	1.11
23:DA:2015:A:H1'	50:D2:2:ALA:HA	1.33	1.08
34:DL:33:ARG:HG3	34:DL:36:LYS:HD3	1.33	1.08

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
2	AB	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	7 45
2	CB	232/234 (99%)	194 (84%)	32 (14%)	6 (3%)	7 45
3	AC	204/206 (99%)	153 (75%)	38 (19%)	13 (6%)	2 20
3	CC	204/206 (99%)	154 (76%)	37 (18%)	13 (6%)	2 20
4	AD	206/208 (99%)	172 (84%)	26 (13%)	8 (4%)	4 34
4	CD	206/208 (99%)	172 (84%)	25 (12%)	9 (4%)	3 30
5	AE	149/151 (99%)	123 (83%)	22 (15%)	4 (3%)	6 44
5	CE	149/151 (99%)	126 (85%)	19 (13%)	4 (3%)	6 44
6	AF	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	19 66
6	CF	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	19 66
7	AG	153/155 (99%)	132 (86%)	18 (12%)	3 (2%)	9 51
7	CG	153/155 (99%)	133 (87%)	17 (11%)	3 (2%)	9 51
8	AH	136/138 (99%)	119 (88%)	17 (12%)	0	100 100
8	CH	136/138 (99%)	119 (88%)	17 (12%)	0	100 100
9	AI	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	7 47
9	CI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	7 47
10	AJ	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	2 21
10	CJ	96/98 (98%)	78 (81%)	12 (12%)	6 (6%)	2 21
11	AK	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	5 39
11	CK	117/119 (98%)	97 (83%)	16 (14%)	4 (3%)	5 39
12	AL	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	3 27
12	CL	122/124 (98%)	94 (77%)	22 (18%)	6 (5%)	3 27
13	AM	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	4 38
13	CM	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	4 38
14	AN	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	2 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	CN	58/60 (97%)	50 (86%)	5 (9%)	3 (5%)	2 25
15	AO	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	8 48
15	CO	86/88 (98%)	77 (90%)	7 (8%)	2 (2%)	8 48
16	AP	81/83 (98%)	65 (80%)	14 (17%)	2 (2%)	7 46
16	CP	81/83 (98%)	65 (80%)	13 (16%)	3 (4%)	4 36
17	AQ	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	19 66
17	CQ	97/99 (98%)	81 (84%)	15 (16%)	1 (1%)	19 66
18	AR	68/70 (97%)	53 (78%)	13 (19%)	2 (3%)	6 42
18	CR	68/70 (97%)	53 (78%)	12 (18%)	3 (4%)	3 30
19	AS	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	1 19
19	CS	76/78 (97%)	57 (75%)	14 (18%)	5 (7%)	1 19
20	AT	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	5 41
20	CT	97/99 (98%)	82 (84%)	12 (12%)	3 (3%)	5 41
21	AU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	3 30
21	CU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	3 30
25	BC	269/271 (99%)	220 (82%)	31 (12%)	18 (7%)	1 19
25	DC	269/271 (99%)	218 (81%)	33 (12%)	18 (7%)	1 19
26	BD	202/204 (99%)	168 (83%)	26 (13%)	8 (4%)	4 33
26	DD	202/204 (99%)	167 (83%)	29 (14%)	6 (3%)	5 42
27	BE	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	4 38
27	DE	200/202 (99%)	165 (82%)	28 (14%)	7 (4%)	4 38
28	BF	179/181 (99%)	134 (75%)	37 (21%)	8 (4%)	3 30
28	DF	179/181 (99%)	133 (74%)	37 (21%)	9 (5%)	3 27
29	BG	157/159 (99%)	126 (80%)	27 (17%)	4 (2%)	7 46
29	DG	157/159 (99%)	125 (80%)	28 (18%)	4 (2%)	7 46
30	BH	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	3 32
30	DH	143/145 (99%)	109 (76%)	28 (20%)	6 (4%)	3 32
31	BI	28/65 (43%)	27 (96%)	1 (4%)	0	100 100
31	DI	28/65 (43%)	27 (96%)	1 (4%)	0	100 100
32	BJ	135/137 (98%)	108 (80%)	19 (14%)	8 (6%)	2 22
32	DJ	135/137 (98%)	108 (80%)	19 (14%)	8 (6%)	2 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
33	BK	120/122 (98%)	105 (88%)	8 (7%)	7 (6%)	2 23
33	DK	120/122 (98%)	107 (89%)	6 (5%)	7 (6%)	2 23
34	BL	144/146 (99%)	94 (65%)	35 (24%)	15 (10%)	1 8
34	DL	144/146 (99%)	92 (64%)	37 (26%)	15 (10%)	1 8
35	BM	134/136 (98%)	98 (73%)	22 (16%)	14 (10%)	1 8
35	DM	134/136 (98%)	97 (72%)	24 (18%)	13 (10%)	1 10
36	BN	115/117 (98%)	97 (84%)	13 (11%)	5 (4%)	3 31
36	DN	115/117 (98%)	97 (84%)	14 (12%)	4 (4%)	4 38
37	BO	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0 4
37	DO	96/98 (98%)	65 (68%)	18 (19%)	13 (14%)	0 4
38	BP	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	3 30
38	DP	135/137 (98%)	99 (73%)	30 (22%)	6 (4%)	3 30
39	BQ	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	11 53
39	DQ	114/116 (98%)	99 (87%)	13 (11%)	2 (2%)	11 53
40	BR	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	1 11
40	DR	99/101 (98%)	71 (72%)	19 (19%)	9 (9%)	1 11
41	BS	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	11 53
41	DS	110/112 (98%)	94 (86%)	14 (13%)	2 (2%)	11 53
42	BT	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	17 63
42	DT	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	17 63
43	BU	98/100 (98%)	65 (66%)	22 (22%)	11 (11%)	0 7
43	DU	98/100 (98%)	63 (64%)	23 (24%)	12 (12%)	0 6
44	BV	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	2 25
44	DV	186/188 (99%)	140 (75%)	36 (19%)	10 (5%)	2 25
45	BW	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	3 33
45	DW	74/76 (97%)	57 (77%)	14 (19%)	3 (4%)	3 33
46	BX	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	1 8
46	DX	86/88 (98%)	57 (66%)	20 (23%)	9 (10%)	1 8
47	BY	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3 27
47	DY	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	3 27
48	BZ	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	11 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	DZ	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	11 53
49	B1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	0 8
49	D1	28/30 (93%)	15 (54%)	10 (36%)	3 (11%)	0 8
50	B2	50/52 (96%)	39 (78%)	8 (16%)	3 (6%)	2 21
50	D2	50/52 (96%)	40 (80%)	6 (12%)	4 (8%)	1 13
51	B3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	0 6
51	D3	42/44 (96%)	35 (83%)	2 (5%)	5 (12%)	0 6
52	B4	46/48 (96%)	42 (91%)	4 (9%)	0	100 100
52	D4	46/48 (96%)	41 (89%)	5 (11%)	0	100 100
53	B5	61/63 (97%)	43 (70%)	13 (21%)	5 (8%)	1 13
53	D5	61/63 (97%)	44 (72%)	13 (21%)	4 (7%)	1 19
All	All	11192/11458 (98%)	8966 (80%)	1699 (15%)	527 (5%)	3 29

5 of 527 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	15	THR
4	AD	30	LYS
4	AD	137	SER
4	AD	138	TYR
4	AD	168	ARG

5.3.2 Protein sidechains (i)

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
2	AB	202/202 (100%)	192 (95%)	10 (5%)	30 69
2	CB	202/202 (100%)	192 (95%)	10 (5%)	30 69
3	AC	160/160 (100%)	154 (96%)	6 (4%)	40 76
3	CC	160/160 (100%)	154 (96%)	6 (4%)	40 76
4	AD	180/180 (100%)	168 (93%)	12 (7%)	20 61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	CD	180/180 (100%)	167 (93%)	13 (7%)	18 57
5	AE	116/116 (100%)	108 (93%)	8 (7%)	19 59
5	CE	116/116 (100%)	108 (93%)	8 (7%)	19 59
6	AF	90/90 (100%)	85 (94%)	5 (6%)	26 66
6	CF	90/90 (100%)	85 (94%)	5 (6%)	26 66
7	AG	126/126 (100%)	126 (100%)	0	100 100
7	CG	126/126 (100%)	126 (100%)	0	100 100
8	AH	119/119 (100%)	114 (96%)	5 (4%)	36 74
8	CH	119/119 (100%)	114 (96%)	5 (4%)	36 74
9	AI	98/98 (100%)	92 (94%)	6 (6%)	23 64
9	CI	98/98 (100%)	92 (94%)	6 (6%)	23 64
10	AJ	88/88 (100%)	79 (90%)	9 (10%)	9 40
10	CJ	88/88 (100%)	79 (90%)	9 (10%)	9 40
11	AK	90/90 (100%)	86 (96%)	4 (4%)	35 73
11	CK	90/90 (100%)	86 (96%)	4 (4%)	35 73
12	AL	104/104 (100%)	94 (90%)	10 (10%)	10 43
12	CL	104/104 (100%)	94 (90%)	10 (10%)	10 43
13	AM	94/94 (100%)	88 (94%)	6 (6%)	22 62
13	CM	94/94 (100%)	88 (94%)	6 (6%)	22 62
14	AN	49/49 (100%)	47 (96%)	2 (4%)	37 74
14	CN	49/49 (100%)	48 (98%)	1 (2%)	63 87
15	AO	79/79 (100%)	75 (95%)	4 (5%)	29 69
15	CO	79/79 (100%)	75 (95%)	4 (5%)	29 69
16	AP	72/72 (100%)	67 (93%)	5 (7%)	19 59
16	CP	72/72 (100%)	68 (94%)	4 (6%)	26 66
17	AQ	94/94 (100%)	92 (98%)	2 (2%)	61 86
17	CQ	94/94 (100%)	92 (98%)	2 (2%)	61 86
18	AR	61/61 (100%)	59 (97%)	2 (3%)	45 79
18	CR	61/61 (100%)	59 (97%)	2 (3%)	45 79
19	AS	69/69 (100%)	60 (87%)	9 (13%)	5 27
19	CS	69/69 (100%)	60 (87%)	9 (13%)	5 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	AT	76/76 (100%)	71 (93%)	5 (7%)	21 61
20	CT	76/76 (100%)	71 (93%)	5 (7%)	21 61
21	AU	19/19 (100%)	18 (95%)	1 (5%)	28 67
21	CU	19/19 (100%)	18 (95%)	1 (5%)	28 67
25	BC	213/213 (100%)	192 (90%)	21 (10%)	10 41
25	DC	213/213 (100%)	192 (90%)	21 (10%)	10 41
26	BD	165/165 (100%)	149 (90%)	16 (10%)	10 42
26	DD	165/165 (100%)	149 (90%)	16 (10%)	10 42
27	BE	161/161 (100%)	148 (92%)	13 (8%)	15 52
27	DE	161/161 (100%)	147 (91%)	14 (9%)	13 48
28	BF	155/155 (100%)	144 (93%)	11 (7%)	18 58
28	DF	155/155 (100%)	144 (93%)	11 (7%)	18 58
29	BG	132/132 (100%)	123 (93%)	9 (7%)	20 60
29	DG	132/132 (100%)	123 (93%)	9 (7%)	20 60
30	BH	122/122 (100%)	115 (94%)	7 (6%)	25 66
30	DH	122/122 (100%)	115 (94%)	7 (6%)	25 66
31	BI	27/53 (51%)	26 (96%)	1 (4%)	41 76
31	DI	27/53 (51%)	26 (96%)	1 (4%)	41 76
32	BJ	116/116 (100%)	103 (89%)	13 (11%)	7 35
32	DJ	116/116 (100%)	103 (89%)	13 (11%)	7 35
33	BK	100/100 (100%)	92 (92%)	8 (8%)	15 52
33	DK	100/100 (100%)	92 (92%)	8 (8%)	15 52
34	BL	112/112 (100%)	87 (78%)	25 (22%)	1 6
34	DL	112/112 (100%)	87 (78%)	25 (22%)	1 6
35	BM	106/106 (100%)	98 (92%)	8 (8%)	17 55
35	DM	106/106 (100%)	98 (92%)	8 (8%)	17 55
36	BN	100/100 (100%)	94 (94%)	6 (6%)	24 64
36	DN	100/100 (100%)	94 (94%)	6 (6%)	24 64
37	BO	77/77 (100%)	68 (88%)	9 (12%)	7 32
37	DO	77/77 (100%)	68 (88%)	9 (12%)	7 32
38	BP	121/121 (100%)	109 (90%)	12 (10%)	10 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	DP	121/121 (100%)	110 (91%)	11 (9%)	12 46
39	BQ	92/92 (100%)	88 (96%)	4 (4%)	35 74
39	DQ	92/92 (100%)	88 (96%)	4 (4%)	35 74
40	BR	82/82 (100%)	77 (94%)	5 (6%)	23 64
40	DR	82/82 (100%)	77 (94%)	5 (6%)	23 64
41	BS	91/91 (100%)	85 (93%)	6 (7%)	21 61
41	DS	91/91 (100%)	85 (93%)	6 (7%)	21 61
42	BT	74/74 (100%)	67 (90%)	7 (10%)	11 43
42	DT	74/74 (100%)	67 (90%)	7 (10%)	11 43
43	BU	84/84 (100%)	78 (93%)	6 (7%)	18 58
43	DU	84/84 (100%)	78 (93%)	6 (7%)	18 58
44	BV	163/163 (100%)	159 (98%)	4 (2%)	55 84
44	DV	163/163 (100%)	159 (98%)	4 (2%)	55 84
45	BW	61/61 (100%)	55 (90%)	6 (10%)	10 42
45	DW	61/61 (100%)	55 (90%)	6 (10%)	10 42
46	BX	73/73 (100%)	61 (84%)	12 (16%)	3 17
46	DX	73/73 (100%)	61 (84%)	12 (16%)	3 17
47	BY	58/58 (100%)	51 (88%)	7 (12%)	6 30
47	DY	58/58 (100%)	51 (88%)	7 (12%)	6 30
48	BZ	51/51 (100%)	49 (96%)	2 (4%)	39 76
48	DZ	51/51 (100%)	49 (96%)	2 (4%)	39 76
49	B1	27/27 (100%)	24 (89%)	3 (11%)	8 35
49	D1	27/27 (100%)	24 (89%)	3 (11%)	8 35
50	B2	45/45 (100%)	43 (96%)	2 (4%)	35 73
50	D2	45/45 (100%)	43 (96%)	2 (4%)	35 73
51	B3	43/43 (100%)	39 (91%)	4 (9%)	11 45
51	D3	43/43 (100%)	39 (91%)	4 (9%)	11 45
52	B4	41/41 (100%)	34 (83%)	7 (17%)	2 15
52	D4	41/41 (100%)	34 (83%)	7 (17%)	2 15
53	B5	53/53 (100%)	51 (96%)	2 (4%)	40 76
53	D5	53/53 (100%)	51 (96%)	2 (4%)	40 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9462/9514 (100%)	8769 (93%)	693 (7%)	17 57

5 of 693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BX	45	ASN
6	CF	98	LEU
43	DU	8	LYS
47	BY	37	PHE
2	CB	116	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 257 such sidechains are listed below:

Mol	Chain	Res	Type
46	BX	19	GLN
5	CE	78	HIS
43	DU	6	HIS
46	BX	66	HIS
53	B5	33	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	204 (13%)	35 (2%)
1	CA	1505/1506 (99%)	205 (13%)	35 (2%)
22	AV	34/35 (97%)	2 (5%)	2 (5%)
22	CV	34/35 (97%)	2 (5%)	2 (5%)
23	BA	2757/2879 (95%)	410 (14%)	69 (2%)
23	DA	2757/2879 (95%)	407 (14%)	70 (2%)
24	BB	118/119 (99%)	16 (13%)	1 (0%)
24	DB	118/119 (99%)	16 (13%)	1 (0%)
All	All	8828/9078 (97%)	1262 (14%)	215 (2%)

5 of 1262 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

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Mol	Chain	Res	Type
1	AA	41	G

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BA	2468	G
1	CA	496	A
23	DA	2098	U
23	BA	2585	U
1	CA	119	A

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2661 ligands modelled in this entry, 2661 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1506/1506 (100%)	0.10	58 (3%) 43 35	66, 119, 257, 429	0
1	CA	1506/1506 (100%)	0.32	99 (6%) 22 16	75, 164, 286, 403	0
2	AB	234/234 (100%)	1.53	80 (34%) 0 0	88, 178, 260, 354	0
2	CB	234/234 (100%)	1.37	73 (31%) 1 1	106, 202, 279, 372	0
3	AC	206/206 (100%)	0.59	22 (10%) 8 7	83, 165, 233, 293	0
3	CC	206/206 (100%)	0.67	32 (15%) 3 3	124, 198, 272, 337	0
4	AD	208/208 (100%)	0.04	4 (1%) 70 60	45, 119, 180, 228	0
4	CD	208/208 (100%)	0.48	20 (9%) 10 9	96, 186, 253, 314	0
5	AE	151/151 (100%)	0.00	3 (1%) 68 59	71, 118, 191, 293	0
5	CE	151/151 (100%)	0.20	6 (3%) 42 33	72, 165, 223, 282	0
6	AF	101/101 (100%)	0.72	19 (18%) 2 2	87, 160, 207, 278	0
6	CF	101/101 (100%)	0.03	5 (4%) 32 25	60, 130, 195, 271	0
7	AG	155/155 (100%)	0.98	30 (19%) 1 2	134, 201, 260, 328	0
7	CG	155/155 (100%)	1.10	34 (21%) 1 1	124, 213, 271, 320	0
8	AH	138/138 (100%)	0.46	15 (10%) 7 7	60, 122, 190, 265	0
8	CH	138/138 (100%)	0.70	19 (13%) 4 4	101, 171, 217, 257	0
9	AI	127/127 (100%)	1.82	49 (38%) 0 0	119, 228, 303, 333	0
9	CI	127/127 (100%)	1.48	39 (30%) 1 1	148, 229, 297, 370	0
10	AJ	98/98 (100%)	2.01	46 (46%) 0 0	113, 203, 294, 334	0
10	CJ	98/98 (100%)	1.92	40 (40%) 0 0	133, 232, 290, 339	0
11	AK	119/119 (100%)	-0.07	9 (7%) 17 14	66, 136, 219, 274	0
11	CK	119/119 (100%)	0.27	8 (6%) 21 16	87, 145, 207, 287	0
12	AL	124/124 (100%)	0.60	9 (7%) 18 14	56, 108, 182, 328	0
12	CL	124/124 (100%)	0.48	12 (9%) 10 9	77, 139, 236, 271	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	116/116 (100%)	1.07	25 (21%) 1 1	129, 216, 277, 325	0
13	CM	116/116 (100%)	2.08	51 (43%) 0 0	119, 238, 307, 372	0
14	AN	60/60 (100%)	1.46	17 (28%) 1 1	94, 178, 243, 278	0
14	CN	60/60 (100%)	1.91	25 (41%) 0 0	110, 207, 261, 344	0
15	AO	88/88 (100%)	-0.06	0 100 100	73, 127, 187, 281	0
15	CO	88/88 (100%)	0.12	5 (5%) 27 21	73, 138, 201, 244	0
16	AP	83/83 (100%)	0.31	4 (4%) 34 27	67, 109, 175, 245	0
16	CP	83/83 (100%)	0.87	23 (27%) 1 1	128, 171, 247, 277	0
17	AQ	99/99 (100%)	-0.12	0 100 100	63, 112, 169, 222	0
17	CQ	99/99 (100%)	0.70	15 (15%) 3 3	99, 155, 196, 228	0
18	AR	70/70 (100%)	1.24	18 (25%) 1 1	82, 149, 241, 325	0
18	CR	70/70 (100%)	0.82	10 (14%) 4 4	76, 145, 204, 232	0
19	AS	78/78 (100%)	1.92	32 (41%) 0 0	133, 212, 274, 295	0
19	CS	78/78 (100%)	2.12	35 (44%) 0 0	173, 235, 302, 347	0
20	AT	99/99 (100%)	0.42	8 (8%) 15 12	65, 131, 220, 241	0
20	CT	99/99 (100%)	2.09	47 (47%) 0 0	103, 178, 284, 301	0
21	AU	24/24 (100%)	2.38	13 (54%) 0 0	122, 220, 292, 333	0
21	CU	24/24 (100%)	2.01	9 (37%) 0 0	173, 236, 317, 346	0
22	AV	35/35 (100%)	1.52	12 (34%) 0 0	96, 223, 325, 366	0
22	CV	35/35 (100%)	1.13	6 (17%) 2 2	117, 192, 362, 386	0
23	BA	2760/2879 (95%)	-0.04	67 (2%) 62 52	38, 86, 205, 371	0
23	DA	2760/2879 (95%)	-0.10	44 (1%) 74 65	33, 77, 196, 377	0
24	BB	119/119 (100%)	-0.02	0 100 100	83, 149, 196, 251	0
24	DB	119/119 (100%)	0.03	6 (5%) 32 25	87, 132, 198, 274	0
25	BC	271/271 (100%)	-0.05	4 (1%) 76 67	24, 81, 150, 209	0
25	DC	271/271 (100%)	-0.30	0 100 100	26, 72, 144, 220	0
26	BD	204/204 (100%)	0.14	3 (1%) 76 67	45, 96, 173, 331	0
26	DD	204/204 (100%)	-0.02	3 (1%) 76 67	36, 90, 189, 305	0
27	BE	202/202 (100%)	0.12	4 (1%) 68 59	32, 94, 172, 311	0
27	DE	202/202 (100%)	0.18	8 (3%) 42 33	20, 85, 182, 249	0
28	BF	181/181 (100%)	0.50	19 (10%) 8 8	107, 202, 262, 297	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	DF	181/181 (100%)	0.48	20 (11%) 7 7	109, 198, 281, 324	0
29	BG	159/159 (100%)	1.28	47 (29%) 1 1	102, 192, 269, 331	0
29	DG	159/159 (100%)	0.20	10 (6%) 23 18	61, 117, 190, 269	0
30	BH	145/145 (100%)	1.78	42 (28%) 1 1	60, 224, 376, 453	0
30	DH	145/145 (100%)	1.73	49 (33%) 0 0	60, 210, 372, 482	0
31	BI	32/65 (49%)	6.39	31 (96%) 0 0	163, 256, 325, 352	0
31	DI	32/65 (49%)	2.47	21 (65%) 0 0	176, 235, 294, 325	0
32	BJ	137/137 (100%)	0.30	3 (2%) 65 55	58, 105, 182, 221	0
32	DJ	137/137 (100%)	0.03	1 (0%) 89 82	55, 101, 170, 219	0
33	BK	122/122 (100%)	-0.22	0 100 100	48, 90, 142, 194	0
33	DK	122/122 (100%)	-0.21	0 100 100	41, 90, 153, 251	0
34	BL	146/146 (100%)	0.50	10 (6%) 20 16	40, 114, 204, 306	0
34	DL	146/146 (100%)	0.42	11 (7%) 17 14	27, 111, 207, 324	0
35	BM	136/136 (100%)	0.12	4 (2%) 55 45	57, 110, 205, 344	0
35	DM	136/136 (100%)	0.41	8 (5%) 26 20	46, 106, 199, 388	0
36	BN	117/117 (100%)	0.14	2 (1%) 73 64	44, 92, 166, 282	0
36	DN	117/117 (100%)	0.09	2 (1%) 73 64	41, 89, 173, 285	0
37	BO	98/98 (100%)	2.05	46 (46%) 0 0	89, 155, 230, 299	0
37	DO	98/98 (100%)	0.73	18 (18%) 2 2	80, 148, 221, 299	0
38	BP	137/137 (100%)	0.30	6 (4%) 38 29	52, 115, 216, 248	0
38	DP	137/137 (100%)	0.37	11 (8%) 15 12	60, 119, 249, 299	0
39	BQ	116/116 (100%)	-0.06	2 (1%) 73 64	43, 88, 163, 244	0
39	DQ	116/116 (100%)	-0.28	0 100 100	34, 84, 154, 205	0
40	BR	101/101 (100%)	-0.18	0 100 100	55, 134, 187, 294	0
40	DR	101/101 (100%)	-0.26	0 100 100	52, 132, 197, 321	0
41	BS	112/112 (100%)	0.48	5 (4%) 37 29	45, 78, 151, 250	0
41	DS	112/112 (100%)	0.03	1 (0%) 85 78	40, 72, 166, 277	0
42	BT	92/92 (100%)	0.09	1 (1%) 82 73	57, 107, 174, 204	0
42	DT	92/92 (100%)	0.10	0 100 100	41, 78, 161, 204	0
43	BU	100/100 (100%)	0.48	12 (12%) 6 6	59, 139, 289, 344	0
43	DU	100/100 (100%)	0.71	10 (10%) 9 9	49, 119, 264, 373	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	BV	188/188 (100%)	0.67	27 (14%) 3 4	80, 160, 224, 277	0
44	DV	188/188 (100%)	0.22	13 (6%) 20 16	67, 154, 220, 254	0
45	BW	76/76 (100%)	-0.07	3 (3%) 43 35	61, 101, 160, 258	0
45	DW	76/76 (100%)	0.20	2 (2%) 59 49	54, 101, 167, 254	0
46	BX	88/88 (100%)	0.06	3 (3%) 49 40	50, 106, 191, 346	0
46	DX	88/88 (100%)	-0.04	1 (1%) 82 73	31, 83, 196, 340	0
47	BY	62/62 (100%)	0.23	6 (9%) 10 9	61, 141, 244, 287	0
47	DY	62/62 (100%)	0.45	5 (8%) 15 12	45, 99, 224, 304	0
48	BZ	59/59 (100%)	1.41	13 (22%) 1 1	47, 102, 174, 342	0
48	DZ	59/59 (100%)	1.43	15 (25%) 1 1	45, 102, 189, 335	0
49	B1	30/30 (100%)	1.78	9 (30%) 1 1	161, 244, 282, 323	0
49	D1	30/30 (100%)	0.96	4 (13%) 4 5	187, 262, 306, 326	0
50	B2	52/52 (100%)	-0.29	1 (1%) 70 60	36, 93, 189, 273	0
50	D2	52/52 (100%)	-0.37	1 (1%) 70 60	24, 93, 214, 262	0
51	B3	44/44 (100%)	6.82	43 (97%) 0 0	151, 254, 304, 322	0
51	D3	44/44 (100%)	7.53	43 (97%) 0 0	191, 247, 298, 313	0
52	B4	48/48 (100%)	0.14	1 (2%) 67 58	43, 66, 132, 297	0
52	D4	48/48 (100%)	-0.27	0 100 100	23, 45, 122, 217	0
53	B5	63/63 (100%)	-0.20	1 (1%) 74 65	47, 94, 171, 222	0
53	D5	63/63 (100%)	0.18	0 100 100	43, 92, 170, 209	0
All	All	20232/20536 (98%)	0.37	1808 (8%) 12 10	20, 120, 258, 482	0

The worst 5 of 1808 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	DU	52	SER	23.5
1	AA	85	U	22.6
30	BH	84	GLY	21.6
30	DH	90	GLY	18.4
1	AA	82	U	17.7

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3321	1/1	0.91	0.72	63.58	110,110,110,110	0
54	MG	AA	1613	1/1	0.96	0.63	60.65	55,55,55,55	0
54	MG	AA	1820	1/1	0.47	1.17	60.51	94,94,94,94	0
54	MG	DA	3646	1/1	0.87	0.67	57.35	45,45,45,45	0
54	MG	BA	2926	1/1	0.80	0.69	55.26	50,50,50,50	0
54	MG	BA	3451	1/1	0.78	0.94	54.98	47,47,47,47	0
54	MG	DA	3689	1/1	0.80	1.08	47.20	67,67,67,67	0
54	MG	DA	3178	1/1	0.88	0.66	42.10	54,54,54,54	0
54	MG	BA	2957	1/1	0.85	0.84	41.63	75,75,75,75	0
54	MG	BA	3040	1/1	0.75	1.23	38.37	76,76,76,76	0
54	MG	BA	3425	1/1	0.86	0.67	38.34	85,85,85,85	0
54	MG	DA	3072	1/1	0.87	0.72	37.98	80,80,80,80	0
54	MG	AA	1860	1/1	0.73	0.86	37.30	138,138,138,138	0
54	MG	BA	3643	1/1	0.68	0.84	34.13	92,92,92,92	0
54	MG	DA	3020	1/1	0.92	0.73	33.61	47,47,47,47	0
54	MG	BA	3239	1/1	0.90	0.80	32.70	62,62,62,62	0
54	MG	BA	3060	1/1	0.91	1.14	31.24	110,110,110,110	0
54	MG	BA	3003	1/1	0.78	0.47	30.71	55,55,55,55	0
54	MG	AA	1800	1/1	0.73	1.10	30.07	69,69,69,69	0
54	MG	BA	2929	1/1	0.92	0.69	29.83	50,50,50,50	0
54	MG	DA	3667	1/1	0.90	0.76	29.82	59,59,59,59	0
54	MG	BA	3073	1/1	0.88	0.34	28.99	63,63,63,63	0
54	MG	DA	3103	1/1	0.63	0.67	28.48	58,58,58,58	0
54	MG	AA	1760	1/1	0.91	0.77	28.16	88,88,88,88	0
54	MG	AA	1846	1/1	0.79	0.40	27.84	88,88,88,88	0
54	MG	DA	3227	1/1	0.93	0.49	27.80	43,43,43,43	0
54	MG	DA	3063	1/1	0.88	0.69	26.99	126,126,126,126	0
54	MG	DA	3629	1/1	0.96	0.77	25.85	89,89,89,89	0
54	MG	DA	3065	1/1	0.88	0.41	25.80	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3340	1/1	0.95	0.58	25.78	85,85,85,85	0
54	MG	DA	3698	1/1	0.72	0.66	25.45	61,61,61,61	0
54	MG	BA	3196	1/1	0.85	0.86	25.32	80,80,80,80	0
54	MG	DA	3603	1/1	0.79	0.69	25.30	64,64,64,64	0
54	MG	BA	2968	1/1	0.89	0.53	25.00	47,47,47,47	0
54	MG	BA	3136	1/1	0.79	0.36	24.64	64,64,64,64	0
54	MG	BA	3048	1/1	0.90	0.69	24.25	70,70,70,70	0
54	MG	DA	2971	1/1	0.94	0.68	23.94	38,38,38,38	0
54	MG	DA	3080	1/1	0.88	0.78	23.25	83,83,83,83	0
54	MG	DA	3650	1/1	0.83	0.43	22.80	55,55,55,55	0
54	MG	DA	2953	1/1	0.81	0.61	22.72	46,46,46,46	0
54	MG	DA	3637	1/1	0.91	0.47	22.35	15,15,15,15	0
54	MG	BA	3023	1/1	0.86	0.70	22.18	57,57,57,57	0
54	MG	CA	1665	1/1	0.77	1.01	22.02	71,71,71,71	0
54	MG	DA	3013	1/1	0.75	0.90	21.61	52,52,52,52	0
54	MG	DA	3472	1/1	0.95	0.66	21.14	95,95,95,95	0
54	MG	BA	3570	1/1	0.66	0.53	20.73	67,67,67,67	0
54	MG	BA	3159	1/1	0.88	0.69	20.12	59,59,59,59	0
54	MG	BA	3070	1/1	0.74	0.39	20.06	85,85,85,85	0
54	MG	AA	1667	1/1	0.91	0.85	20.06	78,78,78,78	0
54	MG	AA	1724	1/1	0.83	0.35	19.96	79,79,79,79	0
54	MG	DA	2957	1/1	0.90	0.63	19.49	40,40,40,40	0
54	MG	DA	3333	1/1	0.75	0.51	19.43	90,90,90,90	0
54	MG	AA	1620	1/1	0.84	0.58	18.63	56,56,56,56	0
54	MG	BA	3020	1/1	0.85	0.60	18.53	88,88,88,88	0
54	MG	DA	2986	1/1	0.87	0.59	18.15	41,41,41,41	0
54	MG	DA	3177	1/1	0.96	0.59	18.11	46,46,46,46	0
54	MG	DA	3633	1/1	0.86	0.43	17.83	83,83,83,83	0
54	MG	BA	3455	1/1	0.99	0.28	17.39	32,32,32,32	0
54	MG	CA	1676	1/1	0.94	0.49	17.34	90,90,90,90	0
54	MG	BA	3626	1/1	0.81	0.60	17.18	64,64,64,64	0
54	MG	BA	3088	1/1	0.95	0.50	16.97	57,57,57,57	0
54	MG	DA	3018	1/1	0.97	0.44	16.78	60,60,60,60	0
54	MG	BA	3021	1/1	0.90	0.53	16.62	66,66,66,66	0
54	MG	DA	3563	1/1	0.92	0.96	16.47	95,95,95,95	0
54	MG	DA	3144	1/1	0.94	0.32	16.36	69,69,69,69	0
54	MG	DA	3684	1/1	0.98	0.37	16.26	69,69,69,69	0
54	MG	BA	2911	1/1	0.92	0.63	16.07	33,33,33,33	0
54	MG	DA	2923	1/1	0.98	0.46	15.97	12,12,12,12	0
54	MG	BA	3058	1/1	0.85	0.48	15.62	78,78,78,78	0
54	MG	BA	3432	1/1	0.97	0.49	15.52	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1875	1/1	0.96	0.64	15.47	63,63,63,63	0
54	MG	BA	3008	1/1	0.83	0.36	15.28	70,70,70,70	0
54	MG	DA	2954	1/1	0.97	0.59	15.08	41,41,41,41	0
54	MG	AA	1631	1/1	0.59	0.43	15.05	76,76,76,76	0
54	MG	DA	3193	1/1	0.82	0.32	15.00	86,86,86,86	0
54	MG	BA	2963	1/1	0.84	0.70	14.97	34,34,34,34	0
54	MG	DA	2947	1/1	0.89	0.48	14.69	37,37,37,37	0
54	MG	BA	2906	1/1	0.98	0.50	14.45	24,24,24,24	0
54	MG	AA	1606	1/1	0.94	0.53	14.29	62,62,62,62	0
54	MG	DC	302	1/1	0.93	0.41	13.88	164,164,164,164	0
54	MG	BA	2939	1/1	0.92	0.52	13.76	47,47,47,47	0
54	MG	BA	3556	1/1	0.92	0.55	13.70	77,77,77,77	0
54	MG	CA	1619	1/1	0.95	0.52	13.66	62,62,62,62	0
54	MG	AA	1664	1/1	0.68	0.44	13.60	80,80,80,80	0
54	MG	DA	3863	1/1	0.84	0.94	13.55	104,104,104,104	0
54	MG	BA	3461	1/1	0.92	0.50	13.45	48,48,48,48	0
54	MG	DA	2913	1/1	0.95	0.67	13.19	21,21,21,21	0
54	MG	DA	3057	1/1	0.83	0.36	13.02	79,79,79,79	0
54	MG	BA	2924	1/1	0.96	0.44	13.02	48,48,48,48	0
54	MG	DA	2901	1/1	0.96	0.53	12.70	9,9,9,9	0
54	MG	BA	3072	1/1	0.94	0.33	12.17	57,57,57,57	0
54	MG	BA	2903	1/1	0.95	0.90	12.11	22,22,22,22	0
54	MG	DA	3154	1/1	0.80	0.39	12.05	50,50,50,50	0
54	MG	BA	3227	1/1	0.94	0.67	11.88	61,61,61,61	0
54	MG	DA	3038	1/1	0.87	0.42	11.71	44,44,44,44	0
54	MG	BA	3122	1/1	0.93	0.24	11.70	56,56,56,56	0
54	MG	BA	2913	1/1	0.94	0.60	11.67	27,27,27,27	0
54	MG	DA	2907	1/1	0.95	0.57	11.53	17,17,17,17	0
54	MG	BA	2920	1/1	0.93	0.41	11.45	24,24,24,24	0
54	MG	DA	2928	1/1	0.93	0.49	11.42	31,31,31,31	0
54	MG	DA	2985	1/1	0.85	0.36	11.42	40,40,40,40	0
54	MG	DA	3511	1/1	0.83	0.51	11.38	52,52,52,52	0
54	MG	AA	1711	1/1	0.91	0.34	11.34	58,58,58,58	0
54	MG	DA	3534	1/1	0.89	0.32	11.31	83,83,83,83	0
54	MG	BA	2954	1/1	0.88	0.27	11.14	73,73,73,73	0
54	MG	AA	1651	1/1	0.93	0.34	10.74	56,56,56,56	0
54	MG	DB	207	1/1	0.97	0.29	10.69	58,58,58,58	0
54	MG	AA	1626	1/1	0.81	0.23	10.68	88,88,88,88	0
54	MG	BA	2916	1/1	0.95	0.47	10.67	37,37,37,37	0
54	MG	DA	3742	1/1	0.94	0.41	10.65	47,47,47,47	0
54	MG	DA	3655	1/1	0.77	0.35	10.59	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3733	1/1	0.63	0.49	10.58	84,84,84,84	0
54	MG	DA	3226	1/1	0.85	0.41	10.35	86,86,86,86	0
54	MG	BA	3597	1/1	0.88	0.28	10.29	56,56,56,56	0
54	MG	BA	2934	1/1	0.94	0.53	10.15	33,33,33,33	0
54	MG	DA	3160	1/1	0.96	0.41	10.09	53,53,53,53	0
54	MG	DA	2902	1/1	0.95	0.55	10.06	17,17,17,17	0
54	MG	AA	1647	1/1	0.96	0.44	9.98	63,63,63,63	0
54	MG	DA	2918	1/1	0.98	0.56	9.89	25,25,25,25	0
54	MG	CA	1680	1/1	0.83	0.41	9.83	63,63,63,63	0
54	MG	DA	2982	1/1	0.94	0.26	9.81	39,39,39,39	0
54	MG	DA	3569	1/1	0.93	0.48	9.71	36,36,36,36	0
54	MG	BA	2907	1/1	0.99	0.35	9.64	15,15,15,15	0
54	MG	BA	3049	1/1	0.91	0.54	9.56	58,58,58,58	0
54	MG	BA	2902	1/1	0.97	0.51	9.46	12,12,12,12	0
54	MG	AA	1628	1/1	0.91	0.45	9.42	86,86,86,86	0
54	MG	CA	1602	1/1	0.86	0.51	9.41	43,43,43,43	0
54	MG	DA	3161	1/1	0.95	0.45	9.39	70,70,70,70	0
54	MG	AA	1685	1/1	0.82	0.39	9.28	64,64,64,64	0
54	MG	BA	2922	1/1	0.97	0.53	9.28	38,38,38,38	0
54	MG	CA	1606	1/1	0.98	0.46	9.26	57,57,57,57	0
54	MG	DA	2908	1/1	0.96	0.46	9.15	20,20,20,20	0
54	MG	BA	3172	1/1	0.89	0.26	9.13	74,74,74,74	0
54	MG	CA	1601	1/1	0.92	0.40	9.02	60,60,60,60	0
54	MG	DA	3024	1/1	0.71	0.37	8.96	58,58,58,58	0
54	MG	DA	2925	1/1	0.97	0.40	8.86	34,34,34,34	0
54	MG	DA	3035	1/1	0.95	0.61	8.86	43,43,43,43	0
54	MG	AA	1681	1/1	0.92	0.41	8.70	65,65,65,65	0
54	MG	DA	3859	1/1	0.94	0.40	8.48	55,55,55,55	0
54	MG	DA	3045	1/1	0.92	0.59	8.48	39,39,39,39	0
54	MG	BA	3150	1/1	0.73	0.61	8.47	97,97,97,97	0
54	MG	DA	2932	1/1	0.98	0.24	8.35	24,24,24,24	0
54	MG	BA	3022	1/1	0.76	0.38	8.25	83,83,83,83	0
54	MG	DA	3059	1/1	0.98	0.34	8.21	39,39,39,39	0
54	MG	DA	3173	1/1	0.87	0.29	7.83	73,73,73,73	0
54	MG	DA	3106	1/1	0.90	0.26	7.78	69,69,69,69	0
54	MG	DA	3158	1/1	0.88	0.40	7.74	42,42,42,42	0
54	MG	BA	3068	1/1	0.90	0.25	7.69	55,55,55,55	0
54	MG	BA	3114	1/1	0.67	0.48	7.67	69,69,69,69	0
54	MG	CA	1891	1/1	0.71	0.43	7.65	113,113,113,113	0
54	MG	DA	3267	1/1	0.69	0.39	7.63	43,43,43,43	0
54	MG	DA	3414	1/1	0.94	0.32	7.60	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	2997	1/1	0.95	0.29	7.54	46,46,46,46	0
54	MG	DA	3074	1/1	0.95	0.32	7.51	43,43,43,43	0
54	MG	DA	2973	1/1	0.99	0.30	7.42	50,50,50,50	0
54	MG	BA	3064	1/1	0.89	0.37	7.36	61,61,61,61	0
54	MG	AA	1828	1/1	0.94	0.38	7.31	82,82,82,82	0
54	MG	DA	3258	1/1	0.96	0.28	7.21	67,67,67,67	0
54	MG	DA	3607	1/1	0.93	0.41	7.18	79,79,79,79	0
54	MG	BA	3004	1/1	0.95	0.28	7.14	49,49,49,49	0
54	MG	BA	3051	1/1	0.97	0.49	7.13	62,62,62,62	0
54	MG	CA	1737	1/1	0.86	0.47	7.12	70,70,70,70	0
54	MG	BA	2923	1/1	0.94	0.49	7.08	13,13,13,13	0
54	MG	DA	3064	1/1	0.96	0.24	6.97	127,127,127,127	0
54	MG	DA	3622	1/1	0.94	0.35	6.84	45,45,45,45	0
54	MG	BA	3187	1/1	0.62	0.75	6.81	73,73,73,73	0
54	MG	DA	3357	1/1	0.98	0.35	6.78	169,169,169,169	0
54	MG	DA	3311	1/1	0.70	0.55	6.70	95,95,95,95	0
54	MG	BA	2945	1/1	0.95	0.29	6.62	56,56,56,56	0
54	MG	BA	2912	1/1	0.89	0.50	6.57	19,19,19,19	0
54	MG	BA	3164	1/1	0.92	0.34	6.47	75,75,75,75	0
54	MG	BA	3442	1/1	0.96	0.51	6.38	26,26,26,26	0
54	MG	AA	1778	1/1	0.85	0.62	6.38	113,113,113,113	0
54	MG	DA	3840	1/1	0.88	0.38	6.37	81,81,81,81	0
54	MG	DA	3180	1/1	0.80	0.30	6.34	78,78,78,78	0
54	MG	BA	3243	1/1	0.80	0.51	6.29	85,85,85,85	0
54	MG	DA	2934	1/1	0.97	0.40	6.27	13,13,13,13	0
54	MG	CA	1733	1/1	0.94	0.56	6.16	78,78,78,78	0
54	MG	BA	2909	1/1	0.98	0.48	6.15	16,16,16,16	0
54	MG	AA	1632	1/1	0.89	0.34	6.08	65,65,65,65	0
54	MG	DA	3360	1/1	0.82	0.33	6.04	107,107,107,107	0
54	MG	BX	102	1/1	0.88	0.35	5.97	103,103,103,103	0
54	MG	BA	3443	1/1	0.98	0.34	5.97	36,36,36,36	0
54	MG	DA	3152	1/1	0.90	0.38	5.96	43,43,43,43	0
54	MG	BA	2919	1/1	0.98	0.32	5.86	14,14,14,14	0
54	MG	AA	1729	1/1	0.72	0.47	5.80	107,107,107,107	0
54	MG	BA	2955	1/1	0.97	0.32	5.80	63,63,63,63	0
54	MG	BA	2943	1/1	0.97	0.17	5.78	34,34,34,34	0
54	MG	BA	3434	1/1	0.97	0.27	5.75	19,19,19,19	0
54	MG	CA	1881	1/1	0.81	0.30	5.67	74,74,74,74	0
54	MG	DA	3056	1/1	0.97	0.24	5.67	25,25,25,25	0
54	MG	BA	3438	1/1	0.97	0.57	5.67	29,29,29,29	0
54	MG	DA	2904	1/1	0.98	0.30	5.63	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	2926	1/1	0.97	0.39	5.60	25,25,25,25	0
54	MG	DA	3048	1/1	0.87	0.29	5.50	51,51,51,51	0
54	MG	BB	218	1/1	0.98	0.36	5.47	79,79,79,79	0
54	MG	BA	3126	1/1	0.86	0.40	5.45	60,60,60,60	0
54	MG	AA	1665	1/1	0.87	0.32	5.45	70,70,70,70	0
54	MG	BA	3110	1/1	0.84	0.48	5.44	72,72,72,72	0
54	MG	AA	1625	1/1	0.94	0.22	5.38	53,53,53,53	0
54	MG	BA	3469	1/1	0.89	0.25	5.38	58,58,58,58	0
54	MG	DA	3005	1/1	0.98	0.36	5.35	41,41,41,41	0
54	MG	DD	301	1/1	0.91	0.50	5.31	39,39,39,39	0
54	MG	BA	3411	1/1	0.96	0.34	5.30	90,90,90,90	0
54	MG	DA	3121	1/1	0.95	0.35	5.23	38,38,38,38	0
54	MG	DA	2906	1/1	0.98	0.32	5.18	16,16,16,16	0
54	MG	DA	3343	1/1	0.78	0.30	5.16	97,97,97,97	0
54	MG	DA	3529	1/1	0.85	0.23	5.13	61,61,61,61	0
54	MG	BA	3673	1/1	0.80	0.28	5.08	92,92,92,92	0
54	MG	DA	3320	1/1	0.86	0.24	5.05	80,80,80,80	0
54	MG	DB	204	1/1	0.89	0.28	5.04	56,56,56,56	0
54	MG	BA	3169	1/1	0.84	0.26	4.99	43,43,43,43	0
54	MG	DA	3672	1/1	0.93	0.17	4.98	80,80,80,80	0
54	MG	BA	2914	1/1	0.96	0.45	4.93	24,24,24,24	0
54	MG	DA	2938	1/1	0.98	0.34	4.93	7,7,7,7	0
54	MG	DB	216	1/1	0.69	0.38	4.92	101,101,101,101	0
54	MG	BA	3575	1/1	0.95	0.38	4.90	59,59,59,59	0
54	MG	CA	1788	1/1	0.91	0.38	4.88	95,95,95,95	0
54	MG	BA	3038	1/1	0.74	0.28	4.81	63,63,63,63	0
54	MG	CA	1651	1/1	0.87	0.40	4.79	111,111,111,111	0
54	MG	DA	3014	1/1	0.91	0.25	4.74	52,52,52,52	0
54	MG	AA	1641	1/1	0.74	0.35	4.68	66,66,66,66	0
54	MG	BA	3327	1/1	0.85	0.79	4.65	86,86,86,86	0
54	MG	BE	302	1/1	0.93	0.44	4.60	93,93,93,93	0
54	MG	BA	3634	1/1	0.49	0.17	4.50	98,98,98,98	0
54	MG	DA	3197	1/1	0.92	0.17	4.47	46,46,46,46	0
54	MG	AA	1720	1/1	0.93	0.83	4.40	101,101,101,101	0
54	MG	DA	2980	1/1	0.98	0.37	4.32	12,12,12,12	0
54	MG	DA	3126	1/1	0.96	0.32	4.31	64,64,64,64	0
54	MG	DA	3851	1/1	0.94	0.27	4.23	74,74,74,74	0
54	MG	DA	3590	1/1	0.90	0.45	4.21	47,47,47,47	0
54	MG	AA	1609	1/1	0.98	0.33	4.18	26,26,26,26	0
54	MG	CA	1862	1/1	0.92	0.43	4.14	96,96,96,96	0
54	MG	AA	1635	1/1	0.99	0.27	4.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3178	1/1	0.93	0.27	4.05	74,74,74,74	0
54	MG	DA	3638	1/1	0.95	0.31	4.04	22,22,22,22	0
54	MG	DA	3415	1/1	0.90	0.48	4.04	66,66,66,66	0
54	MG	BA	2990	1/1	0.94	0.43	4.03	35,35,35,35	0
54	MG	DA	3506	1/1	0.87	0.40	3.90	101,101,101,101	0
54	MG	BA	3289	1/1	0.96	0.39	3.90	61,61,61,61	0
54	MG	DA	3310	1/1	0.85	0.34	3.74	54,54,54,54	0
54	MG	DA	3108	1/1	0.88	0.26	3.74	54,54,54,54	0
54	MG	BA	3471	1/1	0.81	0.27	3.71	70,70,70,70	0
54	MG	BA	3098	1/1	0.95	0.27	3.69	90,90,90,90	0
54	MG	DA	3353	1/1	0.89	0.25	3.63	105,105,105,105	0
54	MG	AT	202	1/1	0.91	0.39	3.59	80,80,80,80	0
54	MG	BA	2991	1/1	0.97	0.22	3.41	42,42,42,42	0
54	MG	DA	3153	1/1	0.97	0.35	3.40	33,33,33,33	0
54	MG	BC	303	1/1	0.83	0.42	3.36	95,95,95,95	0
54	MG	DA	3455	1/1	0.94	0.90	3.34	97,97,97,97	0
54	MG	BA	3019	1/1	0.74	0.23	3.29	67,67,67,67	0
54	MG	DA	3052	1/1	0.97	0.27	3.11	50,50,50,50	0
54	MG	DA	3329	1/1	0.86	0.17	3.08	96,96,96,96	0
54	MG	BA	3238	1/1	0.92	0.44	3.06	49,49,49,49	0
54	MG	AA	1603	1/1	0.95	0.50	3.05	37,37,37,37	0
54	MG	BA	3047	1/1	0.93	0.23	3.05	72,72,72,72	0
54	MG	CA	1915	1/1	0.97	0.41	3.03	58,58,58,58	0
54	MG	BA	2975	1/1	0.98	0.26	3.00	58,58,58,58	0
54	MG	DA	2927	1/1	0.98	0.25	2.97	18,18,18,18	0
54	MG	AA	1870	1/1	0.93	0.25	2.91	98,98,98,98	0
54	MG	DA	3082	1/1	0.98	0.41	2.89	68,68,68,68	0
54	MG	DA	3736	1/1	0.95	0.23	2.87	134,134,134,134	0
54	MG	AD	303	1/1	0.94	0.47	2.87	68,68,68,68	0
54	MG	DA	3771	1/1	0.80	0.35	2.86	58,58,58,58	0
54	MG	DJ	205	1/1	0.88	0.50	2.76	91,91,91,91	0
54	MG	DW	101	1/1	0.85	0.33	2.75	56,56,56,56	0
54	MG	DA	3599	1/1	0.91	0.27	2.71	58,58,58,58	0
54	MG	BA	2981	1/1	0.96	0.26	2.70	56,56,56,56	0
54	MG	DA	3172	1/1	0.98	0.24	2.70	88,88,88,88	0
54	MG	DA	3268	1/1	0.92	0.25	2.67	51,51,51,51	0
54	MG	DA	3658	1/1	0.96	0.34	2.55	23,23,23,23	0
54	MG	DA	3289	1/1	0.91	0.26	2.55	44,44,44,44	0
54	MG	DA	3185	1/1	0.94	0.26	2.54	54,54,54,54	0
54	MG	BA	3334	1/1	0.96	0.24	2.52	60,60,60,60	0
54	MG	DA	2975	1/1	0.92	0.26	2.51	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1760	1/1	0.81	0.27	2.48	66,66,66,66	0
54	MG	BA	2931	1/1	0.96	0.39	2.45	49,49,49,49	0
54	MG	DA	3098	1/1	0.96	0.24	2.44	46,46,46,46	0
54	MG	DA	3412	1/1	0.95	0.29	2.41	86,86,86,86	0
54	MG	AA	1630	1/1	0.81	0.27	2.39	81,81,81,81	0
54	MG	DX	101	1/1	0.85	0.37	2.38	103,103,103,103	0
54	MG	AA	1615	1/1	0.97	0.35	2.37	67,67,67,67	0
54	MG	BM	203	1/1	0.92	0.47	2.35	90,90,90,90	0
54	MG	BA	3013	1/1	0.96	0.40	2.29	21,21,21,21	0
54	MG	CA	1659	1/1	0.90	0.36	2.29	100,100,100,100	0
54	MG	CA	1688	1/1	0.54	0.26	2.24	80,80,80,80	0
54	MG	BA	3459	1/1	0.92	0.34	2.24	30,30,30,30	0
54	MG	DA	3606	1/1	0.89	0.26	2.22	68,68,68,68	0
54	MG	AA	1610	1/1	0.91	0.36	2.19	29,29,29,29	0
54	MG	DA	3605	1/1	0.83	0.27	2.17	103,103,103,103	0
54	MG	DA	3431	1/1	0.94	0.24	2.16	94,94,94,94	0
54	MG	BA	3301	1/1	0.78	0.38	2.15	58,58,58,58	0
54	MG	BA	3467	1/1	0.96	0.38	2.10	30,30,30,30	0
54	MG	DA	3028	1/1	0.95	0.35	2.07	58,58,58,58	0
54	MG	DA	2943	1/1	0.98	0.28	2.07	5,5,5,5	0
54	MG	DA	3010	1/1	0.90	0.23	2.06	72,72,72,72	0
54	MG	CA	1943	1/1	0.81	0.39	2.04	87,87,87,87	0
54	MG	DA	3015	1/1	0.94	0.26	2.03	33,33,33,33	0
54	MG	DA	3589	1/1	0.97	0.26	2.00	51,51,51,51	0
54	MG	BA	3356	1/1	0.96	0.28	1.99	33,33,33,33	0
54	MG	DA	3142	1/1	0.93	0.27	1.99	61,61,61,61	0
54	MG	DA	3750	1/1	0.91	0.45	1.99	87,87,87,87	0
54	MG	DA	3040	1/1	0.78	0.34	1.98	76,76,76,76	0
54	MG	BA	3252	1/1	0.85	0.28	1.96	60,60,60,60	0
54	MG	AA	1719	1/1	0.94	0.24	1.96	66,66,66,66	0
54	MG	BA	3175	1/1	0.80	0.43	1.94	71,71,71,71	0
54	MG	BA	2960	1/1	0.95	0.54	1.90	39,39,39,39	0
54	MG	CA	1675	1/1	0.93	0.24	1.90	74,74,74,74	0
54	MG	BA	2917	1/1	0.99	0.26	1.89	6,6,6,6	0
54	MG	AA	1601	1/1	0.96	0.24	1.89	35,35,35,35	0
54	MG	BB	220	1/1	0.83	0.33	1.84	75,75,75,75	0
54	MG	BA	3237	1/1	0.81	0.30	1.81	64,64,64,64	0
54	MG	BA	3030	1/1	0.89	0.18	1.79	61,61,61,61	0
54	MG	BA	3515	1/1	0.82	0.38	1.77	54,54,54,54	0
54	MG	DA	3361	1/1	0.95	0.12	1.74	69,69,69,69	0
54	MG	DA	3410	1/1	0.81	0.32	1.72	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CN	102	1/1	0.91	1.05	1.70	134,134,134,134	0
54	MG	DA	3250	1/1	0.65	0.27	1.67	70,70,70,70	0
54	MG	BA	3256	1/1	0.75	0.17	1.66	105,105,105,105	0
54	MG	DS	201	1/1	0.84	0.37	1.57	98,98,98,98	0
54	MG	DA	3554	1/1	0.84	0.30	1.50	136,136,136,136	0
54	MG	DA	3146	1/1	0.96	0.22	1.47	31,31,31,31	0
54	MG	CA	1944	1/1	0.88	0.32	1.43	66,66,66,66	0
54	MG	DA	3186	1/1	0.89	0.41	1.40	82,82,82,82	0
54	MG	BM	202	1/1	0.95	0.30	1.39	85,85,85,85	0
54	MG	DA	3514	1/1	0.89	0.23	1.34	68,68,68,68	0
54	MG	CA	1921	1/1	0.87	0.21	1.25	97,97,97,97	0
54	MG	DA	3307	1/1	0.93	0.21	1.21	84,84,84,84	0
54	MG	DA	3176	1/1	0.94	0.31	1.20	50,50,50,50	0
54	MG	DA	3283	1/1	0.88	0.27	1.19	71,71,71,71	0
54	MG	AA	1614	1/1	0.81	0.20	1.09	68,68,68,68	0
54	MG	CA	1781	1/1	0.93	0.22	1.08	76,76,76,76	0
54	MG	BA	3430	1/1	0.97	0.27	1.07	6,6,6,6	0
54	MG	CA	1826	1/1	0.86	0.31	1.02	97,97,97,97	0
54	MG	BA	2948	1/1	0.90	0.27	0.99	62,62,62,62	0
54	MG	BA	3677	1/1	0.87	0.26	0.98	72,72,72,72	0
54	MG	DA	3625	1/1	0.94	0.32	0.97	84,84,84,84	0
54	MG	BA	3574	1/1	0.95	0.18	0.89	62,62,62,62	0
54	MG	DA	3632	1/1	0.73	0.29	0.88	111,111,111,111	0
54	MG	DA	3044	1/1	0.90	0.19	0.83	45,45,45,45	0
54	MG	DA	3099	1/1	0.92	0.18	0.81	49,49,49,49	0
54	MG	AA	1784	1/1	0.72	0.42	0.80	89,89,89,89	0
54	MG	CA	1762	1/1	0.96	0.21	0.76	114,114,114,114	0
54	MG	CA	1607	1/1	0.93	0.18	0.75	62,62,62,62	0
54	MG	DA	2990	1/1	0.95	0.21	0.74	20,20,20,20	0
54	MG	DA	3037	1/1	0.93	0.18	0.74	44,44,44,44	0
54	MG	DA	3484	1/1	0.96	0.25	0.72	21,21,21,21	0
54	MG	B5	101	1/1	0.91	0.47	0.68	78,78,78,78	0
54	MG	DA	3125	1/1	0.96	0.20	0.66	36,36,36,36	0
54	MG	BA	3107	1/1	0.99	0.31	0.66	25,25,25,25	0
54	MG	DB	215	1/1	0.86	0.28	0.60	103,103,103,103	0
54	MG	CM	201	1/1	0.92	0.89	0.59	85,85,85,85	0
54	MG	DD	305	1/1	0.76	0.41	0.57	52,52,52,52	0
54	MG	DA	3641	1/1	0.95	0.25	0.55	13,13,13,13	0
54	MG	AE	202	1/1	0.85	0.21	0.50	173,173,173,173	0
54	MG	DJ	204	1/1	0.93	0.50	0.48	32,32,32,32	0
54	MG	CA	1702	1/1	0.96	0.24	0.47	114,114,114,114	0
54	MG	BA	2933	1/1	0.95	0.24	0.45	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3307	1/1	0.94	0.19	0.43	63,63,63,63	0
54	MG	D4	102	1/1	0.88	0.23	0.42	65,65,65,65	0
54	MG	DA	3104	1/1	0.89	0.24	0.41	49,49,49,49	0
54	MG	DA	3680	1/1	0.96	0.20	0.41	41,41,41,41	0
54	MG	DA	3050	1/1	0.98	0.21	0.35	89,89,89,89	0
54	MG	CA	1950	1/1	0.77	0.36	0.35	107,107,107,107	0
54	MG	BA	2942	1/1	0.88	0.21	0.35	19,19,19,19	0
54	MG	CA	1690	1/1	0.86	0.16	0.32	65,65,65,65	0
54	MG	BA	3403	1/1	0.86	0.26	0.31	106,106,106,106	0
54	MG	DA	2972	1/1	0.97	0.19	0.29	37,37,37,37	0
54	MG	DA	3137	1/1	0.94	0.29	0.28	29,29,29,29	0
54	MG	DA	3613	1/1	0.55	0.32	0.27	121,121,121,121	0
54	MG	BA	3547	1/1	0.96	0.20	0.26	87,87,87,87	0
54	MG	BJ	202	1/1	0.94	0.31	0.24	69,69,69,69	0
54	MG	CD	304	1/1	0.89	0.50	0.22	108,108,108,108	0
54	MG	AA	1649	1/1	0.77	0.16	0.21	74,74,74,74	0
54	MG	CA	1657	1/1	0.79	0.17	0.20	60,60,60,60	0
54	MG	DA	2999	1/1	0.93	0.15	0.19	69,69,69,69	0
54	MG	DA	2995	1/1	0.95	0.21	0.17	26,26,26,26	0
54	MG	DA	2984	1/1	0.97	0.22	0.17	22,22,22,22	0
54	MG	BA	2988	1/1	0.97	0.21	0.15	40,40,40,40	0
54	MG	BA	3546	1/1	0.96	0.20	0.15	67,67,67,67	0
54	MG	BA	3370	1/1	0.79	0.27	0.13	76,76,76,76	0
54	MG	BA	3615	1/1	0.93	0.18	0.11	93,93,93,93	0
54	MG	DA	3634	1/1	0.84	1.08	0.10	106,106,106,106	0
54	MG	BA	2936	1/1	0.95	0.18	0.06	32,32,32,32	0
54	MG	DB	212	1/1	0.92	0.24	0.05	85,85,85,85	0
54	MG	DA	3001	1/1	0.89	0.18	0.03	25,25,25,25	0
54	MG	BA	3562	1/1	0.91	0.20	-0.01	40,40,40,40	0
54	MG	AA	1841	1/1	0.95	0.17	-0.01	83,83,83,83	0
54	MG	BA	2973	1/1	0.82	0.15	-0.02	60,60,60,60	0
54	MG	DA	3326	1/1	0.94	0.32	-0.04	81,81,81,81	0
54	MG	CA	1764	1/1	0.75	0.15	-0.16	65,65,65,65	0
54	MG	BA	2989	1/1	0.94	0.20	-0.16	50,50,50,50	0
55	ZN	AD	301	1/1	0.98	0.29	-0.21	51,51,51,51	0
54	MG	BW	101	1/1	0.91	0.20	-0.22	57,57,57,57	0
54	MG	AA	1658	1/1	0.81	0.18	-0.23	84,84,84,84	0
54	MG	BA	3522	1/1	0.89	0.27	-0.23	54,54,54,54	0
54	MG	AA	1835	1/1	0.94	0.23	-0.26	158,158,158,158	0
54	MG	DQ	201	1/1	0.88	0.23	-0.27	57,57,57,57	0
54	MG	CA	1811	1/1	-0.03	0.28	-0.28	181,181,181,181	0
54	MG	BA	3131	1/1	0.92	0.15	-0.28	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DL	202	1/1	0.64	0.23	-0.32	146,146,146,146	0
54	MG	CA	1620	1/1	0.94	0.20	-0.33	51,51,51,51	0
54	MG	AA	1660	1/1	0.87	0.17	-0.37	122,122,122,122	0
54	MG	DA	3338	1/1	0.98	0.14	-0.38	123,123,123,123	0
54	MG	BA	3482	1/1	0.95	0.21	-0.39	40,40,40,40	0
54	MG	AA	1624	1/1	0.96	0.18	-0.40	58,58,58,58	0
54	MG	BX	101	1/1	0.91	0.21	-0.41	71,71,71,71	0
54	MG	DK	201	1/1	0.86	0.16	-0.48	87,87,87,87	0
54	MG	BA	3056	1/1	0.94	0.19	-0.49	31,31,31,31	0
54	MG	CA	1854	1/1	0.87	0.14	-0.50	111,111,111,111	0
54	MG	BA	3099	1/1	0.93	0.11	-0.52	56,56,56,56	0
54	MG	CK	201	1/1	0.78	0.17	-0.60	136,136,136,136	0
54	MG	AB	301	1/1	0.94	0.30	-0.61	92,92,92,92	0
54	MG	DA	2978	1/1	0.94	0.24	-0.62	23,23,23,23	0
54	MG	BA	3125	1/1	0.91	0.15	-0.63	78,78,78,78	0
54	MG	AM	201	1/1	0.76	0.23	-0.69	126,126,126,126	0
54	MG	BA	3535	1/1	0.95	0.21	-0.70	95,95,95,95	0
54	MG	DA	3281	1/1	0.96	0.16	-0.71	62,62,62,62	0
54	MG	CA	1710	1/1	0.79	0.16	-0.72	169,169,169,169	0
54	MG	AB	302	1/1	0.96	0.24	-0.74	57,57,57,57	0
54	MG	CA	1689	1/1	0.91	0.14	-0.74	130,130,130,130	0
54	MG	DA	3016	1/1	0.98	0.18	-0.76	47,47,47,47	0
54	MG	BA	3104	1/1	0.93	0.15	-0.77	49,49,49,49	0
54	MG	DI	101	1/1	0.79	0.29	-0.79	104,104,104,104	0
54	MG	DP	201	1/1	0.92	0.26	-0.79	72,72,72,72	0
55	ZN	CN	101	1/1	0.83	0.20	-0.82	244,244,244,244	0
54	MG	DA	3023	1/1	0.98	0.15	-0.83	23,23,23,23	0
54	MG	DA	3214	1/1	0.99	0.17	-0.85	34,34,34,34	0
54	MG	CA	1703	1/1	0.81	0.21	-0.95	113,113,113,113	0
54	MG	BA	3241	1/1	0.95	0.13	-0.99	69,69,69,69	0
54	MG	BA	3581	1/1	0.99	0.14	-1.01	127,127,127,127	0
54	MG	DA	3796	1/1	0.95	0.15	-1.03	67,67,67,67	0
54	MG	DA	3000	1/1	0.92	0.20	-1.03	23,23,23,23	0
54	MG	DA	2941	1/1	0.90	0.18	-1.05	21,21,21,21	0
54	MG	AA	1701	1/1	0.82	0.19	-1.13	84,84,84,84	0
54	MG	BA	2980	1/1	0.96	0.18	-1.15	51,51,51,51	0
54	MG	DA	3306	1/1	0.83	0.15	-1.19	152,152,152,152	0
54	MG	DA	3119	1/1	0.96	0.15	-1.20	74,74,74,74	0
54	MG	BA	3123	1/1	0.90	0.14	-1.21	40,40,40,40	0
55	ZN	AN	101	1/1	0.95	0.13	-1.21	144,144,144,144	0
54	MG	B2	101	1/1	0.93	0.11	-1.22	27,27,27,27	0
54	MG	CA	1747	1/1	0.90	0.17	-1.26	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AE	201	1/1	0.86	0.11	-1.27	123,123,123,123	0
54	MG	AA	1802	1/1	0.91	0.09	-1.33	62,62,62,62	0
54	MG	CA	1860	1/1	0.94	0.21	-1.33	68,68,68,68	0
54	MG	AA	1644	1/1	0.92	0.14	-1.33	62,62,62,62	0
54	MG	BA	3014	1/1	0.92	0.08	-1.36	45,45,45,45	0
54	MG	BA	2982	1/1	0.94	0.12	-1.37	38,38,38,38	0
54	MG	BA	2950	1/1	0.98	0.16	-1.37	68,68,68,68	0
54	MG	CA	1616	1/1	0.96	0.14	-1.48	94,94,94,94	0
54	MG	DE	301	1/1	0.86	0.17	-1.50	32,32,32,32	0
54	MG	DA	2963	1/1	0.87	0.10	-1.61	32,32,32,32	0
54	MG	DB	217	1/1	0.95	0.09	-1.62	93,93,93,93	0
54	MG	CA	1720	1/1	0.90	0.22	-1.65	69,69,69,69	0
54	MG	CA	1937	1/1	0.96	0.27	-1.69	100,100,100,100	0
54	MG	CA	1749	1/1	0.98	0.11	-1.70	77,77,77,77	0
54	MG	BE	301	1/1	0.77	0.13	-1.82	75,75,75,75	0
54	MG	AS	101	1/1	0.40	0.12	-1.84	106,106,106,106	0
54	MG	BA	3477	1/1	0.96	0.13	-1.88	50,50,50,50	0
54	MG	DA	3117	1/1	0.96	0.12	-1.93	31,31,31,31	0
54	MG	DX	102	1/1	0.92	0.12	-1.96	91,91,91,91	0
54	MG	BA	3412	1/1	0.98	0.13	-1.96	49,49,49,49	0
54	MG	AD	302	1/1	0.85	0.18	-1.97	76,76,76,76	0
54	MG	DA	3139	1/1	0.97	0.15	-2.05	40,40,40,40	0
54	MG	CC	301	1/1	0.78	0.09	-2.05	93,93,93,93	0
54	MG	DB	219	1/1	0.89	0.17	-2.16	73,73,73,73	0
54	MG	DA	3591	1/1	0.95	0.10	-2.21	90,90,90,90	0
54	MG	AA	1684	1/1	0.91	0.11	-2.26	71,71,71,71	0
54	MG	DA	2948	1/1	0.99	0.13	-2.50	21,21,21,21	0
55	ZN	CD	301	1/1	0.94	0.28	-2.51	116,116,116,116	0
54	MG	DA	3120	1/1	0.87	0.10	-2.62	61,61,61,61	0
54	MG	DA	3242	1/1	0.91	0.11	-2.65	59,59,59,59	0
54	MG	BA	3080	1/1	0.94	0.11	-2.69	43,43,43,43	0
54	MG	BA	3387	1/1	0.96	0.13	-2.77	84,84,84,84	0
54	MG	BA	2966	1/1	0.98	0.14	-2.81	38,38,38,38	0
54	MG	BA	3154	1/1	0.94	0.08	-3.45	139,139,139,139	0
54	MG	AA	1634	1/1	0.97	0.10	-3.47	48,48,48,48	0
54	MG	DA	3130	1/1	0.96	0.08	-3.51	68,68,68,68	0
54	MG	DA	3184	1/1	0.93	0.12	-3.67	38,38,38,38	0
54	MG	CA	1770	1/1	0.80	0.09	-4.19	125,125,125,125	0
54	MG	D2	102	1/1	0.90	0.08	-4.21	42,42,42,42	0
54	MG	BA	3015	1/1	0.97	0.10	-7.40	55,55,55,55	0
54	MG	DA	3301	1/1	0.92	0.68	-	87,87,87,87	0
54	MG	DA	3279	1/1	0.89	0.37	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3422	1/1	0.72	0.62	-	62,62,62,62	0
54	MG	DA	3195	1/1	0.88	0.25	-	83,83,83,83	0
54	MG	DB	227	1/1	0.91	0.16	-	104,104,104,104	0
54	MG	BA	3505	1/1	0.80	0.29	-	81,81,81,81	0
54	MG	DA	3224	1/1	0.81	0.40	-	55,55,55,55	0
54	MG	BA	3589	1/1	0.34	0.19	-	105,105,105,105	0
54	MG	DA	3461	1/1	0.82	0.38	-	88,88,88,88	0
54	MG	BA	3408	1/1	0.93	0.51	-	86,86,86,86	0
54	MG	DV	203	1/1	0.92	0.15	-	128,128,128,128	0
54	MG	CA	1755	1/1	0.95	0.45	-	69,69,69,69	0
54	MG	DA	3649	1/1	0.92	1.06	-	50,50,50,50	0
54	MG	BA	3151	1/1	0.88	0.45	-	70,70,70,70	0
54	MG	BA	3517	1/1	0.94	0.42	-	87,87,87,87	0
54	MG	CA	1894	1/1	0.88	0.47	-	97,97,97,97	0
54	MG	AK	202	1/1	0.77	0.10	-	101,101,101,101	0
54	MG	BA	2956	1/1	0.85	0.63	-	49,49,49,49	0
54	MG	DA	3748	1/1	0.88	0.24	-	61,61,61,61	0
54	MG	DA	3707	1/1	0.85	0.20	-	54,54,54,54	0
54	MG	CA	1784	1/1	0.90	0.24	-	94,94,94,94	0
54	MG	BA	3250	1/1	0.86	0.13	-	67,67,67,67	0
54	MG	CA	1857	1/1	0.95	0.33	-	76,76,76,76	0
54	MG	DA	3490	1/1	0.94	0.21	-	70,70,70,70	0
54	MG	DA	3252	1/1	0.92	0.13	-	52,52,52,52	0
54	MG	CA	1869	1/1	0.93	0.08	-	96,96,96,96	0
54	MG	BA	2977	1/1	0.97	0.40	-	69,69,69,69	0
54	MG	DA	3546	1/1	0.91	0.20	-	56,56,56,56	0
54	MG	BA	3468	1/1	0.79	0.55	-	57,57,57,57	0
54	MG	DA	3492	1/1	0.92	0.18	-	102,102,102,102	0
54	MG	D5	103	1/1	0.90	0.38	-	71,71,71,71	0
54	MG	BA	2949	1/1	0.85	0.21	-	65,65,65,65	0
54	MG	BA	3364	1/1	0.90	0.36	-	107,107,107,107	0
54	MG	DA	3619	1/1	0.85	0.95	-	83,83,83,83	0
54	MG	DA	3566	1/1	0.82	0.29	-	91,91,91,91	0
54	MG	CA	1630	1/1	0.97	0.25	-	49,49,49,49	0
54	MG	DA	3442	1/1	0.89	0.63	-	71,71,71,71	0
54	MG	DA	3300	1/1	0.95	0.23	-	46,46,46,46	0
54	MG	BA	3044	1/1	0.87	0.26	-	39,39,39,39	0
54	MG	CA	1906	1/1	0.82	0.32	-	80,80,80,80	0
54	MG	AA	1821	1/1	0.87	0.51	-	91,91,91,91	0
54	MG	DA	3820	1/1	0.90	0.94	-	59,59,59,59	0
54	MG	BA	3319	1/1	0.95	0.16	-	79,79,79,79	0
54	MG	DA	3365	1/1	0.85	0.34	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1852	1/1	0.92	0.78	-	84,84,84,84	0
54	MG	CA	1832	1/1	0.95	0.11	-	92,92,92,92	0
54	MG	CA	1821	1/1	0.93	0.50	-	96,96,96,96	0
54	MG	BA	2915	1/1	0.92	0.34	-	20,20,20,20	0
54	MG	CA	1748	1/1	0.88	0.21	-	115,115,115,115	0
54	MG	CA	1609	1/1	0.96	0.25	-	66,66,66,66	0
54	MG	DA	3702	1/1	0.72	0.60	-	74,74,74,74	0
54	MG	BA	3413	1/1	0.76	0.41	-	65,65,65,65	0
54	MG	AA	1775	1/1	0.96	0.11	-	105,105,105,105	0
54	MG	BA	3053	1/1	0.90	0.45	-	69,69,69,69	0
54	MG	BA	3065	1/1	0.95	0.22	-	59,59,59,59	0
54	MG	DA	3149	1/1	0.94	0.25	-	60,60,60,60	0
54	MG	DA	2924	1/1	0.80	0.51	-	68,68,68,68	0
54	MG	B2	103	1/1	0.84	0.09	-	75,75,75,75	0
54	MG	BA	3541	1/1	0.81	0.69	-	89,89,89,89	0
54	MG	BA	3519	1/1	0.91	0.15	-	50,50,50,50	0
54	MG	DA	3731	1/1	0.95	0.14	-	60,60,60,60	0
54	MG	DA	3550	1/1	0.91	0.14	-	65,65,65,65	0
54	MG	BA	3127	1/1	0.88	0.77	-	61,61,61,61	0
54	MG	DA	3577	1/1	0.92	0.40	-	73,73,73,73	0
54	MG	DA	3089	1/1	0.96	0.40	-	71,71,71,71	0
54	MG	AV	6207	1/1	0.91	0.11	-	78,78,78,78	0
54	MG	BA	3623	1/1	0.67	0.65	-	64,64,64,64	0
54	MG	CA	1729	1/1	0.91	0.16	-	58,58,58,58	0
54	MG	CA	1899	1/1	0.72	0.10	-	98,98,98,98	0
54	MG	BA	2928	1/1	0.95	0.51	-	28,28,28,28	0
54	MG	CQ	202	1/1	0.90	0.20	-	79,79,79,79	0
54	MG	DA	3664	1/1	0.56	1.62	-	109,109,109,109	0
54	MG	DA	3332	1/1	0.66	0.79	-	88,88,88,88	0
54	MG	CA	1647	1/1	0.82	0.27	-	94,94,94,94	0
54	MG	DA	2921	1/1	0.95	0.13	-	32,32,32,32	0
54	MG	CA	1797	1/1	0.70	0.27	-	133,133,133,133	0
54	MG	DA	3653	1/1	0.92	0.52	-	51,51,51,51	0
54	MG	BA	3233	1/1	0.98	0.61	-	97,97,97,97	0
54	MG	CA	1823	1/1	0.96	0.12	-	61,61,61,61	0
54	MG	CA	1671	1/1	0.98	0.26	-	51,51,51,51	0
54	MG	BA	3426	1/1	0.77	0.35	-	87,87,87,87	0
54	MG	BA	3369	1/1	0.95	0.30	-	108,108,108,108	0
54	MG	DA	2976	1/1	0.78	1.34	-	68,68,68,68	0
54	MG	CF	201	1/1	0.65	0.24	-	131,131,131,131	0
54	MG	BA	3166	1/1	0.75	0.90	-	86,86,86,86	0
54	MG	BA	3460	1/1	0.93	0.22	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1642	1/1	0.95	0.18	-	79,79,79,79	0
54	MG	DA	3165	1/1	0.97	0.11	-	59,59,59,59	0
54	MG	DB	225	1/1	0.78	0.18	-	72,72,72,72	0
54	MG	AA	1748	1/1	0.86	0.21	-	56,56,56,56	0
54	MG	DA	3500	1/1	0.88	0.23	-	108,108,108,108	0
54	MG	AA	1779	1/1	0.90	0.71	-	108,108,108,108	0
54	MG	CA	1715	1/1	0.97	0.42	-	107,107,107,107	0
54	MG	DP	202	1/1	0.70	0.10	-	90,90,90,90	0
54	MG	BA	3205	1/1	0.83	0.48	-	70,70,70,70	0
54	MG	DA	3437	1/1	0.81	0.66	-	120,120,120,120	0
54	MG	DA	3374	1/1	0.99	0.14	-	80,80,80,80	0
54	MG	DA	3218	1/1	0.94	0.11	-	79,79,79,79	0
54	MG	CA	1684	1/1	0.93	0.49	-	63,63,63,63	0
54	MG	BA	3039	1/1	0.93	0.14	-	54,54,54,54	0
54	MG	BA	3636	1/1	0.93	0.77	-	76,76,76,76	0
54	MG	DA	3787	1/1	0.72	1.21	-	114,114,114,114	0
54	MG	BA	3320	1/1	0.93	0.41	-	71,71,71,71	0
54	MG	CA	1752	1/1	0.92	0.33	-	71,71,71,71	0
54	MG	DA	3156	1/1	0.90	0.21	-	52,52,52,52	0
54	MG	CA	1707	1/1	0.95	0.14	-	102,102,102,102	0
54	MG	BA	3341	1/1	0.12	0.66	-	125,125,125,125	0
54	MG	BA	3218	1/1	0.89	0.24	-	55,55,55,55	0
54	MG	DA	3439	1/1	0.94	0.27	-	52,52,52,52	0
54	MG	DA	3369	1/1	0.99	0.10	-	99,99,99,99	0
54	MG	AA	1810	1/1	0.96	0.24	-	86,86,86,86	0
54	MG	BA	3026	1/1	0.79	0.15	-	68,68,68,68	0
54	MG	BA	3216	1/1	0.92	0.18	-	87,87,87,87	0
54	MG	DA	3244	1/1	0.84	0.55	-	85,85,85,85	0
54	MG	DA	3836	1/1	0.20	0.63	-	135,135,135,135	0
54	MG	AA	1607	1/1	0.81	0.60	-	46,46,46,46	0
54	MG	CA	1683	1/1	0.84	0.34	-	72,72,72,72	0
54	MG	BA	3470	1/1	0.86	0.30	-	71,71,71,71	0
54	MG	DA	3384	1/1	0.83	0.30	-	84,84,84,84	0
54	MG	DA	3179	1/1	0.62	0.57	-	105,105,105,105	0
54	MG	DJ	206	1/1	0.88	0.14	-	135,135,135,135	0
54	MG	DA	3303	1/1	0.96	0.36	-	67,67,67,67	0
54	MG	DA	2945	1/1	0.94	0.58	-	29,29,29,29	0
54	MG	CA	1816	1/1	0.82	0.41	-	107,107,107,107	0
54	MG	AA	1811	1/1	0.93	0.19	-	61,61,61,61	0
54	MG	CA	1952	1/1	0.81	0.29	-	88,88,88,88	0
54	MG	DA	3521	1/1	0.93	0.24	-	101,101,101,101	0
54	MG	BA	3305	1/1	0.89	0.10	-	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3849	1/1	0.88	0.17	-	89,89,89,89	0
54	MG	CA	1901	1/1	0.89	0.30	-	76,76,76,76	0
54	MG	DA	3069	1/1	0.79	0.46	-	61,61,61,61	0
54	MG	CA	1837	1/1	0.75	0.61	-	83,83,83,83	0
54	MG	DV	204	1/1	0.85	0.28	-	96,96,96,96	0
54	MG	DA	3071	1/1	0.99	0.16	-	49,49,49,49	0
54	MG	BA	3016	1/1	0.95	0.50	-	54,54,54,54	0
54	MG	BA	3595	1/1	0.83	0.34	-	108,108,108,108	0
54	MG	DA	3295	1/1	0.77	0.40	-	107,107,107,107	0
54	MG	BA	3423	1/1	0.95	0.39	-	72,72,72,72	0
54	MG	CA	1819	1/1	0.83	0.26	-	109,109,109,109	0
54	MG	DA	3525	1/1	0.95	0.75	-	73,73,73,73	0
54	MG	DD	303	1/1	0.72	0.17	-	70,70,70,70	0
54	MG	BA	3496	1/1	0.82	0.16	-	67,67,67,67	0
54	MG	DA	3123	1/1	0.93	0.42	-	59,59,59,59	0
54	MG	DA	3597	1/1	0.95	0.13	-	124,124,124,124	0
54	MG	BA	3361	1/1	0.83	0.27	-	154,154,154,154	0
54	MG	CA	1709	1/1	0.95	0.05	-	107,107,107,107	0
54	MG	DA	2959	1/1	0.92	0.30	-	42,42,42,42	0
54	MG	DA	3196	1/1	0.96	0.20	-	84,84,84,84	0
54	MG	BA	3100	1/1	0.94	0.31	-	79,79,79,79	0
54	MG	BA	3322	1/1	0.79	0.36	-	71,71,71,71	0
54	MG	DA	3533	1/1	0.88	0.25	-	60,60,60,60	0
54	MG	DA	3710	1/1	0.97	0.15	-	92,92,92,92	0
54	MG	DA	3386	1/1	0.93	0.13	-	76,76,76,76	0
54	MG	CA	1829	1/1	0.95	0.13	-	89,89,89,89	0
54	MG	DA	3094	1/1	0.89	0.41	-	67,67,67,67	0
54	MG	DA	3174	1/1	0.94	0.18	-	66,66,66,66	0
54	MG	AA	1674	1/1	0.82	0.95	-	113,113,113,113	0
54	MG	AG	202	1/1	0.82	0.31	-	129,129,129,129	0
54	MG	DA	3535	1/1	0.81	0.31	-	107,107,107,107	0
54	MG	AA	1663	1/1	0.90	0.22	-	54,54,54,54	0
54	MG	BA	3456	1/1	0.95	0.38	-	64,64,64,64	0
54	MG	BA	3464	1/1	0.70	0.73	-	67,67,67,67	0
54	MG	CA	1790	1/1	0.80	0.28	-	132,132,132,132	0
54	MG	DA	3743	1/1	0.71	0.27	-	105,105,105,105	0
54	MG	DA	3636	1/1	0.98	0.42	-	12,12,12,12	0
54	MG	BA	3475	1/1	0.77	1.13	-	67,67,67,67	0
54	MG	DA	3257	1/1	0.94	0.15	-	48,48,48,48	0
54	MG	DA	3447	1/1	0.92	0.25	-	73,73,73,73	0
54	MG	DB	205	1/1	0.94	0.32	-	78,78,78,78	0
54	MG	BA	3417	1/1	0.93	0.18	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	2946	1/1	0.97	0.21	-	37,37,37,37	0
54	MG	DA	3479	1/1	0.84	0.20	-	130,130,130,130	0
54	MG	CA	1807	1/1	0.73	0.37	-	125,125,125,125	0
54	MG	AV	6205	1/1	0.92	0.12	-	107,107,107,107	0
54	MG	DA	3436	1/1	0.72	1.02	-	101,101,101,101	0
54	MG	BA	3057	1/1	0.99	0.14	-	64,64,64,64	0
54	MG	BP	202	1/1	0.89	0.13	-	84,84,84,84	0
54	MG	AA	1670	1/1	0.57	0.14	-	93,93,93,93	0
54	MG	CA	1670	1/1	0.94	0.36	-	106,106,106,106	0
54	MG	CA	1672	1/1	0.95	0.14	-	137,137,137,137	0
54	MG	CA	1613	1/1	0.89	0.62	-	68,68,68,68	0
54	MG	AO	101	1/1	0.77	0.09	-	115,115,115,115	0
54	MG	CA	1835	1/1	0.93	0.23	-	76,76,76,76	0
54	MG	BA	3106	1/1	-0.09	0.22	-	142,142,142,142	0
54	MG	BA	2908	1/1	0.95	0.44	-	26,26,26,26	0
54	MG	DA	3434	1/1	0.91	0.27	-	89,89,89,89	0
54	MG	DA	3097	1/1	0.98	0.30	-	55,55,55,55	0
54	MG	CA	1961	1/1	0.98	0.12	-	63,63,63,63	0
54	MG	DV	202	1/1	0.72	0.34	-	115,115,115,115	0
54	MG	AA	1627	1/1	0.93	0.60	-	59,59,59,59	0
54	MG	BA	3630	1/1	0.90	0.37	-	151,151,151,151	0
54	MG	BA	3582	1/1	0.89	0.30	-	102,102,102,102	0
54	MG	CA	1624	1/1	0.95	0.43	-	94,94,94,94	0
54	MG	CA	1697	1/1	0.89	0.08	-	83,83,83,83	0
54	MG	AA	1680	1/1	0.57	0.42	-	140,140,140,140	0
54	MG	CA	1718	1/1	0.95	0.27	-	109,109,109,109	0
54	MG	AA	1650	1/1	0.99	0.22	-	92,92,92,92	0
54	MG	BA	3678	1/1	0.93	0.53	-	122,122,122,122	0
54	MG	DB	214	1/1	0.96	0.21	-	72,72,72,72	0
54	MG	AA	1739	1/1	0.91	0.27	-	81,81,81,81	0
54	MG	BB	216	1/1	0.54	0.69	-	154,154,154,154	0
54	MG	BA	3404	1/1	0.88	0.21	-	80,80,80,80	0
54	MG	BA	3362	1/1	0.76	0.93	-	130,130,130,130	0
54	MG	DA	3693	1/1	0.87	0.31	-	63,63,63,63	0
54	MG	DA	3383	1/1	0.77	0.34	-	112,112,112,112	0
54	MG	AA	1669	1/1	0.94	0.39	-	54,54,54,54	0
54	MG	AA	1611	1/1	0.88	0.45	-	55,55,55,55	0
54	MG	BA	3148	1/1	0.79	0.28	-	62,62,62,62	0
54	MG	BA	3349	1/1	0.68	0.33	-	95,95,95,95	0
54	MG	DA	3055	1/1	0.93	0.34	-	59,59,59,59	0
54	MG	BA	3399	1/1	0.84	0.38	-	104,104,104,104	0
54	MG	BA	3232	1/1	0.94	0.27	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1628	1/1	0.89	0.63	-	84,84,84,84	0
54	MG	DA	3493	1/1	0.95	0.39	-	59,59,59,59	0
54	MG	DB	203	1/1	0.87	0.16	-	69,69,69,69	0
54	MG	BA	3001	1/1	0.85	0.37	-	65,65,65,65	0
54	MG	DA	3349	1/1	0.92	0.17	-	116,116,116,116	0
54	MG	BA	3197	1/1	0.74	0.18	-	84,84,84,84	0
54	MG	CA	1809	1/1	0.96	0.21	-	92,92,92,92	0
54	MG	BA	3018	1/1	0.62	0.84	-	88,88,88,88	0
54	MG	DA	3265	1/1	0.91	0.67	-	138,138,138,138	0
54	MG	DA	3340	1/1	0.71	0.33	-	59,59,59,59	0
54	MG	DA	3705	1/1	0.86	0.20	-	86,86,86,86	0
54	MG	DQ	202	1/1	0.82	0.20	-	97,97,97,97	0
54	MG	DA	3800	1/1	0.80	0.36	-	95,95,95,95	0
54	MG	DA	3854	1/1	0.87	0.10	-	124,124,124,124	0
54	MG	DA	3312	1/1	0.68	0.16	-	130,130,130,130	0
54	MG	DA	3448	1/1	0.96	0.17	-	99,99,99,99	0
54	MG	DB	224	1/1	0.97	0.26	-	95,95,95,95	0
54	MG	AA	1662	1/1	0.90	0.56	-	78,78,78,78	0
54	MG	CA	1822	1/1	0.90	0.38	-	93,93,93,93	0
54	MG	BA	3045	1/1	0.64	0.38	-	94,94,94,94	0
54	MG	BA	3651	1/1	0.84	0.49	-	77,77,77,77	0
54	MG	BA	2967	1/1	0.92	0.41	-	51,51,51,51	0
54	MG	DA	3560	1/1	0.85	0.44	-	83,83,83,83	0
54	MG	BA	3529	1/1	0.86	0.27	-	79,79,79,79	0
54	MG	AA	1721	1/1	0.95	0.32	-	56,56,56,56	0
54	MG	DA	3726	1/1	0.74	0.29	-	106,106,106,106	0
54	MG	DA	3392	1/1	0.90	0.50	-	76,76,76,76	0
54	MG	DA	3537	1/1	0.70	0.43	-	101,101,101,101	0
54	MG	DA	3665	1/1	0.47	0.87	-	137,137,137,137	0
54	MG	DA	3395	1/1	0.93	0.27	-	75,75,75,75	0
54	MG	BY	103	1/1	0.78	0.22	-	95,95,95,95	0
54	MG	DA	3469	1/1	0.91	0.40	-	83,83,83,83	0
54	MG	CA	1641	1/1	0.71	0.40	-	79,79,79,79	0
54	MG	BB	223	1/1	0.95	0.17	-	94,94,94,94	0
54	MG	BA	3344	1/1	0.86	0.36	-	99,99,99,99	0
54	MG	DA	3235	1/1	0.99	0.20	-	59,59,59,59	0
54	MG	BA	3625	1/1	0.85	0.25	-	53,53,53,53	0
54	MG	BA	3383	1/1	0.90	0.25	-	66,66,66,66	0
54	MG	BA	3199	1/1	0.89	0.33	-	61,61,61,61	0
54	MG	CA	1928	1/1	0.56	0.54	-	117,117,117,117	0
54	MG	AA	1866	1/1	0.65	0.58	-	108,108,108,108	0
54	MG	BA	3179	1/1	0.93	0.21	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1741	1/1	0.71	0.40	-	112,112,112,112	0
54	MG	BA	3497	1/1	0.92	0.23	-	61,61,61,61	0
54	MG	CA	1802	1/1	0.99	0.03	-	94,94,94,94	0
54	MG	BB	224	1/1	0.83	0.36	-	140,140,140,140	0
54	MG	BA	3247	1/1	0.90	0.25	-	109,109,109,109	0
54	MG	CA	1799	1/1	0.84	0.18	-	109,109,109,109	0
54	MG	DA	3403	1/1	0.85	0.31	-	56,56,56,56	0
54	MG	DA	3579	1/1	0.96	0.54	-	80,80,80,80	0
54	MG	DB	223	1/1	0.83	0.17	-	82,82,82,82	0
54	MG	DA	3068	1/1	0.80	0.53	-	64,64,64,64	0
54	MG	DA	3728	1/1	0.86	0.68	-	83,83,83,83	0
54	MG	BA	3527	1/1	0.79	0.52	-	65,65,65,65	0
54	MG	BA	3138	1/1	0.81	0.31	-	88,88,88,88	0
54	MG	BA	3602	1/1	0.85	0.73	-	98,98,98,98	0
54	MG	BA	3617	1/1	0.90	0.14	-	96,96,96,96	0
54	MG	BA	3275	1/1	0.92	0.24	-	68,68,68,68	0
54	MG	BA	3591	1/1	0.94	0.22	-	99,99,99,99	0
54	MG	DA	3757	1/1	0.97	0.14	-	89,89,89,89	0
54	MG	DA	2910	1/1	0.97	0.68	-	38,38,38,38	0
54	MG	DA	3536	1/1	0.97	0.16	-	92,92,92,92	0
54	MG	DA	3458	1/1	0.86	0.09	-	95,95,95,95	0
54	MG	DL	203	1/1	0.88	0.33	-	66,66,66,66	0
54	MG	BA	3409	1/1	0.97	0.15	-	51,51,51,51	0
54	MG	DA	3819	1/1	0.90	0.58	-	130,130,130,130	0
54	MG	CA	1971	1/1	0.84	0.43	-	86,86,86,86	0
54	MG	DA	3688	1/1	0.78	0.57	-	50,50,50,50	0
54	MG	DA	3440	1/1	0.96	0.46	-	125,125,125,125	0
54	MG	DA	2983	1/1	0.94	0.40	-	52,52,52,52	0
54	MG	CC	303	1/1	0.52	0.23	-	147,147,147,147	0
54	MG	AA	1756	1/1	0.96	0.23	-	111,111,111,111	0
54	MG	DA	2915	1/1	0.92	0.47	-	49,49,49,49	0
54	MG	DA	2905	1/1	0.98	0.33	-	18,18,18,18	0
54	MG	BA	3561	1/1	0.95	0.14	-	75,75,75,75	0
54	MG	BB	215	1/1	0.93	0.39	-	82,82,82,82	0
54	MG	CA	1849	1/1	0.93	0.08	-	167,167,167,167	0
54	MG	BA	2984	1/1	0.90	0.20	-	50,50,50,50	0
54	MG	DA	3163	1/1	0.85	0.31	-	113,113,113,113	0
54	MG	DA	3237	1/1	0.84	0.73	-	64,64,64,64	0
54	MG	BA	3201	1/1	0.82	0.43	-	107,107,107,107	0
54	MG	BA	3346	1/1	0.90	0.15	-	136,136,136,136	0
54	MG	DA	3549	1/1	0.87	0.32	-	115,115,115,115	0
54	MG	DA	3273	1/1	0.90	0.13	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3386	1/1	0.98	0.36	-	134,134,134,134	0
54	MG	CA	1847	1/1	0.94	0.16	-	58,58,58,58	0
54	MG	DA	3669	1/1	0.72	0.46	-	61,61,61,61	0
54	MG	BA	3091	1/1	0.89	0.22	-	72,72,72,72	0
54	MG	AA	1769	1/1	0.84	0.49	-	118,118,118,118	0
54	MG	BA	3324	1/1	0.76	0.38	-	109,109,109,109	0
54	MG	DA	3592	1/1	0.90	0.12	-	114,114,114,114	0
54	MG	BA	3242	1/1	0.78	0.15	-	112,112,112,112	0
54	MG	DA	3766	1/1	0.64	0.14	-	123,123,123,123	0
54	MG	BA	3299	1/1	0.91	0.15	-	72,72,72,72	0
54	MG	DA	3612	1/1	0.92	0.16	-	74,74,74,74	0
54	MG	DA	3513	1/1	0.99	0.34	-	30,30,30,30	0
54	MG	DA	3229	1/1	0.92	0.22	-	59,59,59,59	0
54	MG	BA	3195	1/1	0.91	0.71	-	91,91,91,91	0
54	MG	DA	3614	1/1	-0.06	0.31	-	128,128,128,128	0
54	MG	DA	3206	1/1	0.92	0.33	-	89,89,89,89	0
54	MG	CA	1712	1/1	0.62	0.25	-	108,108,108,108	0
54	MG	DA	3212	1/1	0.93	0.44	-	75,75,75,75	0
54	MG	CA	1652	1/1	0.96	0.19	-	87,87,87,87	0
54	MG	BA	3593	1/1	0.74	0.14	-	81,81,81,81	0
54	MG	DA	3833	1/1	0.93	0.43	-	73,73,73,73	0
54	MG	CA	1732	1/1	0.70	0.82	-	78,78,78,78	0
54	MG	CA	1945	1/1	0.92	0.64	-	95,95,95,95	0
54	MG	BA	3317	1/1	0.96	0.17	-	84,84,84,84	0
54	MG	DA	3223	1/1	0.79	0.10	-	83,83,83,83	0
54	MG	CA	1663	1/1	0.90	0.31	-	128,128,128,128	0
54	MG	AF	201	1/1	0.84	0.14	-	90,90,90,90	0
54	MG	CA	1743	1/1	0.90	0.14	-	88,88,88,88	0
54	MG	DA	3508	1/1	0.94	0.17	-	70,70,70,70	0
54	MG	CA	1817	1/1	0.95	0.23	-	89,89,89,89	0
54	MG	DA	3687	1/1	0.91	0.18	-	57,57,57,57	0
54	MG	AA	1872	1/1	0.95	0.51	-	88,88,88,88	0
54	MG	CA	1863	1/1	0.81	0.14	-	125,125,125,125	0
54	MG	DA	3675	1/1	0.80	0.62	-	46,46,46,46	0
54	MG	DA	3582	1/1	0.94	0.16	-	85,85,85,85	0
54	MG	DA	3418	1/1	0.74	0.24	-	65,65,65,65	0
54	MG	BB	219	1/1	0.84	0.09	-	69,69,69,69	0
54	MG	DA	3352	1/1	0.95	0.21	-	121,121,121,121	0
54	MG	BA	3401	1/1	0.91	0.27	-	85,85,85,85	0
54	MG	AA	1783	1/1	0.96	0.23	-	123,123,123,123	0
54	MG	BA	3359	1/1	0.97	0.12	-	89,89,89,89	0
54	MG	BA	3502	1/1	0.76	0.12	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3217	1/1	0.88	0.22	-	55,55,55,55	0
54	MG	CA	1792	1/1	0.86	0.31	-	93,93,93,93	0
54	MG	AA	1648	1/1	0.97	0.49	-	90,90,90,90	0
54	MG	BA	3257	1/1	0.73	1.02	-	108,108,108,108	0
54	MG	BA	3407	1/1	0.88	0.30	-	79,79,79,79	0
54	MG	CE	202	1/1	0.72	0.23	-	80,80,80,80	0
54	MG	DA	3083	1/1	0.95	0.25	-	120,120,120,120	0
54	MG	BA	3263	1/1	0.87	0.32	-	107,107,107,107	0
54	MG	DA	3769	1/1	0.65	0.35	-	90,90,90,90	0
54	MG	BA	3300	1/1	0.96	0.32	-	93,93,93,93	0
54	MG	BA	3285	1/1	0.95	0.11	-	91,91,91,91	0
54	MG	DA	3362	1/1	0.91	0.29	-	78,78,78,78	0
54	MG	DA	3709	1/1	0.93	0.75	-	75,75,75,75	0
54	MG	DA	3814	1/1	0.73	0.17	-	186,186,186,186	0
54	MG	CA	1827	1/1	0.95	0.25	-	82,82,82,82	0
54	MG	BA	3600	1/1	0.79	0.14	-	93,93,93,93	0
54	MG	DA	3405	1/1	0.94	0.87	-	67,67,67,67	0
54	MG	DB	237	1/1	0.74	0.81	-	109,109,109,109	0
54	MG	DA	3565	1/1	0.96	0.17	-	97,97,97,97	0
54	MG	BA	3566	1/1	0.90	0.31	-	72,72,72,72	0
54	MG	CA	1872	1/1	0.93	0.47	-	84,84,84,84	0
54	MG	DA	3644	1/1	0.90	0.50	-	75,75,75,75	0
54	MG	CA	1911	1/1	0.73	0.76	-	90,90,90,90	0
54	MG	BA	3347	1/1	0.89	0.16	-	77,77,77,77	0
54	MG	BA	3005	1/1	0.99	0.76	-	53,53,53,53	0
54	MG	DA	3545	1/1	0.70	0.70	-	94,94,94,94	0
54	MG	BA	3029	1/1	0.97	0.33	-	41,41,41,41	0
54	MG	BA	3587	1/1	0.90	0.27	-	77,77,77,77	0
54	MG	BA	3093	1/1	0.89	0.39	-	67,67,67,67	0
54	MG	DA	3350	1/1	0.92	0.09	-	95,95,95,95	0
54	MG	DA	2939	1/1	0.98	0.40	-	21,21,21,21	0
54	MG	BA	3598	1/1	0.91	0.10	-	100,100,100,100	0
54	MG	BA	3077	1/1	0.82	0.51	-	55,55,55,55	0
54	MG	DA	3804	1/1	0.93	0.32	-	72,72,72,72	0
54	MG	BA	2952	1/1	0.93	0.19	-	59,59,59,59	0
54	MG	DA	3245	1/1	0.92	0.79	-	100,100,100,100	0
54	MG	AA	1686	1/1	0.92	0.47	-	65,65,65,65	0
54	MG	BA	3130	1/1	0.93	0.21	-	47,47,47,47	0
54	MG	DA	3093	1/1	0.88	0.35	-	47,47,47,47	0
54	MG	AA	1766	1/1	0.89	0.24	-	106,106,106,106	0
54	MG	BA	3108	1/1	0.81	0.50	-	72,72,72,72	0
54	MG	CA	1643	1/1	0.77	0.19	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1859	1/1	0.89	0.21	-	87,87,87,87	0
54	MG	BB	213	1/1	0.90	0.41	-	111,111,111,111	0
54	MG	BA	3453	1/1	0.96	0.27	-	27,27,27,27	0
54	MG	DA	3264	1/1	0.89	0.12	-	78,78,78,78	0
54	MG	DA	3406	1/1	0.93	0.20	-	59,59,59,59	0
54	MG	DA	3115	1/1	0.96	0.18	-	58,58,58,58	0
54	MG	BA	2944	1/1	0.92	0.51	-	47,47,47,47	0
54	MG	CA	1938	1/1	0.80	0.20	-	81,81,81,81	0
54	MG	AV	6202	1/1	0.71	0.08	-	97,97,97,97	0
54	MG	DA	3230	1/1	0.97	0.25	-	80,80,80,80	0
54	MG	DA	2903	1/1	0.99	0.24	-	16,16,16,16	0
54	MG	CA	1605	1/1	0.96	0.64	-	54,54,54,54	0
54	MG	BA	3094	1/1	0.76	0.27	-	63,63,63,63	0
54	MG	DA	3556	1/1	0.96	0.15	-	110,110,110,110	0
54	MG	BA	3113	1/1	0.97	0.53	-	59,59,59,59	0
54	MG	DA	2937	1/1	0.94	0.43	-	43,43,43,43	0
54	MG	DA	3553	1/1	0.94	0.14	-	91,91,91,91	0
54	MG	DA	3084	1/1	0.91	0.85	-	65,65,65,65	0
54	MG	BA	3444	1/1	0.97	0.32	-	26,26,26,26	0
54	MG	DA	3138	1/1	0.93	0.30	-	81,81,81,81	0
54	MG	BA	3111	1/1	0.91	0.72	-	64,64,64,64	0
54	MG	DA	3397	1/1	0.81	0.92	-	124,124,124,124	0
54	MG	DD	304	1/1	0.73	0.96	-	94,94,94,94	0
54	MG	BA	3537	1/1	0.88	0.19	-	60,60,60,60	0
54	MG	CA	1831	1/1	0.93	0.44	-	90,90,90,90	0
54	MG	AD	304	1/1	0.68	0.44	-	113,113,113,113	0
54	MG	DA	3512	1/1	0.91	0.35	-	159,159,159,159	0
54	MG	DA	3711	1/1	0.83	0.44	-	84,84,84,84	0
54	MG	CA	1721	1/1	0.88	0.91	-	118,118,118,118	0
54	MG	BA	3255	1/1	0.86	0.57	-	101,101,101,101	0
54	MG	BA	3063	1/1	0.96	0.92	-	85,85,85,85	0
54	MG	BA	3633	1/1	0.63	0.49	-	88,88,88,88	0
54	MG	DA	3085	1/1	0.91	0.46	-	68,68,68,68	0
54	MG	DA	2956	1/1	0.90	0.43	-	44,44,44,44	0
54	MG	BA	3182	1/1	0.95	0.19	-	78,78,78,78	0
54	MG	AA	1676	1/1	0.95	0.14	-	90,90,90,90	0
54	MG	DA	3122	1/1	0.64	0.27	-	93,93,93,93	0
54	MG	DA	3054	1/1	0.95	1.00	-	72,72,72,72	0
54	MG	BA	3590	1/1	0.65	0.34	-	119,119,119,119	0
54	MG	DA	3813	1/1	0.94	0.15	-	50,50,50,50	0
54	MG	BA	3081	1/1	0.91	0.21	-	67,67,67,67	0
54	MG	AA	1689	1/1	0.92	0.62	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1957	1/1	0.97	0.43	-	73,73,73,73	0
54	MG	AA	1823	1/1	0.79	0.63	-	148,148,148,148	0
54	MG	DA	3239	1/1	0.93	0.18	-	126,126,126,126	0
54	MG	AL	202	1/1	0.84	0.12	-	67,67,67,67	0
54	MG	AA	1770	1/1	0.91	0.21	-	76,76,76,76	0
54	MG	AA	1762	1/1	0.90	0.55	-	91,91,91,91	0
54	MG	AA	1797	1/1	0.89	0.48	-	72,72,72,72	0
54	MG	AA	1768	1/1	0.95	0.80	-	87,87,87,87	0
54	MG	DA	3699	1/1	0.58	0.12	-	96,96,96,96	0
54	MG	AA	1771	1/1	0.71	1.16	-	111,111,111,111	0
54	MG	DA	3542	1/1	0.95	0.24	-	65,65,65,65	0
54	MG	BA	3627	1/1	0.82	0.34	-	67,67,67,67	0
54	MG	DA	3659	1/1	0.87	1.14	-	61,61,61,61	0
54	MG	BA	2978	1/1	0.76	0.71	-	58,58,58,58	0
54	MG	CA	1907	1/1	0.88	0.44	-	87,87,87,87	0
54	MG	CA	1897	1/1	0.76	0.81	-	74,74,74,74	0
54	MG	DA	3188	1/1	0.81	0.53	-	69,69,69,69	0
54	MG	BA	3224	1/1	0.97	0.25	-	97,97,97,97	0
54	MG	BA	3543	1/1	0.86	0.30	-	76,76,76,76	0
54	MG	BA	3032	1/1	0.82	0.37	-	76,76,76,76	0
54	MG	DA	3200	1/1	0.95	0.30	-	97,97,97,97	0
54	MG	CA	1820	1/1	0.73	1.15	-	99,99,99,99	0
54	MG	BA	3416	1/1	0.77	0.12	-	83,83,83,83	0
54	MG	DK	203	1/1	0.83	0.24	-	73,73,73,73	0
54	MG	DA	3236	1/1	0.96	0.15	-	75,75,75,75	0
54	MG	BA	3296	1/1	0.97	0.22	-	71,71,71,71	0
54	MG	DA	2967	1/1	0.96	0.33	-	34,34,34,34	0
54	MG	CA	1836	1/1	0.98	0.43	-	98,98,98,98	0
54	MG	AA	1692	1/1	0.93	0.16	-	89,89,89,89	0
54	MG	DA	3821	1/1	0.92	0.34	-	79,79,79,79	0
54	MG	DA	3732	1/1	0.82	0.32	-	81,81,81,81	0
54	MG	BA	3559	1/1	0.79	0.76	-	70,70,70,70	0
54	MG	DA	3253	1/1	0.90	0.22	-	70,70,70,70	0
54	MG	CA	1776	1/1	0.90	0.13	-	118,118,118,118	0
54	MG	DD	302	1/1	0.89	0.21	-	61,61,61,61	0
54	MG	DA	3839	1/1	0.68	0.30	-	86,86,86,86	0
54	MG	BA	3279	1/1	0.99	0.06	-	85,85,85,85	0
54	MG	CA	1841	1/1	0.90	0.18	-	95,95,95,95	0
54	MG	AA	1671	1/1	0.95	0.13	-	74,74,74,74	0
54	MG	DB	208	1/1	0.92	0.16	-	86,86,86,86	0
54	MG	BA	3601	1/1	0.96	0.20	-	76,76,76,76	0
54	MG	CA	1934	1/1	0.95	0.12	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	2946	1/1	0.97	0.51	-	25,25,25,25	0
54	MG	AA	1816	1/1	0.88	0.88	-	89,89,89,89	0
54	MG	AA	1799	1/1	0.81	0.52	-	58,58,58,58	0
54	MG	CA	1734	1/1	0.74	0.87	-	90,90,90,90	0
54	MG	AA	1750	1/1	0.91	0.30	-	128,128,128,128	0
54	MG	AA	1818	1/1	0.75	0.23	-	76,76,76,76	0
54	MG	CA	1757	1/1	0.97	0.18	-	102,102,102,102	0
54	MG	DA	3183	1/1	0.98	0.33	-	76,76,76,76	0
54	MG	DA	3611	1/1	0.95	0.77	-	74,74,74,74	0
54	MG	BA	3282	1/1	0.76	0.40	-	98,98,98,98	0
54	MG	DA	3358	1/1	0.96	0.30	-	83,83,83,83	0
54	MG	BA	3583	1/1	0.96	0.70	-	105,105,105,105	0
54	MG	BA	3354	1/1	0.53	0.56	-	123,123,123,123	0
54	MG	DA	3049	1/1	0.98	0.52	-	43,43,43,43	0
54	MG	BA	3314	1/1	0.96	0.20	-	69,69,69,69	0
54	MG	CA	1959	1/1	0.96	0.09	-	106,106,106,106	0
54	MG	BA	3665	1/1	0.91	0.25	-	123,123,123,123	0
54	MG	BA	3516	1/1	0.66	0.39	-	100,100,100,100	0
54	MG	DA	3824	1/1	0.94	0.25	-	113,113,113,113	0
54	MG	AA	1848	1/1	0.88	0.34	-	77,77,77,77	0
54	MG	DA	3523	1/1	0.96	0.13	-	77,77,77,77	0
54	MG	BB	210	1/1	0.91	0.29	-	82,82,82,82	0
54	MG	DA	3348	1/1	0.87	0.10	-	83,83,83,83	0
54	MG	CA	1925	1/1	0.86	0.37	-	77,77,77,77	0
54	MG	DA	3786	1/1	0.79	0.90	-	104,104,104,104	0
54	MG	DA	3425	1/1	0.80	0.25	-	113,113,113,113	0
54	MG	DA	3474	1/1	0.62	1.06	-	81,81,81,81	0
54	MG	DA	3282	1/1	0.90	0.55	-	69,69,69,69	0
54	MG	CB	301	1/1	0.82	0.22	-	115,115,115,115	0
54	MG	AI	201	1/1	0.92	0.19	-	70,70,70,70	0
54	MG	CA	1699	1/1	0.97	0.10	-	76,76,76,76	0
54	MG	AA	1702	1/1	0.95	0.15	-	56,56,56,56	0
54	MG	CA	1868	1/1	0.94	0.30	-	71,71,71,71	0
54	MG	BA	3610	1/1	0.88	0.90	-	80,80,80,80	0
54	MG	AA	1754	1/1	0.95	0.16	-	98,98,98,98	0
54	MG	CA	1661	1/1	0.94	0.11	-	80,80,80,80	0
54	MG	CA	1830	1/1	0.80	0.26	-	82,82,82,82	0
54	MG	AA	1725	1/1	0.94	0.24	-	93,93,93,93	0
54	MG	CA	1794	1/1	0.99	0.12	-	122,122,122,122	0
54	MG	CA	1825	1/1	0.92	0.46	-	97,97,97,97	0
54	MG	DA	2944	1/1	0.93	0.43	-	25,25,25,25	0
54	MG	DA	3487	1/1	0.92	0.40	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3293	1/1	0.96	0.24	-	60,60,60,60	0
54	MG	BA	3135	1/1	0.83	0.24	-	61,61,61,61	0
54	MG	DA	3216	1/1	0.92	0.54	-	91,91,91,91	0
54	MG	CO	104	1/1	0.63	0.24	-	99,99,99,99	0
54	MG	AA	1633	1/1	0.83	0.29	-	123,123,123,123	0
54	MG	AA	1851	1/1	0.91	0.62	-	93,93,93,93	0
54	MG	DA	3712	1/1	0.82	0.20	-	41,41,41,41	0
54	MG	BA	3538	1/1	0.93	0.25	-	75,75,75,75	0
54	MG	BA	2987	1/1	0.85	0.06	-	79,79,79,79	0
54	MG	DA	3147	1/1	0.88	0.47	-	86,86,86,86	0
54	MG	BC	301	1/1	0.86	0.80	-	60,60,60,60	0
54	MG	BA	3638	1/1	0.89	0.85	-	127,127,127,127	0
54	MG	BA	3398	1/1	0.93	0.28	-	74,74,74,74	0
54	MG	DA	3586	1/1	0.89	0.32	-	79,79,79,79	0
54	MG	CA	1874	1/1	0.78	0.38	-	76,76,76,76	0
54	MG	DA	3031	1/1	0.90	0.62	-	79,79,79,79	0
54	MG	AA	1753	1/1	0.85	0.60	-	103,103,103,103	0
54	MG	BA	3229	1/1	0.75	0.27	-	90,90,90,90	0
54	MG	DB	221	1/1	0.95	0.29	-	98,98,98,98	0
54	MG	AA	1687	1/1	0.85	0.70	-	108,108,108,108	0
54	MG	BA	3312	1/1	0.97	0.69	-	71,71,71,71	0
54	MG	DA	3783	1/1	0.96	0.13	-	63,63,63,63	0
54	MG	BA	3392	1/1	0.80	0.27	-	108,108,108,108	0
54	MG	DA	3430	1/1	0.96	0.27	-	103,103,103,103	0
54	MG	CD	302	1/1	0.83	0.13	-	74,74,74,74	0
54	MG	CA	1774	1/1	0.90	0.27	-	79,79,79,79	0
54	MG	AA	1791	1/1	0.92	0.08	-	106,106,106,106	0
54	MG	DA	3208	1/1	0.97	0.28	-	56,56,56,56	0
54	MG	BA	3302	1/1	0.93	0.34	-	84,84,84,84	0
54	MG	CA	1913	1/1	0.89	0.19	-	109,109,109,109	0
54	MG	D1	101	1/1	0.65	0.39	-	80,80,80,80	0
54	MG	BA	3609	1/1	0.93	0.16	-	65,65,65,65	0
54	MG	CA	1954	1/1	0.85	0.08	-	89,89,89,89	0
54	MG	BA	3552	1/1	0.87	0.11	-	99,99,99,99	0
54	MG	CA	1812	1/1	0.93	0.74	-	92,92,92,92	0
54	MG	DA	3578	1/1	0.69	0.29	-	96,96,96,96	0
54	MG	BA	3372	1/1	0.74	1.46	-	123,123,123,123	0
54	MG	BB	206	1/1	0.83	0.47	-	125,125,125,125	0
54	MG	BA	3389	1/1	0.92	0.30	-	66,66,66,66	0
54	MG	DA	3530	1/1	0.88	0.32	-	71,71,71,71	0
54	MG	AA	1796	1/1	0.91	0.62	-	106,106,106,106	0
54	MG	BA	3680	1/1	0.71	0.76	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3518	1/1	0.96	0.24	-	102,102,102,102	0
54	MG	DA	3155	1/1	0.78	0.29	-	70,70,70,70	0
54	MG	DA	3370	1/1	0.86	1.28	-	92,92,92,92	0
54	MG	BA	3298	1/1	0.97	0.22	-	126,126,126,126	0
54	MG	DA	3808	1/1	0.85	0.32	-	116,116,116,116	0
54	MG	DA	3744	1/1	0.92	0.24	-	64,64,64,64	0
54	MG	DA	3714	1/1	0.90	0.07	-	96,96,96,96	0
54	MG	BA	3200	1/1	0.98	0.26	-	93,93,93,93	0
54	MG	BA	3465	1/1	0.91	0.32	-	31,31,31,31	0
54	MG	AA	1728	1/1	0.80	0.29	-	71,71,71,71	0
54	MG	BA	2969	1/1	0.94	0.56	-	69,69,69,69	0
54	MG	BA	3284	1/1	0.76	0.24	-	95,95,95,95	0
54	MG	BA	3212	1/1	0.89	0.27	-	67,67,67,67	0
54	MG	BA	3318	1/1	0.87	0.48	-	73,73,73,73	0
54	MG	DA	3278	1/1	0.74	0.74	-	99,99,99,99	0
54	MG	CA	1604	1/1	0.96	0.48	-	43,43,43,43	0
54	MG	BA	3668	1/1	0.68	0.47	-	97,97,97,97	0
54	MG	DA	3494	1/1	0.88	0.29	-	63,63,63,63	0
54	MG	DA	3488	1/1	0.96	0.29	-	102,102,102,102	0
54	MG	BA	3436	1/1	0.97	0.53	-	38,38,38,38	0
54	MG	DA	3433	1/1	0.93	0.25	-	67,67,67,67	0
54	MG	CL	202	1/1	0.97	0.07	-	105,105,105,105	0
54	MG	BA	3115	1/1	0.87	0.44	-	76,76,76,76	0
54	MG	DA	3324	1/1	0.92	0.25	-	95,95,95,95	0
54	MG	AA	1792	1/1	0.79	0.10	-	101,101,101,101	0
54	MG	DA	3075	1/1	0.84	0.19	-	50,50,50,50	0
54	MG	DA	3661	1/1	0.95	0.64	-	98,98,98,98	0
54	MG	CA	1636	1/1	0.95	0.08	-	98,98,98,98	0
54	MG	DA	3211	1/1	0.75	0.37	-	64,64,64,64	0
54	MG	BA	3657	1/1	0.82	0.43	-	84,84,84,84	0
54	MG	BA	3155	1/1	0.75	0.93	-	99,99,99,99	0
54	MG	DA	3325	1/1	0.92	0.25	-	66,66,66,66	0
54	MG	BA	3420	1/1	0.72	0.53	-	94,94,94,94	0
54	MG	DA	3076	1/1	0.94	0.13	-	78,78,78,78	0
54	MG	CA	1808	1/1	0.94	0.14	-	98,98,98,98	0
54	MG	CA	1864	1/1	0.95	0.21	-	90,90,90,90	0
54	MG	BA	3422	1/1	0.91	0.18	-	93,93,93,93	0
54	MG	CA	1664	1/1	0.98	0.09	-	85,85,85,85	0
54	MG	DA	2993	1/1	0.86	0.38	-	47,47,47,47	0
54	MG	BA	3395	1/1	0.94	0.40	-	84,84,84,84	0
54	MG	AA	1654	1/1	0.94	0.28	-	99,99,99,99	0
54	MG	BA	3577	1/1	0.95	0.32	-	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1706	1/1	0.96	0.46	-	78,78,78,78	0
54	MG	DB	240	1/1	0.90	0.17	-	123,123,123,123	0
54	MG	AA	1742	1/1	0.93	0.14	-	90,90,90,90	0
54	MG	BA	2986	1/1	0.96	0.72	-	54,54,54,54	0
54	MG	DA	3302	1/1	0.87	0.73	-	102,102,102,102	0
54	MG	DA	3380	1/1	0.80	0.21	-	84,84,84,84	0
54	MG	BA	3181	1/1	0.92	0.21	-	62,62,62,62	0
54	MG	DA	3393	1/1	0.88	0.40	-	77,77,77,77	0
54	MG	BA	3132	1/1	0.68	0.26	-	66,66,66,66	0
54	MG	AV	6208	1/1	0.96	0.38	-	79,79,79,79	0
54	MG	CE	203	1/1	0.70	0.12	-	79,79,79,79	0
54	MG	CG	203	1/1	0.80	0.22	-	100,100,100,100	0
54	MG	BA	3028	1/1	0.85	1.61	-	61,61,61,61	0
54	MG	DA	2912	1/1	0.94	0.41	-	19,19,19,19	0
54	MG	BR	201	1/1	0.89	0.07	-	75,75,75,75	0
54	MG	AA	1677	1/1	0.97	0.17	-	50,50,50,50	0
54	MG	DA	3723	1/1	0.88	0.31	-	67,67,67,67	0
54	MG	DA	3682	1/1	0.91	0.23	-	59,59,59,59	0
54	MG	AA	1855	1/1	0.93	0.34	-	81,81,81,81	0
54	MG	DA	3201	1/1	0.98	0.05	-	46,46,46,46	0
54	MG	BA	3355	1/1	0.96	0.22	-	72,72,72,72	0
54	MG	BA	3231	1/1	0.94	0.29	-	64,64,64,64	0
54	MG	CB	302	1/1	0.92	0.21	-	112,112,112,112	0
54	MG	CA	1892	1/1	0.90	0.65	-	114,114,114,114	0
54	MG	BA	3283	1/1	0.84	0.26	-	100,100,100,100	0
54	MG	BA	3539	1/1	0.85	0.42	-	97,97,97,97	0
54	MG	BA	3345	1/1	0.92	0.26	-	71,71,71,71	0
54	MG	DA	3148	1/1	0.92	0.12	-	94,94,94,94	0
54	MG	CA	1722	1/1	0.74	0.30	-	116,116,116,116	0
54	MG	BA	3331	1/1	0.95	0.86	-	66,66,66,66	0
54	MG	AA	1878	1/1	0.77	0.09	-	92,92,92,92	0
54	MG	DA	3456	1/1	0.96	0.47	-	121,121,121,121	0
54	MG	CA	1923	1/1	0.93	0.31	-	74,74,74,74	0
54	MG	AA	1623	1/1	0.66	0.16	-	99,99,99,99	0
54	MG	DA	3845	1/1	0.90	0.23	-	94,94,94,94	0
54	MG	BA	3565	1/1	0.97	0.25	-	104,104,104,104	0
54	MG	DA	3269	1/1	0.93	0.19	-	109,109,109,109	0
54	MG	DA	3219	1/1	0.90	0.14	-	60,60,60,60	0
54	MG	BA	3511	1/1	0.82	1.01	-	78,78,78,78	0
54	MG	AA	1819	1/1	0.81	0.45	-	73,73,73,73	0
54	MG	AA	1801	1/1	0.93	0.89	-	71,71,71,71	0
54	MG	AA	1747	1/1	0.88	0.45	-	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3716	1/1	0.82	0.58	-	78,78,78,78	0
54	MG	BA	2925	1/1	0.98	0.29	-	12,12,12,12	0
54	MG	DA	3368	1/1	0.88	0.25	-	98,98,98,98	0
54	MG	DB	202	1/1	0.96	0.30	-	33,33,33,33	0
54	MG	DA	3794	1/1	0.92	0.23	-	104,104,104,104	0
54	MG	DA	3809	1/1	0.76	1.09	-	84,84,84,84	0
54	MG	CA	1706	1/1	0.89	0.82	-	106,106,106,106	0
54	MG	BA	2953	1/1	0.96	0.18	-	45,45,45,45	0
54	MG	DA	3411	1/1	0.79	0.51	-	68,68,68,68	0
54	MG	DA	3290	1/1	0.90	0.15	-	61,61,61,61	0
54	MG	AA	1803	1/1	0.83	0.49	-	69,69,69,69	0
54	MG	CA	1895	1/1	0.92	0.73	-	88,88,88,88	0
54	MG	AA	1789	1/1	0.82	0.41	-	106,106,106,106	0
54	MG	BA	3207	1/1	0.94	0.37	-	70,70,70,70	0
54	MG	DA	3547	1/1	0.98	0.40	-	115,115,115,115	0
54	MG	DA	3112	1/1	0.94	0.27	-	91,91,91,91	0
54	MG	AA	1765	1/1	0.94	0.14	-	91,91,91,91	0
54	MG	DA	3191	1/1	0.89	0.23	-	62,62,62,62	0
54	MG	DA	3651	1/1	0.91	0.37	-	51,51,51,51	0
54	MG	AA	1794	1/1	0.94	0.15	-	112,112,112,112	0
54	MG	DA	3507	1/1	0.97	0.65	-	70,70,70,70	0
54	MG	BA	2959	1/1	0.96	0.31	-	40,40,40,40	0
54	MG	DA	3576	1/1	0.94	0.49	-	99,99,99,99	0
54	MG	BA	3292	1/1	0.88	0.24	-	71,71,71,71	0
54	MG	BA	3335	1/1	0.85	0.89	-	80,80,80,80	0
54	MG	DA	3081	1/1	0.83	0.68	-	67,67,67,67	0
54	MG	DB	218	1/1	0.94	0.10	-	113,113,113,113	0
54	MG	DA	3798	1/1	0.95	0.43	-	88,88,88,88	0
54	MG	DA	3315	1/1	0.94	0.40	-	58,58,58,58	0
54	MG	DA	3450	1/1	0.76	0.72	-	81,81,81,81	0
54	MG	DA	3642	1/1	0.91	0.45	-	52,52,52,52	0
54	MG	CA	1834	1/1	0.94	0.17	-	81,81,81,81	0
54	MG	DA	3145	1/1	0.94	0.16	-	100,100,100,100	0
54	MG	CA	1900	1/1	0.81	0.23	-	86,86,86,86	0
54	MG	DA	3133	1/1	0.98	0.18	-	114,114,114,114	0
54	MG	DF	201	1/1	0.79	0.32	-	70,70,70,70	0
54	MG	CA	1844	1/1	0.85	0.41	-	78,78,78,78	0
54	MG	DA	3822	1/1	0.91	0.11	-	70,70,70,70	0
54	MG	AA	1602	1/1	0.95	0.89	-	45,45,45,45	0
54	MG	AA	1864	1/1	0.83	0.17	-	75,75,75,75	0
54	MG	BA	3209	1/1	0.92	0.60	-	81,81,81,81	0
54	MG	BA	2951	1/1	0.90	0.84	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3168	1/1	0.98	0.27	-	20,20,20,20	0
54	MG	DB	222	1/1	0.95	0.19	-	137,137,137,137	0
54	MG	BA	3472	1/1	0.95	0.51	-	65,65,65,65	0
54	MG	DA	3187	1/1	0.92	0.23	-	114,114,114,114	0
54	MG	AA	1703	1/1	0.93	0.45	-	63,63,63,63	0
54	MG	BA	3614	1/1	0.68	0.11	-	112,112,112,112	0
54	MG	DA	3841	1/1	0.81	0.40	-	80,80,80,80	0
54	MG	DA	3587	1/1	0.74	0.12	-	113,113,113,113	0
54	MG	DA	3313	1/1	0.89	0.54	-	78,78,78,78	0
54	MG	CA	1779	1/1	0.96	0.28	-	79,79,79,79	0
54	MG	BA	3521	1/1	0.89	0.19	-	88,88,88,88	0
54	MG	CA	1611	1/1	0.94	0.30	-	128,128,128,128	0
54	MG	BA	3528	1/1	0.87	0.22	-	73,73,73,73	0
54	MG	BY	101	1/1	0.73	0.34	-	42,42,42,42	0
54	MG	DA	3510	1/1	0.96	0.23	-	64,64,64,64	0
54	MG	DA	3213	1/1	0.99	0.25	-	59,59,59,59	0
54	MG	BB	214	1/1	0.88	0.65	-	84,84,84,84	0
54	MG	AA	1712	1/1	0.66	0.19	-	105,105,105,105	0
54	MG	AA	1716	1/1	0.80	0.32	-	96,96,96,96	0
54	MG	DA	2914	1/1	0.97	0.44	-	23,23,23,23	0
54	MG	CA	1618	1/1	0.91	0.69	-	84,84,84,84	0
54	MG	DA	3759	1/1	0.79	0.53	-	97,97,97,97	0
54	MG	BT	101	1/1	0.86	0.89	-	101,101,101,101	0
54	MG	CV	6201	1/1	0.72	0.10	-	95,95,95,95	0
54	MG	CA	1855	1/1	0.93	0.31	-	107,107,107,107	0
54	MG	CA	1625	1/1	0.86	0.51	-	67,67,67,67	0
54	MG	DA	3670	1/1	0.85	0.61	-	83,83,83,83	0
54	MG	DA	3134	1/1	0.92	0.75	-	69,69,69,69	0
54	MG	BA	3548	1/1	0.83	0.32	-	61,61,61,61	0
54	MG	CA	1851	1/1	0.95	0.48	-	103,103,103,103	0
54	MG	AA	1655	1/1	0.90	0.73	-	58,58,58,58	0
54	MG	DA	3708	1/1	0.80	0.18	-	63,63,63,63	0
54	MG	BA	3160	1/1	0.93	0.63	-	87,87,87,87	0
54	MG	DA	3596	1/1	0.82	0.81	-	113,113,113,113	0
54	MG	CA	1914	1/1	0.89	0.13	-	97,97,97,97	0
54	MG	DA	2964	1/1	0.95	0.46	-	45,45,45,45	0
54	MG	DA	3420	1/1	0.82	0.21	-	110,110,110,110	0
54	MG	DA	3136	1/1	0.97	0.21	-	57,57,57,57	0
54	MG	DA	3697	1/1	0.75	0.34	-	92,92,92,92	0
54	MG	DA	2981	1/1	0.95	0.30	-	40,40,40,40	0
54	MG	DA	3857	1/1	0.91	0.23	-	98,98,98,98	0
54	MG	DA	3396	1/1	0.96	0.28	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3603	1/1	0.91	0.22	-	86,86,86,86	0
54	MG	DA	3169	1/1	0.94	0.30	-	54,54,54,54	0
54	MG	BA	3531	1/1	0.68	0.14	-	91,91,91,91	0
54	MG	DA	3855	1/1	0.86	0.33	-	104,104,104,104	0
54	MG	BA	2962	1/1	0.77	0.30	-	54,54,54,54	0
54	MG	DA	3571	1/1	0.81	1.03	-	72,72,72,72	0
54	MG	CA	1687	1/1	0.91	1.14	-	63,63,63,63	0
54	MG	DA	3404	1/1	0.90	0.28	-	79,79,79,79	0
54	MG	DA	3285	1/1	0.93	0.52	-	65,65,65,65	0
54	MG	BA	3184	1/1	0.79	0.61	-	67,67,67,67	0
54	MG	DA	3539	1/1	0.62	0.16	-	81,81,81,81	0
54	MG	DA	3829	1/1	0.88	0.08	-	96,96,96,96	0
54	MG	AA	1621	1/1	0.74	0.66	-	71,71,71,71	0
54	MG	BB	201	1/1	0.94	0.48	-	63,63,63,63	0
54	MG	DV	201	1/1	0.84	0.20	-	90,90,90,90	0
54	MG	DA	3305	1/1	0.96	0.28	-	99,99,99,99	0
54	MG	BA	3397	1/1	0.52	0.40	-	125,125,125,125	0
54	MG	BA	3554	1/1	0.93	0.94	-	90,90,90,90	0
54	MG	AA	1617	1/1	0.83	0.59	-	84,84,84,84	0
54	MG	BA	3514	1/1	0.85	0.19	-	83,83,83,83	0
54	MG	AT	201	1/1	0.97	0.09	-	103,103,103,103	0
54	MG	DA	3078	1/1	0.97	0.44	-	48,48,48,48	0
54	MG	BA	3271	1/1	0.95	0.19	-	83,83,83,83	0
54	MG	BA	3445	1/1	0.84	0.46	-	61,61,61,61	0
54	MG	AA	1782	1/1	0.92	0.25	-	104,104,104,104	0
54	MG	DA	3551	1/1	0.91	0.22	-	80,80,80,80	0
54	MG	CA	1947	1/1	0.85	0.21	-	136,136,136,136	0
54	MG	BA	3635	1/1	0.90	0.28	-	113,113,113,113	0
54	MG	BA	3326	1/1	0.96	0.20	-	82,82,82,82	0
54	MG	AA	1865	1/1	0.88	0.12	-	107,107,107,107	0
54	MG	AA	1808	1/1	0.52	0.21	-	97,97,97,97	0
54	MG	DA	3727	1/1	0.85	0.33	-	88,88,88,88	0
54	MG	DA	3760	1/1	0.92	0.27	-	97,97,97,97	0
54	MG	AA	1629	1/1	0.83	0.43	-	66,66,66,66	0
54	MG	AA	1735	1/1	0.85	0.06	-	68,68,68,68	0
54	MG	CA	1735	1/1	0.62	0.52	-	77,77,77,77	0
54	MG	DB	211	1/1	0.96	0.07	-	65,65,65,65	0
54	MG	CC	304	1/1	0.83	0.21	-	121,121,121,121	0
54	MG	BA	2998	1/1	0.95	0.10	-	75,75,75,75	0
54	MG	DA	3203	1/1	0.92	0.10	-	67,67,67,67	0
54	MG	CA	1654	1/1	0.89	0.20	-	78,78,78,78	0
54	MG	DA	3060	1/1	0.96	0.48	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3328	1/1	0.93	0.33	-	85,85,85,85	0
54	MG	BA	3007	1/1	0.95	0.06	-	98,98,98,98	0
54	MG	BA	3036	1/1	0.91	1.45	-	57,57,57,57	0
54	MG	DA	3751	1/1	0.93	0.21	-	76,76,76,76	0
54	MG	BA	3586	1/1	0.85	0.28	-	97,97,97,97	0
54	MG	AA	1751	1/1	0.88	0.13	-	88,88,88,88	0
54	MG	AA	1675	1/1	0.93	0.27	-	82,82,82,82	0
54	MG	BA	3675	1/1	0.92	0.09	-	120,120,120,120	0
54	MG	CA	1724	1/1	0.48	0.58	-	124,124,124,124	0
54	MG	DA	3643	1/1	0.94	0.48	-	40,40,40,40	0
54	MG	DA	3438	1/1	0.94	0.22	-	54,54,54,54	0
54	MG	DA	3538	1/1	0.73	0.70	-	66,66,66,66	0
54	MG	BA	3185	1/1	0.80	0.40	-	85,85,85,85	0
54	MG	BA	3661	1/1	0.92	0.09	-	82,82,82,82	0
54	MG	BA	3240	1/1	0.93	0.38	-	157,157,157,157	0
54	MG	DA	3058	1/1	0.97	0.14	-	56,56,56,56	0
54	MG	DA	3445	1/1	0.88	0.15	-	137,137,137,137	0
54	MG	CA	1882	1/1	0.47	0.14	-	135,135,135,135	0
54	MG	CA	1929	1/1	0.87	0.48	-	95,95,95,95	0
54	MG	BA	3488	1/1	0.92	0.36	-	53,53,53,53	0
54	MG	AA	1763	1/1	0.92	0.06	-	121,121,121,121	0
54	MG	BA	3082	1/1	0.95	0.14	-	38,38,38,38	0
54	MG	BB	211	1/1	0.83	0.45	-	85,85,85,85	0
54	MG	AA	1608	1/1	0.94	0.41	-	46,46,46,46	0
54	MG	CA	1621	1/1	0.91	0.17	-	67,67,67,67	0
54	MG	CA	1936	1/1	0.94	0.40	-	102,102,102,102	0
54	MG	CA	1698	1/1	0.91	0.16	-	123,123,123,123	0
54	MG	DA	3701	1/1	0.91	0.21	-	56,56,56,56	0
54	MG	CA	1614	1/1	0.76	0.55	-	66,66,66,66	0
54	MG	BA	3644	1/1	0.90	0.37	-	86,86,86,86	0
54	MG	BA	3594	1/1	0.62	0.17	-	129,129,129,129	0
54	MG	DA	3222	1/1	0.88	0.49	-	112,112,112,112	0
54	MG	AA	1646	1/1	0.92	0.67	-	89,89,89,89	0
54	MG	DA	3398	1/1	0.98	0.17	-	80,80,80,80	0
54	MG	CA	1843	1/1	0.78	0.16	-	109,109,109,109	0
54	MG	DA	2917	1/1	0.81	0.18	-	71,71,71,71	0
54	MG	DA	3095	1/1	0.89	0.55	-	72,72,72,72	0
54	MG	BM	201	1/1	0.89	0.28	-	50,50,50,50	0
54	MG	CA	1958	1/1	0.65	0.62	-	125,125,125,125	0
54	MG	BA	3213	1/1	0.91	0.15	-	102,102,102,102	0
54	MG	BA	3315	1/1	0.87	0.15	-	84,84,84,84	0
54	MG	DA	3773	1/1	0.91	0.50	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1645	1/1	0.96	0.15	-	80,80,80,80	0
54	MG	DA	3385	1/1	0.75	0.46	-	69,69,69,69	0
54	MG	CA	1876	1/1	0.91	0.17	-	69,69,69,69	0
54	MG	DA	2969	1/1	0.95	0.50	-	39,39,39,39	0
54	MG	CA	1685	1/1	0.56	0.33	-	109,109,109,109	0
54	MG	BA	3286	1/1	0.89	0.20	-	68,68,68,68	0
54	MG	BA	3501	1/1	0.81	1.80	-	105,105,105,105	0
54	MG	DA	2977	1/1	0.98	0.57	-	49,49,49,49	0
54	MG	DA	3626	1/1	0.98	0.21	-	106,106,106,106	0
54	MG	BC	302	1/1	0.67	0.48	-	82,82,82,82	0
54	MG	DA	3555	1/1	0.95	0.54	-	61,61,61,61	0
54	MG	DA	3446	1/1	0.96	0.21	-	57,57,57,57	0
54	MG	AA	1781	1/1	0.87	0.20	-	92,92,92,92	0
54	MG	DA	3342	1/1	0.68	0.94	-	112,112,112,112	0
54	MG	BA	3580	1/1	0.86	0.64	-	94,94,94,94	0
54	MG	BA	3183	1/1	0.76	0.17	-	68,68,68,68	0
54	MG	CL	201	1/1	0.84	0.14	-	99,99,99,99	0
54	MG	BB	227	1/1	0.90	0.43	-	80,80,80,80	0
54	MG	BA	3158	1/1	0.81	0.96	-	99,99,99,99	0
54	MG	DA	3780	1/1	0.78	0.30	-	67,67,67,67	0
54	MG	CA	1669	1/1	0.93	0.17	-	76,76,76,76	0
54	MG	AA	1714	1/1	0.84	0.81	-	81,81,81,81	0
54	MG	DA	3749	1/1	0.81	0.74	-	59,59,59,59	0
54	MG	DA	3561	1/1	0.92	0.29	-	85,85,85,85	0
54	MG	DA	3495	1/1	0.90	0.27	-	111,111,111,111	0
54	MG	BA	3142	1/1	0.94	0.22	-	47,47,47,47	0
54	MG	DA	3346	1/1	0.99	0.15	-	68,68,68,68	0
54	MG	DA	3322	1/1	0.96	0.15	-	65,65,65,65	0
54	MG	DA	2920	1/1	0.96	0.29	-	14,14,14,14	0
54	MG	DB	226	1/1	0.83	0.14	-	73,73,73,73	0
54	MG	DA	3167	1/1	0.90	0.45	-	58,58,58,58	0
54	MG	CA	1785	1/1	0.89	0.26	-	76,76,76,76	0
54	MG	DA	3275	1/1	0.95	0.53	-	92,92,92,92	0
54	MG	CA	1650	1/1	0.47	0.28	-	111,111,111,111	0
54	MG	CA	1617	1/1	0.80	0.19	-	104,104,104,104	0
54	MG	CA	1926	1/1	0.98	0.30	-	76,76,76,76	0
54	MG	AA	1805	1/1	0.64	0.51	-	66,66,66,66	0
54	MG	BA	3447	1/1	0.91	0.80	-	39,39,39,39	0
54	MG	AA	1746	1/1	0.95	0.05	-	86,86,86,86	0
54	MG	DA	3763	1/1	0.97	0.26	-	57,57,57,57	0
54	MG	BB	221	1/1	0.84	0.35	-	89,89,89,89	0
54	MG	CA	1964	1/1	0.95	0.21	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3042	1/1	0.85	0.29	-	81,81,81,81	0
54	MG	D2	101	1/1	0.67	1.19	-	78,78,78,78	0
54	MG	BA	3440	1/1	0.97	0.41	-	23,23,23,23	0
54	MG	DA	3788	1/1	0.94	0.33	-	92,92,92,92	0
54	MG	AA	1697	1/1	0.86	0.81	-	73,73,73,73	0
54	MG	AA	1749	1/1	0.89	0.24	-	90,90,90,90	0
54	MG	BA	3572	1/1	0.94	0.09	-	87,87,87,87	0
54	MG	DA	3012	1/1	0.95	0.28	-	48,48,48,48	0
54	MG	DA	3304	1/1	0.80	0.28	-	85,85,85,85	0
54	MG	AA	1638	1/1	0.96	0.24	-	89,89,89,89	0
54	MG	BA	3012	1/1	0.84	0.89	-	71,71,71,71	0
54	MG	CA	1887	1/1	0.93	0.15	-	75,75,75,75	0
54	MG	DA	3124	1/1	0.98	0.40	-	51,51,51,51	0
54	MG	DA	3467	1/1	0.99	0.14	-	97,97,97,97	0
54	MG	DA	3818	1/1	0.89	0.16	-	78,78,78,78	0
54	MG	DA	3330	1/1	0.75	0.40	-	100,100,100,100	0
54	MG	CB	303	1/1	0.80	0.10	-	122,122,122,122	0
54	MG	CA	1972	1/1	0.93	0.29	-	67,67,67,67	0
54	MG	BA	3659	1/1	0.86	0.28	-	68,68,68,68	0
54	MG	CA	1750	1/1	0.90	0.27	-	87,87,87,87	0
54	MG	DA	3347	1/1	0.90	0.58	-	67,67,67,67	0
54	MG	AA	1863	1/1	0.94	0.15	-	119,119,119,119	0
54	MG	DA	2952	1/1	0.89	0.47	-	25,25,25,25	0
54	MG	BA	3585	1/1	0.76	0.51	-	69,69,69,69	0
54	MG	DA	3621	1/1	0.73	0.20	-	88,88,88,88	0
54	MG	BA	3323	1/1	0.68	0.32	-	98,98,98,98	0
54	MG	BA	3545	1/1	0.80	0.60	-	59,59,59,59	0
54	MG	CA	1815	1/1	0.92	0.39	-	97,97,97,97	0
54	MG	DK	202	1/1	0.73	0.28	-	69,69,69,69	0
54	MG	DA	3408	1/1	0.88	0.23	-	109,109,109,109	0
54	MG	CA	1839	1/1	0.86	0.35	-	92,92,92,92	0
54	MG	BA	3367	1/1	0.93	0.22	-	74,74,74,74	0
54	MG	BA	3478	1/1	0.85	0.77	-	78,78,78,78	0
54	MG	DA	3505	1/1	0.79	0.40	-	105,105,105,105	0
54	MG	DA	3795	1/1	0.83	0.48	-	80,80,80,80	0
54	MG	BA	2995	1/1	0.76	0.84	-	57,57,57,57	0
54	MG	BA	3251	1/1	0.90	0.54	-	95,95,95,95	0
54	MG	CA	1730	1/1	0.72	0.19	-	112,112,112,112	0
54	MG	BA	3141	1/1	0.90	0.65	-	91,91,91,91	0
54	MG	AA	1744	1/1	0.70	0.17	-	96,96,96,96	0
54	MG	BA	3303	1/1	0.94	0.22	-	157,157,157,157	0
54	MG	DA	2994	1/1	0.95	0.33	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1777	1/1	0.97	0.34	-	98,98,98,98	0
54	MG	DA	3816	1/1	0.93	0.19	-	52,52,52,52	0
54	MG	AA	1656	1/1	0.83	0.57	-	86,86,86,86	0
54	MG	DA	2992	1/1	0.95	0.39	-	60,60,60,60	0
54	MG	DA	3453	1/1	0.86	0.63	-	87,87,87,87	0
54	MG	DA	3314	1/1	0.85	0.37	-	105,105,105,105	0
54	MG	CA	1800	1/1	0.86	0.18	-	89,89,89,89	0
54	MG	BA	3629	1/1	0.81	0.34	-	86,86,86,86	0
54	MG	DA	3231	1/1	0.77	0.48	-	81,81,81,81	0
54	MG	DA	3113	1/1	0.84	0.16	-	66,66,66,66	0
54	MG	DA	3345	1/1	0.90	0.28	-	88,88,88,88	0
54	MG	AA	1673	1/1	0.92	0.28	-	95,95,95,95	0
54	MG	BO	201	1/1	0.91	0.13	-	70,70,70,70	0
54	MG	BA	3628	1/1	0.94	0.10	-	102,102,102,102	0
54	MG	BA	3287	1/1	0.77	0.33	-	83,83,83,83	0
54	MG	AA	1758	1/1	0.95	0.62	-	69,69,69,69	0
54	MG	BA	3493	1/1	0.79	0.48	-	75,75,75,75	0
54	MG	DA	3150	1/1	0.99	0.12	-	56,56,56,56	0
54	MG	DA	3482	1/1	0.93	0.18	-	69,69,69,69	0
54	MG	DA	3166	1/1	0.86	0.09	-	73,73,73,73	0
54	MG	DA	3240	1/1	0.95	0.16	-	69,69,69,69	0
54	MG	CA	1778	1/1	0.78	0.32	-	94,94,94,94	0
54	MG	DA	3364	1/1	0.94	0.52	-	75,75,75,75	0
54	MG	BJ	203	1/1	0.73	0.23	-	89,89,89,89	0
54	MG	AA	1622	1/1	0.88	0.54	-	62,62,62,62	0
54	MG	DA	3768	1/1	0.73	0.48	-	102,102,102,102	0
54	MG	DA	3738	1/1	0.92	0.20	-	91,91,91,91	0
54	MG	DA	3777	1/1	0.98	0.29	-	90,90,90,90	0
54	MG	BA	2999	1/1	0.96	0.53	-	39,39,39,39	0
54	MG	BK	201	1/1	0.59	0.19	-	77,77,77,77	0
54	MG	BA	3479	1/1	0.82	0.25	-	69,69,69,69	0
54	MG	DA	3465	1/1	0.89	0.27	-	105,105,105,105	0
54	MG	BA	3428	1/1	0.97	0.26	-	90,90,90,90	0
54	MG	CA	1631	1/1	0.91	0.54	-	82,82,82,82	0
54	MG	DJ	202	1/1	0.86	0.37	-	126,126,126,126	0
54	MG	DA	3700	1/1	0.66	1.31	-	96,96,96,96	0
54	MG	BA	3050	1/1	0.88	0.57	-	57,57,57,57	0
54	MG	BA	3061	1/1	0.97	0.13	-	54,54,54,54	0
54	MG	DA	3753	1/1	0.88	0.38	-	79,79,79,79	0
54	MG	AA	1853	1/1	0.82	0.10	-	86,86,86,86	0
54	MG	BA	3473	1/1	0.91	1.49	-	70,70,70,70	0
54	MG	BA	3450	1/1	0.94	0.64	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3424	1/1	0.98	0.33	-	115,115,115,115	0
54	MG	CV	6202	1/1	0.82	0.12	-	108,108,108,108	0
54	MG	DA	3003	1/1	0.90	0.56	-	51,51,51,51	0
54	MG	BA	3330	1/1	0.84	0.60	-	101,101,101,101	0
54	MG	BB	225	1/1	0.82	1.22	-	96,96,96,96	0
54	MG	BA	3391	1/1	0.91	0.36	-	93,93,93,93	0
54	MG	DA	2965	1/1	0.95	0.60	-	34,34,34,34	0
54	MG	DJ	201	1/1	0.93	0.30	-	61,61,61,61	0
54	MG	CA	1768	1/1	0.87	0.20	-	123,123,123,123	0
54	MG	DA	2989	1/1	0.83	0.36	-	39,39,39,39	0
54	MG	DA	3604	1/1	0.91	0.16	-	103,103,103,103	0
54	MG	AA	1817	1/1	0.92	0.83	-	84,84,84,84	0
54	MG	BA	3437	1/1	0.98	0.53	-	42,42,42,42	0
54	MG	CA	1772	1/1	0.96	0.14	-	112,112,112,112	0
54	MG	DA	3686	1/1	0.90	0.18	-	52,52,52,52	0
54	MG	DA	3129	1/1	0.93	0.45	-	93,93,93,93	0
54	MG	DA	3255	1/1	0.76	0.44	-	70,70,70,70	0
54	MG	DA	3025	1/1	0.81	0.56	-	80,80,80,80	0
54	MG	BA	3337	1/1	0.95	0.18	-	77,77,77,77	0
54	MG	BA	3655	1/1	0.96	0.17	-	92,92,92,92	0
54	MG	DA	2951	1/1	0.89	0.67	-	56,56,56,56	0
54	MG	DA	3558	1/1	0.87	0.27	-	148,148,148,148	0
54	MG	CA	1655	1/1	0.98	0.26	-	100,100,100,100	0
54	MG	DO	201	1/1	0.82	0.53	-	55,55,55,55	0
54	MG	AA	1777	1/1	0.91	0.30	-	49,49,49,49	0
54	MG	DA	3034	1/1	0.77	0.53	-	89,89,89,89	0
54	MG	BA	3489	1/1	0.90	0.18	-	73,73,73,73	0
54	MG	BA	3495	1/1	0.92	0.11	-	74,74,74,74	0
54	MG	DA	3718	1/1	0.94	0.22	-	70,70,70,70	0
54	MG	CA	1653	1/1	0.88	0.16	-	133,133,133,133	0
54	MG	DA	3496	1/1	0.84	0.38	-	95,95,95,95	0
54	MG	BA	3280	1/1	0.79	0.42	-	61,61,61,61	0
54	MG	BA	3219	1/1	0.97	0.15	-	80,80,80,80	0
54	MG	BA	3338	1/1	0.94	0.19	-	78,78,78,78	0
54	MG	BA	3248	1/1	0.87	0.52	-	82,82,82,82	0
54	MG	BA	3624	1/1	0.93	0.12	-	82,82,82,82	0
54	MG	DB	231	1/1	0.86	0.33	-	117,117,117,117	0
54	MG	DA	3220	1/1	0.94	0.17	-	98,98,98,98	0
54	MG	CA	1932	1/1	0.79	0.13	-	84,84,84,84	0
54	MG	BA	3571	1/1	0.96	0.15	-	74,74,74,74	0
54	MG	DA	3540	1/1	0.86	0.21	-	93,93,93,93	0
54	MG	CA	1956	1/1	0.89	0.27	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3198	1/1	0.67	0.38	-	85,85,85,85	0
54	MG	BA	3188	1/1	0.95	0.19	-	103,103,103,103	0
54	MG	BA	3365	1/1	0.94	0.12	-	131,131,131,131	0
54	MG	DA	3595	1/1	0.91	0.20	-	61,61,61,61	0
54	MG	AN	102	1/1	0.76	0.83	-	91,91,91,91	0
54	MG	BA	3350	1/1	0.86	0.38	-	66,66,66,66	0
54	MG	BA	3062	1/1	0.89	0.53	-	79,79,79,79	0
54	MG	CA	1904	1/1	0.88	0.32	-	97,97,97,97	0
54	MG	AA	1723	1/1	0.90	0.26	-	126,126,126,126	0
54	MG	DA	2933	1/1	0.97	0.32	-	25,25,25,25	0
54	MG	CA	1632	1/1	0.88	0.46	-	59,59,59,59	0
54	MG	AA	1875	1/1	0.88	0.22	-	97,97,97,97	0
54	MG	DA	3734	1/1	0.92	0.38	-	76,76,76,76	0
54	MG	BA	3017	1/1	0.89	0.22	-	55,55,55,55	0
54	MG	DA	3681	1/1	0.96	0.23	-	78,78,78,78	0
54	MG	DA	3259	1/1	0.79	0.15	-	87,87,87,87	0
54	MG	BA	3119	1/1	0.92	0.63	-	73,73,73,73	0
54	MG	BA	2937	1/1	0.90	0.13	-	56,56,56,56	0
54	MG	AA	1733	1/1	0.93	0.20	-	89,89,89,89	0
54	MG	DA	2931	1/1	0.98	0.40	-	21,21,21,21	0
54	MG	DC	303	1/1	0.87	0.88	-	80,80,80,80	0
54	MG	DA	3299	1/1	0.89	0.40	-	104,104,104,104	0
54	MG	CA	1828	1/1	0.91	0.39	-	88,88,88,88	0
54	MG	BA	3452	1/1	0.99	0.25	-	41,41,41,41	0
54	MG	DA	3423	1/1	0.92	0.28	-	79,79,79,79	0
54	MG	DA	3373	1/1	0.87	0.10	-	78,78,78,78	0
54	MG	DA	3102	1/1	0.86	0.26	-	50,50,50,50	0
54	MG	DA	3562	1/1	0.94	0.20	-	60,60,60,60	0
54	MG	DA	3483	1/1	0.98	0.45	-	63,63,63,63	0
54	MG	AA	1867	1/1	0.93	0.18	-	114,114,114,114	0
54	MG	BA	3400	1/1	0.77	0.55	-	83,83,83,83	0
54	MG	DA	3298	1/1	0.89	1.05	-	72,72,72,72	0
54	MG	DA	3140	1/1	0.95	0.73	-	50,50,50,50	0
54	MG	BA	3382	1/1	0.79	0.14	-	85,85,85,85	0
54	MG	DA	3274	1/1	0.87	0.13	-	116,116,116,116	0
54	MG	DA	3574	1/1	0.87	0.26	-	152,152,152,152	0
54	MG	AA	1715	1/1	0.90	0.23	-	58,58,58,58	0
54	MG	DA	3199	1/1	0.97	0.09	-	108,108,108,108	0
54	MG	DB	243	1/1	0.62	0.35	-	101,101,101,101	0
54	MG	CA	1786	1/1	0.92	0.33	-	94,94,94,94	0
54	MG	DA	3703	1/1	0.88	0.37	-	60,60,60,60	0
54	MG	BA	3211	1/1	0.74	0.42	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1930	1/1	0.90	0.10	-	89,89,89,89	0
54	MG	AA	1708	1/1	0.84	0.37	-	137,137,137,137	0
54	MG	DA	3444	1/1	0.88	0.38	-	72,72,72,72	0
54	MG	DA	3761	1/1	0.96	0.11	-	100,100,100,100	0
54	MG	CA	1677	1/1	0.95	0.45	-	93,93,93,93	0
54	MG	AA	1757	1/1	0.91	0.14	-	98,98,98,98	0
54	MG	DA	3601	1/1	0.95	0.20	-	59,59,59,59	0
54	MG	DA	3401	1/1	0.94	0.31	-	100,100,100,100	0
54	MG	DG	201	1/1	0.79	0.19	-	108,108,108,108	0
54	MG	BA	3096	1/1	0.88	0.33	-	76,76,76,76	0
54	MG	CA	1693	1/1	0.95	0.87	-	95,95,95,95	0
54	MG	CA	1856	1/1	0.83	1.38	-	118,118,118,118	0
54	MG	DA	3740	1/1	0.88	0.10	-	99,99,99,99	0
54	MG	DA	3387	1/1	0.94	0.12	-	124,124,124,124	0
54	MG	BA	3599	1/1	0.44	0.25	-	94,94,94,94	0
54	MG	DA	3842	1/1	0.84	0.37	-	105,105,105,105	0
54	MG	BA	3306	1/1	0.86	0.25	-	78,78,78,78	0
54	MG	CA	1711	1/1	0.84	0.48	-	76,76,76,76	0
54	MG	DA	3217	1/1	0.85	0.31	-	59,59,59,59	0
54	MG	DA	3033	1/1	0.88	0.51	-	79,79,79,79	0
54	MG	AA	1854	1/1	0.60	0.56	-	114,114,114,114	0
54	MG	BA	3086	1/1	0.94	0.11	-	63,63,63,63	0
54	MG	BA	3378	1/1	0.77	0.47	-	80,80,80,80	0
54	MG	BA	3325	1/1	0.99	0.22	-	168,168,168,168	0
54	MG	DA	3789	1/1	0.97	0.15	-	56,56,56,56	0
54	MG	CA	1793	1/1	0.96	0.19	-	125,125,125,125	0
54	MG	DA	3460	1/1	0.96	0.45	-	86,86,86,86	0
54	MG	CA	1883	1/1	0.88	0.38	-	75,75,75,75	0
54	MG	DA	3478	1/1	0.95	0.33	-	48,48,48,48	0
54	MG	AH	201	1/1	0.83	0.28	-	78,78,78,78	0
54	MG	BA	3492	1/1	0.96	0.17	-	70,70,70,70	0
54	MG	AA	1640	1/1	0.94	0.29	-	58,58,58,58	0
54	MG	DA	3790	1/1	0.94	0.48	-	63,63,63,63	0
54	MG	DL	201	1/1	0.98	0.10	-	7,7,7,7	0
54	MG	BA	3137	1/1	0.94	0.29	-	90,90,90,90	0
54	MG	BA	3568	1/1	0.93	0.35	-	69,69,69,69	0
54	MG	BA	3619	1/1	0.98	0.20	-	145,145,145,145	0
54	MG	AA	1850	1/1	0.94	0.70	-	70,70,70,70	0
54	MG	DA	3210	1/1	0.79	0.18	-	92,92,92,92	0
54	MG	BA	3208	1/1	0.83	0.45	-	96,96,96,96	0
54	MG	DE	302	1/1	0.77	0.41	-	83,83,83,83	0
54	MG	CA	1941	1/1	0.81	0.19	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	2916	1/1	0.97	0.47	-	15,15,15,15	0
54	MG	CA	1910	1/1	0.95	0.20	-	109,109,109,109	0
54	MG	AA	1858	1/1	0.89	0.08	-	86,86,86,86	0
54	MG	DA	3779	1/1	0.91	0.23	-	81,81,81,81	0
54	MG	AG	201	1/1	0.82	0.09	-	106,106,106,106	0
54	MG	AA	1732	1/1	0.96	0.13	-	104,104,104,104	0
54	MG	BA	3384	1/1	0.83	0.30	-	93,93,93,93	0
54	MG	DA	3162	1/1	0.90	0.38	-	30,30,30,30	0
54	MG	DA	3292	1/1	0.93	1.15	-	73,73,73,73	0
54	MG	DA	3261	1/1	0.95	0.29	-	57,57,57,57	0
54	MG	DA	3583	1/1	0.83	0.49	-	119,119,119,119	0
54	MG	AA	1833	1/1	0.94	0.43	-	75,75,75,75	0
54	MG	BA	2974	1/1	0.89	0.31	-	81,81,81,81	0
54	MG	DA	3584	1/1	0.88	0.46	-	130,130,130,130	0
54	MG	BU	201	1/1	0.91	0.36	-	70,70,70,70	0
54	MG	AO	103	1/1	0.93	0.10	-	111,111,111,111	0
54	MG	BA	3304	1/1	0.90	0.58	-	100,100,100,100	0
54	MG	CA	1701	1/1	0.91	0.70	-	83,83,83,83	0
54	MG	CA	1717	1/1	0.73	0.67	-	103,103,103,103	0
54	MG	BA	3226	1/1	0.82	0.36	-	59,59,59,59	0
54	MG	DA	3399	1/1	0.95	0.17	-	75,75,75,75	0
54	MG	AA	1731	1/1	0.85	0.32	-	83,83,83,83	0
54	MG	DA	3079	1/1	0.88	0.35	-	51,51,51,51	0
54	MG	DA	3207	1/1	0.89	0.29	-	43,43,43,43	0
54	MG	DA	3077	1/1	0.98	0.09	-	33,33,33,33	0
54	MG	DA	3409	1/1	0.66	0.24	-	110,110,110,110	0
54	MG	DA	3377	1/1	0.78	0.31	-	107,107,107,107	0
54	MG	BA	2910	1/1	0.92	0.39	-	17,17,17,17	0
54	MG	DA	2958	1/1	0.95	0.07	-	31,31,31,31	0
54	MG	CA	1935	1/1	0.88	0.26	-	101,101,101,101	0
54	MG	CA	1939	1/1	0.85	0.07	-	144,144,144,144	0
54	MG	BA	3410	1/1	0.87	0.46	-	112,112,112,112	0
54	MG	DA	3280	1/1	0.84	0.15	-	85,85,85,85	0
54	MG	DB	213	1/1	0.70	0.17	-	113,113,113,113	0
54	MG	DA	3834	1/1	0.98	0.13	-	60,60,60,60	0
54	MG	DA	3692	1/1	0.74	0.68	-	86,86,86,86	0
54	MG	CA	1678	1/1	0.66	0.39	-	81,81,81,81	0
54	MG	CA	1738	1/1	0.84	0.23	-	93,93,93,93	0
54	MG	BA	3637	1/1	0.95	0.18	-	105,105,105,105	0
54	MG	CA	1905	1/1	0.98	0.28	-	130,130,130,130	0
54	MG	CA	1885	1/1	0.83	0.37	-	75,75,75,75	0
54	MG	AA	1679	1/1	0.99	0.34	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1786	1/1	0.87	0.65	-	119,119,119,119	0
54	MG	DA	3100	1/1	0.88	0.14	-	78,78,78,78	0
54	MG	AA	1619	1/1	0.85	0.27	-	57,57,57,57	0
54	MG	CA	1898	1/1	0.75	0.85	-	87,87,87,87	0
54	MG	DA	3277	1/1	0.75	0.27	-	59,59,59,59	0
54	MG	DA	3557	1/1	0.94	0.12	-	128,128,128,128	0
54	MG	DA	3532	1/1	0.70	0.33	-	106,106,106,106	0
54	MG	CC	306	1/1	0.71	0.40	-	117,117,117,117	0
54	MG	DA	3762	1/1	0.69	0.78	-	103,103,103,103	0
54	MG	DA	3608	1/1	0.87	0.33	-	128,128,128,128	0
54	MG	CA	1648	1/1	0.93	0.43	-	61,61,61,61	0
54	MG	DA	3504	1/1	0.92	0.44	-	97,97,97,97	0
54	MG	DA	3600	1/1	0.63	0.07	-	86,86,86,86	0
54	MG	CA	1805	1/1	0.98	0.09	-	94,94,94,94	0
54	MG	DA	3805	1/1	0.89	0.10	-	70,70,70,70	0
54	MG	DA	3645	1/1	0.97	0.28	-	23,23,23,23	0
54	MG	CA	1608	1/1	0.98	0.35	-	121,121,121,121	0
54	MG	DA	3486	1/1	0.94	0.54	-	124,124,124,124	0
54	MG	BA	3385	1/1	0.29	0.20	-	125,125,125,125	0
54	MG	DA	3778	1/1	0.89	0.52	-	80,80,80,80	0
54	MG	BA	3103	1/1	0.94	0.87	-	74,74,74,74	0
54	MG	DA	3308	1/1	0.91	0.15	-	83,83,83,83	0
54	MG	BA	3117	1/1	0.76	0.47	-	91,91,91,91	0
54	MG	DA	3515	1/1	0.89	0.51	-	73,73,73,73	0
54	MG	CA	1656	1/1	0.97	0.05	-	78,78,78,78	0
54	MG	AA	1840	1/1	0.99	0.05	-	91,91,91,91	0
54	MG	DA	3690	1/1	0.95	0.51	-	70,70,70,70	0
54	MG	D2	103	1/1	0.65	0.51	-	56,56,56,56	0
54	MG	DA	3351	1/1	0.89	0.30	-	89,89,89,89	0
54	MG	DA	3011	1/1	0.98	0.12	-	36,36,36,36	0
54	MG	BA	3203	1/1	0.85	0.14	-	67,67,67,67	0
54	MG	DA	3341	1/1	0.91	0.24	-	75,75,75,75	0
54	MG	DA	3543	1/1	0.91	0.20	-	87,87,87,87	0
54	MG	BA	3084	1/1	0.96	0.37	-	82,82,82,82	0
54	MG	DA	3588	1/1	0.33	0.42	-	96,96,96,96	0
54	MG	CA	1833	1/1	0.89	0.28	-	79,79,79,79	0
54	MG	DA	3030	1/1	0.86	0.28	-	73,73,73,73	0
54	MG	DA	3061	1/1	0.83	0.24	-	55,55,55,55	0
54	MG	DA	3238	1/1	0.88	0.33	-	56,56,56,56	0
54	MG	DA	3454	1/1	0.95	0.36	-	81,81,81,81	0
54	MG	BA	3612	1/1	0.82	0.35	-	85,85,85,85	0
54	MG	BA	3647	1/1	0.86	0.62	-	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3725	1/1	0.90	0.45	-	65,65,65,65	0
54	MG	CA	1726	1/1	0.96	0.29	-	49,49,49,49	0
54	MG	BA	3265	1/1	0.86	0.16	-	53,53,53,53	0
54	MG	BA	3253	1/1	0.87	0.18	-	88,88,88,88	0
54	MG	DY	101	1/1	0.85	0.30	-	12,12,12,12	0
54	MG	DB	209	1/1	0.83	0.33	-	103,103,103,103	0
54	MG	BA	3266	1/1	0.90	0.13	-	104,104,104,104	0
54	MG	CA	1744	1/1	0.97	0.24	-	80,80,80,80	0
54	MG	DA	3811	1/1	0.94	0.17	-	60,60,60,60	0
54	MG	BA	3484	1/1	0.93	0.20	-	56,56,56,56	0
54	MG	DY	102	1/1	0.88	0.38	-	69,69,69,69	0
54	MG	DA	3067	1/1	0.74	0.69	-	91,91,91,91	0
54	MG	BA	3368	1/1	0.91	0.07	-	58,58,58,58	0
54	MG	BA	3622	1/1	0.94	0.27	-	90,90,90,90	0
54	MG	CA	1951	1/1	0.39	0.21	-	87,87,87,87	0
54	MG	CA	1666	1/1	0.75	0.33	-	104,104,104,104	0
54	MG	DA	3323	1/1	0.68	1.21	-	78,78,78,78	0
54	MG	DA	3552	1/1	0.93	0.17	-	68,68,68,68	0
54	MG	AA	1752	1/1	0.88	0.24	-	94,94,94,94	0
54	MG	BA	3328	1/1	0.92	0.28	-	80,80,80,80	0
54	MG	DA	3354	1/1	0.85	0.50	-	79,79,79,79	0
54	MG	DA	3477	1/1	0.94	0.16	-	78,78,78,78	0
54	MG	DA	3616	1/1	0.85	0.46	-	103,103,103,103	0
54	MG	BA	3278	1/1	0.93	0.28	-	88,88,88,88	0
54	MG	DA	3356	1/1	0.91	0.17	-	70,70,70,70	0
54	MG	CA	1814	1/1	0.94	0.33	-	47,47,47,47	0
54	MG	BA	3249	1/1	0.91	0.26	-	36,36,36,36	0
54	MG	DA	3572	1/1	0.94	0.14	-	93,93,93,93	0
54	MG	DA	3131	1/1	0.96	0.10	-	63,63,63,63	0
54	MG	CA	1888	1/1	0.61	0.13	-	109,109,109,109	0
54	MG	DA	3317	1/1	0.84	0.29	-	96,96,96,96	0
54	MG	CA	1804	1/1	0.92	2.12	-	100,100,100,100	0
54	MG	BA	3632	1/1	0.93	0.57	-	61,61,61,61	0
54	MG	DA	3652	1/1	0.75	0.58	-	66,66,66,66	0
54	MG	BB	204	1/1	0.96	0.33	-	102,102,102,102	0
54	MG	CA	1963	1/1	0.94	0.17	-	99,99,99,99	0
54	MG	BA	3089	1/1	0.91	0.49	-	69,69,69,69	0
54	MG	DA	3462	1/1	0.79	0.39	-	83,83,83,83	0
54	MG	CA	1649	1/1	0.89	1.00	-	96,96,96,96	0
54	MG	AA	1727	1/1	0.97	0.37	-	104,104,104,104	0
54	MG	BA	3170	1/1	0.96	0.34	-	87,87,87,87	0
54	MG	BA	3156	1/1	0.91	0.42	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3043	1/1	0.75	0.32	-	50,50,50,50	0
54	MG	CA	1691	1/1	0.94	0.07	-	92,92,92,92	0
54	MG	BA	3133	1/1	0.77	0.41	-	86,86,86,86	0
54	MG	DA	3679	1/1	0.86	0.34	-	50,50,50,50	0
54	MG	BA	3190	1/1	0.86	0.35	-	72,72,72,72	0
54	MG	DA	3190	1/1	0.94	0.43	-	69,69,69,69	0
54	MG	CA	1716	1/1	0.96	0.20	-	89,89,89,89	0
54	MG	BA	3336	1/1	0.89	0.73	-	87,87,87,87	0
54	MG	DA	3378	1/1	0.90	0.36	-	68,68,68,68	0
54	MG	DA	3674	1/1	0.97	0.54	-	47,47,47,47	0
54	MG	DA	3135	1/1	0.88	0.13	-	114,114,114,114	0
54	MG	DJ	203	1/1	0.92	0.84	-	84,84,84,84	0
54	MG	DA	3548	1/1	0.96	0.86	-	110,110,110,110	0
54	MG	DA	3837	1/1	0.74	0.35	-	95,95,95,95	0
54	MG	DA	3847	1/1	0.90	0.28	-	91,91,91,91	0
54	MG	CA	1639	1/1	0.96	0.38	-	59,59,59,59	0
54	MG	DA	3843	1/1	0.92	0.60	-	55,55,55,55	0
54	MG	BA	3153	1/1	0.82	0.24	-	79,79,79,79	0
54	MG	DA	3720	1/1	0.85	0.40	-	79,79,79,79	0
54	MG	AA	1717	1/1	0.32	1.41	-	103,103,103,103	0
54	MG	DA	3594	1/1	0.71	0.20	-	58,58,58,58	0
54	MG	BS	201	1/1	0.94	0.20	-	52,52,52,52	0
54	MG	DA	3164	1/1	0.98	0.22	-	83,83,83,83	0
54	MG	BA	3494	1/1	0.93	0.39	-	66,66,66,66	0
54	MG	BA	3466	1/1	0.83	0.52	-	61,61,61,61	0
54	MG	CA	1708	1/1	0.95	0.13	-	60,60,60,60	0
54	MG	BA	3524	1/1	0.92	0.12	-	107,107,107,107	0
54	MG	BA	3194	1/1	0.85	0.40	-	64,64,64,64	0
54	MG	DA	3559	1/1	0.85	1.17	-	92,92,92,92	0
54	MG	BA	3054	1/1	0.93	0.15	-	65,65,65,65	0
54	MG	CA	1725	1/1	0.85	0.08	-	82,82,82,82	0
54	MG	DE	303	1/1	0.90	0.20	-	81,81,81,81	0
54	MG	DA	3827	1/1	0.83	0.24	-	103,103,103,103	0
54	MG	DA	3198	1/1	0.87	0.31	-	65,65,65,65	0
54	MG	BA	3415	1/1	0.91	0.41	-	128,128,128,128	0
54	MG	CA	1756	1/1	0.88	0.26	-	84,84,84,84	0
54	MG	CA	1795	1/1	0.82	0.20	-	131,131,131,131	0
54	MG	BA	3640	1/1	0.56	0.31	-	97,97,97,97	0
54	MG	BA	3192	1/1	0.91	0.57	-	110,110,110,110	0
54	MG	BA	3162	1/1	0.92	0.08	-	86,86,86,86	0
54	MG	AA	1804	1/1	0.90	1.50	-	80,80,80,80	0
54	MG	AA	1824	1/1	0.75	0.29	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3041	1/1	0.88	0.36	-	62,62,62,62	0
54	MG	BA	3510	1/1	0.64	0.43	-	86,86,86,86	0
54	MG	BA	3352	1/1	0.93	0.33	-	80,80,80,80	0
54	MG	BA	3342	1/1	0.73	0.37	-	62,62,62,62	0
54	MG	DA	3862	1/1	0.67	0.70	-	119,119,119,119	0
54	MG	AA	1693	1/1	0.80	0.46	-	83,83,83,83	0
54	MG	DA	3581	1/1	0.97	0.12	-	68,68,68,68	0
54	MG	DA	3006	1/1	0.94	0.27	-	60,60,60,60	0
54	MG	DA	3498	1/1	0.98	0.50	-	51,51,51,51	0
54	MG	CA	1858	1/1	0.84	0.87	-	107,107,107,107	0
54	MG	BA	3264	1/1	0.91	0.09	-	87,87,87,87	0
54	MG	AA	1873	1/1	0.86	0.49	-	105,105,105,105	0
54	MG	DU	201	1/1	0.85	0.09	-	84,84,84,84	0
54	MG	DA	3181	1/1	0.86	0.13	-	96,96,96,96	0
54	MG	AA	1604	1/1	0.91	0.46	-	62,62,62,62	0
54	MG	BA	2935	1/1	0.98	0.40	-	26,26,26,26	0
54	MG	D5	102	1/1	0.87	0.24	-	59,59,59,59	0
54	MG	DA	3666	1/1	0.77	0.31	-	81,81,81,81	0
54	MG	BA	3095	1/1	0.54	0.59	-	96,96,96,96	0
54	MG	BA	3186	1/1	0.89	0.20	-	85,85,85,85	0
54	MG	BA	3244	1/1	0.97	0.17	-	79,79,79,79	0
54	MG	BA	3549	1/1	0.65	1.60	-	87,87,87,87	0
54	MG	DA	3568	1/1	0.99	0.10	-	78,78,78,78	0
54	MG	DA	3706	1/1	0.95	0.16	-	75,75,75,75	0
54	MG	CE	201	1/1	0.89	0.13	-	117,117,117,117	0
54	MG	BA	3258	1/1	0.94	0.20	-	78,78,78,78	0
54	MG	DA	3598	1/1	0.83	0.13	-	108,108,108,108	0
54	MG	DA	3838	1/1	0.92	0.48	-	117,117,117,117	0
54	MG	CA	1840	1/1	0.96	0.30	-	76,76,76,76	0
54	MG	DA	3331	1/1	0.94	0.15	-	90,90,90,90	0
54	MG	DA	3573	1/1	0.78	0.43	-	85,85,85,85	0
54	MG	AQ	203	1/1	0.85	0.20	-	101,101,101,101	0
54	MG	AE	205	1/1	0.94	0.43	-	106,106,106,106	0
54	MG	CA	1623	1/1	0.80	0.40	-	93,93,93,93	0
54	MG	DA	3825	1/1	0.90	0.38	-	103,103,103,103	0
54	MG	BA	3071	1/1	0.91	0.21	-	71,71,71,71	0
54	MG	DA	3531	1/1	0.89	0.35	-	93,93,93,93	0
54	MG	DA	3175	1/1	0.87	0.10	-	102,102,102,102	0
54	MG	CA	1728	1/1	0.99	0.15	-	120,120,120,120	0
54	MG	DA	3228	1/1	0.84	0.32	-	54,54,54,54	0
54	MG	BB	217	1/1	0.75	0.34	-	72,72,72,72	0
54	MG	BA	3025	1/1	0.95	0.49	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3466	1/1	0.94	0.08	-	117,117,117,117	0
54	MG	DA	3828	1/1	0.79	0.24	-	85,85,85,85	0
54	MG	DB	201	1/1	0.93	0.27	-	44,44,44,44	0
54	MG	CA	1813	1/1	0.95	0.17	-	107,107,107,107	0
54	MG	BA	3483	1/1	0.94	0.32	-	71,71,71,71	0
54	MG	DA	3755	1/1	0.86	0.30	-	89,89,89,89	0
54	MG	DA	3204	1/1	0.88	0.50	-	53,53,53,53	0
54	MG	AA	1755	1/1	0.77	0.16	-	98,98,98,98	0
54	MG	CA	1873	1/1	0.92	0.44	-	58,58,58,58	0
54	MG	AA	1695	1/1	0.85	0.12	-	96,96,96,96	0
54	MG	BB	212	1/1	0.87	0.23	-	107,107,107,107	0
54	MG	DA	3807	1/1	0.91	0.26	-	61,61,61,61	0
54	MG	DA	3602	1/1	0.89	0.39	-	91,91,91,91	0
54	MG	AA	1718	1/1	0.93	0.21	-	63,63,63,63	0
54	MG	BA	2965	1/1	0.98	0.23	-	51,51,51,51	0
54	MG	DA	2942	1/1	0.93	0.92	-	54,54,54,54	0
54	MG	CA	1969	1/1	0.87	0.60	-	124,124,124,124	0
54	MG	CM	202	1/1	0.16	0.91	-	164,164,164,164	0
54	MG	AA	1809	1/1	0.92	0.75	-	94,94,94,94	0
54	MG	DA	3407	1/1	0.91	0.17	-	108,108,108,108	0
54	MG	BA	3608	1/1	0.81	0.32	-	101,101,101,101	0
54	MG	BA	2918	1/1	0.96	0.61	-	43,43,43,43	0
54	MG	DA	3189	1/1	0.91	0.22	-	73,73,73,73	0
54	MG	BA	3555	1/1	0.84	0.57	-	66,66,66,66	0
54	MG	BA	3480	1/1	0.89	1.07	-	79,79,79,79	0
54	MG	DA	3564	1/1	0.74	0.13	-	77,77,77,77	0
54	MG	DA	3476	1/1	0.71	0.56	-	87,87,87,87	0
54	MG	DA	2919	1/1	0.98	0.33	-	12,12,12,12	0
54	MG	AA	1730	1/1	0.66	0.37	-	107,107,107,107	0
54	MG	CA	1731	1/1	0.98	0.14	-	76,76,76,76	0
54	MG	BA	3002	1/1	0.89	1.37	-	96,96,96,96	0
54	MG	DA	3151	1/1	0.88	0.26	-	76,76,76,76	0
54	MG	AA	1745	1/1	0.99	0.42	-	119,119,119,119	0
54	MG	BA	3429	1/1	0.89	0.38	-	79,79,79,79	0
54	MG	BA	3000	1/1	0.89	0.46	-	49,49,49,49	0
54	MG	BA	2971	1/1	0.84	0.24	-	76,76,76,76	0
54	MG	DA	3812	1/1	0.94	0.22	-	87,87,87,87	0
54	MG	BA	3551	1/1	0.87	0.17	-	95,95,95,95	0
54	MG	DA	2955	1/1	0.99	0.58	-	45,45,45,45	0
54	MG	DA	3767	1/1	0.72	0.33	-	73,73,73,73	0
54	MG	DA	3339	1/1	0.84	0.22	-	81,81,81,81	0
54	MG	DC	301	1/1	0.94	0.73	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3660	1/1	0.82	0.34	-	65,65,65,65	0
54	MG	CA	1903	1/1	0.67	0.26	-	84,84,84,84	0
54	MG	DA	3861	1/1	0.89	0.30	-	90,90,90,90	0
54	MG	DA	3628	1/1	0.95	0.32	-	56,56,56,56	0
54	MG	BA	3512	1/1	0.85	0.34	-	77,77,77,77	0
54	MG	BA	3530	1/1	0.93	0.28	-	65,65,65,65	0
54	MG	DA	3355	1/1	0.70	0.42	-	76,76,76,76	0
54	MG	AA	1834	1/1	0.81	1.43	-	77,77,77,77	0
54	MG	BA	2932	1/1	0.98	0.86	-	44,44,44,44	0
54	MG	BA	3333	1/1	0.95	0.48	-	54,54,54,54	0
54	MG	BA	3165	1/1	0.92	0.15	-	73,73,73,73	0
54	MG	BA	3542	1/1	0.93	0.18	-	102,102,102,102	0
54	MG	AA	1737	1/1	0.90	0.25	-	111,111,111,111	0
54	MG	DA	3752	1/1	0.82	0.39	-	74,74,74,74	0
54	MG	DA	2962	1/1	0.87	0.19	-	37,37,37,37	0
54	MG	DA	2979	1/1	0.99	0.20	-	16,16,16,16	0
54	MG	BA	3373	1/1	0.82	0.36	-	61,61,61,61	0
54	MG	BA	3173	1/1	0.86	0.51	-	87,87,87,87	0
54	MG	AA	1826	1/1	0.96	0.38	-	75,75,75,75	0
54	MG	DA	3663	1/1	0.71	0.46	-	75,75,75,75	0
54	MG	DA	3724	1/1	0.91	0.25	-	109,109,109,109	0
54	MG	DA	3848	1/1	0.81	0.96	-	105,105,105,105	0
54	MG	DA	3337	1/1	0.75	0.37	-	88,88,88,88	0
54	MG	DA	3375	1/1	0.91	0.30	-	63,63,63,63	0
54	MG	BA	3486	1/1	0.95	0.20	-	60,60,60,60	0
54	MG	DA	3276	1/1	0.95	0.56	-	86,86,86,86	0
54	MG	DA	3027	1/1	0.97	0.28	-	53,53,53,53	0
54	MG	CA	1787	1/1	0.97	0.76	-	37,37,37,37	0
54	MG	BA	3560	1/1	0.95	0.62	-	74,74,74,74	0
54	MG	DA	3194	1/1	0.93	0.44	-	74,74,74,74	0
54	MG	DA	3271	1/1	0.68	0.35	-	99,99,99,99	0
54	MG	BA	3639	1/1	0.97	0.23	-	88,88,88,88	0
54	MG	AA	1869	1/1	0.99	0.08	-	74,74,74,74	0
54	MG	BA	3507	1/1	0.80	0.32	-	68,68,68,68	0
54	MG	CA	1746	1/1	0.88	0.24	-	141,141,141,141	0
54	MG	BA	3544	1/1	0.87	0.39	-	81,81,81,81	0
54	MG	BA	3024	1/1	0.95	0.37	-	52,52,52,52	0
54	MG	DA	3719	1/1	0.94	0.33	-	84,84,84,84	0
54	MG	BP	201	1/1	0.92	0.18	-	122,122,122,122	0
54	MG	DA	3246	1/1	0.92	0.12	-	57,57,57,57	0
54	MG	CA	1824	1/1	0.87	0.21	-	123,123,123,123	0
54	MG	BA	3134	1/1	0.75	0.41	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AA	1661	1/1	0.87	0.16	-	51,51,51,51	0
54	MG	DA	2996	1/1	0.96	0.45	-	32,32,32,32	0
54	MG	DA	3835	1/1	0.94	0.35	-	111,111,111,111	0
54	MG	CA	1739	1/1	0.92	0.15	-	102,102,102,102	0
54	MG	CC	308	1/1	0.79	0.25	-	110,110,110,110	0
54	MG	BA	3206	1/1	0.72	0.23	-	96,96,96,96	0
54	MG	AA	1618	1/1	0.95	0.62	-	71,71,71,71	0
54	MG	BA	3267	1/1	0.90	0.49	-	65,65,65,65	0
54	MG	CG	202	1/1	0.78	0.62	-	131,131,131,131	0
54	MG	DA	3657	1/1	0.83	0.76	-	57,57,57,57	0
54	MG	DA	3334	1/1	0.95	0.30	-	53,53,53,53	0
54	MG	AA	1795	1/1	0.90	0.34	-	111,111,111,111	0
54	MG	DA	3635	1/1	0.94	0.12	-	73,73,73,73	0
54	MG	CA	1637	1/1	0.83	0.09	-	98,98,98,98	0
54	MG	BA	3374	1/1	0.91	0.36	-	108,108,108,108	0
54	MG	DA	2940	1/1	0.96	0.50	-	31,31,31,31	0
54	MG	DA	3695	1/1	0.89	0.28	-	76,76,76,76	0
54	MG	AA	1672	1/1	0.81	0.67	-	78,78,78,78	0
54	MG	BA	3376	1/1	0.85	0.34	-	123,123,123,123	0
54	MG	DA	3002	1/1	0.90	0.16	-	52,52,52,52	0
54	MG	CA	1922	1/1	0.93	0.08	-	127,127,127,127	0
54	MG	DA	3022	1/1	0.88	0.24	-	35,35,35,35	0
54	MG	BA	3152	1/1	0.84	0.12	-	76,76,76,76	0
54	MG	BA	3358	1/1	0.85	0.41	-	81,81,81,81	0
54	MG	AE	204	1/1	0.91	0.23	-	74,74,74,74	0
54	MG	BA	3090	1/1	0.80	0.44	-	84,84,84,84	0
54	MG	BA	3228	1/1	0.97	0.13	-	42,42,42,42	0
54	MG	AA	1764	1/1	0.84	0.62	-	99,99,99,99	0
54	MG	DA	3202	1/1	0.94	0.20	-	76,76,76,76	0
54	MG	AA	1871	1/1	0.65	0.13	-	110,110,110,110	0
54	MG	CE	204	1/1	0.74	0.34	-	109,109,109,109	0
54	MG	DD	306	1/1	0.72	0.18	-	107,107,107,107	0
54	MG	CA	1896	1/1	0.73	0.34	-	70,70,70,70	0
54	MG	CA	1946	1/1	0.94	0.14	-	137,137,137,137	0
54	MG	DA	3417	1/1	0.79	0.65	-	72,72,72,72	0
54	MG	DA	3344	1/1	0.97	0.16	-	75,75,75,75	0
54	MG	CA	1919	1/1	0.68	0.22	-	145,145,145,145	0
54	MG	DA	3363	1/1	0.94	0.17	-	74,74,74,74	0
54	MG	AA	1847	1/1	0.78	0.33	-	90,90,90,90	0
54	MG	AA	1713	1/1	0.98	0.38	-	98,98,98,98	0
54	MG	CV	6205	1/1	0.21	0.11	-	159,159,159,159	0
54	MG	CA	1754	1/1	0.90	0.86	-	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3476	1/1	0.85	0.33	-	53,53,53,53	0
54	MG	CA	1660	1/1	0.88	0.14	-	158,158,158,158	0
54	MG	AA	1798	1/1	0.96	0.45	-	46,46,46,46	0
54	MG	DA	3107	1/1	0.95	0.14	-	50,50,50,50	0
54	MG	AO	102	1/1	0.72	0.34	-	114,114,114,114	0
54	MG	AA	1774	1/1	0.92	0.10	-	70,70,70,70	0
54	MG	DA	3624	1/1	0.88	0.27	-	92,92,92,92	0
54	MG	CA	1948	1/1	0.89	0.07	-	99,99,99,99	0
54	MG	AA	1837	1/1	0.94	0.39	-	115,115,115,115	0
54	MG	DA	3501	1/1	0.82	0.25	-	96,96,96,96	0
54	MG	CA	1629	1/1	0.86	0.34	-	93,93,93,93	0
54	MG	AA	1657	1/1	0.93	0.54	-	79,79,79,79	0
54	MG	DA	3359	1/1	0.71	0.31	-	96,96,96,96	0
54	MG	AA	1836	1/1	0.96	0.08	-	91,91,91,91	0
54	MG	AA	1736	1/1	0.94	0.14	-	112,112,112,112	0
54	MG	CA	1933	1/1	0.73	0.24	-	137,137,137,137	0
54	MG	CA	1640	1/1	0.73	1.18	-	133,133,133,133	0
54	MG	BA	3079	1/1	0.97	0.10	-	73,73,73,73	0
54	MG	DA	3435	1/1	0.92	0.33	-	97,97,97,97	0
54	MG	BA	3254	1/1	0.96	0.34	-	68,68,68,68	0
54	MG	BA	3274	1/1	0.70	0.73	-	98,98,98,98	0
54	MG	BA	3116	1/1	0.92	0.17	-	70,70,70,70	0
54	MG	BA	3118	1/1	0.95	0.14	-	95,95,95,95	0
54	MG	DA	3522	1/1	0.81	0.52	-	147,147,147,147	0
54	MG	CG	201	1/1	0.73	0.48	-	104,104,104,104	0
54	MG	DA	3182	1/1	0.83	0.29	-	63,63,63,63	0
54	MG	CA	1806	1/1	0.94	0.18	-	110,110,110,110	0
54	MG	AA	1690	1/1	0.76	0.30	-	88,88,88,88	0
54	MG	CA	1884	1/1	0.77	0.23	-	99,99,99,99	0
54	MG	CA	1705	1/1	0.90	0.37	-	122,122,122,122	0
54	MG	DA	2935	1/1	0.97	0.50	-	23,23,23,23	0
54	MG	BA	2961	1/1	0.98	0.62	-	51,51,51,51	0
54	MG	BA	3508	1/1	0.87	0.15	-	90,90,90,90	0
54	MG	DB	236	1/1	0.72	0.18	-	84,84,84,84	0
54	MG	AA	1653	1/1	0.74	0.07	-	102,102,102,102	0
54	MG	BA	3112	1/1	0.84	0.30	-	65,65,65,65	0
54	MG	CA	1758	1/1	0.89	0.22	-	77,77,77,77	0
54	MG	DA	3497	1/1	0.53	0.73	-	62,62,62,62	0
54	MG	BA	3405	1/1	0.94	0.16	-	68,68,68,68	0
54	MG	DA	3765	1/1	0.94	0.18	-	64,64,64,64	0
54	MG	DA	3775	1/1	0.87	0.21	-	98,98,98,98	0
54	MG	D5	101	1/1	0.92	0.19	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AK	201	1/1	0.87	0.33	-	101,101,101,101	0
54	MG	BA	3124	1/1	0.77	0.14	-	87,87,87,87	0
54	MG	BA	3579	1/1	0.94	0.73	-	107,107,107,107	0
54	MG	AA	1849	1/1	0.88	0.31	-	79,79,79,79	0
54	MG	DA	3070	1/1	0.83	0.05	-	85,85,85,85	0
54	MG	BA	3353	1/1	0.84	0.47	-	85,85,85,85	0
54	MG	AA	1815	1/1	0.72	1.70	-	78,78,78,78	0
54	MG	DA	3715	1/1	0.90	0.30	-	57,57,57,57	0
54	MG	DA	3288	1/1	0.90	0.15	-	104,104,104,104	0
54	MG	BA	3343	1/1	0.91	0.25	-	87,87,87,87	0
54	MG	BB	226	1/1	0.67	0.71	-	98,98,98,98	0
54	MG	DA	3096	1/1	0.88	0.51	-	59,59,59,59	0
54	MG	CA	1801	1/1	0.95	0.25	-	82,82,82,82	0
54	MG	DA	2968	1/1	0.96	0.63	-	36,36,36,36	0
54	MG	BB	207	1/1	0.97	0.16	-	111,111,111,111	0
54	MG	DA	3735	1/1	0.82	0.17	-	97,97,97,97	0
54	MG	BA	3037	1/1	0.92	0.24	-	62,62,62,62	0
54	MG	AB	303	1/1	0.61	0.26	-	108,108,108,108	0
54	MG	DB	228	1/1	0.84	0.28	-	88,88,88,88	0
54	MG	DB	206	1/1	0.96	0.27	-	63,63,63,63	0
54	MG	BA	3225	1/1	0.96	0.32	-	54,54,54,54	0
54	MG	DA	3782	1/1	0.94	0.42	-	67,67,67,67	0
54	MG	DA	3623	1/1	0.97	0.41	-	104,104,104,104	0
54	MG	B4	101	1/1	0.89	0.28	-	91,91,91,91	0
54	MG	DA	3721	1/1	0.70	0.80	-	88,88,88,88	0
54	MG	AC	302	1/1	0.90	0.33	-	71,71,71,71	0
54	MG	DA	3503	1/1	0.87	0.28	-	91,91,91,91	0
54	MG	BA	3491	1/1	0.93	0.47	-	79,79,79,79	0
54	MG	AA	1868	1/1	0.80	0.28	-	101,101,101,101	0
54	MG	DA	3580	1/1	0.88	0.32	-	162,162,162,162	0
54	MG	BA	3652	1/1	0.83	0.35	-	109,109,109,109	0
54	MG	CC	305	1/1	0.96	0.08	-	93,93,93,93	0
54	MG	BJ	201	1/1	0.79	0.17	-	75,75,75,75	0
54	MG	BH	201	1/1	0.91	0.24	-	107,107,107,107	0
54	MG	AA	1637	1/1	0.93	0.16	-	62,62,62,62	0
54	MG	DA	3004	1/1	0.95	0.21	-	38,38,38,38	0
54	MG	BA	3268	1/1	0.93	0.64	-	84,84,84,84	0
54	MG	DA	3631	1/1	0.99	0.04	-	73,73,73,73	0
54	MG	AA	1812	1/1	0.94	0.93	-	81,81,81,81	0
54	MG	CA	1635	1/1	0.62	0.36	-	99,99,99,99	0
54	MG	CA	1908	1/1	0.73	0.43	-	104,104,104,104	0
54	MG	DA	3221	1/1	0.94	0.23	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3668	1/1	0.79	0.56	-	133,133,133,133	0
54	MG	AA	1793	1/1	0.88	0.25	-	68,68,68,68	0
54	MG	DA	3116	1/1	0.90	0.47	-	52,52,52,52	0
54	MG	BA	3161	1/1	0.94	0.34	-	64,64,64,64	0
54	MG	CA	1622	1/1	0.61	0.82	-	77,77,77,77	0
54	MG	DA	3815	1/1	0.98	0.53	-	74,74,74,74	0
54	MG	DA	3741	1/1	0.84	0.18	-	84,84,84,84	0
54	MG	BA	2930	1/1	0.93	0.40	-	47,47,47,47	0
54	MG	DB	241	1/1	0.90	0.13	-	90,90,90,90	0
54	MG	DA	3043	1/1	0.96	0.14	-	59,59,59,59	0
54	MG	DA	3570	1/1	0.65	0.59	-	90,90,90,90	0
54	MG	DA	3225	1/1	0.72	0.11	-	139,139,139,139	0
54	MG	BA	3674	1/1	0.95	0.37	-	55,55,55,55	0
54	MG	BA	3664	1/1	0.94	0.10	-	69,69,69,69	0
54	MG	DA	3293	1/1	0.94	0.23	-	66,66,66,66	0
54	MG	AV	6206	1/1	0.84	0.20	-	87,87,87,87	0
54	MG	CA	1853	1/1	0.92	0.18	-	113,113,113,113	0
54	MG	AA	1776	1/1	0.92	0.37	-	108,108,108,108	0
54	MG	BA	3396	1/1	0.95	0.15	-	108,108,108,108	0
54	MG	DA	3171	1/1	0.89	0.14	-	93,93,93,93	0
54	MG	BA	3066	1/1	0.83	1.05	-	91,91,91,91	0
54	MG	DB	242	1/1	0.89	0.09	-	113,113,113,113	0
54	MG	AQ	202	1/1	0.91	0.13	-	85,85,85,85	0
54	MG	DA	3764	1/1	0.90	0.35	-	80,80,80,80	0
54	MG	DA	3797	1/1	0.79	0.26	-	101,101,101,101	0
54	MG	DA	3593	1/1	0.97	0.43	-	125,125,125,125	0
54	MG	BA	3676	1/1	0.95	0.11	-	112,112,112,112	0
54	MG	DA	3864	1/1	0.95	0.37	-	53,53,53,53	0
54	MG	BA	3269	1/1	0.84	0.71	-	104,104,104,104	0
54	MG	DA	3168	1/1	0.93	0.63	-	67,67,67,67	0
54	MG	AA	1743	1/1	0.86	0.53	-	140,140,140,140	0
54	MG	AA	1659	1/1	0.87	0.52	-	74,74,74,74	0
54	MG	CA	1723	1/1	0.84	0.74	-	85,85,85,85	0
54	MG	DA	3132	1/1	0.86	0.57	-	62,62,62,62	0
54	MG	CA	1766	1/1	0.77	0.12	-	77,77,77,77	0
54	MG	BA	3431	1/1	0.97	0.33	-	26,26,26,26	0
54	MG	BA	3235	1/1	0.89	0.26	-	54,54,54,54	0
54	MG	DA	3294	1/1	0.97	0.17	-	36,36,36,36	0
54	MG	BA	3078	1/1	0.87	0.27	-	104,104,104,104	0
54	MG	DA	3413	1/1	0.96	0.23	-	60,60,60,60	0
54	MG	BA	3525	1/1	0.77	0.36	-	67,67,67,67	0
54	MG	DA	3830	1/1	0.89	0.18	-	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3215	1/1	0.85	0.65	-	64,64,64,64	0
54	MG	DB	234	1/1	0.57	0.16	-	105,105,105,105	0
54	MG	BA	3261	1/1	0.75	1.47	-	92,92,92,92	0
54	MG	CA	1902	1/1	0.86	0.18	-	77,77,77,77	0
54	MG	BA	3139	1/1	0.94	0.40	-	100,100,100,100	0
54	MG	DA	3673	1/1	0.81	0.20	-	85,85,85,85	0
54	MG	DA	3066	1/1	0.95	0.24	-	114,114,114,114	0
54	MG	BA	3189	1/1	0.82	0.29	-	76,76,76,76	0
54	MG	DA	3400	1/1	0.93	0.11	-	127,127,127,127	0
54	MG	BA	3427	1/1	0.95	0.10	-	74,74,74,74	0
54	MG	CA	1931	1/1	0.94	0.09	-	99,99,99,99	0
54	MG	DA	3516	1/1	0.88	0.33	-	73,73,73,73	0
54	MG	BA	3500	1/1	0.95	0.29	-	72,72,72,72	0
54	MG	DA	3747	1/1	0.92	0.21	-	78,78,78,78	0
54	MG	DA	3615	1/1	0.96	0.20	-	99,99,99,99	0
54	MG	DA	3799	1/1	0.87	0.36	-	96,96,96,96	0
54	MG	BA	3393	1/1	0.63	0.48	-	136,136,136,136	0
54	MG	CO	103	1/1	0.85	0.99	-	203,203,203,203	0
54	MG	CA	1848	1/1	0.96	0.29	-	96,96,96,96	0
54	MG	DA	3256	1/1	0.94	0.44	-	65,65,65,65	0
54	MG	DA	3691	1/1	0.70	0.62	-	96,96,96,96	0
54	MG	CO	102	1/1	0.50	0.49	-	103,103,103,103	0
54	MG	CA	1880	1/1	0.85	1.03	-	83,83,83,83	0
54	MG	DA	3009	1/1	0.93	0.30	-	54,54,54,54	0
54	MG	BA	3083	1/1	0.89	0.08	-	70,70,70,70	0
54	MG	CA	1970	1/1	0.98	0.08	-	98,98,98,98	0
54	MG	CC	302	1/1	0.98	0.20	-	79,79,79,79	0
54	MG	CA	1662	1/1	0.96	0.13	-	84,84,84,84	0
54	MG	DM	1400	1/1	0.82	0.45	-	106,106,106,106	0
54	MG	CA	1909	1/1	0.72	0.23	-	135,135,135,135	0
54	MG	DA	3485	1/1	0.95	0.31	-	119,119,119,119	0
54	MG	BA	3290	1/1	0.89	0.25	-	79,79,79,79	0
54	MG	BA	3085	1/1	0.92	0.34	-	53,53,53,53	0
54	MG	CA	1694	1/1	0.73	0.12	-	79,79,79,79	0
54	MG	DA	3249	1/1	0.93	0.11	-	111,111,111,111	0
54	MG	BA	3490	1/1	0.96	0.09	-	67,67,67,67	0
54	MG	AA	1709	1/1	0.90	0.58	-	87,87,87,87	0
54	MG	DA	3157	1/1	0.98	0.18	-	33,33,33,33	0
54	MG	CA	1612	1/1	0.75	0.34	-	76,76,76,76	0
54	MG	DA	3019	1/1	0.95	0.28	-	48,48,48,48	0
54	MG	BB	209	1/1	0.93	0.17	-	61,61,61,61	0
54	MG	DA	3114	1/1	0.83	0.38	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1667	1/1	0.94	0.29	-	77,77,77,77	0
54	MG	DA	3232	1/1	0.97	0.13	-	67,67,67,67	0
54	MG	CA	1713	1/1	0.93	0.12	-	92,92,92,92	0
54	MG	DA	3737	1/1	0.93	0.71	-	136,136,136,136	0
54	MG	D4	101	1/1	0.90	0.22	-	55,55,55,55	0
54	MG	DB	233	1/1	0.94	0.42	-	67,67,67,67	0
54	MG	AA	1740	1/1	0.86	0.13	-	76,76,76,76	0
54	MG	CA	1780	1/1	0.86	0.15	-	93,93,93,93	0
54	MG	DA	3319	1/1	0.91	0.30	-	38,38,38,38	0
54	MG	AA	1636	1/1	0.82	0.11	-	96,96,96,96	0
54	MG	BA	3076	1/1	0.89	0.51	-	68,68,68,68	0
54	MG	B3	101	1/1	0.80	0.16	-	96,96,96,96	0
54	MG	BA	3439	1/1	0.96	0.39	-	17,17,17,17	0
54	MG	BA	3419	1/1	0.90	0.30	-	67,67,67,67	0
54	MG	AA	1788	1/1	0.88	0.13	-	148,148,148,148	0
54	MG	DA	3528	1/1	0.98	0.08	-	87,87,87,87	0
54	MG	BA	3667	1/1	0.97	0.16	-	85,85,85,85	0
54	MG	BA	3097	1/1	0.95	0.27	-	57,57,57,57	0
54	MG	DA	3792	1/1	0.93	0.35	-	40,40,40,40	0
54	MG	CA	1714	1/1	0.80	0.36	-	123,123,123,123	0
54	MG	DA	3520	1/1	0.85	0.20	-	133,133,133,133	0
54	MG	DA	3470	1/1	0.95	0.21	-	127,127,127,127	0
54	MG	BA	3067	1/1	0.74	0.49	-	103,103,103,103	0
54	MG	CL	203	1/1	0.58	0.23	-	123,123,123,123	0
54	MG	BA	3120	1/1	0.73	0.11	-	85,85,85,85	0
54	MG	BA	2905	1/1	0.98	0.63	-	19,19,19,19	0
54	MG	BA	3245	1/1	0.95	0.32	-	95,95,95,95	0
54	MG	DA	3101	1/1	0.81	0.46	-	75,75,75,75	0
54	MG	CA	1924	1/1	0.89	0.19	-	116,116,116,116	0
54	MG	AA	1726	1/1	0.87	0.12	-	103,103,103,103	0
54	MG	DA	2961	1/1	0.92	0.42	-	58,58,58,58	0
54	MG	DA	3388	1/1	0.94	0.24	-	51,51,51,51	0
54	MG	BA	3055	1/1	0.75	0.62	-	78,78,78,78	0
54	MG	AA	1790	1/1	0.66	0.12	-	109,109,109,109	0
54	MG	AA	1704	1/1	0.94	0.16	-	77,77,77,77	0
54	MG	BB	205	1/1	0.89	0.14	-	108,108,108,108	0
54	MG	BA	3222	1/1	0.81	0.24	-	86,86,86,86	0
54	MG	AA	1876	1/1	0.78	0.12	-	80,80,80,80	0
54	MG	DA	3801	1/1	0.85	0.30	-	83,83,83,83	0
54	MG	CA	1692	1/1	0.91	1.05	-	115,115,115,115	0
54	MG	DA	3449	1/1	0.95	0.15	-	79,79,79,79	0
54	MG	AA	1652	1/1	0.83	0.33	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1765	1/1	0.89	0.19	-	95,95,95,95	0
54	MG	CA	1949	1/1	0.64	0.21	-	98,98,98,98	0
54	MG	DA	3853	1/1	0.81	0.28	-	114,114,114,114	0
54	MG	BA	3291	1/1	0.85	0.39	-	102,102,102,102	0
54	MG	BA	3009	1/1	0.90	0.43	-	73,73,73,73	0
54	MG	CA	1918	1/1	0.81	0.68	-	84,84,84,84	0
54	MG	BA	3499	1/1	0.93	0.29	-	66,66,66,66	0
54	MG	BA	3204	1/1	0.76	0.55	-	68,68,68,68	0
54	MG	CA	1962	1/1	0.46	0.19	-	96,96,96,96	0
54	MG	DA	3502	1/1	0.82	0.34	-	93,93,93,93	0
54	MG	BV	201	1/1	0.92	0.27	-	98,98,98,98	0
54	MG	AV	6203	1/1	0.96	0.15	-	62,62,62,62	0
54	MG	BA	2947	1/1	0.93	0.73	-	37,37,37,37	0
54	MG	DA	3856	1/1	0.98	0.49	-	86,86,86,86	0
54	MG	AA	1861	1/1	0.82	0.22	-	81,81,81,81	0
54	MG	BA	2993	1/1	0.88	0.48	-	49,49,49,49	0
54	MG	AA	1772	1/1	0.91	0.31	-	111,111,111,111	0
54	MG	BA	3167	1/1	0.82	0.63	-	87,87,87,87	0
54	MG	DA	3683	1/1	0.87	0.34	-	58,58,58,58	0
54	MG	BA	3606	1/1	0.73	0.68	-	118,118,118,118	0
54	MG	DA	3263	1/1	0.91	0.17	-	55,55,55,55	0
54	MG	B2	102	1/1	0.86	0.72	-	65,65,65,65	0
54	MG	AA	1682	1/1	0.93	0.16	-	91,91,91,91	0
54	MG	BA	3616	1/1	0.84	0.23	-	89,89,89,89	0
54	MG	AA	1691	1/1	0.97	0.11	-	69,69,69,69	0
54	MG	BA	3366	1/1	0.89	0.32	-	80,80,80,80	0
54	MG	BA	3270	1/1	0.89	0.14	-	93,93,93,93	0
54	MG	BA	3390	1/1	0.93	0.09	-	103,103,103,103	0
54	MG	DA	3567	1/1	0.86	1.01	-	87,87,87,87	0
54	MG	DA	3327	1/1	0.85	0.27	-	79,79,79,79	0
54	MG	BA	3140	1/1	0.83	0.34	-	62,62,62,62	0
54	MG	BB	222	1/1	0.96	0.23	-	112,112,112,112	0
54	MG	DA	3802	1/1	0.95	0.14	-	84,84,84,84	0
54	MG	DA	3286	1/1	0.90	0.23	-	76,76,76,76	0
54	MG	BN	202	1/1	0.91	0.66	-	78,78,78,78	0
54	MG	CV	6207	1/1	0.92	0.20	-	94,94,94,94	0
54	MG	DA	3021	1/1	0.70	1.25	-	68,68,68,68	0
54	MG	CA	1955	1/1	0.94	0.28	-	98,98,98,98	0
54	MG	BA	3596	1/1	0.81	0.23	-	71,71,71,71	0
54	MG	AA	1605	1/1	0.92	0.17	-	65,65,65,65	0
54	MG	DA	3817	1/1	0.86	0.40	-	76,76,76,76	0
54	MG	BA	2970	1/1	0.81	0.42	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1610	1/1	0.94	0.44	-	90,90,90,90	0
54	MG	CE	205	1/1	0.95	0.49	-	104,104,104,104	0
54	MG	BA	3230	1/1	0.93	0.23	-	111,111,111,111	0
54	MG	DA	2949	1/1	0.94	0.37	-	52,52,52,52	0
54	MG	DB	220	1/1	0.71	0.24	-	75,75,75,75	0
54	MG	BA	3059	1/1	0.96	0.64	-	48,48,48,48	0
54	MG	AA	1773	1/1	0.91	0.08	-	97,97,97,97	0
54	MG	AA	1738	1/1	0.74	0.44	-	104,104,104,104	0
54	MG	DB	238	1/1	0.91	0.16	-	74,74,74,74	0
54	MG	DA	3008	1/1	0.95	0.15	-	50,50,50,50	0
54	MG	CA	1769	1/1	0.97	0.13	-	67,67,67,67	0
54	MG	DA	3402	1/1	0.75	0.26	-	95,95,95,95	0
54	MG	DA	3678	1/1	0.93	0.22	-	58,58,58,58	0
54	MG	BA	3297	1/1	0.77	0.68	-	98,98,98,98	0
54	MG	BA	2976	1/1	0.93	0.30	-	65,65,65,65	0
54	MG	DA	3806	1/1	0.97	0.17	-	92,92,92,92	0
54	MG	BA	3607	1/1	0.84	0.76	-	62,62,62,62	0
54	MG	BA	3558	1/1	0.74	0.36	-	91,91,91,91	0
54	MG	AA	1707	1/1	0.92	0.82	-	86,86,86,86	0
54	MG	CA	1682	1/1	0.93	0.54	-	88,88,88,88	0
54	MG	BA	3441	1/1	0.97	0.37	-	35,35,35,35	0
54	MG	CA	1674	1/1	0.91	0.58	-	70,70,70,70	0
54	MG	DA	3524	1/1	0.95	0.12	-	87,87,87,87	0
54	MG	DA	3480	1/1	0.94	0.15	-	76,76,76,76	0
54	MG	DA	3776	1/1	0.97	0.24	-	172,172,172,172	0
54	MG	DA	3826	1/1	0.70	0.17	-	100,100,100,100	0
54	MG	BA	3645	1/1	0.91	0.22	-	69,69,69,69	0
54	MG	CA	1603	1/1	0.92	0.54	-	48,48,48,48	0
54	MG	D4	104	1/1	0.79	0.28	-	76,76,76,76	0
54	MG	CA	1890	1/1	0.86	0.58	-	78,78,78,78	0
54	MG	DA	3254	1/1	0.72	0.67	-	71,71,71,71	0
54	MG	BA	3532	1/1	0.59	0.24	-	107,107,107,107	0
54	MG	DB	230	1/1	0.50	0.68	-	114,114,114,114	0
54	MG	BA	3380	1/1	0.90	0.26	-	55,55,55,55	0
54	MG	BA	3052	1/1	0.49	0.85	-	73,73,73,73	0
54	MG	DA	3234	1/1	0.69	0.36	-	64,64,64,64	0
54	MG	DB	229	1/1	0.69	0.57	-	134,134,134,134	0
54	MG	DA	3858	1/1	0.83	0.32	-	58,58,58,58	0
54	MG	AA	1785	1/1	0.65	0.98	-	117,117,117,117	0
54	MG	BA	3576	1/1	0.77	0.67	-	83,83,83,83	0
54	MG	BA	3513	1/1	0.91	0.16	-	74,74,74,74	0
54	MG	BA	3177	1/1	0.91	0.08	-	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3654	1/1	0.86	0.33	-	122,122,122,122	0
54	MG	DA	3713	1/1	0.78	0.56	-	96,96,96,96	0
54	MG	BA	3105	1/1	0.70	0.18	-	72,72,72,72	0
54	MG	BA	3550	1/1	0.92	0.18	-	79,79,79,79	0
54	MG	DA	3272	1/1	0.92	0.56	-	87,87,87,87	0
54	MG	BA	3613	1/1	0.70	0.21	-	103,103,103,103	0
54	MG	DG	203	1/1	0.65	0.20	-	98,98,98,98	0
54	MG	BA	3277	1/1	0.82	0.34	-	110,110,110,110	0
54	MG	BA	3681	1/1	0.80	0.26	-	95,95,95,95	0
54	MG	CL	204	1/1	0.81	0.25	-	86,86,86,86	0
54	MG	CA	1850	1/1	0.91	0.25	-	129,129,129,129	0
54	MG	CA	1763	1/1	0.58	0.09	-	90,90,90,90	0
54	MG	BA	3564	1/1	0.86	0.76	-	146,146,146,146	0
54	MG	DA	3860	1/1	0.71	0.28	-	78,78,78,78	0
54	MG	CA	1942	1/1	0.97	0.20	-	104,104,104,104	0
54	MG	BA	3446	1/1	0.94	0.42	-	53,53,53,53	0
54	MG	BA	3329	1/1	0.92	0.29	-	113,113,113,113	0
54	MG	CA	1673	1/1	0.98	0.49	-	61,61,61,61	0
54	MG	AA	1616	1/1	0.97	0.65	-	54,54,54,54	0
54	MG	AA	1694	1/1	0.95	0.10	-	71,71,71,71	0
54	MG	CA	1960	1/1	0.82	0.15	-	91,91,91,91	0
54	MG	BV	202	1/1	0.73	0.09	-	75,75,75,75	0
54	MG	BA	3260	1/1	0.94	0.35	-	64,64,64,64	0
54	MG	CA	1877	1/1	0.82	0.26	-	126,126,126,126	0
54	MG	AA	1879	1/1	0.88	0.62	-	119,119,119,119	0
54	MG	AA	1780	1/1	0.90	0.06	-	101,101,101,101	0
54	MG	BA	3180	1/1	0.86	0.34	-	88,88,88,88	0
54	MG	BA	2992	1/1	0.93	0.13	-	69,69,69,69	0
54	MG	DA	3336	1/1	0.89	1.01	-	70,70,70,70	0
54	MG	DA	3247	1/1	0.93	0.14	-	92,92,92,92	0
54	MG	CA	1917	1/1	0.77	0.30	-	105,105,105,105	0
54	MG	DA	3739	1/1	0.98	0.18	-	133,133,133,133	0
54	MG	BA	3592	1/1	0.63	0.53	-	79,79,79,79	0
54	MG	CA	1803	1/1	0.91	0.61	-	99,99,99,99	0
54	MG	DA	3671	1/1	0.89	1.12	-	69,69,69,69	0
54	MG	BA	3553	1/1	0.94	0.17	-	72,72,72,72	0
54	MG	BA	3421	1/1	0.88	0.20	-	80,80,80,80	0
54	MG	CA	1742	1/1	0.94	0.16	-	91,91,91,91	0
54	MG	BA	2979	1/1	0.88	0.14	-	86,86,86,86	0
54	MG	CA	1745	1/1	0.89	0.19	-	77,77,77,77	0
54	MG	BA	3653	1/1	0.79	0.43	-	82,82,82,82	0
54	MG	DA	3092	1/1	0.95	0.54	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3376	1/1	0.91	0.25	-	44,44,44,44	0
54	MG	AA	1838	1/1	0.85	0.64	-	77,77,77,77	0
54	MG	BA	3294	1/1	0.90	0.32	-	89,89,89,89	0
54	MG	BA	3129	1/1	0.79	0.25	-	98,98,98,98	0
54	MG	BA	3046	1/1	0.94	0.25	-	65,65,65,65	0
54	MG	BA	3363	1/1	0.93	0.33	-	113,113,113,113	0
54	MG	DA	3617	1/1	0.96	0.30	-	59,59,59,59	0
54	MG	DA	3318	1/1	0.93	0.25	-	77,77,77,77	0
54	MG	BA	3147	1/1	0.80	0.34	-	123,123,123,123	0
54	MG	BA	3357	1/1	0.76	0.38	-	80,80,80,80	0
54	MG	BA	3377	1/1	0.92	0.47	-	68,68,68,68	0
54	MG	BA	3339	1/1	0.71	0.23	-	103,103,103,103	0
54	MG	BA	3220	1/1	0.80	0.33	-	79,79,79,79	0
54	MG	AA	1877	1/1	0.89	1.48	-	102,102,102,102	0
54	MG	BA	3246	1/1	0.92	0.34	-	164,164,164,164	0
54	MG	BA	3145	1/1	0.89	0.59	-	74,74,74,74	0
54	MG	CA	1861	1/1	0.96	0.28	-	64,64,64,64	0
54	MG	CA	1842	1/1	0.82	0.41	-	103,103,103,103	0
54	MG	DA	3704	1/1	0.92	0.75	-	68,68,68,68	0
54	MG	DA	3694	1/1	0.90	0.20	-	64,64,64,64	0
54	MG	CA	1783	1/1	0.98	0.12	-	139,139,139,139	0
54	MG	DA	3241	1/1	0.85	0.09	-	76,76,76,76	0
54	MG	BA	3567	1/1	0.93	0.20	-	126,126,126,126	0
54	MG	DA	3105	1/1	0.69	0.41	-	87,87,87,87	0
54	MG	DB	235	1/1	0.81	0.41	-	91,91,91,91	0
54	MG	BA	3620	1/1	0.89	0.57	-	88,88,88,88	0
54	MG	CA	1940	1/1	0.94	0.16	-	72,72,72,72	0
54	MG	CA	1927	1/1	0.95	0.18	-	88,88,88,88	0
54	MG	DA	3676	1/1	0.80	0.23	-	92,92,92,92	0
54	MG	BA	2904	1/1	0.85	0.31	-	40,40,40,40	0
54	MG	CA	1965	1/1	0.94	0.36	-	78,78,78,78	0
54	MG	BA	3611	1/1	0.89	0.28	-	75,75,75,75	0
54	MG	DA	2970	1/1	0.96	0.25	-	29,29,29,29	0
54	MG	BA	3433	1/1	0.97	0.69	-	21,21,21,21	0
54	MG	BA	3646	1/1	0.80	0.28	-	82,82,82,82	0
54	MG	BA	3406	1/1	0.80	0.77	-	88,88,88,88	0
54	MG	DA	3209	1/1	0.74	1.22	-	94,94,94,94	0
54	MG	DA	3831	1/1	0.89	0.30	-	66,66,66,66	0
54	MG	DA	3846	1/1	0.89	0.24	-	94,94,94,94	0
54	MG	DA	3784	1/1	0.86	0.07	-	108,108,108,108	0
54	MG	BA	3075	1/1	0.74	0.13	-	60,60,60,60	0
54	MG	CD	303	1/1	0.84	0.21	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DG	202	1/1	0.63	0.13	-	102,102,102,102	0
54	MG	DA	3526	1/1	0.91	0.18	-	84,84,84,84	0
54	MG	DA	3371	1/1	0.90	0.30	-	53,53,53,53	0
54	MG	BA	3485	1/1	0.93	0.53	-	72,72,72,72	0
54	MG	DA	3046	1/1	0.85	0.35	-	37,37,37,37	0
54	MG	BA	3481	1/1	0.96	0.39	-	71,71,71,71	0
54	MG	DA	3026	1/1	0.74	0.42	-	83,83,83,83	0
54	MG	BA	3031	1/1	0.94	0.55	-	80,80,80,80	0
54	MG	CA	1771	1/1	0.90	0.17	-	98,98,98,98	0
54	MG	CA	1798	1/1	0.87	0.26	-	111,111,111,111	0
54	MG	BA	3557	1/1	0.83	0.36	-	67,67,67,67	0
54	MG	AA	1642	1/1	0.84	0.63	-	100,100,100,100	0
54	MG	AQ	201	1/1	0.72	0.30	-	90,90,90,90	0
54	MG	BA	3504	1/1	0.80	0.52	-	94,94,94,94	0
54	MG	AA	1699	1/1	0.88	0.34	-	57,57,57,57	0
54	MG	DA	3620	1/1	0.97	0.30	-	115,115,115,115	0
54	MG	DA	3260	1/1	0.86	1.20	-	90,90,90,90	0
54	MG	DA	2960	1/1	0.97	0.32	-	33,33,33,33	0
54	MG	BA	2996	1/1	0.90	0.27	-	125,125,125,125	0
54	MG	CA	1668	1/1	0.89	0.25	-	86,86,86,86	0
54	MG	DA	3758	1/1	0.91	0.31	-	60,60,60,60	0
54	MG	BA	2940	1/1	0.94	0.33	-	30,30,30,30	0
54	MG	DA	3382	1/1	0.90	0.42	-	92,92,92,92	0
54	MG	CA	1867	1/1	0.45	0.59	-	123,123,123,123	0
54	MG	CC	307	1/1	0.53	0.18	-	108,108,108,108	0
54	MG	CA	1696	1/1	0.82	0.16	-	75,75,75,75	0
54	MG	DA	3609	1/1	0.72	0.36	-	113,113,113,113	0
54	MG	BA	3394	1/1	0.92	0.53	-	95,95,95,95	0
54	MG	DA	3251	1/1	0.79	0.15	-	77,77,77,77	0
54	MG	DX	103	1/1	0.88	0.29	-	60,60,60,60	0
54	MG	BA	2927	1/1	0.86	0.24	-	25,25,25,25	0
54	MG	DA	3087	1/1	0.70	0.70	-	71,71,71,71	0
54	MG	DA	3262	1/1	0.87	0.58	-	73,73,73,73	0
54	MG	AA	1688	1/1	0.40	0.44	-	140,140,140,140	0
54	MG	DA	3086	1/1	0.61	0.46	-	71,71,71,71	0
54	MG	BA	3414	1/1	0.31	1.52	-	137,137,137,137	0
54	MG	DA	3032	1/1	0.96	0.64	-	80,80,80,80	0
54	MG	BA	2983	1/1	0.97	0.10	-	44,44,44,44	0
54	MG	DA	3585	1/1	0.81	0.24	-	154,154,154,154	0
54	MG	DA	3426	1/1	0.96	0.19	-	96,96,96,96	0
54	MG	AA	1839	1/1	0.74	0.41	-	69,69,69,69	0
54	MG	BA	3463	1/1	0.97	0.41	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3388	1/1	0.87	0.52	-	66,66,66,66	0
54	MG	DA	2974	1/1	0.98	0.26	-	60,60,60,60	0
54	MG	BA	3649	1/1	0.95	0.15	-	67,67,67,67	0
54	MG	BA	3669	1/1	0.91	0.17	-	84,84,84,84	0
54	MG	DA	3475	1/1	0.62	0.68	-	120,120,120,120	0
54	MG	CA	1773	1/1	0.98	0.24	-	97,97,97,97	0
54	MG	CA	1912	1/1	0.70	0.29	-	138,138,138,138	0
54	MG	BA	3662	1/1	0.82	0.22	-	108,108,108,108	0
54	MG	BA	3518	1/1	0.95	0.69	-	81,81,81,81	0
54	MG	DA	2929	1/1	0.96	0.48	-	21,21,21,21	0
54	MG	DA	3499	1/1	0.91	0.62	-	87,87,87,87	0
54	MG	BA	3011	1/1	0.97	0.25	-	51,51,51,51	0
54	MG	CL	205	1/1	0.95	0.26	-	97,97,97,97	0
54	MG	CA	1878	1/1	0.96	0.41	-	82,82,82,82	0
54	MG	BA	3143	1/1	0.97	0.12	-	48,48,48,48	0
54	MG	DA	3823	1/1	0.96	0.51	-	84,84,84,84	0
54	MG	BA	3144	1/1	0.96	0.09	-	148,148,148,148	0
54	MG	AA	1645	1/1	0.90	0.06	-	138,138,138,138	0
54	MG	BA	3027	1/1	0.88	0.28	-	72,72,72,72	0
54	MG	CA	1700	1/1	0.94	0.16	-	129,129,129,129	0
54	MG	DA	3287	1/1	0.86	0.07	-	104,104,104,104	0
54	MG	BA	3534	1/1	0.81	0.42	-	82,82,82,82	0
54	MG	BB	202	1/1	0.85	0.44	-	48,48,48,48	0
54	MG	AA	1856	1/1	0.89	0.39	-	58,58,58,58	0
54	MG	BA	3371	1/1	0.84	0.29	-	114,114,114,114	0
54	MG	BA	3540	1/1	0.86	0.27	-	80,80,80,80	0
54	MG	BF	201	1/1	0.93	0.08	-	122,122,122,122	0
54	MG	CA	1767	1/1	0.93	0.42	-	72,72,72,72	0
54	MG	DA	3791	1/1	0.88	0.28	-	108,108,108,108	0
54	MG	DA	3640	1/1	0.98	0.25	-	24,24,24,24	0
54	MG	DA	3309	1/1	0.93	0.21	-	127,127,127,127	0
54	MG	CA	1886	1/1	0.70	0.32	-	105,105,105,105	0
54	MG	AA	1767	1/1	0.90	0.14	-	118,118,118,118	0
54	MG	DA	3509	1/1	0.81	0.14	-	148,148,148,148	0
54	MG	DA	3159	1/1	0.93	0.43	-	106,106,106,106	0
54	MG	DA	2966	1/1	0.97	0.19	-	39,39,39,39	0
54	MG	BA	3234	1/1	0.86	0.42	-	73,73,73,73	0
54	MG	BA	3656	1/1	0.93	0.22	-	107,107,107,107	0
54	MG	DA	2911	1/1	0.94	0.38	-	11,11,11,11	0
54	MG	DA	3143	1/1	0.83	0.25	-	67,67,67,67	0
54	MG	BA	3128	1/1	0.98	0.18	-	65,65,65,65	0
54	MG	AA	1845	1/1	0.96	0.06	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3321	1/1	0.98	0.22	-	179,179,179,179	0
54	MG	CA	1633	1/1	0.93	0.21	-	85,85,85,85	0
54	MG	BA	3375	1/1	0.92	0.28	-	62,62,62,62	0
54	MG	BA	3462	1/1	0.79	0.61	-	80,80,80,80	0
54	MG	DA	2991	1/1	0.99	0.21	-	36,36,36,36	0
54	MG	DA	2930	1/1	0.99	0.49	-	34,34,34,34	0
54	MG	DA	3471	1/1	0.56	0.30	-	104,104,104,104	0
54	MG	DA	3648	1/1	0.80	0.48	-	60,60,60,60	0
54	MG	DS	202	1/1	0.95	0.52	-	62,62,62,62	0
54	MG	BA	3604	1/1	0.69	0.29	-	89,89,89,89	0
54	MG	AA	1710	1/1	0.87	0.52	-	84,84,84,84	0
54	MG	AA	1829	1/1	0.90	0.13	-	64,64,64,64	0
54	MG	DA	3774	1/1	0.94	0.30	-	74,74,74,74	0
54	MG	AA	1696	1/1	0.94	0.05	-	120,120,120,120	0
54	MG	DA	3451	1/1	0.93	0.35	-	80,80,80,80	0
54	MG	BA	3642	1/1	0.83	0.18	-	98,98,98,98	0
54	MG	DA	3243	1/1	0.98	0.12	-	59,59,59,59	0
54	MG	DA	3391	1/1	0.94	0.37	-	82,82,82,82	0
54	MG	BA	3498	1/1	0.81	0.97	-	67,67,67,67	0
54	MG	BA	2994	1/1	0.84	0.55	-	90,90,90,90	0
54	MG	CA	1966	1/1	0.92	0.30	-	97,97,97,97	0
54	MG	DB	239	1/1	0.73	0.17	-	107,107,107,107	0
54	MG	CA	1646	1/1	0.95	0.21	-	115,115,115,115	0
54	MG	DA	3367	1/1	0.74	0.92	-	97,97,97,97	0
54	MG	DA	3517	1/1	0.78	0.21	-	102,102,102,102	0
54	MG	AA	1643	1/1	0.86	0.19	-	63,63,63,63	0
54	MG	BA	3618	1/1	0.90	0.22	-	76,76,76,76	0
54	MG	DA	3088	1/1	0.90	0.09	-	83,83,83,83	0
54	MG	DA	3481	1/1	0.97	0.29	-	77,77,77,77	0
54	MG	CA	1615	1/1	0.94	0.20	-	70,70,70,70	0
54	MG	BA	3648	1/1	0.82	0.31	-	63,63,63,63	0
54	MG	BA	3171	1/1	0.90	0.10	-	127,127,127,127	0
54	MG	BA	3533	1/1	0.93	0.20	-	83,83,83,83	0
54	MG	DA	3464	1/1	0.88	0.12	-	133,133,133,133	0
54	MG	DA	3007	1/1	0.88	0.36	-	44,44,44,44	0
54	MG	DA	3017	1/1	0.96	0.33	-	38,38,38,38	0
54	MG	CA	1736	1/1	0.82	0.25	-	73,73,73,73	0
54	MG	DA	3463	1/1	0.71	0.42	-	69,69,69,69	0
54	MG	BA	3351	1/1	0.90	0.76	-	116,116,116,116	0
54	MG	DA	2909	1/1	0.95	0.61	-	22,22,22,22	0
54	MG	CA	1740	1/1	0.76	0.14	-	117,117,117,117	0
54	MG	BA	3663	1/1	0.90	0.31	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BV	203	1/1	0.92	0.09	-	104,104,104,104	0
54	MG	DA	3291	1/1	0.82	0.27	-	57,57,57,57	0
54	MG	DA	3424	1/1	0.76	0.19	-	90,90,90,90	0
54	MG	BA	3520	1/1	0.63	0.87	-	95,95,95,95	0
54	MG	BA	3578	1/1	0.93	0.10	-	74,74,74,74	0
54	MG	BA	3621	1/1	0.83	0.58	-	107,107,107,107	0
54	MG	BA	2997	1/1	0.94	0.71	-	81,81,81,81	0
54	MG	BA	3526	1/1	0.89	0.18	-	66,66,66,66	0
54	MG	DA	3421	1/1	0.89	0.15	-	63,63,63,63	0
54	MG	AA	1831	1/1	0.95	0.40	-	67,67,67,67	0
54	MG	CA	1759	1/1	0.90	0.32	-	89,89,89,89	0
54	MG	DA	3296	1/1	0.96	0.24	-	70,70,70,70	0
54	MG	BA	3309	1/1	0.90	0.26	-	84,84,84,84	0
54	MG	BA	3660	1/1	0.95	0.15	-	119,119,119,119	0
54	MG	BA	2941	1/1	0.96	0.34	-	31,31,31,31	0
54	MG	CA	1775	1/1	0.94	0.17	-	64,64,64,64	0
54	MG	DA	3781	1/1	0.80	0.34	-	55,55,55,55	0
54	MG	AA	1807	1/1	0.82	0.51	-	76,76,76,76	0
54	MG	DA	3772	1/1	0.98	0.21	-	114,114,114,114	0
54	MG	BA	3163	1/1	0.79	0.45	-	87,87,87,87	0
54	MG	DA	3647	1/1	0.99	0.75	-	54,54,54,54	0
54	MG	CA	1889	1/1	0.67	0.33	-	74,74,74,74	0
54	MG	CA	1681	1/1	0.97	0.20	-	66,66,66,66	0
54	MG	AA	1761	1/1	0.96	0.10	-	68,68,68,68	0
54	MG	BA	3457	1/1	0.94	0.37	-	48,48,48,48	0
54	MG	CA	1644	1/1	0.91	0.15	-	94,94,94,94	0
54	MG	AA	1705	1/1	0.70	0.57	-	62,62,62,62	0
54	MG	BA	3679	1/1	0.96	0.29	-	75,75,75,75	0
54	MG	DA	3284	1/1	0.96	0.20	-	79,79,79,79	0
54	MG	DA	3803	1/1	0.56	0.51	-	123,123,123,123	0
54	MG	BA	3316	1/1	0.87	0.44	-	97,97,97,97	0
54	MG	DA	3029	1/1	0.80	0.37	-	74,74,74,74	0
54	MG	BA	3402	1/1	0.75	0.33	-	90,90,90,90	0
54	MG	DA	3297	1/1	0.88	0.55	-	76,76,76,76	0
54	MG	BA	3360	1/1	0.95	0.20	-	75,75,75,75	0
54	MG	DA	3575	1/1	0.95	0.38	-	85,85,85,85	0
54	MG	DA	3443	1/1	0.97	0.15	-	92,92,92,92	0
54	MG	BB	203	1/1	0.89	0.75	-	74,74,74,74	0
54	MG	AA	1832	1/1	0.96	0.46	-	66,66,66,66	0
54	MG	BA	3381	1/1	0.90	0.63	-	82,82,82,82	0
54	MG	DA	3654	1/1	0.97	0.28	-	59,59,59,59	0
54	MG	DA	3051	1/1	0.92	0.30	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	AV	6201	1/1	0.91	0.57	-	67,67,67,67	0
54	MG	BA	3259	1/1	0.92	0.08	-	105,105,105,105	0
54	MG	DA	3627	1/1	0.88	0.60	-	63,63,63,63	0
54	MG	CA	1866	1/1	0.96	0.21	-	102,102,102,102	0
54	MG	BA	3671	1/1	0.93	0.25	-	100,100,100,100	0
54	MG	CA	1879	1/1	0.95	0.17	-	76,76,76,76	0
54	MG	BA	3563	1/1	0.74	0.38	-	58,58,58,58	0
54	MG	BA	3474	1/1	0.94	0.33	-	72,72,72,72	0
54	MG	BA	3569	1/1	0.80	0.13	-	116,116,116,116	0
54	MG	BA	3295	1/1	0.89	0.30	-	60,60,60,60	0
54	MG	DA	3127	1/1	0.85	0.45	-	76,76,76,76	0
54	MG	DA	3541	1/1	0.92	0.19	-	76,76,76,76	0
54	MG	DA	3109	1/1	0.74	0.32	-	88,88,88,88	0
54	MG	BA	3313	1/1	0.94	0.18	-	67,67,67,67	0
54	MG	BA	3092	1/1	0.82	0.70	-	123,123,123,123	0
54	MG	DA	3073	1/1	0.96	0.24	-	69,69,69,69	0
54	MG	DA	3832	1/1	0.73	0.30	-	77,77,77,77	0
54	MG	BA	3087	1/1	0.92	1.47	-	84,84,84,84	0
54	MG	DA	3390	1/1	0.76	0.78	-	72,72,72,72	0
54	MG	BA	3666	1/1	0.93	0.19	-	72,72,72,72	0
54	MG	DA	3366	1/1	0.80	0.39	-	73,73,73,73	0
54	MG	BA	3449	1/1	0.94	0.57	-	31,31,31,31	0
54	MG	AA	1830	1/1	0.08	0.86	-	105,105,105,105	0
54	MG	BA	3458	1/1	0.97	0.11	-	77,77,77,77	0
54	MG	DA	3746	1/1	0.95	0.11	-	94,94,94,94	0
54	MG	BA	3509	1/1	0.92	0.17	-	64,64,64,64	0
54	MG	DA	3630	1/1	0.92	0.23	-	101,101,101,101	0
54	MG	BA	3176	1/1	0.92	0.29	-	53,53,53,53	0
54	MG	BA	3276	1/1	0.97	0.07	-	67,67,67,67	0
54	MG	AA	1844	1/1	0.37	1.02	-	121,121,121,121	0
54	MG	CA	1658	1/1	0.88	0.26	-	94,94,94,94	0
54	MG	BN	201	1/1	0.96	0.28	-	49,49,49,49	0
54	MG	DA	3729	1/1	0.93	0.17	-	81,81,81,81	0
54	MG	CA	1796	1/1	0.81	0.38	-	87,87,87,87	0
54	MG	AA	1857	1/1	0.88	0.14	-	103,103,103,103	0
54	MG	DA	3270	1/1	0.93	0.24	-	82,82,82,82	0
54	MG	BA	2972	1/1	0.85	0.33	-	61,61,61,61	0
54	MG	DA	3468	1/1	0.65	0.49	-	79,79,79,79	0
54	MG	DA	3047	1/1	0.78	0.46	-	74,74,74,74	0
54	MG	DA	3745	1/1	0.96	0.25	-	109,109,109,109	0
54	MG	BA	3010	1/1	0.94	0.07	-	73,73,73,73	0
54	MG	BB	208	1/1	0.96	0.11	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	BA	3487	1/1	0.84	0.41	-	90,90,90,90	0
54	MG	BA	3588	1/1	0.82	0.74	-	52,52,52,52	0
54	MG	BA	3262	1/1	0.83	0.14	-	75,75,75,75	0
54	MG	AA	1639	1/1	0.91	0.60	-	54,54,54,54	0
54	MG	CA	1638	1/1	0.84	0.06	-	101,101,101,101	0
54	MG	DA	3519	1/1	0.96	0.38	-	74,74,74,74	0
54	MG	CA	1810	1/1	0.92	0.09	-	99,99,99,99	0
54	MG	DA	3527	1/1	0.94	0.17	-	104,104,104,104	0
54	MG	DA	3656	1/1	0.96	0.29	-	36,36,36,36	0
54	MG	BA	3034	1/1	0.98	0.98	-	69,69,69,69	0
54	MG	BA	3191	1/1	0.94	0.95	-	90,90,90,90	0
54	MG	DA	2998	1/1	0.95	0.26	-	36,36,36,36	0
54	MG	CA	1967	1/1	0.83	0.33	-	93,93,93,93	0
54	MG	DA	3372	1/1	0.98	0.16	-	90,90,90,90	0
54	MG	BA	3332	1/1	0.91	0.20	-	65,65,65,65	0
54	MG	DA	3379	1/1	0.95	0.04	-	78,78,78,78	0
54	MG	BA	3672	1/1	0.92	0.30	-	92,92,92,92	0
54	MG	BA	3174	1/1	0.86	0.30	-	67,67,67,67	0
54	MG	AA	1612	1/1	0.92	0.58	-	39,39,39,39	0
54	MG	DA	3770	1/1	0.85	0.17	-	79,79,79,79	0
54	MG	BA	3202	1/1	0.79	0.34	-	126,126,126,126	0
54	MG	DA	3754	1/1	0.30	0.37	-	121,121,121,121	0
54	MG	AA	1862	1/1	0.87	0.66	-	84,84,84,84	0
54	MG	BA	3435	1/1	0.98	0.38	-	29,29,29,29	0
54	MG	BA	3641	1/1	0.93	0.15	-	95,95,95,95	0
54	MG	BA	3311	1/1	0.98	0.17	-	87,87,87,87	0
54	MG	DA	3062	1/1	0.92	0.28	-	129,129,129,129	0
54	MG	BA	3288	1/1	0.77	0.53	-	113,113,113,113	0
54	MG	AA	1825	1/1	0.87	0.98	-	79,79,79,79	0
54	MG	DA	3696	1/1	0.92	0.15	-	82,82,82,82	0
54	MG	BA	3281	1/1	0.96	0.72	-	123,123,123,123	0
54	MG	DN	201	1/1	0.95	0.07	-	88,88,88,88	0
54	MG	BA	2958	1/1	0.91	0.60	-	46,46,46,46	0
54	MG	DA	3452	1/1	0.77	0.53	-	74,74,74,74	0
54	MG	CA	1791	1/1	0.92	0.84	-	93,93,93,93	0
54	MG	D3	101	1/1	0.85	0.14	-	90,90,90,90	0
54	MG	DA	3677	1/1	0.93	0.23	-	60,60,60,60	0
54	MG	DA	3459	1/1	0.99	0.16	-	61,61,61,61	0
54	MG	BA	3236	1/1	0.91	0.23	-	56,56,56,56	0
54	MG	DA	3544	1/1	0.94	0.27	-	53,53,53,53	0
54	MG	CF	202	1/1	0.82	0.22	-	83,83,83,83	0
54	MG	DA	3427	1/1	0.88	0.38	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1627	1/1	0.77	1.09	-	99,99,99,99	0
54	MG	BU	202	1/1	0.78	0.25	-	74,74,74,74	0
54	MG	BA	3193	1/1	0.98	0.29	-	81,81,81,81	0
54	MG	DA	3610	1/1	0.89	0.57	-	81,81,81,81	0
54	MG	CA	1845	1/1	0.75	1.93	-	100,100,100,100	0
54	MG	DA	2950	1/1	0.98	0.23	-	33,33,33,33	0
54	MG	CL	206	1/1	0.77	0.16	-	87,87,87,87	0
54	MG	CA	1838	1/1	0.97	0.14	-	94,94,94,94	0
54	MG	BA	3221	1/1	0.88	0.45	-	141,141,141,141	0
54	MG	CA	1920	1/1	0.98	0.28	-	87,87,87,87	0
54	MG	CA	1626	1/1	0.88	0.54	-	68,68,68,68	0
54	MG	DA	3793	1/1	0.85	0.25	-	106,106,106,106	0
54	MG	AA	1700	1/1	0.59	0.38	-	114,114,114,114	0
54	MG	CA	1753	1/1	0.91	0.32	-	97,97,97,97	0
54	MG	CA	1852	1/1	0.82	0.38	-	101,101,101,101	0
54	MG	DA	3717	1/1	0.91	0.26	-	65,65,65,65	0
54	MG	BA	3223	1/1	0.94	0.16	-	76,76,76,76	0
54	MG	DA	3722	1/1	0.97	0.17	-	138,138,138,138	0
54	MG	CV	6206	1/1	0.93	0.08	-	107,107,107,107	0
54	MG	DA	2987	1/1	0.91	0.27	-	28,28,28,28	0
54	MG	AA	1806	1/1	0.89	0.34	-	65,65,65,65	0
54	MG	DB	210	1/1	0.94	0.10	-	92,92,92,92	0
54	MG	DA	3316	1/1	0.93	0.16	-	94,94,94,94	0
54	MG	BA	2921	1/1	0.98	0.27	-	17,17,17,17	0
54	MG	BA	2985	1/1	0.89	0.54	-	43,43,43,43	0
54	MG	CA	1719	1/1	0.81	0.43	-	78,78,78,78	0
54	MG	CA	1871	1/1	0.97	0.49	-	76,76,76,76	0
54	MG	BA	3454	1/1	0.93	0.19	-	41,41,41,41	0
54	MG	DA	3491	1/1	0.82	1.22	-	99,99,99,99	0
54	MG	DB	232	1/1	0.85	0.21	-	84,84,84,84	0
54	MG	CA	1818	1/1	0.82	0.42	-	91,91,91,91	0
54	MG	AA	1678	1/1	0.90	0.20	-	78,78,78,78	0
54	MG	CQ	201	1/1	0.84	0.38	-	103,103,103,103	0
54	MG	DA	3785	1/1	0.89	0.25	-	109,109,109,109	0
54	MG	AA	1874	1/1	0.81	0.11	-	87,87,87,87	0
54	MG	BA	3670	1/1	0.83	0.73	-	90,90,90,90	0
54	MG	BA	2938	1/1	0.97	0.46	-	51,51,51,51	0
54	MG	DA	3110	1/1	0.95	0.24	-	65,65,65,65	0
54	MG	BA	3102	1/1	0.88	0.35	-	72,72,72,72	0
54	MG	AE	203	1/1	0.78	0.12	-	91,91,91,91	0
54	MG	BA	3146	1/1	0.87	0.05	-	99,99,99,99	0
54	MG	DA	3039	1/1	0.95	0.11	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3730	1/1	0.64	0.28	-	61,61,61,61	0
54	MG	DA	3457	1/1	0.85	0.28	-	86,86,86,86	0
54	MG	DA	3266	1/1	0.93	0.16	-	85,85,85,85	0
54	MG	BA	3042	1/1	0.76	0.88	-	92,92,92,92	0
54	MG	DA	3128	1/1	0.91	0.46	-	85,85,85,85	0
54	MG	DA	3053	1/1	0.97	0.47	-	63,63,63,63	0
54	MG	DA	3432	1/1	0.63	0.27	-	84,84,84,84	0
54	MG	CA	1859	1/1	0.88	0.25	-	93,93,93,93	0
54	MG	BA	3149	1/1	0.92	0.36	-	65,65,65,65	0
54	MG	CA	1634	1/1	0.91	0.42	-	78,78,78,78	0
54	MG	BA	3074	1/1	0.97	0.38	-	87,87,87,87	0
54	MG	DA	3381	1/1	0.95	0.23	-	49,49,49,49	0
54	MG	AA	1666	1/1	0.74	0.56	-	93,93,93,93	0
54	MG	CA	1789	1/1	0.93	0.21	-	103,103,103,103	0
54	MG	BA	3273	1/1	0.78	0.36	-	73,73,73,73	0
54	MG	DA	3756	1/1	0.72	0.68	-	80,80,80,80	0
54	MG	CA	1727	1/1	0.91	0.15	-	76,76,76,76	0
54	MG	DA	3844	1/1	0.70	0.21	-	132,132,132,132	0
54	MG	DF	202	1/1	0.97	0.19	-	129,129,129,129	0
54	MG	BI	101	1/1	0.59	0.33	-	109,109,109,109	0
54	MG	AV	6204	1/1	0.54	0.13	-	124,124,124,124	0
54	MG	BT	102	1/1	0.90	0.23	-	66,66,66,66	0
54	MG	DA	3192	1/1	0.94	0.18	-	49,49,49,49	0
54	MG	DA	3489	1/1	0.93	0.29	-	97,97,97,97	0
54	MG	BA	2901	1/1	0.99	0.63	-	8,8,8,8	0
54	MG	CA	1916	1/1	0.88	0.38	-	118,118,118,118	0
54	MG	DA	3215	1/1	0.84	0.39	-	73,73,73,73	0
54	MG	DA	3205	1/1	0.71	0.51	-	97,97,97,97	0
54	MG	AA	1734	1/1	0.76	0.21	-	96,96,96,96	0
54	MG	AA	1722	1/1	0.82	0.51	-	53,53,53,53	0
54	MG	DA	3141	1/1	0.95	0.44	-	57,57,57,57	0
54	MG	CV	6204	1/1	0.93	0.13	-	112,112,112,112	0
54	MG	DA	3685	1/1	0.82	0.39	-	82,82,82,82	0
54	MG	BA	3605	1/1	0.76	0.42	-	69,69,69,69	0
54	MG	DA	3041	1/1	0.91	0.23	-	76,76,76,76	0
54	MG	BA	3523	1/1	0.89	1.59	-	99,99,99,99	0
54	MG	D4	103	1/1	0.95	0.27	-	73,73,73,73	0
54	MG	DA	3170	1/1	0.95	0.41	-	56,56,56,56	0
54	MG	CA	1953	1/1	0.93	0.24	-	120,120,120,120	0
54	MG	CA	1846	1/1	0.93	0.30	-	135,135,135,135	0
54	MG	DA	3852	1/1	0.63	0.20	-	80,80,80,80	0
54	MG	BA	3584	1/1	0.96	0.15	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	DA	3618	1/1	0.76	0.54	-	129,129,129,129	0
54	MG	DA	3419	1/1	0.94	0.13	-	60,60,60,60	0
54	MG	AA	1698	1/1	0.99	0.13	-	88,88,88,88	0
54	MG	DA	3233	1/1	0.92	0.29	-	67,67,67,67	0
54	MG	BA	3379	1/1	0.96	0.21	-	86,86,86,86	0
54	MG	DA	3639	1/1	0.97	0.35	-	26,26,26,26	0
54	MG	BA	3310	1/1	0.75	0.44	-	109,109,109,109	0
54	MG	DA	3394	1/1	0.96	0.53	-	110,110,110,110	0
54	MG	BA	3418	1/1	0.52	0.42	-	88,88,88,88	0
54	MG	BA	3658	1/1	0.96	0.29	-	68,68,68,68	0
54	MG	CA	1782	1/1	0.92	0.07	-	80,80,80,80	0
54	MG	CA	1761	1/1	0.94	0.95	-	88,88,88,88	0
54	MG	AA	1787	1/1	0.67	0.51	-	68,68,68,68	0
54	MG	BA	3506	1/1	0.95	0.36	-	89,89,89,89	0
54	MG	DA	3416	1/1	0.94	0.25	-	101,101,101,101	0
54	MG	DA	3118	1/1	0.89	0.43	-	50,50,50,50	0
54	MG	BA	3308	1/1	0.70	0.21	-	99,99,99,99	0
54	MG	CA	1751	1/1	0.87	0.09	-	117,117,117,117	0
54	MG	DA	3850	1/1	0.87	0.41	-	52,52,52,52	0
54	MG	DA	2936	1/1	0.90	0.12	-	42,42,42,42	0
54	MG	AA	1813	1/1	0.96	0.12	-	76,76,76,76	0
54	MG	BA	3006	1/1	0.87	0.57	-	61,61,61,61	0
54	MG	CA	1741	1/1	0.93	0.28	-	100,100,100,100	0
54	MG	AA	1843	1/1	0.67	1.09	-	126,126,126,126	0
54	MG	AA	1759	1/1	0.82	0.48	-	110,110,110,110	0
54	MG	BA	3650	1/1	0.89	0.31	-	69,69,69,69	0
54	MG	BA	3033	1/1	0.75	0.43	-	77,77,77,77	0
54	MG	BA	3121	1/1	0.91	0.22	-	69,69,69,69	0
54	MG	DA	3428	1/1	0.80	0.38	-	71,71,71,71	0
54	MG	BA	2964	1/1	0.94	0.35	-	43,43,43,43	0
54	MG	DA	3111	1/1	0.89	0.13	-	84,84,84,84	0
54	MG	AA	1668	1/1	0.93	0.17	-	77,77,77,77	0
54	MG	BA	3157	1/1	0.87	0.18	-	94,94,94,94	0
54	MG	BA	3069	1/1	0.95	0.26	-	52,52,52,52	0
54	MG	AA	1814	1/1	0.89	0.12	-	82,82,82,82	0
54	MG	DA	3036	1/1	0.90	0.21	-	72,72,72,72	0
54	MG	BA	3348	1/1	0.89	0.38	-	107,107,107,107	0
54	MG	DA	3810	1/1	0.97	0.05	-	102,102,102,102	0
54	MG	BA	3573	1/1	0.94	0.17	-	58,58,58,58	0
54	MG	DA	3473	1/1	0.94	0.47	-	61,61,61,61	0
54	MG	BY	102	1/1	0.97	0.11	-	110,110,110,110	0
54	MG	DA	3441	1/1	0.93	0.15	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
54	MG	CA	1679	1/1	0.88	0.53	-	89,89,89,89	0
54	MG	BA	3109	1/1	0.83	0.48	-	77,77,77,77	0
54	MG	AL	201	1/1	0.92	0.21	-	109,109,109,109	0
54	MG	DA	3090	1/1	0.89	0.42	-	59,59,59,59	0
54	MG	BA	3035	1/1	0.97	0.23	-	57,57,57,57	0
54	MG	CA	1865	1/1	0.98	0.57	-	93,93,93,93	0
54	MG	CA	1968	1/1	0.90	0.15	-	87,87,87,87	0
54	MG	DA	2922	1/1	0.90	0.46	-	37,37,37,37	0
54	MG	CV	6203	1/1	0.85	0.38	-	80,80,80,80	0
54	MG	BA	3214	1/1	0.88	0.80	-	79,79,79,79	0
54	MG	BA	3503	1/1	0.89	0.83	-	90,90,90,90	0
54	MG	DA	2988	1/1	0.80	0.43	-	23,23,23,23	0
54	MG	DA	3335	1/1	0.94	0.10	-	46,46,46,46	0
54	MG	BA	3536	1/1	0.82	0.34	-	83,83,83,83	0
54	MG	CA	1870	1/1	0.97	0.20	-	94,94,94,94	0
54	MG	AA	1683	1/1	0.97	0.46	-	64,64,64,64	0
54	MG	BA	3272	1/1	0.84	0.79	-	81,81,81,81	0
54	MG	CA	1686	1/1	0.96	0.07	-	82,82,82,82	0
54	MG	BA	3210	1/1	0.91	0.06	-	86,86,86,86	0
54	MG	DA	3389	1/1	0.90	0.17	-	76,76,76,76	0
54	MG	CO	101	1/1	0.38	0.19	-	127,127,127,127	0
54	MG	AC	301	1/1	0.83	0.22	-	104,104,104,104	0
54	MG	BA	3448	1/1	0.89	0.47	-	51,51,51,51	0
54	MG	CA	1695	1/1	0.96	0.18	-	65,65,65,65	0
54	MG	DA	3091	1/1	0.91	0.32	-	127,127,127,127	0
54	MG	BA	3101	1/1	0.81	0.88	-	74,74,74,74	0
54	MG	AA	1827	1/1	0.92	0.28	-	71,71,71,71	0
54	MG	AA	1822	1/1	0.94	0.21	-	92,92,92,92	0
54	MG	DA	3429	1/1	0.97	0.15	-	79,79,79,79	0
54	MG	CA	1704	1/1	0.13	0.49	-	140,140,140,140	0
54	MG	AA	1842	1/1	0.93	0.89	-	69,69,69,69	0
54	MG	DA	3662	1/1	0.65	0.80	-	71,71,71,71	0
54	MG	BA	3631	1/1	0.88	0.12	-	85,85,85,85	0
54	MG	DA	3248	1/1	0.72	0.16	-	80,80,80,80	0
54	MG	CA	1893	1/1	0.73	0.15	-	127,127,127,127	0

6.5 Other polymers (i)

There are no such residues in this entry.