



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 10:21 AM EST

PDB ID : 4V8B  
Title : Crystal structure analysis of ribosomal decoding (near-cognate tRNA-leu complex).  
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.  
Deposited on : unknown  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345



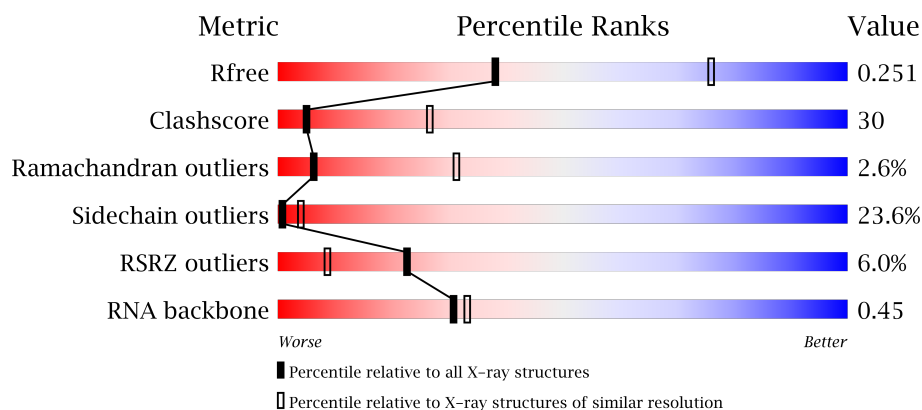
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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

Mol	Chain	Length	Quality of chain
1	AA	1506	<div> <div>32%</div> <div>48%</div> <div>19%</div> <div>.</div> </div>
1	CA	1506	<div> <div>30%</div> <div>47%</div> <div>22%</div> <div>.</div> </div>
2	AE	256	<div> <div>4%</div> <div>32%</div> <div>46%</div> <div>14%</div> <div>7%</div> </div>
2	CE	256	<div> <div>10%</div> <div>34%</div> <div>41%</div> <div>16%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	

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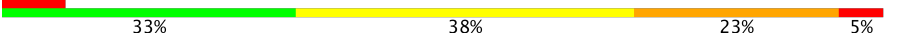
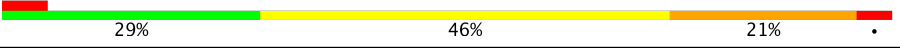

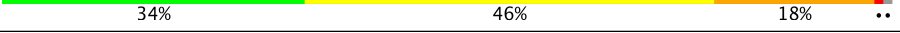


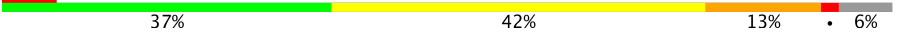
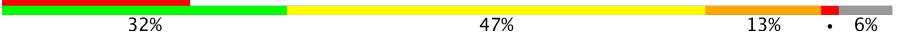
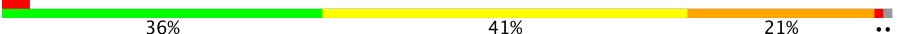








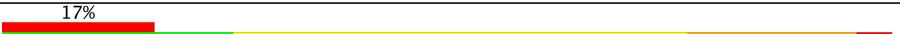




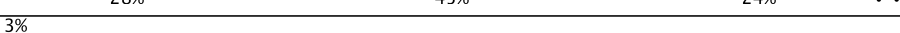
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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	87	
22	CB	87	
23	AC	77	
23	AD	77	
23	CC	77	
23	CD	77	
24	A1	10	
24	C1	10	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39	BR	146	

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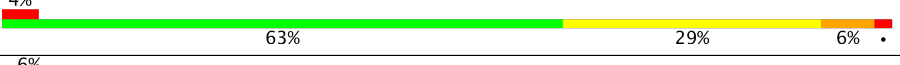
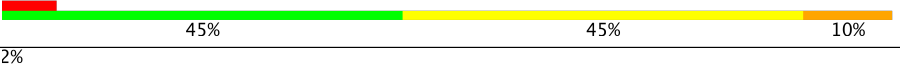
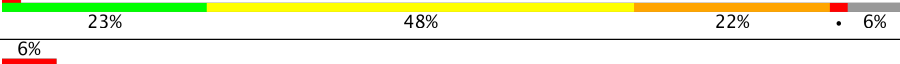
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Mol	Chain	Length	Quality of chain
39	DR	146	
40	B1	118	
40	D1	118	
41	B2	101	
41	D2	101	
42	BS	113	
42	DS	113	
43	BT	96	
43	DT	96	
44	BU	110	
44	DU	110	
45	BV	206	
45	DV	206	
46	B3	85	
46	D3	85	
47	BZ	98	
47	DZ	98	
48	BW	72	
48	DW	72	
49	BX	60	
49	DX	60	
50	B4	71	
50	D4	71	
51	B5	60	
51	D5	60	

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Mol	Chain	Length	Quality of chain
52	B6	54	
52	D6	54	
53	B7	49	
53	D7	49	
54	B8	65	
54	D8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1601	-	-	-	X
55	MG	AA	1602	-	-	-	X
55	MG	AA	1605	-	-	-	X
55	MG	AA	1608	-	-	-	X
55	MG	AA	1610	-	-	-	X
55	MG	AA	1619	-	-	-	X
55	MG	AA	1628	-	-	-	X
55	MG	AA	1632	-	-	-	X
55	MG	AA	1635	-	-	-	X
55	MG	AA	1636	-	-	-	X
55	MG	AA	1639	-	-	-	X
55	MG	AA	1645	-	-	-	X
55	MG	AA	1651	-	-	-	X
55	MG	AA	1658	-	-	-	X
55	MG	AA	1661	-	-	-	X
55	MG	AA	1663	-	-	-	X
55	MG	AA	1667	-	-	-	X
55	MG	AA	1678	-	-	-	X
55	MG	AA	1679	-	-	-	X
55	MG	AA	1682	-	-	-	X
55	MG	AA	1686	-	-	-	X
55	MG	AA	1691	-	-	-	X
55	MG	AA	1699	-	-	-	X
55	MG	AA	1711	-	-	-	X
55	MG	AA	1712	-	-	-	X
55	MG	AA	1717	-	-	-	X
55	MG	AA	1722	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1762	-	-	-	X
55	MG	AA	1783	-	-	-	X
55	MG	AA	1789	-	-	-	X
55	MG	AA	1795	-	-	-	X
55	MG	AA	1822	-	-	-	X
55	MG	AA	1825	-	-	-	X
55	MG	AA	1836	-	-	-	X
55	MG	AA	1837	-	-	-	X
55	MG	AC	101	-	-	-	X
55	MG	AC	107	-	-	-	X
55	MG	B0	201	-	-	-	X
55	MG	B1	201	-	-	-	X
55	MG	BA	3001	-	-	-	X
55	MG	BA	3002	-	-	-	X
55	MG	BA	3004	-	-	-	X
55	MG	BA	3005	-	-	-	X
55	MG	BA	3007	-	-	-	X
55	MG	BA	3008	-	-	-	X
55	MG	BA	3012	-	-	-	X
55	MG	BA	3014	-	-	-	X
55	MG	BA	3016	-	-	-	X
55	MG	BA	3018	-	-	-	X
55	MG	BA	3020	-	-	-	X
55	MG	BA	3021	-	-	-	X
55	MG	BA	3024	-	-	-	X
55	MG	BA	3025	-	-	-	X
55	MG	BA	3027	-	-	-	X
55	MG	BA	3029	-	-	-	X
55	MG	BA	3031	-	-	-	X
55	MG	BA	3032	-	-	-	X
55	MG	BA	3033	-	-	-	X
55	MG	BA	3037	-	-	-	X
55	MG	BA	3040	-	-	-	X
55	MG	BA	3044	-	-	-	X
55	MG	BA	3046	-	-	-	X
55	MG	BA	3049	-	-	-	X
55	MG	BA	3052	-	-	-	X
55	MG	BA	3055	-	-	-	X
55	MG	BA	3056	-	-	-	X
55	MG	BA	3061	-	-	-	X
55	MG	BA	3062	-	-	-	X
55	MG	BA	3064	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3066	-	-	-	X
55	MG	BA	3067	-	-	-	X
55	MG	BA	3076	-	-	-	X
55	MG	BA	3080	-	-	-	X
55	MG	BA	3082	-	-	-	X
55	MG	BA	3090	-	-	-	X
55	MG	BA	3091	-	-	-	X
55	MG	BA	3092	-	-	-	X
55	MG	BA	3093	-	-	-	X
55	MG	BA	3095	-	-	-	X
55	MG	BA	3096	-	-	-	X
55	MG	BA	3098	-	-	-	X
55	MG	BA	3100	-	-	-	X
55	MG	BA	3102	-	-	-	X
55	MG	BA	3104	-	-	-	X
55	MG	BA	3108	-	-	-	X
55	MG	BA	3109	-	-	-	X
55	MG	BA	3119	-	-	-	X
55	MG	BA	3124	-	-	-	X
55	MG	BA	3125	-	-	-	X
55	MG	BA	3126	-	-	-	X
55	MG	BA	3130	-	-	-	X
55	MG	BA	3133	-	-	-	X
55	MG	BA	3137	-	-	-	X
55	MG	BA	3138	-	-	-	X
55	MG	BA	3144	-	-	-	X
55	MG	BA	3146	-	-	-	X
55	MG	BA	3153	-	-	-	X
55	MG	BA	3154	-	-	-	X
55	MG	BA	3156	-	-	-	X
55	MG	BA	3157	-	-	-	X
55	MG	BA	3158	-	-	-	X
55	MG	BA	3160	-	-	-	X
55	MG	BA	3162	-	-	-	X
55	MG	BA	3163	-	-	-	X
55	MG	BA	3169	-	-	-	X
55	MG	BA	3172	-	-	-	X
55	MG	BA	3173	-	-	-	X
55	MG	BA	3178	-	-	-	X
55	MG	BA	3181	-	-	-	X
55	MG	BA	3183	-	-	-	X
55	MG	BA	3184	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3186	-	-	-	X
55	MG	BA	3187	-	-	-	X
55	MG	BA	3190	-	-	-	X
55	MG	BA	3195	-	-	-	X
55	MG	BA	3196	-	-	-	X
55	MG	BA	3197	-	-	-	X
55	MG	BA	3199	-	-	-	X
55	MG	BA	3206	-	-	-	X
55	MG	BA	3207	-	-	-	X
55	MG	BA	3211	-	-	-	X
55	MG	BA	3216	-	-	-	X
55	MG	BA	3226	-	-	-	X
55	MG	BA	3245	-	-	-	X
55	MG	BA	3249	-	-	-	X
55	MG	BA	3256	-	-	-	X
55	MG	BA	3258	-	-	-	X
55	MG	BA	3259	-	-	-	X
55	MG	BA	3262	-	-	-	X
55	MG	BA	3269	-	-	-	X
55	MG	BA	3270	-	-	-	X
55	MG	BA	3274	-	-	-	X
55	MG	BA	3275	-	-	-	X
55	MG	BA	3287	-	-	-	X
55	MG	BA	3289	-	-	-	X
55	MG	BA	3293	-	-	-	X
55	MG	BA	3297	-	-	-	X
55	MG	BA	3302	-	-	-	X
55	MG	BA	3304	-	-	-	X
55	MG	BA	3307	-	-	-	X
55	MG	BA	3308	-	-	-	X
55	MG	BA	3314	-	-	-	X
55	MG	BA	3319	-	-	-	X
55	MG	BA	3344	-	-	-	X
55	MG	BA	3345	-	-	-	X
55	MG	BA	3346	-	-	-	X
55	MG	BA	3353	-	-	-	X
55	MG	BA	3361	-	-	-	X
55	MG	BA	3365	-	-	-	X
55	MG	BA	3367	-	-	-	X
55	MG	BA	3375	-	-	-	X
55	MG	BA	3378	-	-	-	X
55	MG	BA	3389	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3393	-	-	-	X
55	MG	BA	3399	-	-	-	X
55	MG	BA	3401	-	-	-	X
55	MG	BA	3411	-	-	-	X
55	MG	BA	3428	-	-	-	X
55	MG	BA	3436	-	-	-	X
55	MG	BA	3442	-	-	-	X
55	MG	BA	3452	-	-	-	X
55	MG	BA	3478	-	-	-	X
55	MG	BA	3484	-	-	-	X
55	MG	BA	3504	-	-	-	X
55	MG	BA	3514	-	-	-	X
55	MG	BA	3516	-	-	-	X
55	MG	BA	3521	-	-	-	X
55	MG	BA	3524	-	-	-	X
55	MG	BA	3528	-	-	-	X
55	MG	BA	3532	-	-	-	X
55	MG	BA	3583	-	-	-	X
55	MG	BA	3584	-	-	-	X
55	MG	BA	3591	-	-	-	X
55	MG	BA	3600	-	-	-	X
55	MG	BA	3610	-	-	-	X
55	MG	BA	3616	-	-	-	X
55	MG	BA	3619	-	-	-	X
55	MG	BB	215	-	-	-	X
55	MG	BB	217	-	-	-	X
55	MG	BE	301	-	-	-	X
55	MG	BO	201	-	-	-	X
55	MG	CA	1604	-	-	-	X
55	MG	CA	1606	-	-	-	X
55	MG	CA	1610	-	-	-	X
55	MG	CA	1622	-	-	-	X
55	MG	CA	1634	-	-	-	X
55	MG	CA	1640	-	-	-	X
55	MG	CA	1646	-	-	-	X
55	MG	CA	1647	-	-	-	X
55	MG	CA	1648	-	-	-	X
55	MG	CA	1650	-	-	-	X
55	MG	CA	1654	-	-	-	X
55	MG	CA	1657	-	-	-	X
55	MG	CA	1668	-	-	-	X
55	MG	CA	1676	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	1678	-	-	-	X
55	MG	CA	1685	-	-	-	X
55	MG	CA	1686	-	-	-	X
55	MG	CA	1690	-	-	-	X
55	MG	CA	1691	-	-	-	X
55	MG	CA	1716	-	-	-	X
55	MG	CA	1719	-	-	-	X
55	MG	CA	1722	-	-	-	X
55	MG	CA	1739	-	-	-	X
55	MG	CA	1749	-	-	-	X
55	MG	CA	1750	-	-	-	X
55	MG	CA	1754	-	-	-	X
55	MG	CA	1755	-	-	-	X
55	MG	CA	1758	-	-	-	X
55	MG	CA	1766	-	-	-	X
55	MG	CA	1771	-	-	-	X
55	MG	CA	1777	-	-	-	X
55	MG	CA	1784	-	-	-	X
55	MG	CA	1785	-	-	-	X
55	MG	CA	1798	-	-	-	X
55	MG	CA	1802	-	-	-	X
55	MG	CA	1803	-	-	-	X
55	MG	CA	1804	-	-	-	X
55	MG	CC	102	-	-	-	X
55	MG	CS	101	-	-	-	X
55	MG	D1	201	-	-	-	X
55	MG	D1	202	-	-	-	X
55	MG	DA	3019	-	-	-	X
55	MG	DA	3033	-	-	-	X
55	MG	DA	3046	-	-	-	X
55	MG	DA	3047	-	-	-	X
55	MG	DA	3052	-	-	-	X
55	MG	DA	3055	-	-	-	X
55	MG	DA	3063	-	-	-	X
55	MG	DA	3069	-	-	-	X
55	MG	DA	3080	-	-	-	X
55	MG	DA	3081	-	-	-	X
55	MG	DA	3085	-	-	-	X
55	MG	DA	3086	-	-	-	X
55	MG	DA	3087	-	-	-	X
55	MG	DA	3094	-	-	-	X
55	MG	DA	3096	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3101	-	-	-	X
55	MG	DA	3103	-	-	-	X
55	MG	DA	3104	-	-	-	X
55	MG	DA	3105	-	-	-	X
55	MG	DA	3110	-	-	-	X
55	MG	DA	3112	-	-	-	X
55	MG	DA	3113	-	-	-	X
55	MG	DA	3114	-	-	-	X
55	MG	DA	3121	-	-	-	X
55	MG	DA	3122	-	-	-	X
55	MG	DA	3125	-	-	-	X
55	MG	DA	3127	-	-	-	X
55	MG	DA	3128	-	-	-	X
55	MG	DA	3129	-	-	-	X
55	MG	DA	3130	-	-	-	X
55	MG	DA	3131	-	-	-	X
55	MG	DA	3132	-	-	-	X
55	MG	DA	3134	-	-	-	X
55	MG	DA	3135	-	-	-	X
55	MG	DA	3143	-	-	-	X
55	MG	DA	3144	-	-	-	X
55	MG	DA	3145	-	-	-	X
55	MG	DA	3150	-	-	-	X
55	MG	DA	3155	-	-	-	X
55	MG	DA	3156	-	-	-	X
55	MG	DA	3157	-	-	-	X
55	MG	DA	3158	-	-	-	X
55	MG	DA	3159	-	-	-	X
55	MG	DA	3161	-	-	-	X
55	MG	DA	3162	-	-	-	X
55	MG	DA	3164	-	-	-	X
55	MG	DA	3165	-	-	-	X
55	MG	DA	3169	-	-	-	X
55	MG	DA	3174	-	-	-	X
55	MG	DA	3176	-	-	-	X
55	MG	DA	3180	-	-	-	X
55	MG	DA	3187	-	-	-	X
55	MG	DA	3188	-	-	-	X
55	MG	DA	3190	-	-	-	X
55	MG	DA	3191	-	-	-	X
55	MG	DA	3196	-	-	-	X
55	MG	DA	3198	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3201	-	-	-	X
55	MG	DA	3204	-	-	-	X
55	MG	DA	3210	-	-	-	X
55	MG	DA	3212	-	-	-	X
55	MG	DA	3213	-	-	-	X
55	MG	DA	3214	-	-	-	X
55	MG	DA	3215	-	-	-	X
55	MG	DA	3218	-	-	-	X
55	MG	DA	3221	-	-	-	X
55	MG	DA	3222	-	-	-	X
55	MG	DA	3224	-	-	-	X
55	MG	DA	3227	-	-	-	X
55	MG	DA	3228	-	-	-	X
55	MG	DA	3230	-	-	-	X
55	MG	DA	3233	-	-	-	X
55	MG	DA	3237	-	-	-	X
55	MG	DA	3239	-	-	-	X
55	MG	DA	3245	-	-	-	X
55	MG	DA	3254	-	-	-	X
55	MG	DA	3260	-	-	-	X
55	MG	DA	3261	-	-	-	X
55	MG	DA	3262	-	-	-	X
55	MG	DA	3263	-	-	-	X
55	MG	DA	3264	-	-	-	X
55	MG	DA	3266	-	-	-	X
55	MG	DA	3274	-	-	-	X
55	MG	DA	3275	-	-	-	X
55	MG	DA	3278	-	-	-	X
55	MG	DA	3281	-	-	-	X
55	MG	DA	3283	-	-	-	X
55	MG	DA	3284	-	-	-	X
55	MG	DA	3285	-	-	-	X
55	MG	DA	3295	-	-	-	X
55	MG	DA	3299	-	-	-	X
55	MG	DA	3303	-	-	-	X
55	MG	DA	3310	-	-	-	X
55	MG	DA	3317	-	-	-	X
55	MG	DA	3319	-	-	-	X
55	MG	DA	3326	-	-	-	X
55	MG	DA	3328	-	-	-	X
55	MG	DA	3331	-	-	-	X
55	MG	DA	3332	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3335	-	-	-	X
55	MG	DA	3337	-	-	-	X
55	MG	DA	3355	-	-	-	X
55	MG	DA	3364	-	-	-	X
55	MG	DA	3369	-	-	-	X
55	MG	DA	3371	-	-	-	X
55	MG	DA	3374	-	-	-	X
55	MG	DA	3376	-	-	-	X
55	MG	DA	3385	-	-	-	X
55	MG	DA	3397	-	-	-	X
55	MG	DA	3399	-	-	-	X
55	MG	DA	3400	-	-	-	X
55	MG	DA	3412	-	-	-	X
55	MG	DA	3420	-	-	-	X
55	MG	DA	3426	-	-	-	X
55	MG	DA	3427	-	-	-	X
55	MG	DA	3433	-	-	-	X
55	MG	DA	3438	-	-	-	X
55	MG	DA	3450	-	-	-	X
55	MG	DA	3452	-	-	-	X
55	MG	DA	3456	-	-	-	X
55	MG	DA	3495	-	-	-	X
55	MG	DA	3513	-	-	-	X
55	MG	DA	3522	-	-	-	X
55	MG	DB	207	-	-	-	X
55	MG	DB	211	-	-	-	X
55	MG	DE	303	-	-	-	X



## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299552 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CG	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	AH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CI	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	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CJ	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	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CK	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	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CN	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	AO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CQ	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	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CR	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	AS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AU	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AX	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
22	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	AD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	18	C	U	CONFLICT	GB AP012306.1
AD	18	C	U	CONFLICT	GB AP012306.1
CC	18	C	U	CONFLICT	GB AP012306.1
CD	18	C	U	CONFLICT	GB AP012306.1

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			
24	C1	10	Total	C	N	O	P	0	0	0
			205	92	26	77	10			

- Molecule 25 is a RNA chain called RNA (2912-MER).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
25	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	EXPRESSION TAG	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	168	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
26	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	D0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
38	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			



- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
45	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
46	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
50	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	D5	58	Total	C	N	O	S	0	0	0
			454	285	89	75	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
53	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
54	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			



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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	623	Total 623	Mg 623	0	0
55	CA	207	Total 207	Mg 207	0	0
55	AB	5	Total 5	Mg 5	0	0
55	B8	1	Total 1	Mg 1	0	0
55	BE	5	Total 5	Mg 5	0	0
55	DU	1	Total 1	Mg 1	0	0
55	B1	1	Total 1	Mg 1	0	0
55	AN	2	Total 2	Mg 2	0	0
55	CN	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0
55	BB	17	Total 17	Mg 17	0	0
55	D3	1	Total 1	Mg 1	0	0
55	BF	3	Total 3	Mg 3	0	0
55	DR	1	Total 1	Mg 1	0	0
55	B2	1	Total 1	Mg 1	0	0
55	AA	242	Total 242	Mg 242	0	0
55	CG	2	Total 2	Mg 2	0	0
55	BU	2	Total 2	Mg 2	0	0
55	A1	2	Total 2	Mg 2	0	0
55	AD	1	Total 1	Mg 1	0	0
55	CC	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DE	3	Total 3	Mg 3	0	0
55	B3	1	Total 1	Mg 1	0	0
55	DA	526	Total 526	Mg 526	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	1	Total 1	Mg 1	0	0
55	BO	2	Total 2	Mg 2	0	0
55	AQ	1	Total 1	Mg 1	0	0
55	D1	2	Total 2	Mg 2	0	0
55	AH	1	Total 1	Mg 1	0	0
55	DP	1	Total 1	Mg 1	0	0
55	AC	9	Total 9	Mg 9	0	0
55	CB	3	Total 3	Mg 3	0	0
55	D5	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	B0	1	Total 1	Mg 1	0	0
55	CS	1	Total 1	Mg 1	0	0
55	DB	14	Total 14	Mg 14	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0

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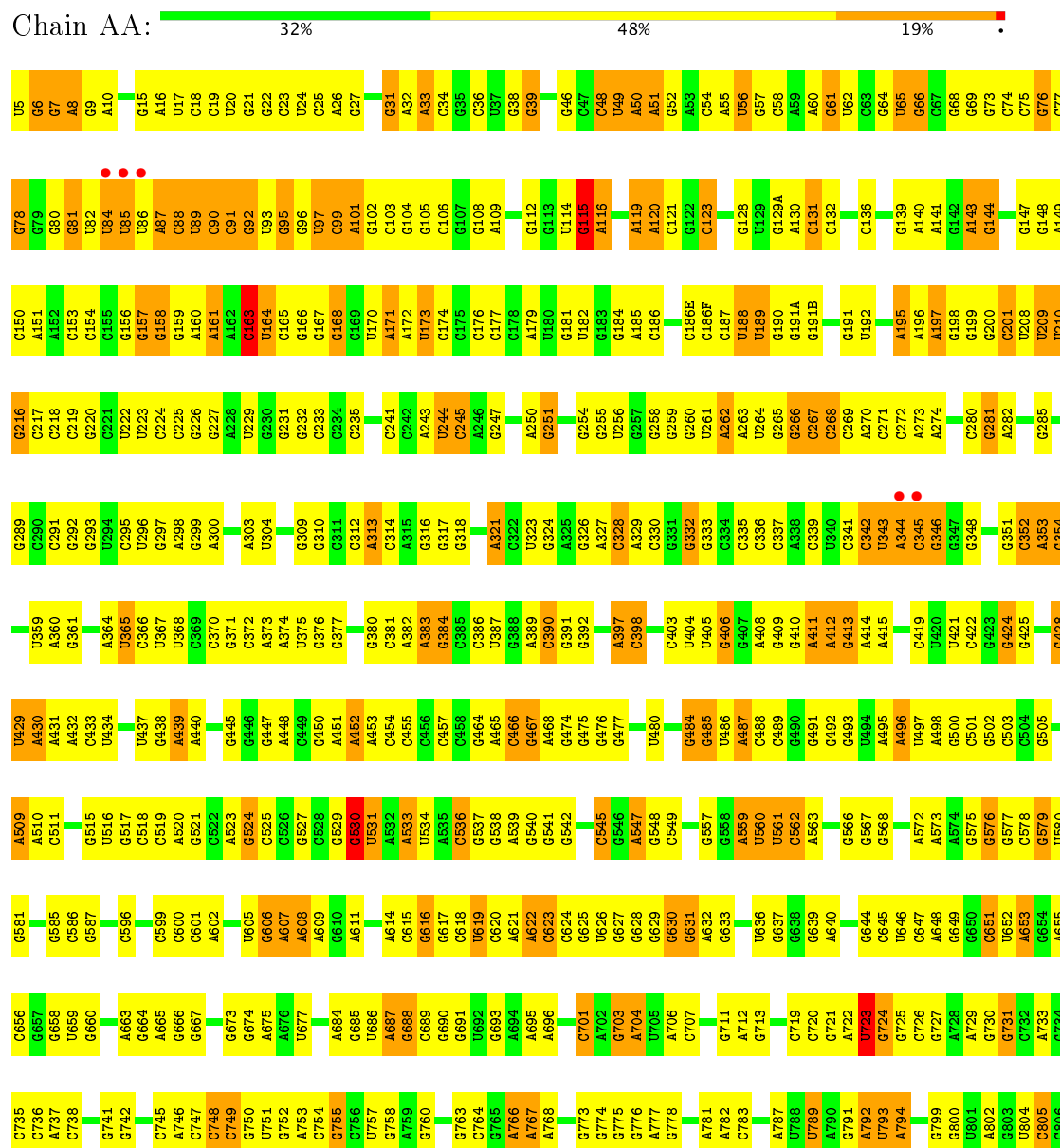
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0



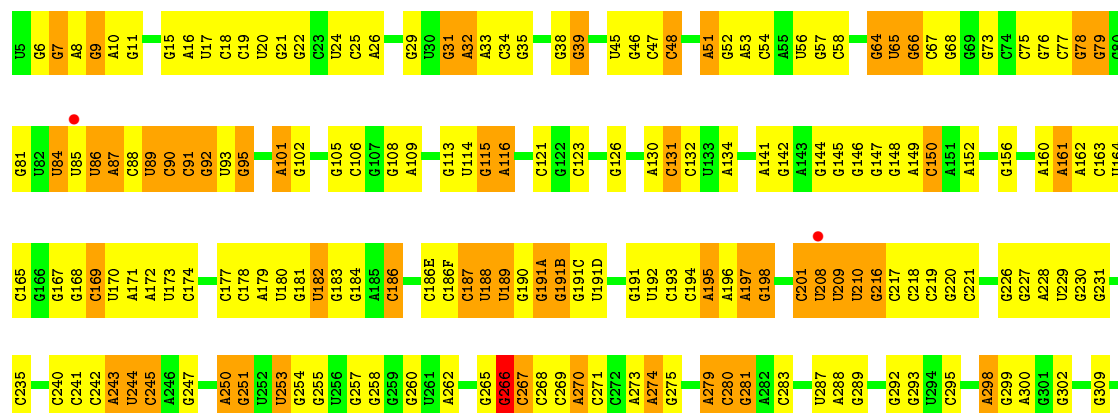
### 3 Residue-property plots

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

- Molecule 1: 16S ribosomal RNA



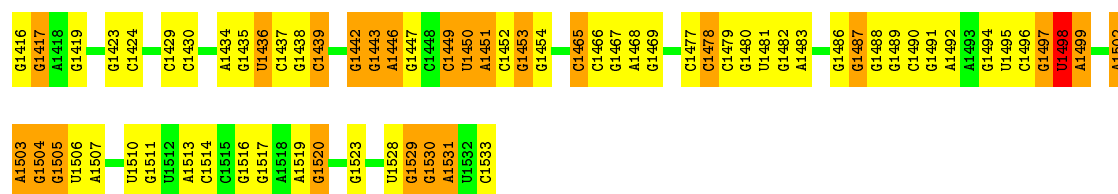




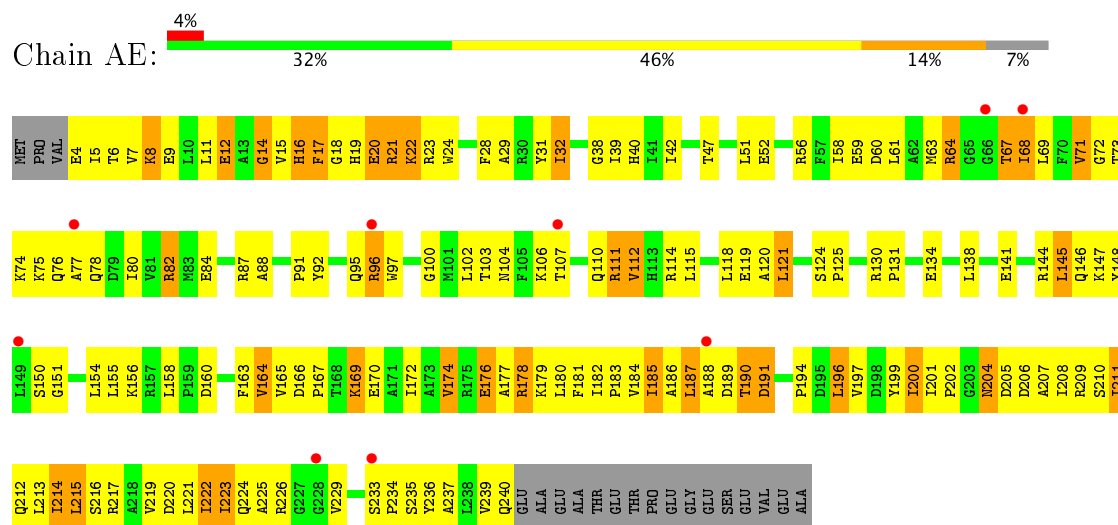




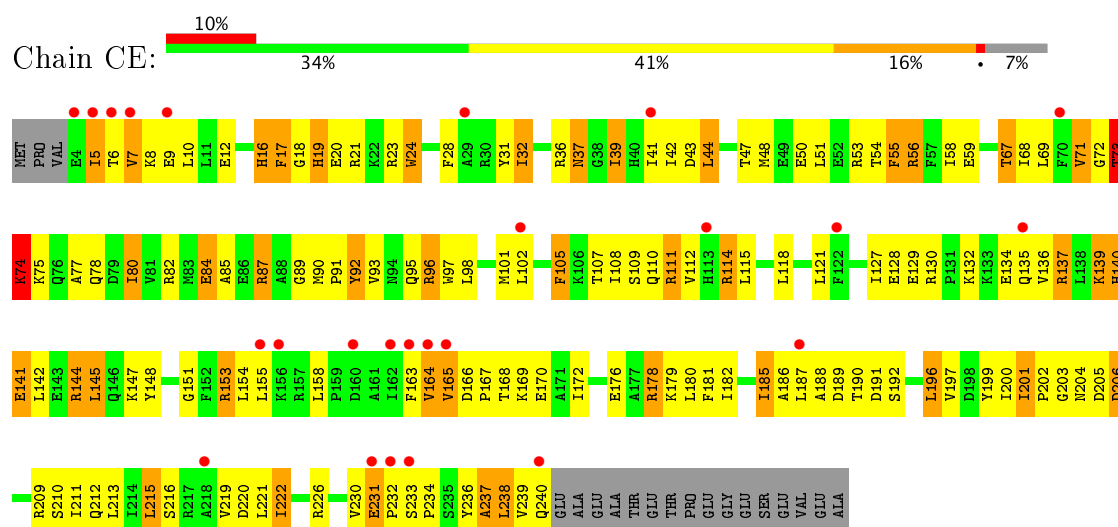




### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



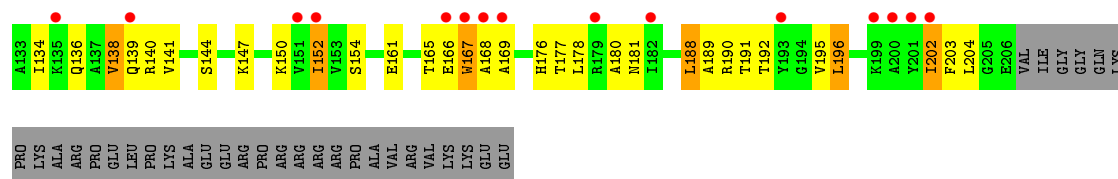
### • Molecule 2: 30S RIBOSOMAL PROTEIN S2



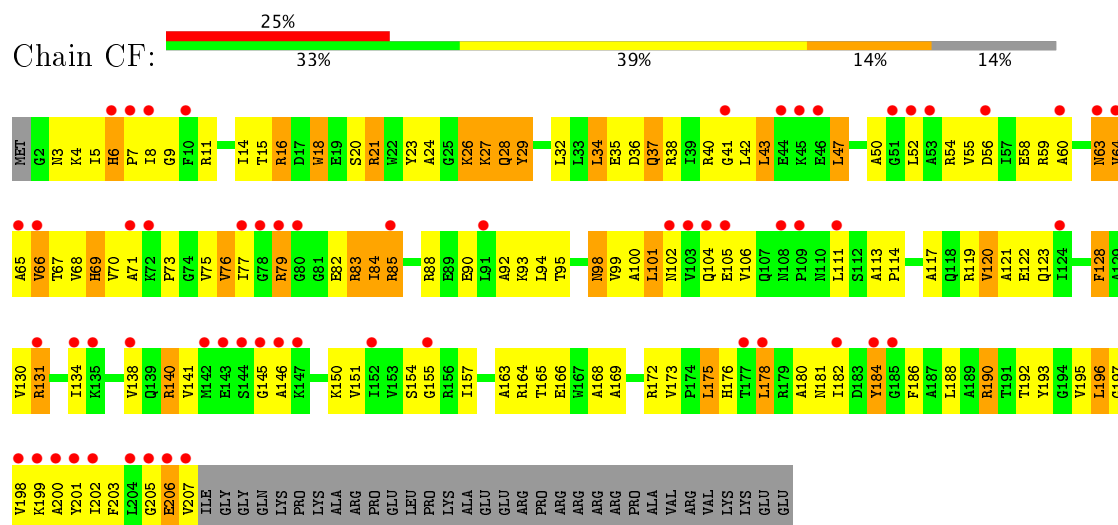
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



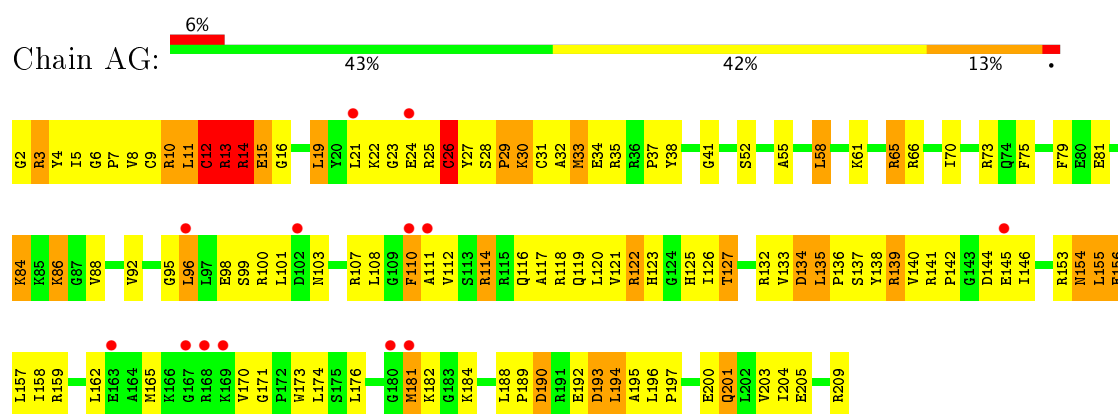




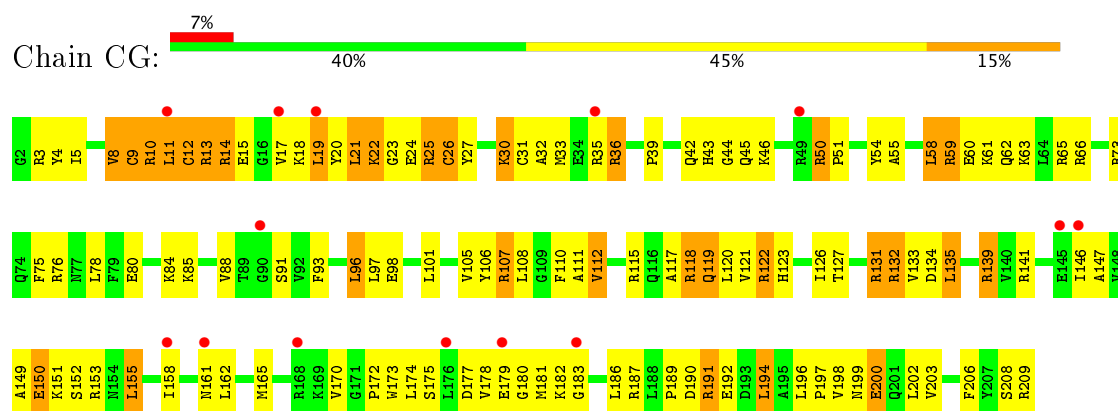
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

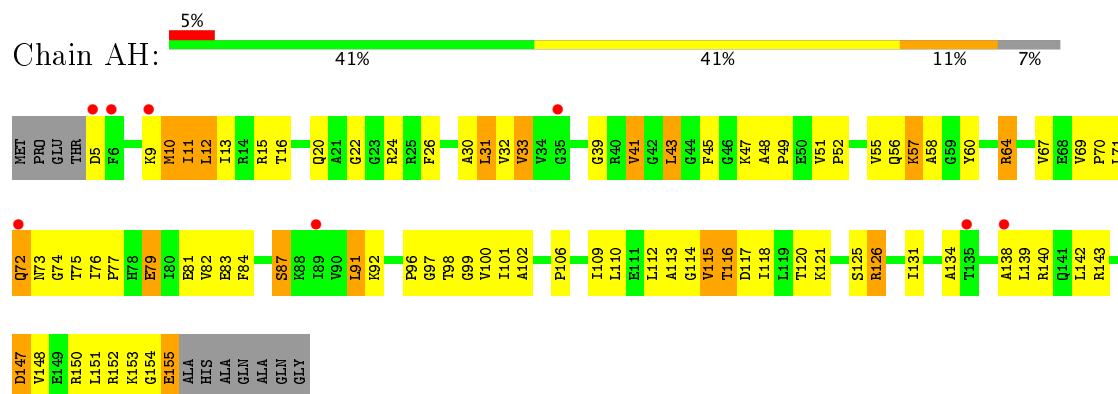


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

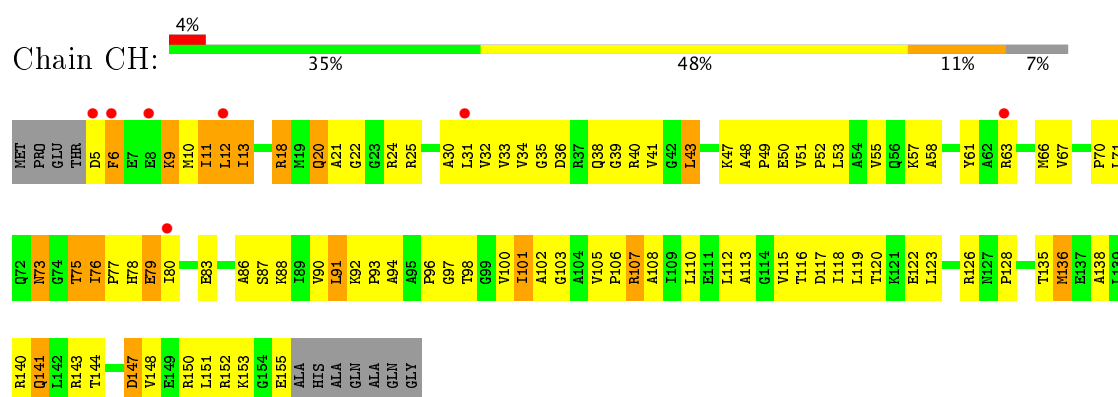




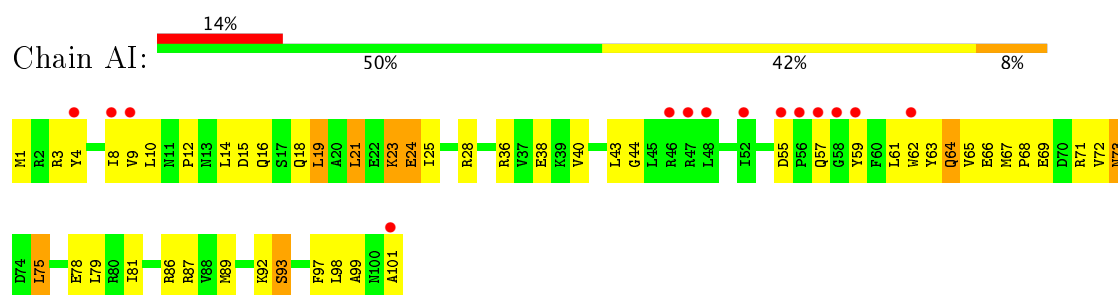
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



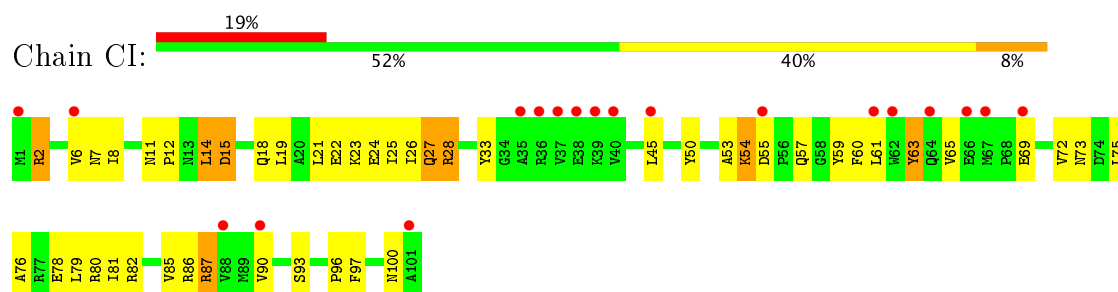
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



- Molecule 6: 30S RIBOSOMAL PROTEIN S6



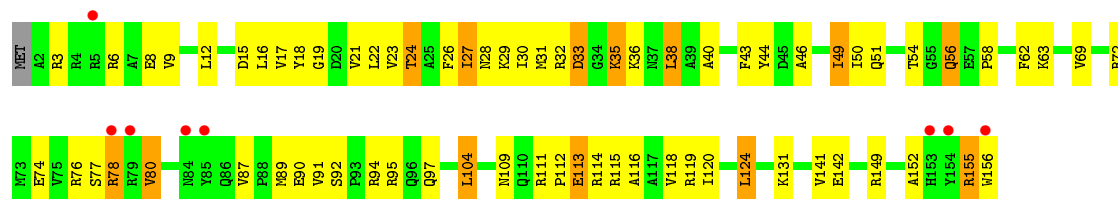
- Molecule 6: 30S RIBOSOMAL PROTEIN S6



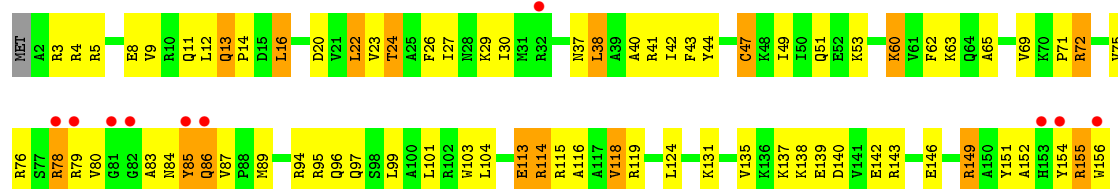
- Molecule 7: 30S RIBOSOMAL PROTEIN S7



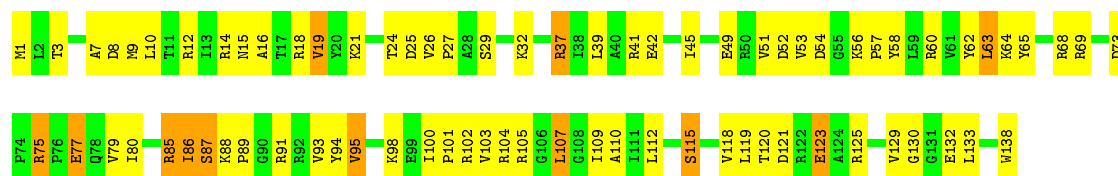




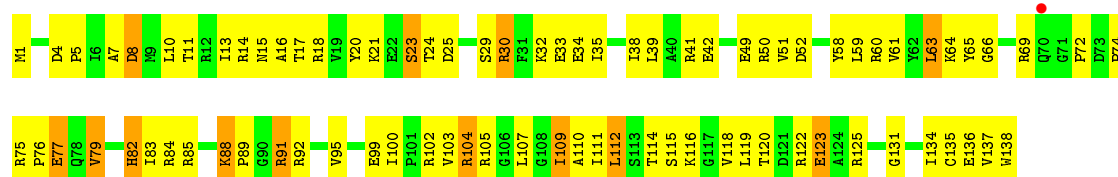
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



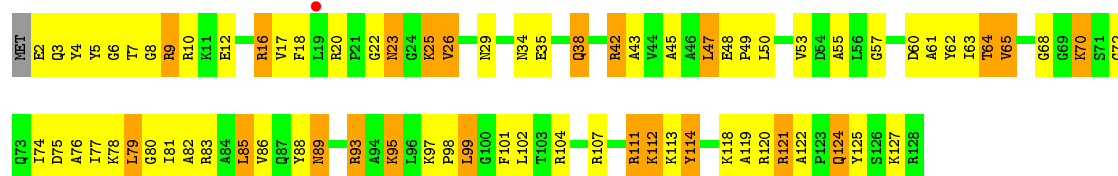
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 8: 30S RIBOSOMAL PROTEIN S8



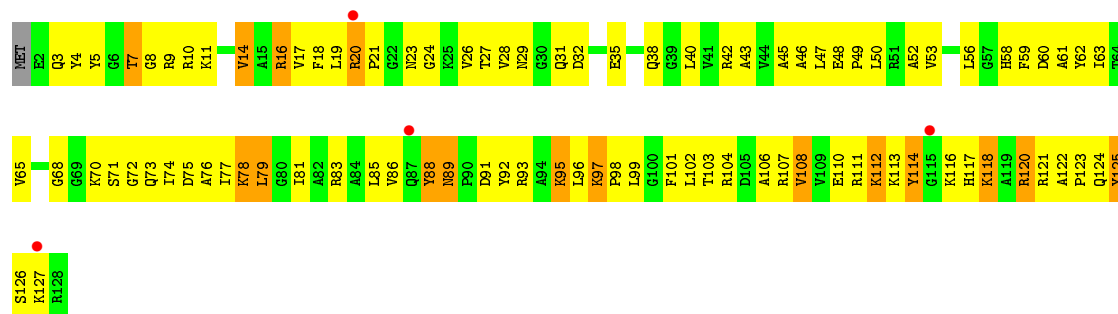
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



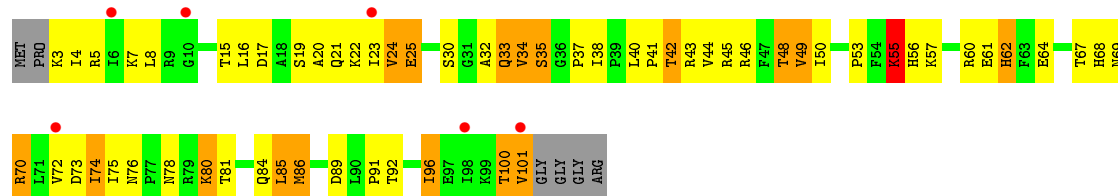
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



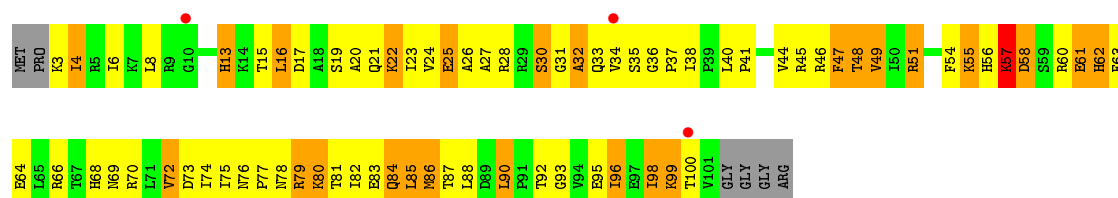




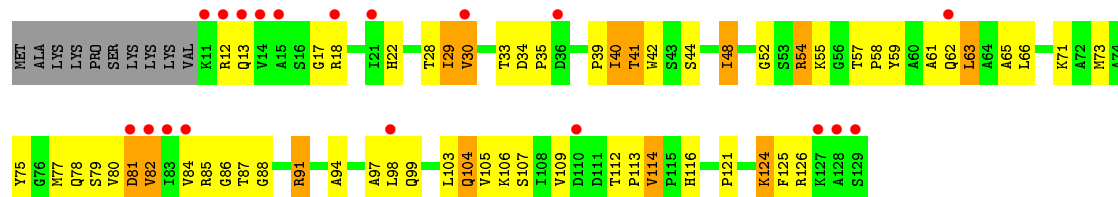
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



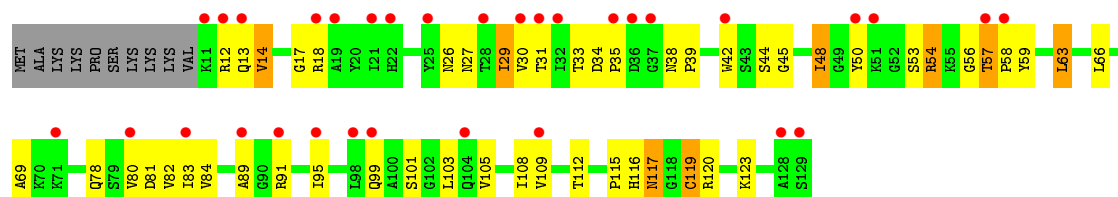
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

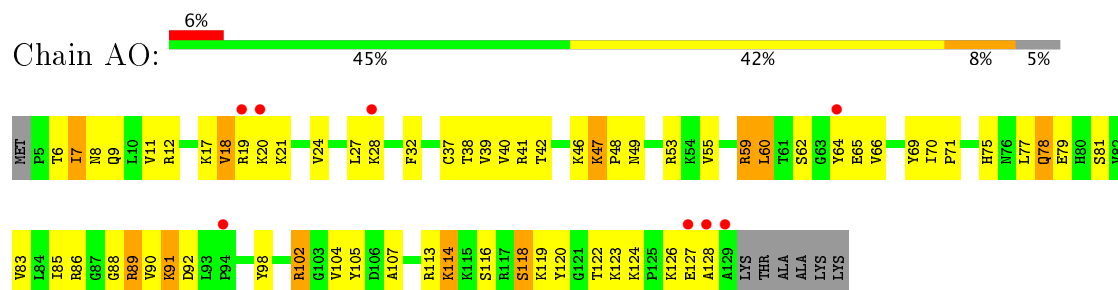


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

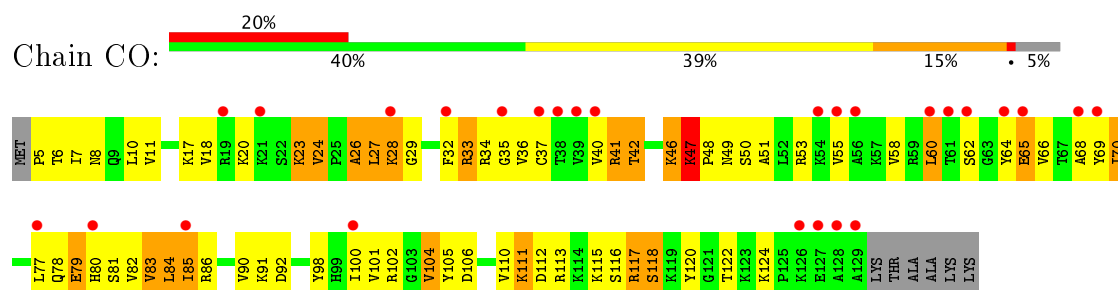




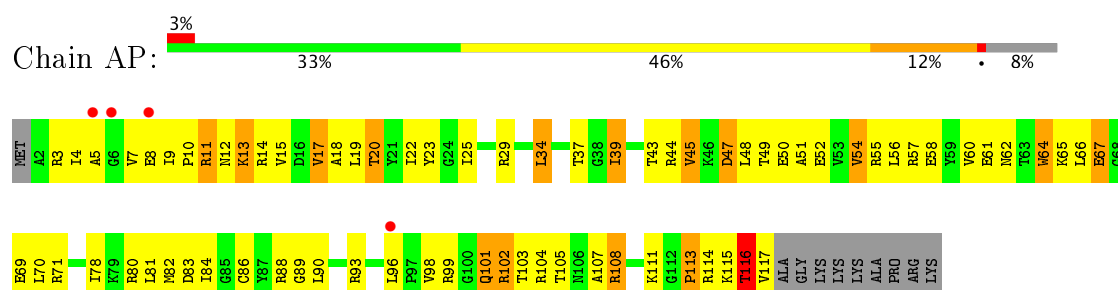
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



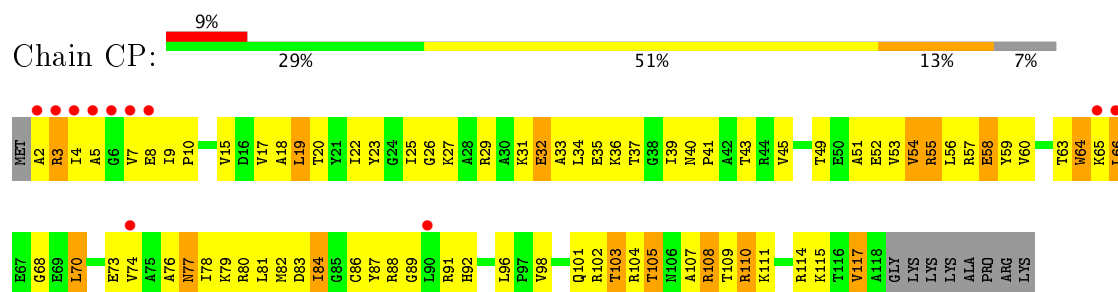
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



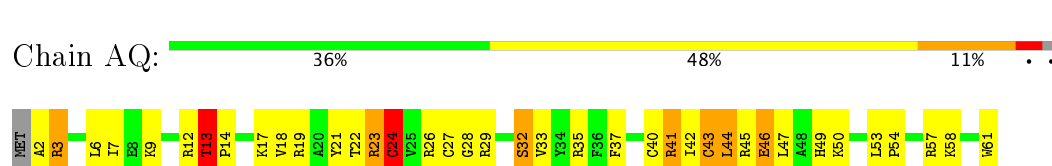
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

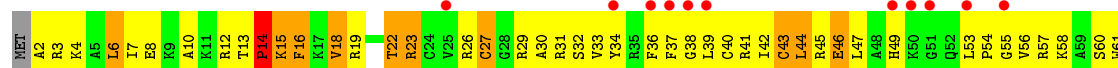


- Molecule 14: 30S RIBOSOMAL PROTEIN S14

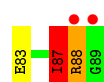
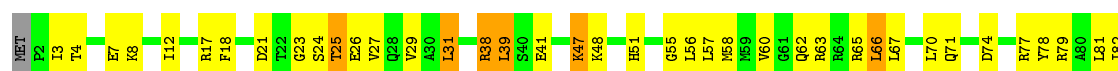


- Molecule 14: 30S RIBOSOMAL PROTEIN S14





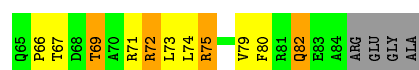
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



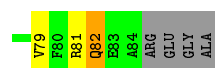
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



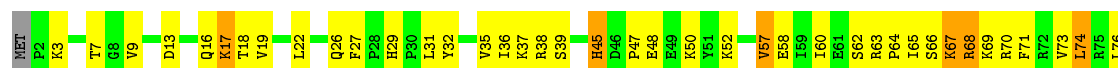
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



- Molecule 16: 30S RIBOSOMAL PROTEIN S16



- Molecule 17: 30S RIBOSOMAL PROTEIN S17

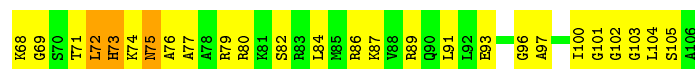








• Molecule 20: 30S RIBOSOMAL PROTEIN S20



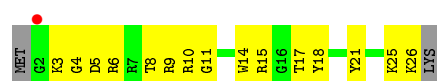
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



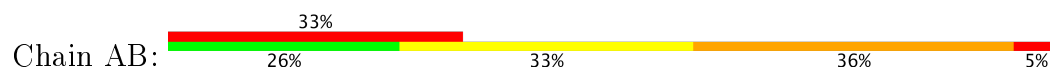
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 21: 30S RIBOSOMAL PROTEIN THX



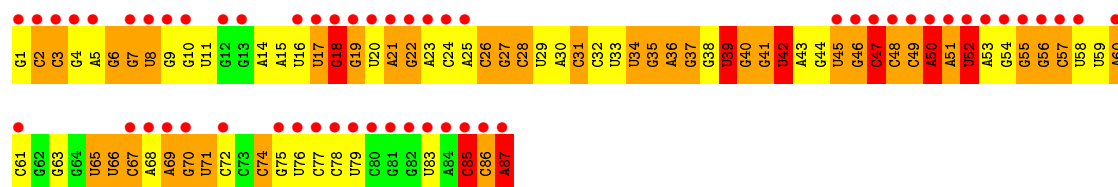
- Molecule 22: tRNA-LEU



- Molecule 22: tRNA-LEU

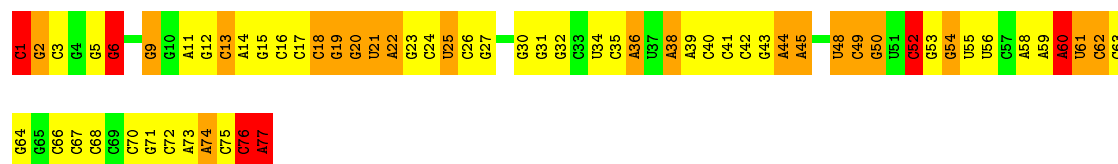






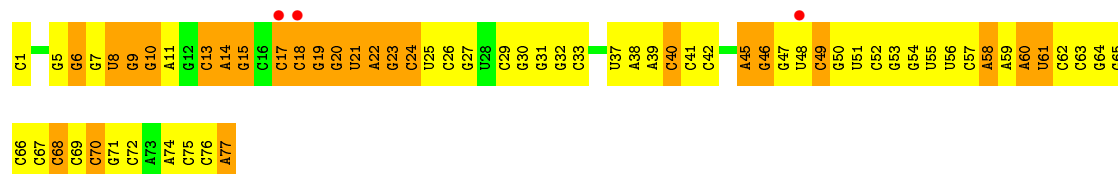
● Molecule 23: TRNA-FMET

Chain AC: 18% 48% 26% 8%



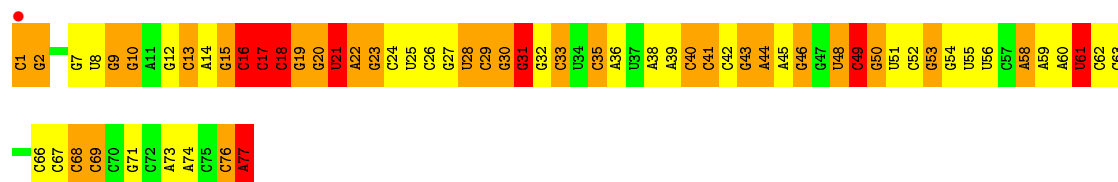
● Molecule 23: TRNA-FMET

Chain AD: 4% 16% 52% 32%



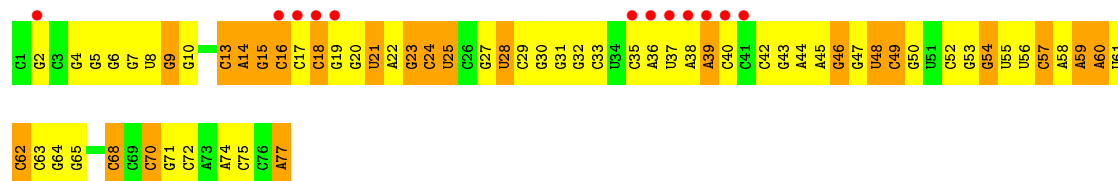
● Molecule 23: TRNA-FMET

Chain CC: 18% 36% 35% 10%



● Molecule 23: TRNA-FMET

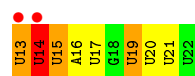
Chain CD: 16% 17% 53% 30%



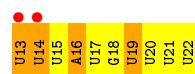
● Molecule 24: MRNA

Chain A1: 20% 20% 40% 30% 10%

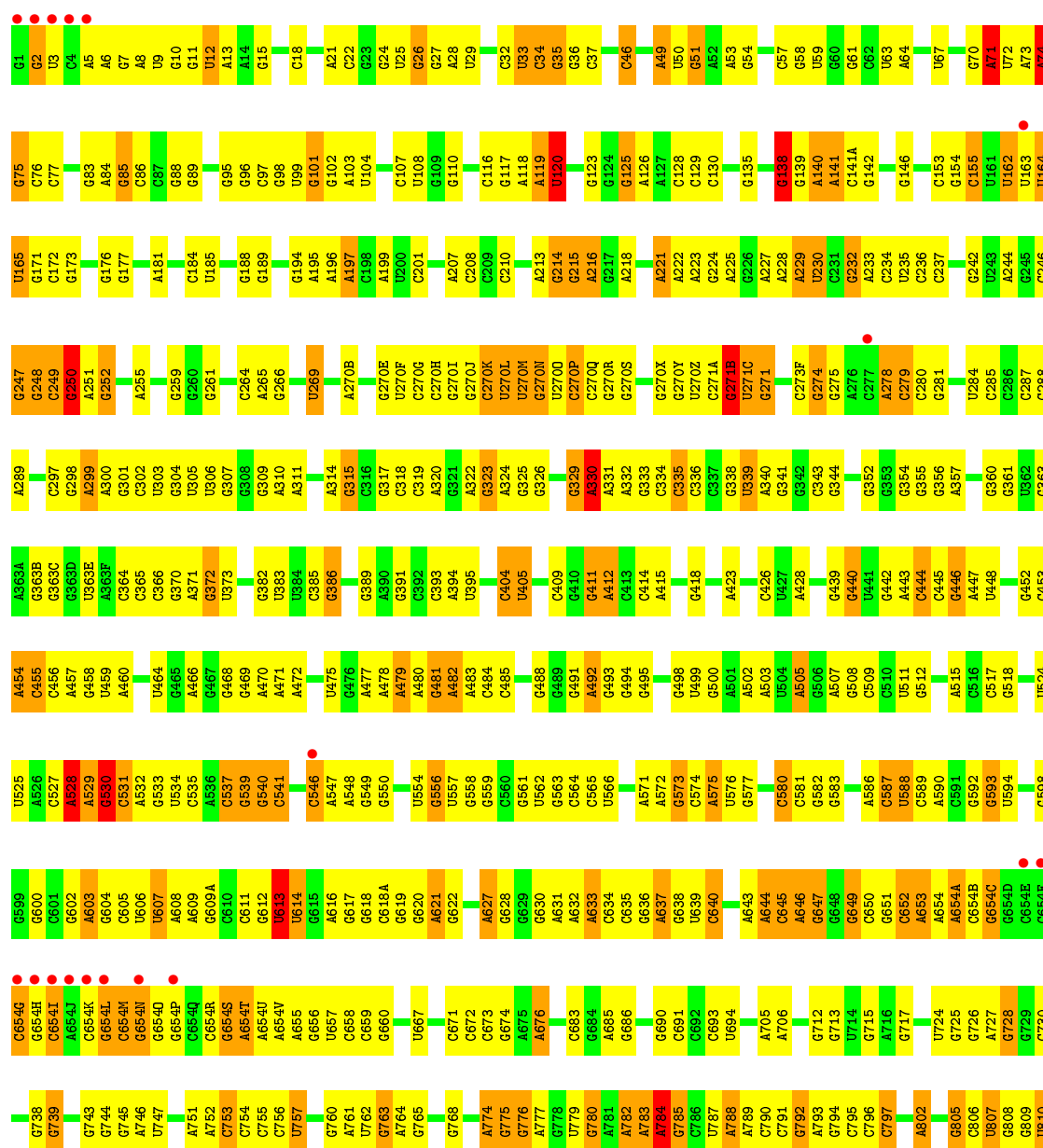




• Molecule 24: MRNA



• Molecule 25: RNA (2912-MER)











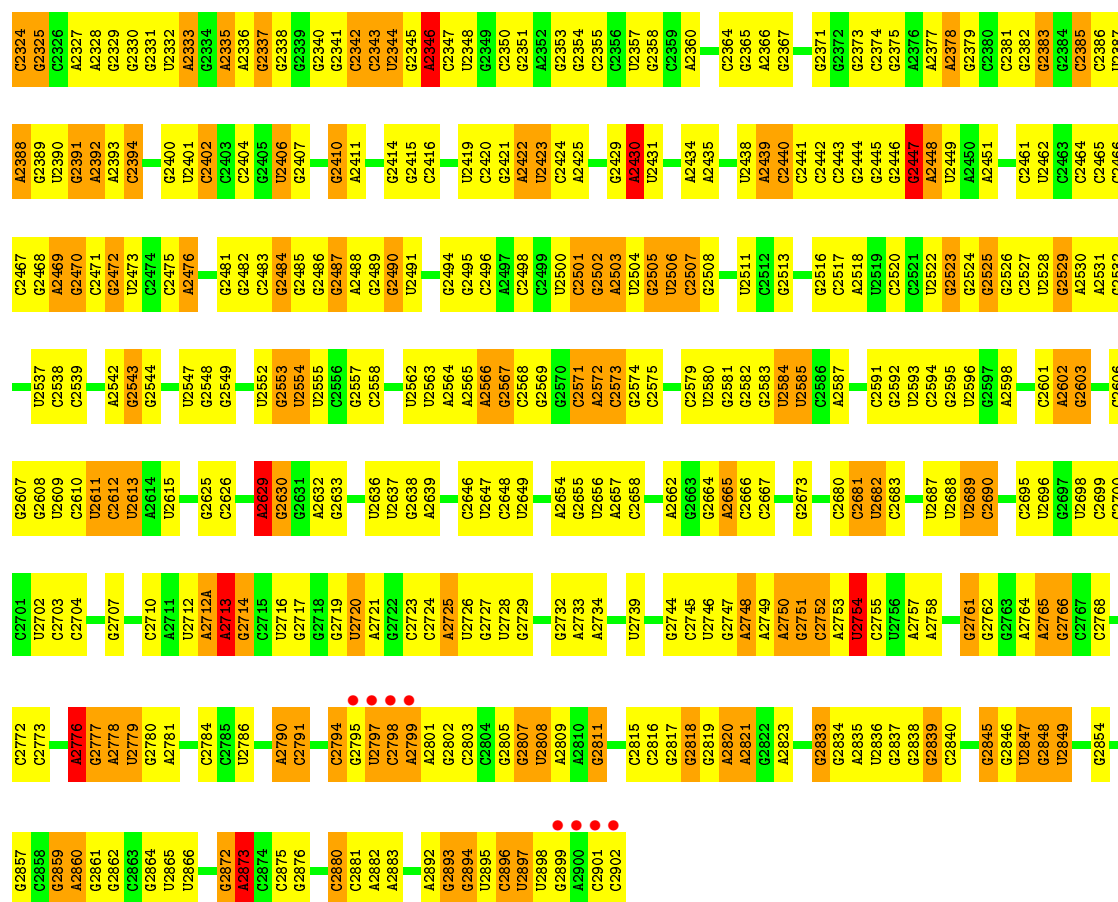




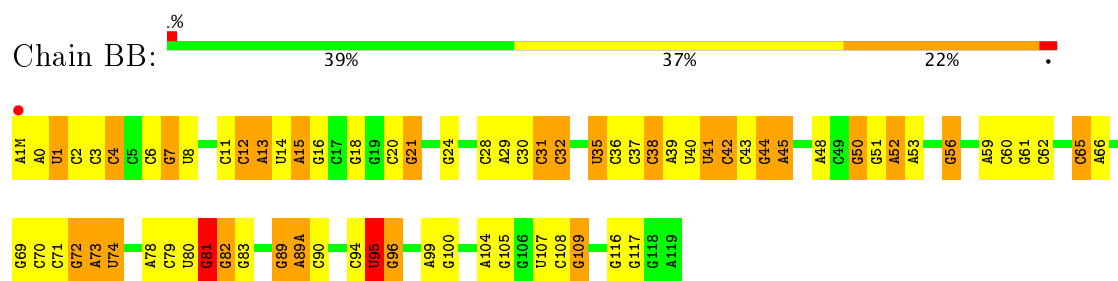


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C2261	G2181	G2120	U2041	U1955	A1884	G1801	G1704	G1623	A1545A	C1476	U1405	U1325	U1249	A1174
C2262	G2182	G2121	A2042	U1956	G1888	A1802	G1705	G1624	C1546	G1477	U1406	U1326	U1250	U1175
C2263	C2122	U2122	C2043	U1957	G1889	U1805	U1706	C1625	C1547	G1478	C1407	G1327	G1251	G1176
C2264	C2185	G2123	G2048	C1957	A1889	U1806	U1716	U1629	C1548	G1479	C1408	G1329	A1253	A1177
A2267	G2187	G2124	G2049	C1958	A1890	G1807	G1717	G1630	A1553	U1482	G1412	G1330	A1254	G1178
A2268	C2188	A2125			G1896	U1808	G1718		A1554	U1483	G1413	A1331	U1255	C1179
A2269	G2189	G2126	G2052	U1963	G1897	G1809	G1719	G1633	C1557	G1484		G1332	U1257	G1180
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G2272	G2192	U2130	C2055	C1967	A1900	A1812	G1728	U1638	G1559	G1487	G1418	G1338	G1265	A1189
G2273	G2193	U2131	G2056	G1968	A1901		A1729	U1639	G1560	G1488	U1420	U1340	U1266	G1190
A2274	U2132	U2132	A2057	A1969	C1902	G1816	U1730	U1640	A1566	U1489	G1421	U1342	G1267	G1191
C2275	G2133	G2133	A2058	U1970	G1903	G1817	G1731	C1640	A1567	U1490	G1422	A1342	U1268	
C2276	U2137	A2134	A2059	A1971		U1818			A1568	G1491			U1269	
C2277	A2198	A2135	A2060	A1972	G1906	A1819	G1741	C1648	A1569	G1492	G1423	G1345	U1270	G1198
C2280	A2199	C2136	G2061	G1973	G1907	A1820	C1742		A1570	C1493	G1424	G1346	G1271	U1199
C2281	C2205	C2137	A2062	C1974	C1908	A1821	G1743	G1651	A1571	A1494	G1425	G1347	G1272	
C2282		C2138	C2063	A1977	C1909	G1826	G1750	G1652		A1495	G1426	G1348	G1273	U1200
C2283	G2208	C2139	C2064			G1827	C1751	G1653	C1575		G1428	A1349	A1272	G1201
C2284	C2209	G2140	C2065	A1978	C1913	G1828		A1655	U1576	C1499	G1429	A1350	A1273	C1202
C2285	G2210	G2141	C2066	C1979	C1914	A1829	G1756	G1656	C1577	G1500	U1430	G1351	G1274	G1203
A2286	G2211	C2142	G2067	G1980	U1915	G1830	U1757	C1657	U1578	C1501	U1431	U1352	A1275	A1204
A2287	G2212	C2143	U2068	A1981	A1916	G1831	G1758	C1658	A1579	C1502	C1432		A1276	U1205
A2288	U2213	U2144	G2069	G1989	U1917	G1832	A1759	U1659	A1580	U1503	U1433	G1356	G1277	
C2289	G2215	C2145	G2070	C1990	A1918	G1833		C1660	G1581	C1504	U1434	G1357	A1278	A1210
C2290	G2216	G2146	A2071	C1991	C1919	A1834	G1770	C1661	G1582	C1505	G1435	G1358	G1279	U1211
G2291	G2219	G2147	U2074	G1992	G1921	A1835	A1762	A1665	A1583	C1506	G1436	A1359	G1283	G1212
G2292	G2224	G2148	U2075	C1993	C1920	G1836	G1764	G1666	C1585	A1507	U1437	A1360	A1284	A1213
C2293	A2225	U2149	U2076	U1994	G1922	A1837		G1667	A1586	A1508	U1438		G1285	A1214
C2296	G2226	G2151		C1999	C1924	G1838	C1767	G1668	A1587	C1509	U1439	A1365	A1286	G1216
C2297	G2227	C2152	A2082	C1999	C1925	G1839	U1768	A1668	C1588	A1510		G1368	G1217	
A2298	G2228	G2153	G2087	G2010	U1926		G1769	A1669	C1589		G1443	U1288	U1287	G1218
G2299	U2232	G2154		U2011	A1928		G1771	U1671	G1593		G1444	G1371	G1219	G1219
G2300	U2233	G2155	U2082	G2012	G1929		G1772	G1672	G1594		C1445	U1372	U1292	A1220
	G2234	G2156	G2093	A2013	G1930		A1773	U1673	G1595			A1378	C1293	C1221
G2303		A2158	C2083	A2014	U1931	A1853	C1774	G1674	A1596			A1379	C1298	G1222
G2304	G2238	G2159	C2087	A2015	A1932	A1854	U1775	C1675	A1597	G1449A	A1449	U1379	G1299	G1223
A2305	G2239	G2160	U2098	U2016	G1933	G1855	G1776	A1676	C1598	C1450	C1450	A1384	U1300	G1224
G2306	C2240	C2161	U2099	U2017	G1934	G1856	U1777	A1677	C1599	C1451	C1451	G1385	A1301	G1225
G2307	A2241	G2162	G2100	G2018	G1935	G1857	U1778	G1678	C1600	A1528		C1386	G1226	
G2308	G2242	C2163			A1936	G1858	U1779		G1601	A1529		C1387		
A2309		C2164	C2103	G2023	A1937	A1859	A1780	C1686	U1602	G1530	U1454	G1388	C1304	G1229
A2310	U2245	G2165	C2104	G2024	A1938	G1860	G1781	C1687	G1606	C1532		G1389	G1309	G1229A
A2311	G2246	G2166	C2105	C2025	U1939	G1861	C1782	U1688	C1607	C1533	G1459	U1390	G1310	G1235
C2312	A2247	U2167	G2106	C2026	U1940	G1862	A1783	A1689	C1608	G1534		U1391	G1311	G1236
C2313	G2248	A2168	C2107	G2027	C1941	G1863	A1784		A1609	U1535		A1392	U1312	A1237
C2314	U2249	A2169	C2108		C1942	U1864	A1785	U1683	A1610	A1536	C1464	A1393	U1313	G1238
G2315	A2170	A2170		A2030	U1943	G1869	G1786	G1694	C1611	C1537	G1465	U1394	U1314	G1239
A2316	C2311	C2171	C2111	A2031	U1944	A1870		G1695	C1612	G1538	G1466	U1396	U1315	U1240
C2317	G2252	U2172	G2032	G1945	A1871	A1872	A1791	G1696	C1613	G1539	C1467	U1397		A1241
G2318	C2318	A2173	U2113	A2033	U1946	G1878		G1697	A1614	G1540				
G2319	G2253	C2174	A2114	C1947	C1947	G1879	U1794	A1698	G1615	U1541				
G2320	C2255	C2175	G2115	G2036	G1948	C1879	C1795	G1699	A1616	G1542	A1471	A1321	G1244	G1244
C2321	A2176	A2176	A2116	G2037	G1949	C1880	U1796	A1700	A1543	G1473	A1472	A1322	U1245	A1246
C2322	C2258	C2177	A2117	G2038	G1950	C1881	C1797	A1701	C1544			G1401	U1323	A1247
C2323	G2259		U2118	C2039	U1951	C1882		G1702				C1403	G1324	

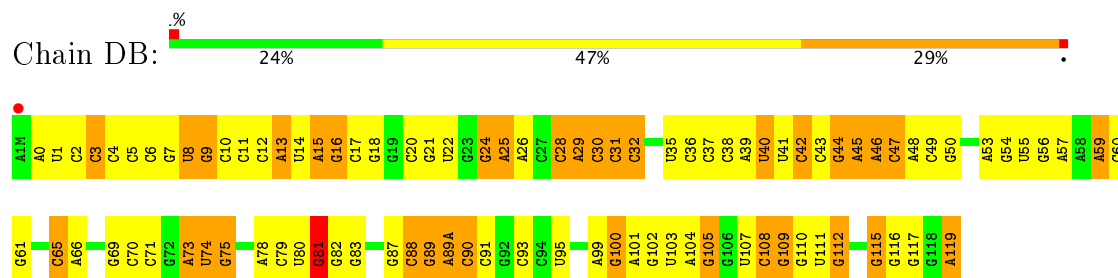




• Molecule 26: 5S RIBOSOMAL RNA



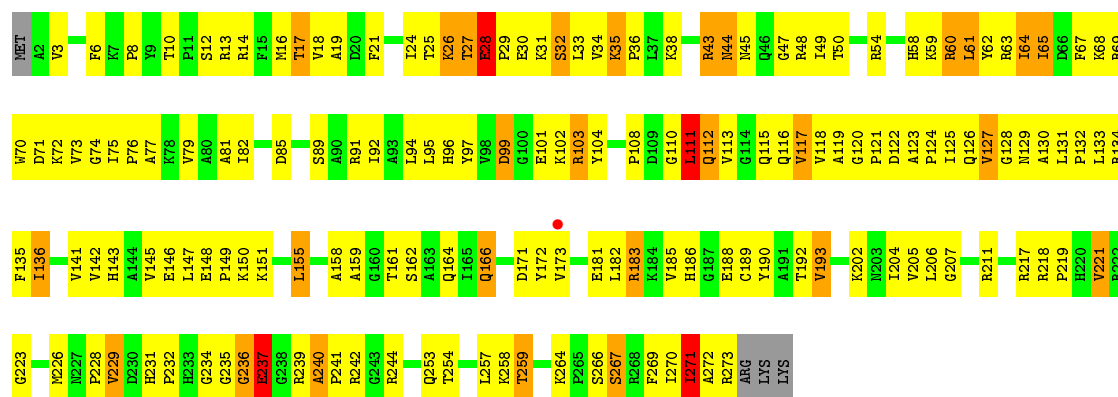
• Molecule 26: 5S RIBOSOMAL RNA



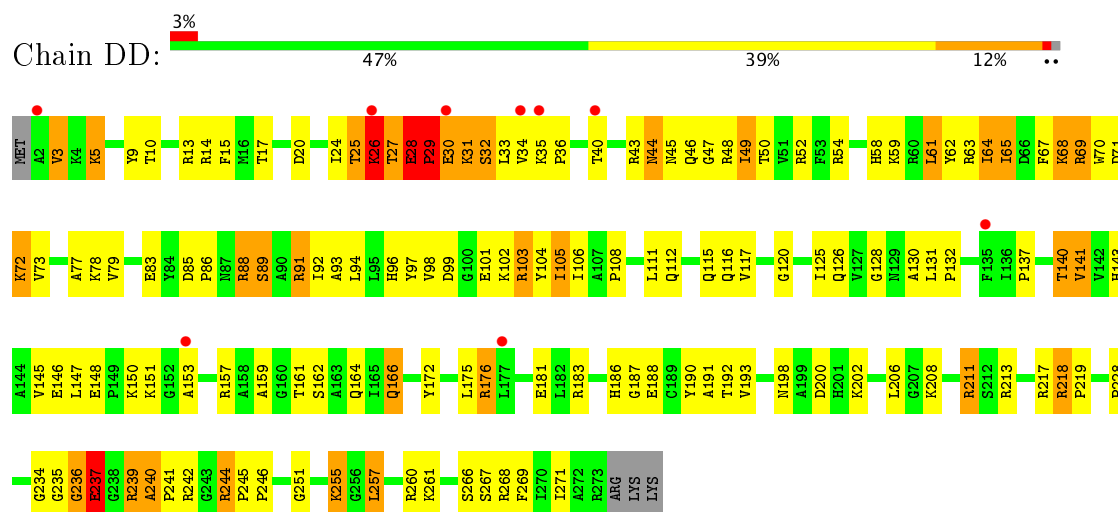
• Molecule 27: 50S ribosomal protein L2



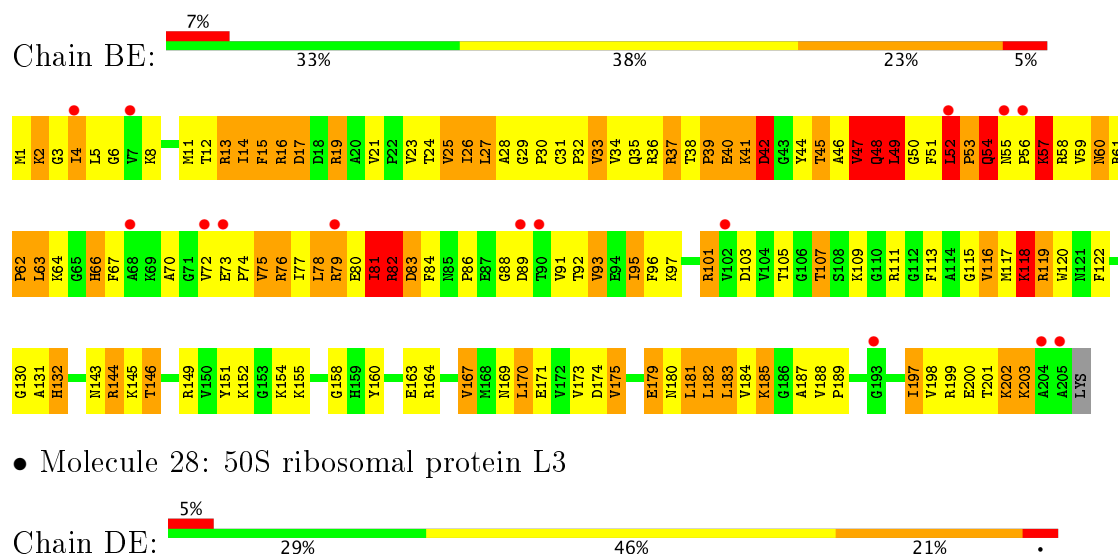




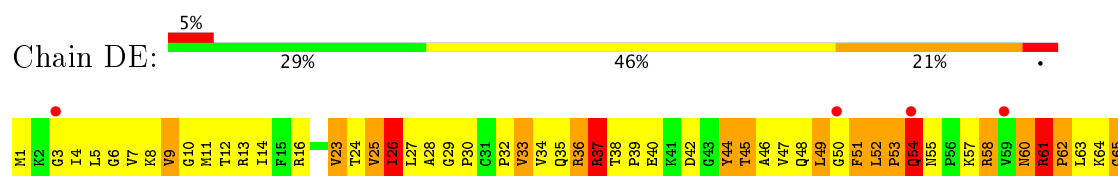
• Molecule 27: 50S ribosomal protein L2



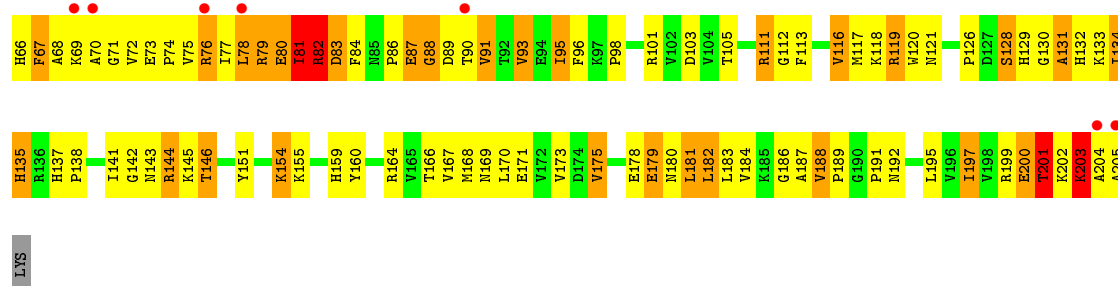
• Molecule 28: 50S ribosomal protein L3



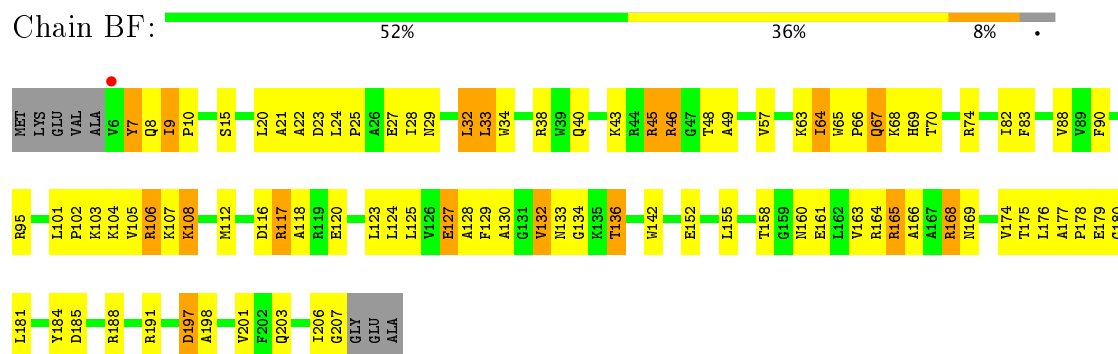
• Molecule 28: 50S ribosomal protein L3



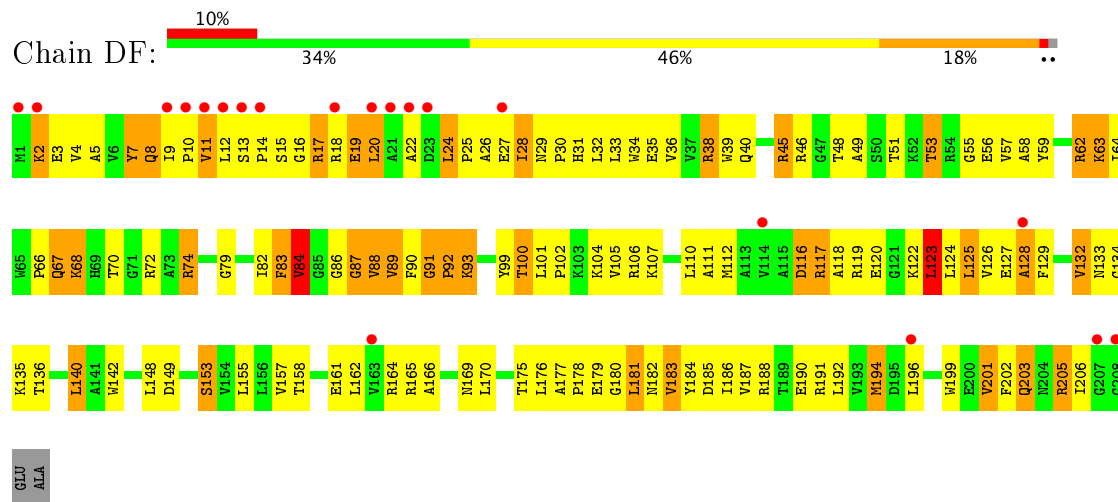




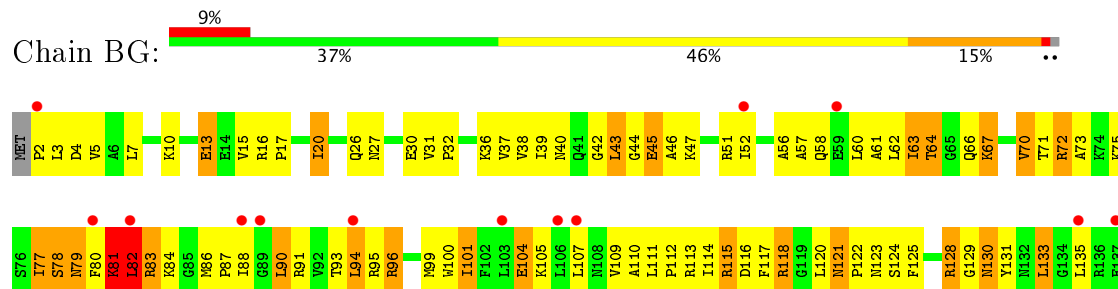
• Molecule 29: 50S ribosomal protein L4



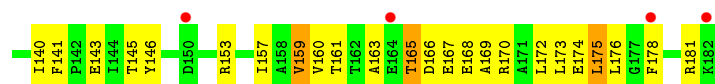
• Molecule 29: 50S ribosomal protein L4



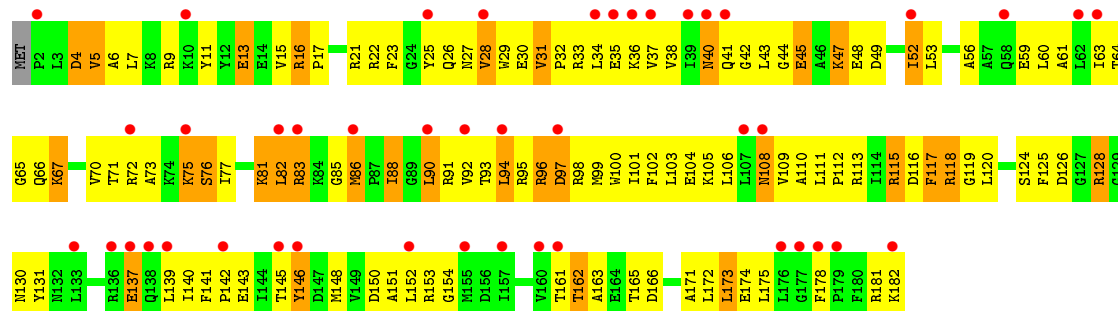
• Molecule 30: 50S ribosomal protein L5



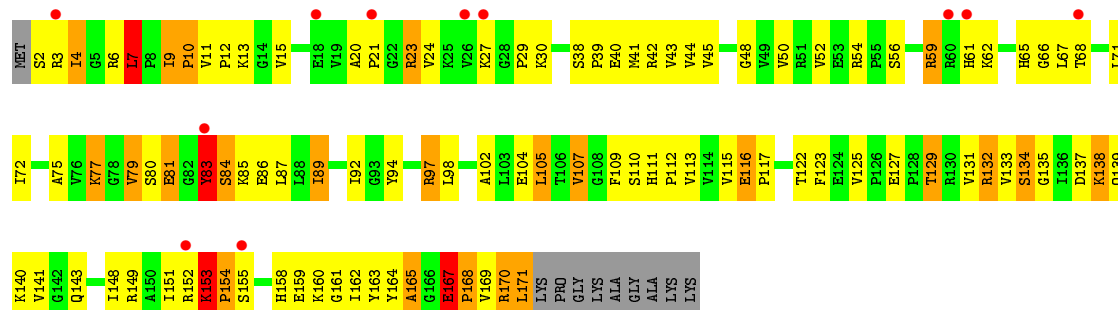




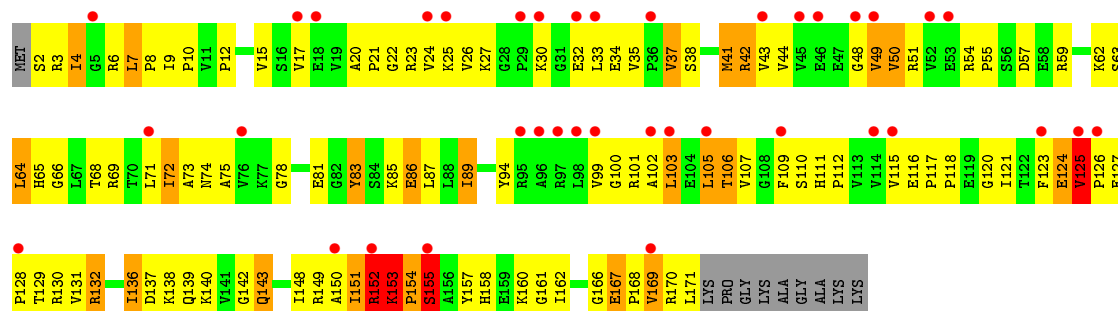
• Molecule 30: 50S ribosomal protein L5



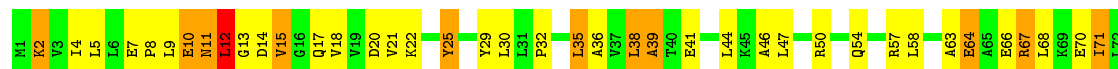
• Molecule 31: 50S ribosomal protein L6



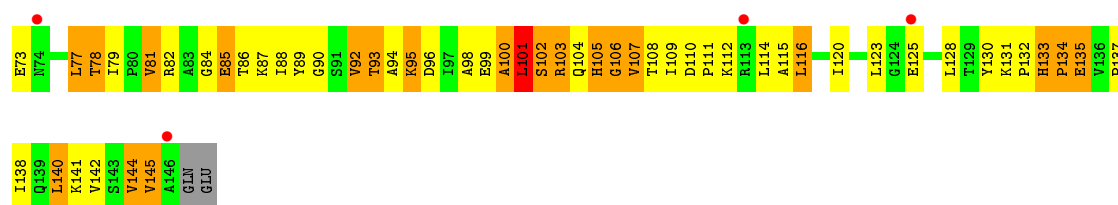
• Molecule 31: 50S ribosomal protein L6



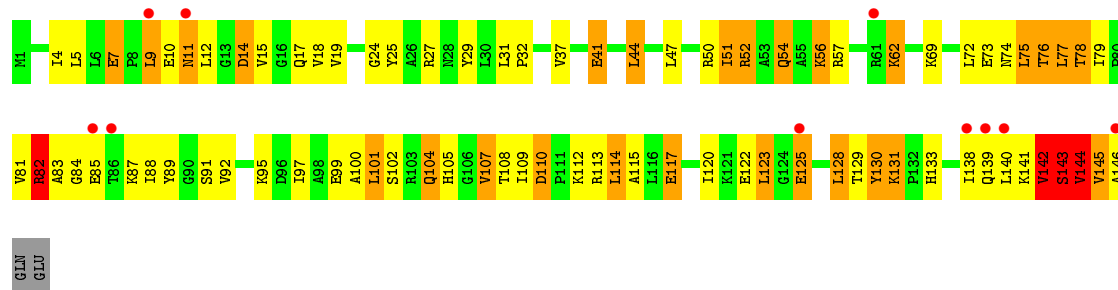
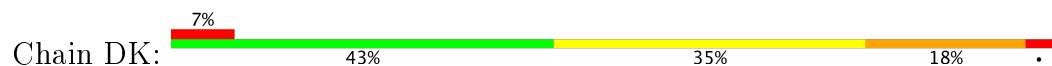
• Molecule 32: 50S ribosomal protein L9



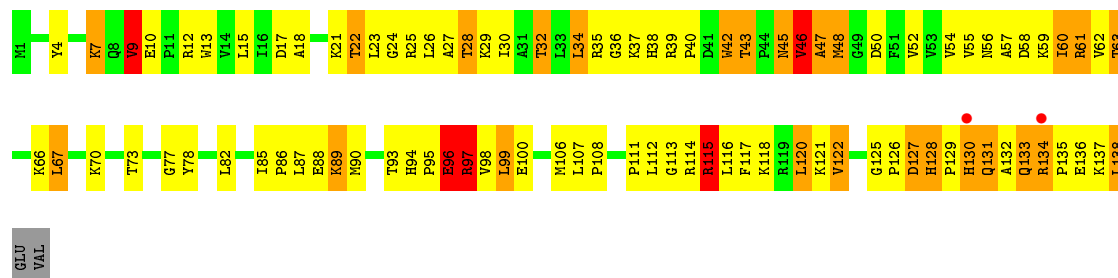




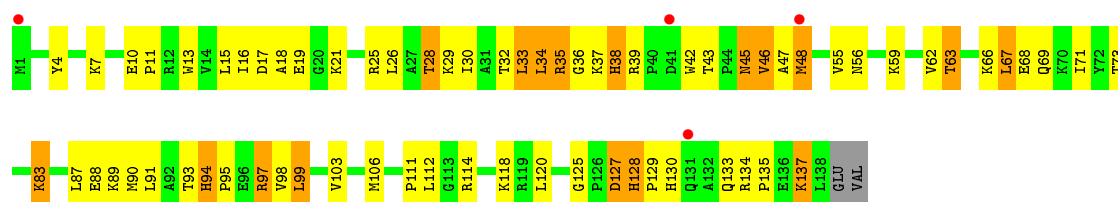
• Molecule 32: 50S ribosomal protein L9



• Molecule 33: 50S ribosomal protein L13



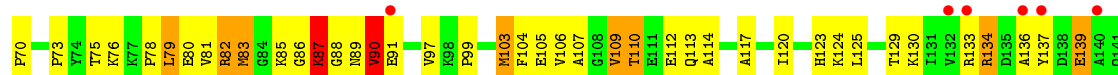
• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

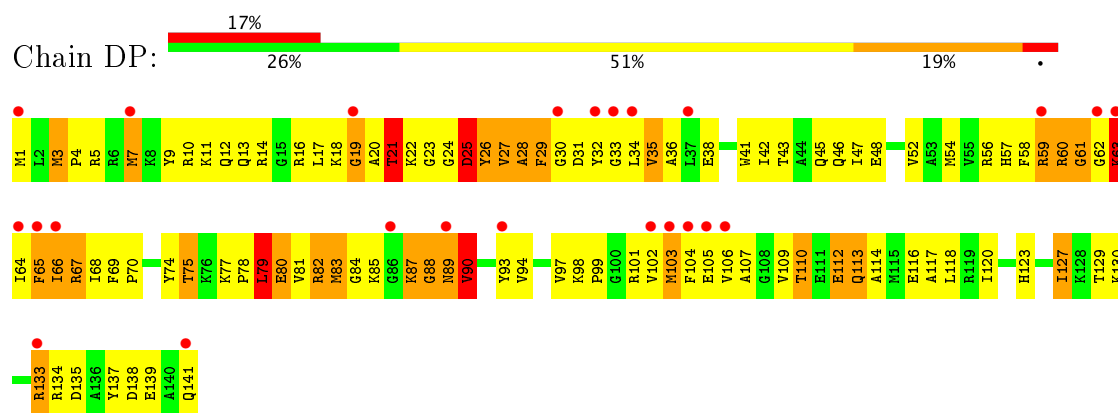




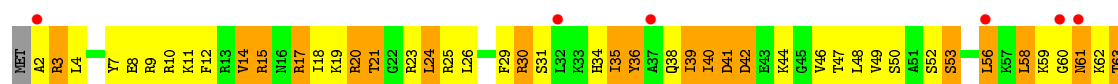




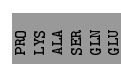
- Molecule 36: 50S ribosomal protein L16



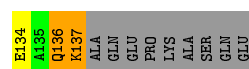
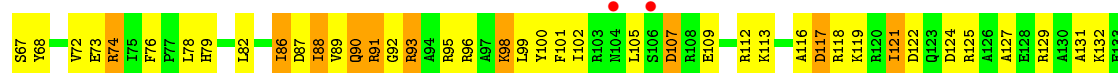




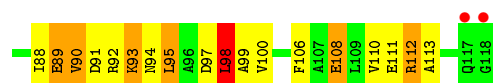
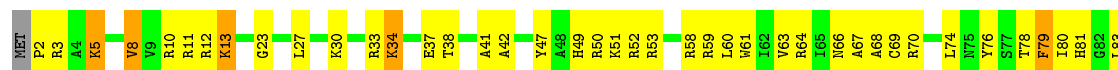
• Molecule 39: 50S ribosomal protein L19



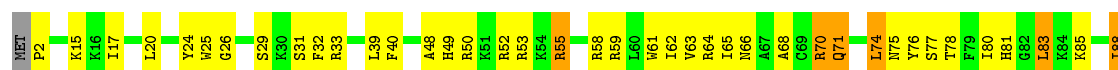
• Molecule 39: 50S ribosomal protein L19



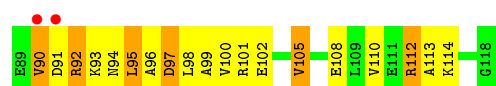
• Molecule 40: 50S ribosomal protein L20



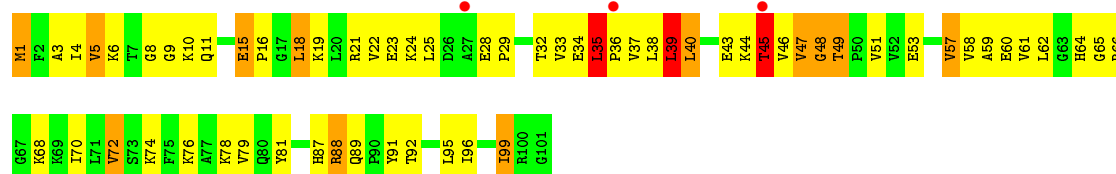
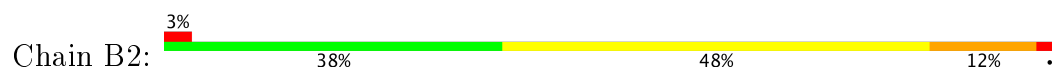
• Molecule 40: 50S ribosomal protein L20



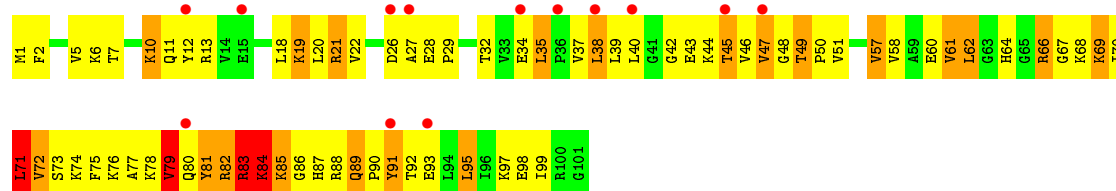




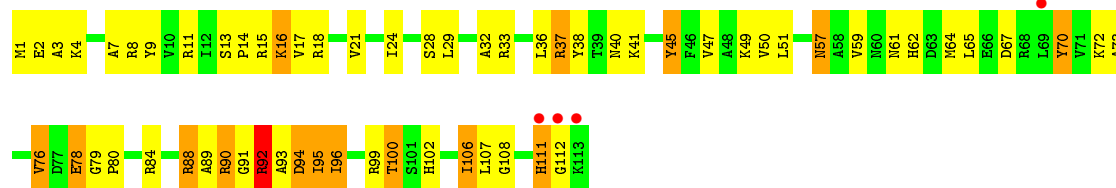
- Molecule 41: 50S ribosomal protein L21



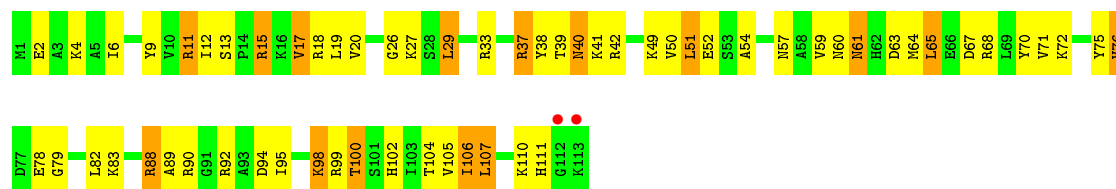
- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22



- Molecule 42: 50S ribosomal protein L22



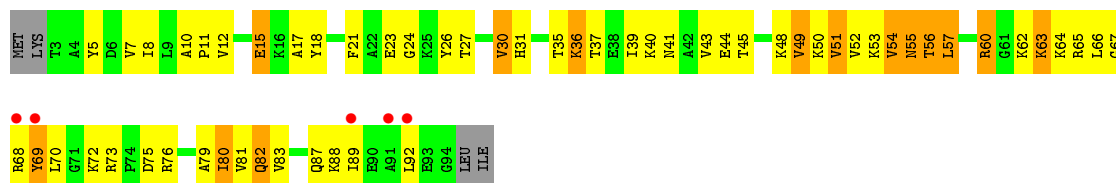
- Molecule 43: 50S ribosomal protein L23



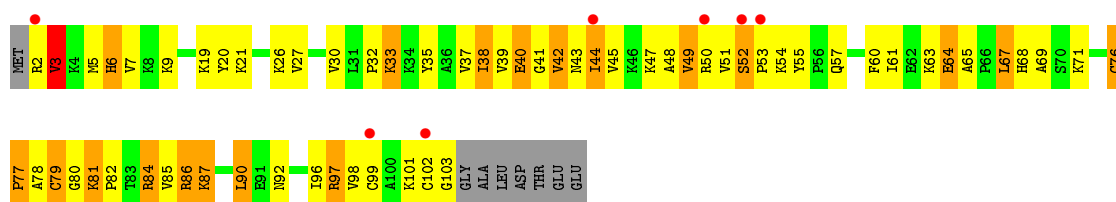




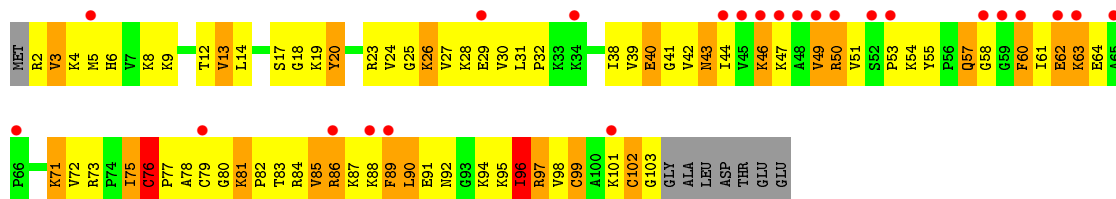
• Molecule 43: 50S ribosomal protein L23



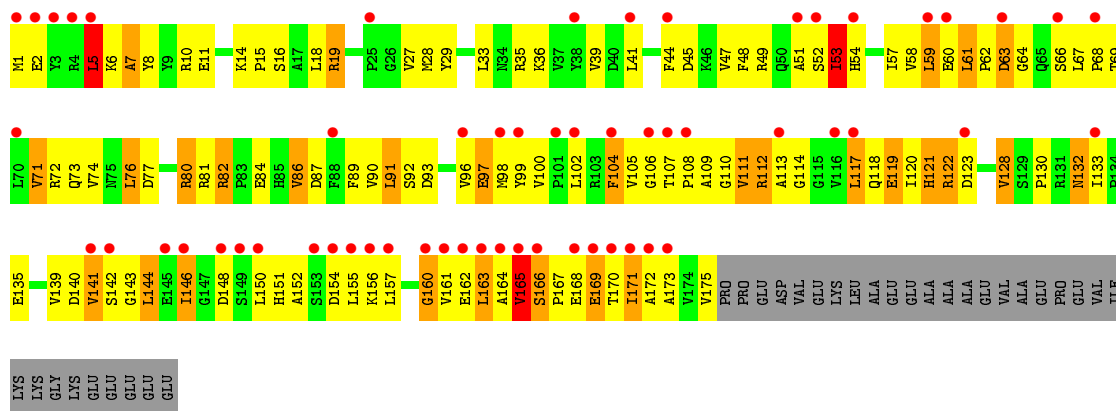
• Molecule 44: 50S ribosomal protein L24



• Molecule 44: 50S ribosomal protein L24

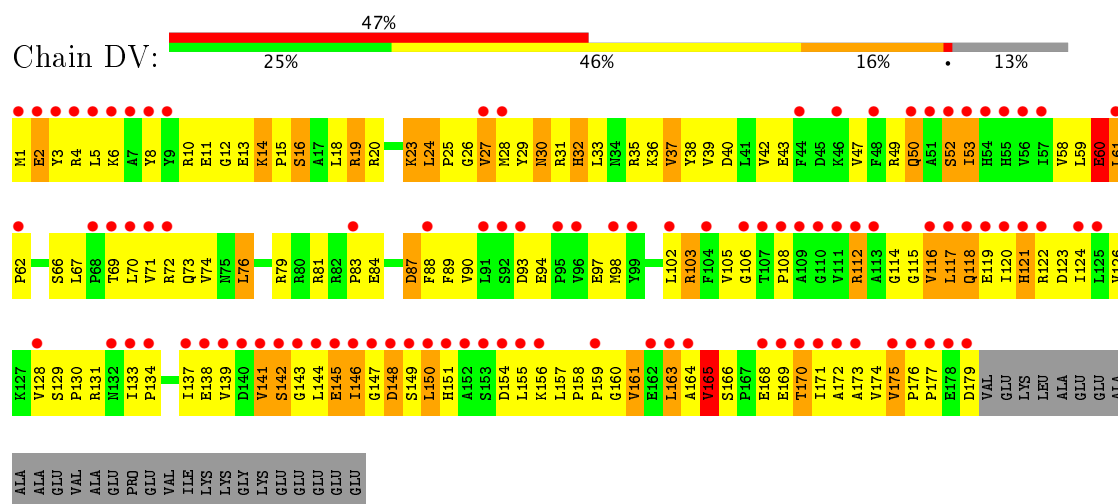


• Molecule 45: 50S ribosomal protein L25

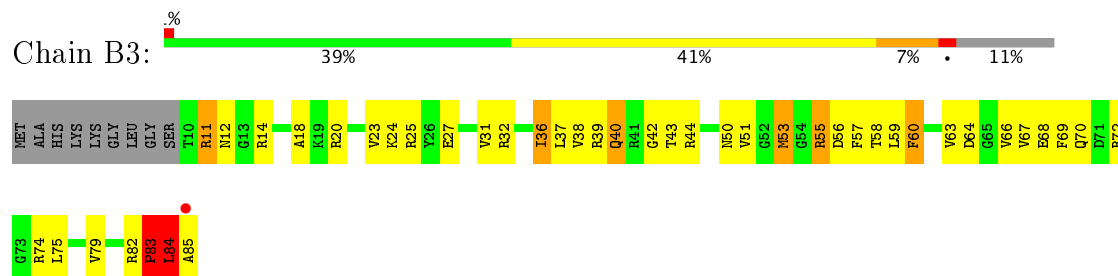




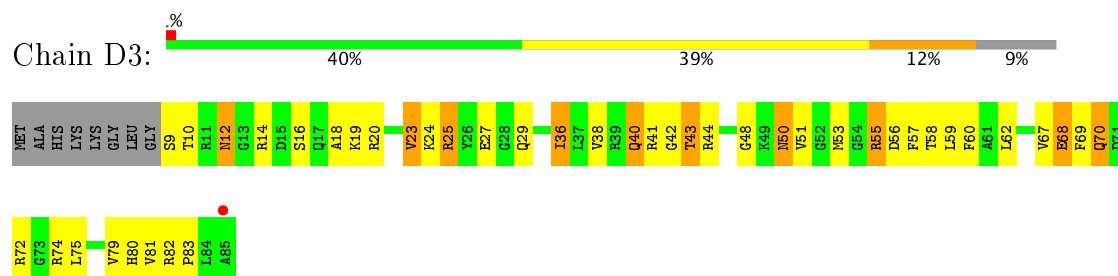
- Molecule 45: 50S ribosomal protein L25



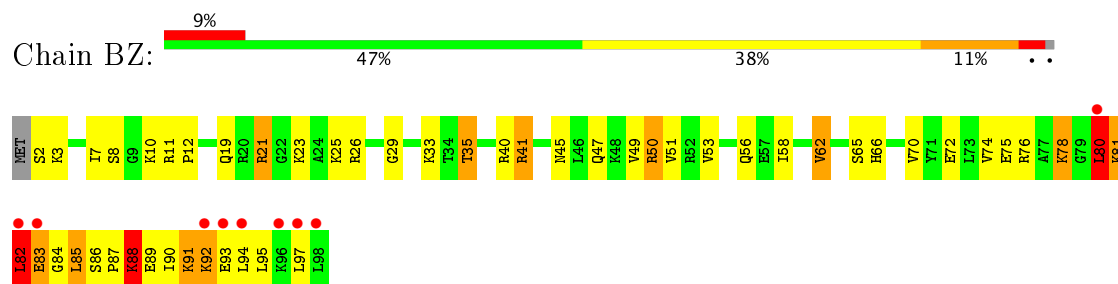
- Molecule 46: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L27



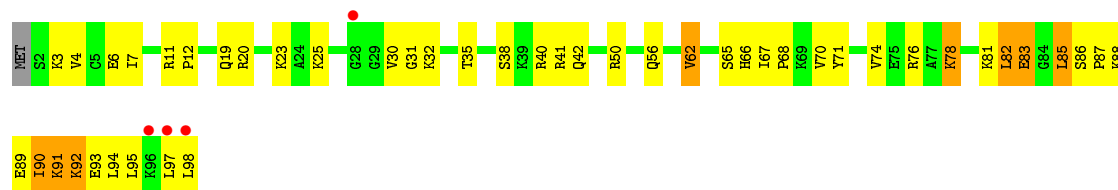
- Molecule 47: 50S ribosomal protein L28



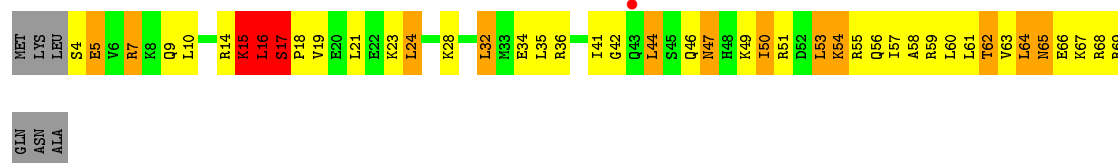
- Molecule 47: 50S ribosomal protein L28



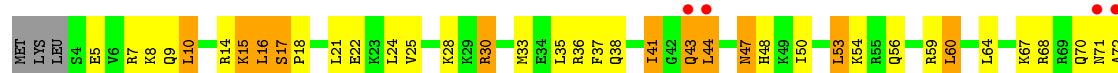
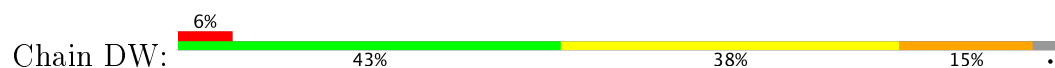




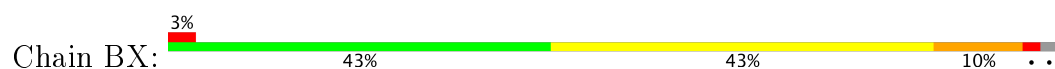
- Molecule 48: 50S ribosomal protein L29



- Molecule 48: 50S ribosomal protein L29



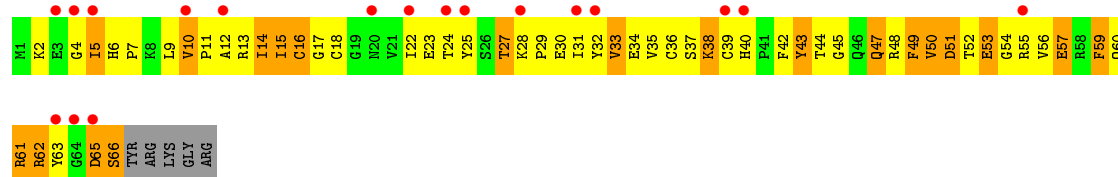
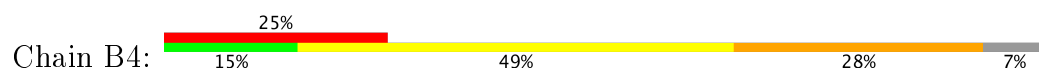
- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30

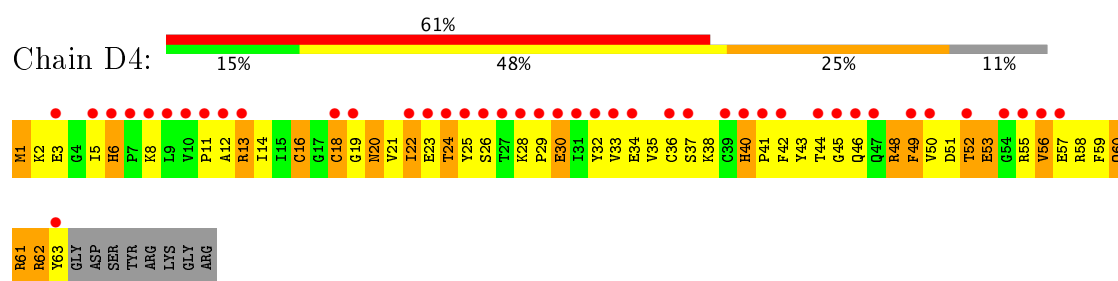


- Molecule 50: 50S ribosomal protein L31

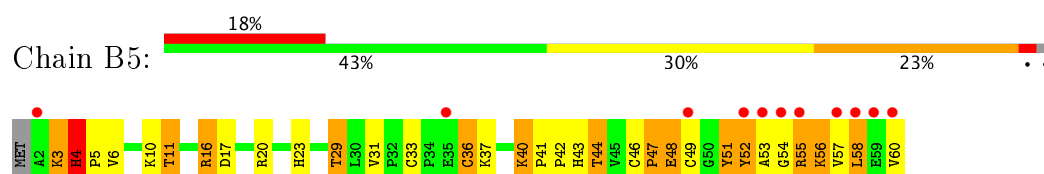


- Molecule 50: 50S ribosomal protein L31

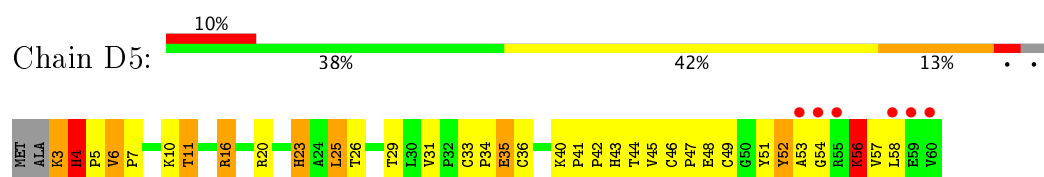




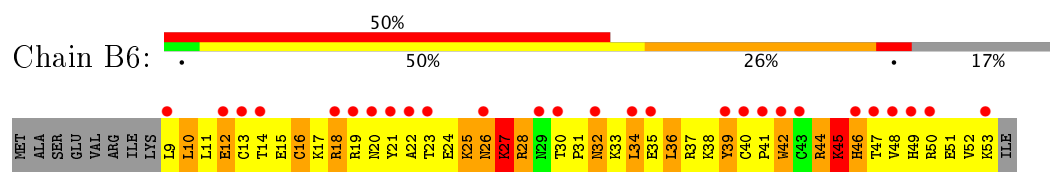
- Molecule 51: 50S ribosomal protein L32



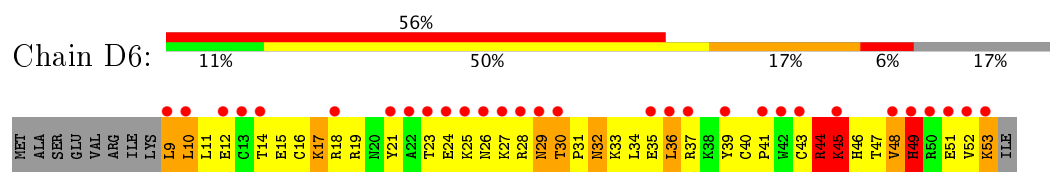
- Molecule 51: 50S ribosomal protein L32



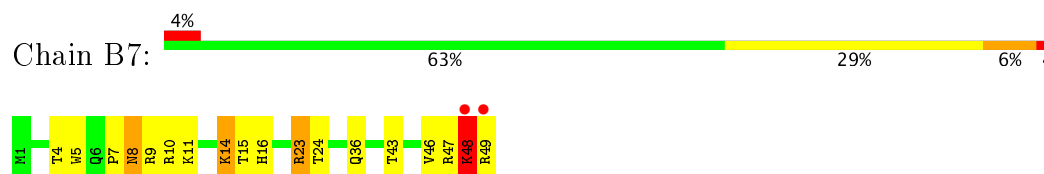
- Molecule 52: 50S ribosomal protein L33



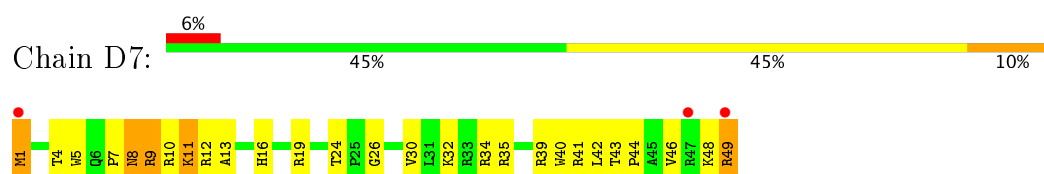
- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



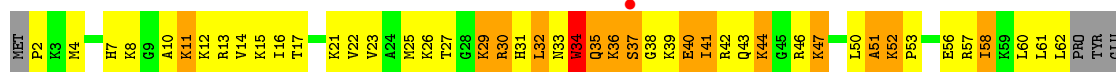
- Molecule 53: 50S ribosomal protein L34





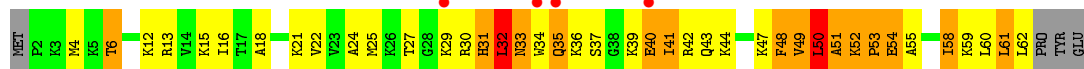
## • Molecule 54: 50S ribosomal protein L35

Chain B8:  2% 23% 48% 22% 6%



## • Molecule 54: 50S ribosomal protein L35

Chain D8:  6% 31% 38% 22% 6%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.00Å 450.05Å 621.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.53 – 3.00 153.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (153.53-3.00) 93.7 (153.53-3.00)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, $R_{free}$	0.211 , 0.272 0.208 , 0.251	Depositor DCC
$R_{free}$ test set	1857 reflections (0.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	299552	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	5/36234 (0.0%)	0.91	68/56554 (0.1%)
1	CA	0.42	1/36237 (0.0%)	0.90	79/56558 (0.1%)
2	AE	0.29	0/1959	0.56	0/2642
2	CE	0.28	0/1959	0.53	0/2642
3	AF	0.33	0/1629	0.53	0/2195
3	CF	0.31	0/1636	0.54	0/2205
4	AG	0.49	2/1733 (0.1%)	0.62	1/2318 (0.0%)
4	CG	0.38	0/1733	0.61	0/2318
5	AH	0.35	0/1171	0.58	0/1576
5	CH	0.34	0/1171	0.56	0/1576
6	AI	0.33	0/856	0.55	0/1154
6	CI	0.32	0/856	0.54	0/1154
7	AJ	0.29	0/1276	0.50	0/1709
7	CJ	0.28	0/1276	0.45	0/1709
8	AK	0.33	0/1136	0.60	0/1527
8	CK	0.27	0/1136	0.51	0/1527
9	AL	0.29	0/1029	0.52	0/1379
9	CL	0.29	0/1029	0.53	0/1379
10	AM	0.31	0/814	0.59	1/1095 (0.1%)
10	CM	0.28	0/814	0.54	0/1095
11	AN	0.33	0/900	0.57	0/1213
11	CN	0.31	0/900	0.56	0/1213
12	AO	0.40	0/991	0.68	1/1327 (0.1%)
12	CO	0.35	0/991	0.60	0/1327
13	AP	0.30	0/938	0.57	0/1258
13	CP	0.28	0/943	0.52	0/1265
14	AQ	0.42	0/501	0.66	1/664 (0.2%)
14	CQ	0.29	0/501	0.58	0/664
15	AR	0.35	0/745	0.58	0/992
15	CR	0.30	0/745	0.51	0/992
16	AS	0.29	0/721	0.53	0/970
16	CS	0.31	0/721	0.58	0/970



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.35	0/847	0.54	0/1131
17	CT	0.31	0/847	0.51	0/1131
18	AU	0.34	0/596	0.64	0/790
18	CU	0.35	0/596	0.59	0/790
19	AV	0.33	0/638	0.59	0/860
19	CV	0.31	0/638	0.65	0/860
20	AW	0.29	0/765	0.52	0/1007
20	CW	0.32	0/765	0.63	0/1007
21	AX	0.28	0/221	0.55	0/288
21	CX	0.28	0/221	0.49	0/288
22	AB	1.15	2/2080 (0.1%)	1.41	25/3242 (0.8%)
22	CB	1.34	6/2080 (0.3%)	1.41	36/3242 (1.1%)
23	AC	1.12	3/1835 (0.2%)	1.69	56/2859 (2.0%)
23	AD	0.57	0/1835	0.97	7/2859 (0.2%)
23	CC	1.08	1/1835 (0.1%)	1.52	44/2859 (1.5%)
23	CD	0.61	0/1835	0.98	5/2859 (0.2%)
24	A1	1.43	2/226 (0.9%)	1.60	7/348 (2.0%)
24	C1	1.57	1/226 (0.4%)	1.73	5/348 (1.4%)
25	BA	0.59	15/70233 (0.0%)	1.07	285/109643 (0.3%)
25	DA	0.52	13/70122 (0.0%)	1.00	265/109469 (0.2%)
26	BB	0.49	0/2928	0.97	9/4568 (0.2%)
26	DB	0.44	0/2928	0.96	7/4568 (0.2%)
27	BD	0.50	0/2165	0.80	2/2919 (0.1%)
27	DD	0.46	0/2165	0.72	0/2919
28	BE	0.38	0/1601	0.67	2/2160 (0.1%)
28	DE	0.38	0/1601	0.69	0/2160
29	BF	0.43	0/1620	0.67	0/2194
29	DF	0.36	0/1662	0.65	0/2249
30	BG	0.36	0/1499	0.60	0/2016
30	DG	0.29	0/1499	0.54	0/2016
31	BH	0.36	0/1332	0.67	1/1802 (0.1%)
31	DH	0.28	0/1332	0.55	0/1802
32	BK	0.34	0/1151	0.68	1/1558 (0.1%)
32	DK	0.33	0/1151	0.66	1/1558 (0.1%)
33	BM	0.42	0/1131	0.69	0/1525
33	DM	0.29	0/1131	0.59	0/1525
34	BN	0.40	0/943	0.64	0/1269
34	DN	0.36	0/943	0.60	0/1269
35	BO	0.39	0/1162	0.76	0/1544
35	DO	0.32	0/1162	0.65	1/1544 (0.1%)
36	BP	0.52	0/1143	0.80	0/1527
36	DP	0.32	0/1143	0.54	0/1527
37	B0	0.39	0/982	0.69	0/1312



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	D0	0.37	0/974	0.64	0/1302
38	BQ	0.42	0/892	0.70	1/1187 (0.1%)
38	DQ	0.30	0/892	0.62	1/1187 (0.1%)
39	BR	0.40	0/1155	0.66	0/1542
39	DR	0.37	0/1155	0.59	0/1542
40	B1	0.42	0/982	0.67	1/1306 (0.1%)
40	D1	0.34	0/982	0.57	0/1306
41	B2	0.42	0/790	0.74	2/1057 (0.2%)
41	D2	0.32	0/790	0.59	0/1057
42	BS	0.37	0/911	0.62	0/1220
42	DS	0.38	0/911	0.64	0/1220
43	BT	0.50	0/739	0.68	0/993
43	DT	0.47	0/739	0.62	0/993
44	BU	0.45	0/798	0.68	0/1064
44	DU	0.41	0/798	0.72	0/1064
45	BV	0.32	0/1427	0.63	0/1935
45	DV	0.28	0/1460	0.56	0/1982
46	B3	0.44	0/615	0.67	0/819
46	D3	0.39	0/621	0.61	0/827
47	BZ	0.42	0/770	0.73	1/1022 (0.1%)
47	DZ	0.39	0/770	0.70	0/1022
48	BW	0.53	0/560	0.72	0/741
48	DW	0.37	0/583	0.63	0/771
49	BX	0.36	0/474	0.64	1/635 (0.2%)
49	DX	0.32	0/474	0.53	0/635
50	B4	0.34	0/545	0.72	1/733 (0.1%)
50	D4	0.32	0/527	0.67	0/709
51	B5	0.43	0/473	0.69	0/639
51	D5	0.34	0/468	0.70	0/632
52	B6	0.43	0/396	0.70	0/529
52	D6	0.33	0/396	0.63	0/529
53	B7	0.46	0/438	0.68	0/575
53	D7	0.40	0/438	0.59	0/575
54	B8	0.52	0/494	0.71	0/649
54	D8	0.38	0/494	0.71	1/649 (0.2%)
All	All	0.51	51/324027 (0.0%)	0.93	919/485226 (0.2%)

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
2	AE	0	3
2	CE	0	5
3	CF	0	1
4	AG	0	1
8	AK	0	1
10	AM	0	1
12	AO	0	2
14	AQ	0	1
14	CQ	0	2
15	AR	0	1
19	CV	0	1
20	CW	0	1
27	BD	0	6
27	DD	0	3
28	BE	0	1
28	DE	0	6
29	DF	0	2
30	BG	0	1
30	DG	0	1
31	BH	0	2
31	DH	0	2
32	BK	0	3
32	DK	0	4
33	BM	0	1
35	BO	0	4
35	DO	0	3
36	BP	0	3
37	D0	0	2
38	BQ	0	1
38	DQ	0	2
39	BR	0	2
40	B1	0	1
40	D1	0	1
41	B2	0	1
43	BT	0	1
44	DU	0	2
45	BV	0	3
45	DV	0	2
46	B3	0	2
48	BW	0	2
48	DW	0	1
50	B4	0	4
50	D4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
51	B5	0	1
51	D5	0	1
52	B6	0	1
52	D6	0	1
53	B7	0	1
54	B8	0	2
54	D8	0	1
All	All	0	99

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	1143	A	N7-C5	-11.10	1.32	1.39
4	AG	12	CYS	CB-SG	10.86	2.00	1.82
25	DA	2873	A	N7-C5	-10.30	1.33	1.39
25	DA	1342	A	N7-C5	-9.87	1.33	1.39
25	BA	2430	A	N9-C4	-9.40	1.32	1.37

The worst 5 of 919 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1899	G	N3-C4-N9	-15.77	116.54	126.00
1	AA	1025	U	C5-C4-O4	-15.29	116.72	125.90
1	AA	1177	G	N9-C4-C5	14.63	111.25	105.40
1	AA	1177	G	C4-C5-N7	-14.21	105.12	110.80
25	DA	1899	G	N3-C4-N9	-13.25	118.05	126.00

There are no chirality outliers.

5 of 99 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AE	14	GLY	Peptide
2	AE	194	PRO	Peptide
2	AE	71	VAL	Peptide
4	AG	29	PRO	Peptide
8	AK	102	ARG	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32369	0	16339	1207	1
1	CA	32372	0	16338	1298	1
2	AE	1924	0	1975	158	0
2	CE	1924	0	1975	180	0
3	AF	1605	0	1668	111	0
3	CF	1612	0	1677	144	0
4	AG	1703	0	1764	146	0
4	CG	1703	0	1763	140	1
5	AH	1155	0	1213	74	0
5	CH	1155	0	1213	91	0
6	AI	843	0	857	39	1
6	CI	843	0	857	45	0
7	AJ	1257	0	1296	68	0
7	CJ	1257	0	1296	74	0
8	AK	1116	0	1177	75	0
8	CK	1116	0	1177	66	0
9	AL	1010	0	1037	99	0
9	CL	1010	0	1037	121	0
10	AM	801	0	849	78	0
10	CM	801	0	849	114	0
11	AN	885	0	904	65	0
11	CN	885	0	904	45	0
12	AO	975	0	1062	62	0
12	CO	975	0	1062	75	0
13	AP	928	0	987	66	0
13	CP	933	0	992	107	0
14	AQ	492	0	529	47	0
14	CQ	492	0	531	68	0
15	AR	734	0	771	38	0
15	CR	734	0	771	35	0
16	AS	705	0	725	79	0
16	CS	705	0	725	45	0
17	AT	834	0	904	55	0
17	CT	834	0	904	41	0
18	AU	591	0	662	30	0
18	CU	591	0	662	47	0
19	AV	624	0	636	71	0
19	CV	624	0	636	91	0
20	AW	763	0	859	73	0
20	CW	763	0	861	56	0
21	AX	217	0	234	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CX	217	0	234	23	0
22	AB	1861	0	938	85	0
22	CB	1861	0	938	99	0
23	AC	1643	0	837	75	0
23	AD	1643	0	837	97	0
23	CC	1643	0	837	91	0
23	CD	1643	0	837	108	0
24	A1	205	0	103	12	0
24	C1	205	0	103	10	0
25	BA	62707	0	31613	2105	0
25	DA	62607	0	31565	2108	1
26	BB	2617	0	1328	94	0
26	DB	2617	0	1328	135	0
27	BD	2115	0	2195	238	0
27	DD	2115	0	2195	211	0
28	BE	1568	0	1634	334	0
28	DE	1568	0	1634	256	0
29	BF	1585	0	1632	119	0
29	DF	1627	0	1680	184	0
30	BG	1474	0	1535	171	0
30	DG	1474	0	1535	148	0
31	BH	1307	0	1382	135	0
31	DH	1307	0	1382	156	1
32	BK	1136	0	1223	99	0
32	DK	1136	0	1223	84	0
33	BM	1104	0	1180	142	0
33	DM	1104	0	1180	87	0
34	BN	933	0	996	63	0
34	DN	933	0	996	51	0
35	BO	1145	0	1228	200	0
35	DO	1145	0	1227	240	0
36	BP	1122	0	1179	95	0
36	DP	1122	0	1179	208	0
37	B0	968	0	1033	78	0
37	D0	960	0	1021	60	0
38	BQ	882	0	943	106	0
38	DQ	882	0	943	120	0
39	BR	1141	0	1202	116	0
39	DR	1141	0	1202	125	0
40	B1	964	0	1022	98	0
40	D1	964	0	1022	94	0
41	B2	779	0	852	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	D2	779	0	852	129	0
42	BS	900	0	964	71	0
42	DS	900	0	964	42	0
43	BT	725	0	778	53	0
43	DT	725	0	778	75	0
44	BU	785	0	878	75	0
44	DU	785	0	878	98	0
45	BV	1397	0	1430	120	0
45	DV	1428	0	1454	162	0
46	B3	607	0	628	50	0
46	D3	613	0	633	52	0
47	BZ	763	0	848	50	0
47	DZ	763	0	848	46	0
48	BW	558	0	610	44	0
48	DW	581	0	629	49	0
49	BX	469	0	518	35	0
49	DX	469	0	518	24	0
50	B4	533	0	522	84	0
50	D4	515	0	510	84	0
51	B5	459	0	480	54	0
51	D5	454	0	475	44	0
52	B6	389	0	404	80	0
52	D6	389	0	404	84	0
53	B7	430	0	480	30	0
53	D7	430	0	480	36	0
54	B8	488	0	558	110	0
54	D8	488	0	558	113	0
55	A1	2	0	0	0	0
55	AA	242	0	0	0	0
55	AB	5	0	0	0	0
55	AC	9	0	0	0	0
55	AD	1	0	0	0	0
55	AG	1	0	0	0	0
55	AH	1	0	0	0	0
55	AN	2	0	0	0	0
55	AQ	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	1	0	0	0	0
55	B2	1	0	0	0	0
55	B3	1	0	0	0	0
55	B5	1	0	0	0	0
55	B7	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B8	1	0	0	0	0
55	BA	623	0	0	0	0
55	BB	17	0	0	0	0
55	BD	1	0	0	0	0
55	BE	5	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BU	2	0	0	0	0
55	CA	207	0	0	0	0
55	CB	3	0	0	0	0
55	CC	8	0	0	0	0
55	CG	2	0	0	0	0
55	CN	1	0	0	0	0
55	CS	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	526	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DR	1	0	0	0	0
55	DU	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299552	0	200910	14872	3

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 30.

The worst 5 of 14872 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:625:G:H4'	16:AS:16:HIS:CD2	1.33	1.61
28:DE:46:ALA:CB	28:DE:82:ARG:HA	1.37	1.55
30:BG:83:ARG:H	30:BG:86:MET:CE	1.24	1.47
36:DP:26:TYR:CE1	36:DP:139:GLU:HB2	1.48	1.45
25:BA:1056:G:N2	25:BA:1103:A:H62	1.13	1.44



All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.90	0.30
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.02	0.18
6:AI:15:ASP:OD2	4:CG:27:TYR:OH[4_555]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	190 (81%)	45 (19%)	0	100	100
2	CE	235/256 (92%)	190 (81%)	41 (17%)	4 (2%)	11	44
3	AF	203/239 (85%)	179 (88%)	24 (12%)	0	100	100
3	CF	204/239 (85%)	179 (88%)	23 (11%)	2 (1%)	18	59
4	AG	206/208 (99%)	179 (87%)	24 (12%)	3 (2%)	12	48
4	CG	206/208 (99%)	179 (87%)	25 (12%)	2 (1%)	18	59
5	AH	149/162 (92%)	137 (92%)	10 (7%)	2 (1%)	14	51
5	CH	149/162 (92%)	139 (93%)	10 (7%)	0	100	100
6	AI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
6	CI	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	AJ	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
7	CJ	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	AK	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	25	67
8	CK	136/138 (99%)	123 (90%)	13 (10%)	0	100	100
9	AL	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	CL	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	AM	97/105 (92%)	86 (89%)	11 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CM	97/105 (92%)	84 (87%)	9 (9%)	4 (4%)	3	19
11	AN	117/129 (91%)	102 (87%)	14 (12%)	1 (1%)	20	62
11	CN	117/129 (91%)	104 (89%)	13 (11%)	0	100	100
12	AO	123/132 (93%)	105 (85%)	16 (13%)	2 (2%)	11	46
12	CO	123/132 (93%)	105 (85%)	15 (12%)	3 (2%)	7	34
13	AP	114/126 (90%)	89 (78%)	23 (20%)	2 (2%)	10	43
13	CP	115/126 (91%)	96 (84%)	17 (15%)	2 (2%)	11	44
14	AQ	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
14	CQ	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	44
15	AR	86/89 (97%)	74 (86%)	11 (13%)	1 (1%)	15	53
15	CR	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	AS	82/88 (93%)	71 (87%)	8 (10%)	3 (4%)	4	22
16	CS	82/88 (93%)	75 (92%)	7 (8%)	0	100	100
17	AT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
17	CT	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	AU	70/88 (80%)	64 (91%)	5 (7%)	1 (1%)	13	49
18	CU	70/88 (80%)	61 (87%)	9 (13%)	0	100	100
19	AV	76/93 (82%)	68 (90%)	6 (8%)	2 (3%)	6	31
19	CV	76/93 (82%)	60 (79%)	12 (16%)	4 (5%)	2	13
20	AW	97/106 (92%)	84 (87%)	13 (13%)	0	100	100
20	CW	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	18	59
21	AX	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
21	CX	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
27	BD	270/276 (98%)	243 (90%)	22 (8%)	5 (2%)	9	41
27	DD	270/276 (98%)	248 (92%)	15 (6%)	7 (3%)	6	31
28	BE	203/206 (98%)	149 (73%)	30 (15%)	24 (12%)	0	2
28	DE	203/206 (98%)	144 (71%)	41 (20%)	18 (9%)	1	4
29	BF	200/210 (95%)	179 (90%)	21 (10%)	0	100	100
29	DF	206/210 (98%)	168 (82%)	30 (15%)	8 (4%)	3	20
30	BG	179/182 (98%)	154 (86%)	20 (11%)	5 (3%)	6	29
30	DG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	28	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	168/180 (93%)	133 (79%)	28 (17%)	7 (4%)	3	18
31	DH	168/180 (93%)	125 (74%)	35 (21%)	8 (5%)	2	16
32	BK	144/148 (97%)	102 (71%)	32 (22%)	10 (7%)	1	7
32	DK	144/148 (97%)	113 (78%)	28 (19%)	3 (2%)	8	38
33	BM	136/140 (97%)	113 (83%)	16 (12%)	7 (5%)	2	14
33	DM	136/140 (97%)	119 (88%)	15 (11%)	2 (2%)	12	48
34	BN	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
34	DN	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	22	64
35	BO	148/150 (99%)	107 (72%)	27 (18%)	14 (10%)	1	3
35	DO	148/150 (99%)	102 (69%)	24 (16%)	22 (15%)	0	1
36	BP	139/141 (99%)	109 (78%)	27 (19%)	3 (2%)	8	36
36	DP	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	2
37	B0	116/118 (98%)	101 (87%)	13 (11%)	2 (2%)	11	44
37	D0	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
38	BQ	109/112 (97%)	86 (79%)	20 (18%)	3 (3%)	6	29
38	DQ	109/112 (97%)	87 (80%)	19 (17%)	3 (3%)	6	29
39	BR	135/146 (92%)	114 (84%)	21 (16%)	0	100	100
39	DR	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	12	48
40	B1	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	20	62
40	D1	115/118 (98%)	101 (88%)	14 (12%)	0	100	100
41	B2	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	9	39
41	D2	99/101 (98%)	78 (79%)	14 (14%)	7 (7%)	1	6
42	BS	111/113 (98%)	97 (87%)	10 (9%)	4 (4%)	4	22
42	DS	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
43	BT	90/96 (94%)	84 (93%)	4 (4%)	2 (2%)	8	36
43	DT	90/96 (94%)	78 (87%)	10 (11%)	2 (2%)	8	36
44	BU	100/110 (91%)	80 (80%)	15 (15%)	5 (5%)	2	15
44	DU	100/110 (91%)	70 (70%)	24 (24%)	6 (6%)	2	10
45	BV	173/206 (84%)	129 (75%)	37 (21%)	7 (4%)	3	20
45	DV	177/206 (86%)	132 (75%)	35 (20%)	10 (6%)	2	12
46	B3	74/85 (87%)	67 (90%)	5 (7%)	2 (3%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	D3	75/85 (88%)	69 (92%)	6 (8%)	0	100	100
47	BZ	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	5	26
47	DZ	95/98 (97%)	84 (88%)	10 (10%)	1 (1%)	17	56
48	BW	64/72 (89%)	58 (91%)	4 (6%)	2 (3%)	5	26
48	DW	67/72 (93%)	60 (90%)	6 (9%)	1 (2%)	12	48
49	BX	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	DX	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
50	B4	64/71 (90%)	41 (64%)	21 (33%)	2 (3%)	5	26
50	D4	61/71 (86%)	32 (52%)	28 (46%)	1 (2%)	11	46
51	B5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	10	43
51	D5	56/60 (93%)	48 (86%)	7 (12%)	1 (2%)	10	43
52	B6	43/54 (80%)	27 (63%)	14 (33%)	2 (5%)	3	16
52	D6	43/54 (80%)	29 (67%)	10 (23%)	4 (9%)	1	4
53	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
53	D7	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
54	B8	59/65 (91%)	47 (80%)	7 (12%)	5 (8%)	1	4
54	D8	59/65 (91%)	40 (68%)	12 (20%)	7 (12%)	0	2
All	All	11335/12052 (94%)	9588 (85%)	1457 (13%)	290 (3%)	6	31

5 of 290 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AG	13	ARG
4	AG	14	ARG
11	AN	82	VAL
16	AS	17	TYR
18	AU	22	VAL

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	155 (76%)	50 (24%)	1	3
2	CE	205/220 (93%)	159 (78%)	46 (22%)	1	5
3	AF	159/188 (85%)	120 (76%)	39 (24%)	1	3
3	CF	160/188 (85%)	124 (78%)	36 (22%)	1	5
4	AG	180/180 (100%)	144 (80%)	36 (20%)	1	8
4	CG	180/180 (100%)	140 (78%)	40 (22%)	1	5
5	AH	116/123 (94%)	88 (76%)	28 (24%)	1	4
5	CH	116/123 (94%)	89 (77%)	27 (23%)	1	4
6	AI	90/90 (100%)	76 (84%)	14 (16%)	3	15
6	CI	90/90 (100%)	74 (82%)	16 (18%)	2	11
7	AJ	126/127 (99%)	104 (82%)	22 (18%)	2	11
7	CJ	126/127 (99%)	89 (71%)	37 (29%)	0	2
8	AK	119/119 (100%)	100 (84%)	19 (16%)	3	14
8	CK	119/119 (100%)	94 (79%)	25 (21%)	1	6
9	AL	98/99 (99%)	70 (71%)	28 (29%)	0	2
9	CL	98/99 (99%)	69 (70%)	29 (30%)	0	2
10	AM	89/92 (97%)	66 (74%)	23 (26%)	0	3
10	CM	89/92 (97%)	60 (67%)	29 (33%)	0	1
11	AN	90/99 (91%)	74 (82%)	16 (18%)	2	11
11	CN	90/99 (91%)	73 (81%)	17 (19%)	2	9
12	AO	104/109 (95%)	88 (85%)	16 (15%)	3	15
12	CO	104/109 (95%)	80 (77%)	24 (23%)	1	4
13	AP	94/101 (93%)	71 (76%)	23 (24%)	1	3
13	CP	94/101 (93%)	75 (80%)	19 (20%)	1	7
14	AQ	49/50 (98%)	33 (67%)	16 (33%)	0	1
14	CQ	49/50 (98%)	39 (80%)	10 (20%)	1	7
15	AR	79/80 (99%)	68 (86%)	11 (14%)	4	18
15	CR	79/80 (99%)	66 (84%)	13 (16%)	2	13
16	AS	72/74 (97%)	53 (74%)	19 (26%)	0	3
16	CS	72/74 (97%)	62 (86%)	10 (14%)	4	18
17	AT	95/97 (98%)	82 (86%)	13 (14%)	4	19
17	CT	95/97 (98%)	89 (94%)	6 (6%)	21	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AU	63/77 (82%)	50 (79%)	13 (21%)	1	7
18	CU	63/77 (82%)	48 (76%)	15 (24%)	1	4
19	AV	67/80 (84%)	47 (70%)	20 (30%)	0	2
19	CV	67/80 (84%)	53 (79%)	14 (21%)	1	6
20	AW	76/82 (93%)	60 (79%)	16 (21%)	1	6
20	CW	76/82 (93%)	55 (72%)	21 (28%)	0	2
21	AX	20/22 (91%)	17 (85%)	3 (15%)	3	16
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	172 (80%)	42 (20%)	1	8
27	DD	214/218 (98%)	162 (76%)	52 (24%)	1	4
28	BE	165/166 (99%)	114 (69%)	51 (31%)	0	1
28	DE	165/166 (99%)	121 (73%)	44 (27%)	0	3
29	BF	161/166 (97%)	129 (80%)	32 (20%)	1	8
29	DF	165/166 (99%)	122 (74%)	43 (26%)	0	3
30	BG	155/156 (99%)	115 (74%)	40 (26%)	0	3
30	DG	155/156 (99%)	113 (73%)	42 (27%)	0	2
31	BH	142/148 (96%)	107 (75%)	35 (25%)	1	3
31	DH	142/148 (96%)	110 (78%)	32 (22%)	1	5
32	BK	122/124 (98%)	91 (75%)	31 (25%)	0	3
32	DK	122/124 (98%)	84 (69%)	38 (31%)	0	1
33	BM	117/119 (98%)	87 (74%)	30 (26%)	0	3
33	DM	117/119 (98%)	96 (82%)	21 (18%)	2	11
34	BN	100/100 (100%)	83 (83%)	17 (17%)	2	12
34	DN	100/100 (100%)	78 (78%)	22 (22%)	1	5
35	BO	116/116 (100%)	78 (67%)	38 (33%)	0	1
35	DO	116/116 (100%)	72 (62%)	44 (38%)	0	1
36	BP	111/111 (100%)	84 (76%)	27 (24%)	1	4
36	DP	111/111 (100%)	85 (77%)	26 (23%)	1	4
37	B0	101/101 (100%)	78 (77%)	23 (23%)	1	5
37	D0	100/101 (99%)	80 (80%)	20 (20%)	1	8
38	BQ	87/88 (99%)	65 (75%)	22 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	DQ	87/88 (99%)	53 (61%)	34 (39%)	0	0
39	BR	120/127 (94%)	92 (77%)	28 (23%)	1	4
39	DR	120/127 (94%)	84 (70%)	36 (30%)	0	2
40	B1	93/94 (99%)	76 (82%)	17 (18%)	2	10
40	D1	93/94 (99%)	80 (86%)	13 (14%)	4	18
41	B2	82/82 (100%)	61 (74%)	21 (26%)	0	3
41	D2	82/82 (100%)	50 (61%)	32 (39%)	0	0
42	BS	92/92 (100%)	72 (78%)	20 (22%)	1	6
42	DS	92/92 (100%)	65 (71%)	27 (29%)	0	2
43	BT	74/78 (95%)	61 (82%)	13 (18%)	2	11
43	DT	74/78 (95%)	57 (77%)	17 (23%)	1	4
44	BU	85/91 (93%)	65 (76%)	20 (24%)	1	4
44	DU	85/91 (93%)	51 (60%)	34 (40%)	0	0
45	BV	154/179 (86%)	116 (75%)	38 (25%)	1	3
45	DV	158/179 (88%)	124 (78%)	34 (22%)	1	6
46	B3	61/67 (91%)	54 (88%)	7 (12%)	6	27
46	D3	62/67 (92%)	47 (76%)	15 (24%)	1	4
47	BZ	82/83 (99%)	64 (78%)	18 (22%)	1	5
47	DZ	82/83 (99%)	64 (78%)	18 (22%)	1	5
48	BW	62/67 (92%)	42 (68%)	20 (32%)	0	1
48	DW	64/67 (96%)	50 (78%)	14 (22%)	1	5
49	BX	51/52 (98%)	41 (80%)	10 (20%)	1	8
49	DX	51/52 (98%)	42 (82%)	9 (18%)	2	11
50	B4	59/63 (94%)	41 (70%)	18 (30%)	0	2
50	D4	57/63 (90%)	38 (67%)	19 (33%)	0	1
51	B5	51/52 (98%)	35 (69%)	16 (31%)	0	1
51	D5	51/52 (98%)	37 (72%)	14 (28%)	0	2
52	B6	44/52 (85%)	27 (61%)	17 (39%)	0	0
52	D6	44/52 (85%)	31 (70%)	13 (30%)	0	2
53	B7	42/42 (100%)	34 (81%)	8 (19%)	2	9
53	D7	42/42 (100%)	32 (76%)	10 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	B8	51/55 (93%)	40 (78%)	11 (22%)	1	6
54	D8	51/55 (93%)	41 (80%)	10 (20%)	1	8
All	All	9579/9996 (96%)	7317 (76%)	2262 (24%)	1	4

5 of 2262 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BX	53	LEU
7	CJ	13	GLN
44	DU	62	GLU
51	B5	48	GLU
3	CF	28	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 255 such sidechains are listed below:

Mol	Chain	Res	Type
48	BW	65	ASN
6	CI	32	ASN
46	D3	12	ASN
49	BX	46	ASN
2	CE	78	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1506 (99%)	375 (24%)	32 (2%)
1	CA	1505/1506 (99%)	409 (27%)	41 (2%)
22	AB	86/87 (98%)	40 (46%)	5 (5%)
22	CB	86/87 (98%)	46 (53%)	2 (2%)
23	AC	77/77 (100%)	23 (29%)	6 (7%)
23	AD	76/77 (98%)	28 (36%)	1 (1%)
23	CC	77/77 (100%)	21 (27%)	5 (6%)
23	CD	76/77 (98%)	26 (34%)	1 (1%)
24	A1	9/10 (90%)	3 (33%)	1 (11%)
24	C1	9/10 (90%)	3 (33%)	0
25	BA	2911/2912 (99%)	713 (24%)	57 (1%)
25	DA	2905/2912 (99%)	763 (26%)	57 (1%)
26	BB	121/122 (99%)	30 (24%)	0
26	DB	121/122 (99%)	39 (32%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9564/9582 (99%)	2519 (26%)	208 (2%)

5 of 2519 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	32	A
1	AA	33	A

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2439	A
1	CA	412	A
25	DA	2275	C
25	BA	2610	C
1	CA	115	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1700 ligands modelled in this entry, 1700 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1506/1506 (100%)	-0.57	5 (0%)	93 82	50, 98, 179, 234	0
1	CA	1506/1506 (100%)	-0.56	4 (0%)	93 82	62, 109, 181, 235	0
2	AE	237/256 (92%)	0.27	9 (3%)	41 17	103, 136, 174, 185	0
2	CE	237/256 (92%)	0.59	25 (10%)	7 3	114, 151, 185, 201	0
3	AF	205/239 (85%)	0.91	34 (16%)	2 1	84, 111, 144, 153	0
3	CF	206/239 (86%)	1.40	59 (28%)	1 0	118, 138, 166, 174	0
4	AG	208/208 (100%)	0.47	13 (6%)	21 7	80, 105, 129, 142	0
4	CG	208/208 (100%)	0.39	14 (6%)	19 7	77, 102, 123, 136	0
5	AH	151/162 (93%)	0.52	8 (5%)	27 11	74, 97, 118, 152	0
5	CH	151/162 (93%)	0.22	7 (4%)	33 13	91, 112, 134, 153	0
6	AI	101/101 (100%)	0.93	14 (13%)	3 1	76, 99, 115, 137	0
6	CI	101/101 (100%)	0.95	19 (18%)	1 1	74, 95, 116, 141	0
7	AJ	155/156 (99%)	-0.08	8 (5%)	28 11	99, 114, 145, 155	0
7	CJ	155/156 (99%)	0.27	10 (6%)	20 7	102, 122, 149, 156	0
8	AK	138/138 (100%)	-0.02	0	100 100	84, 103, 117, 122	0
8	CK	138/138 (100%)	-0.21	1 (0%)	87 67	94, 116, 128, 136	0
9	AL	127/128 (99%)	-0.31	1 (0%)	86 64	85, 133, 153, 160	0
9	CL	127/128 (99%)	-0.02	4 (3%)	49 22	107, 145, 160, 164	0
10	AM	99/105 (94%)	0.38	6 (6%)	22 8	81, 132, 162, 165	0
10	CM	99/105 (94%)	0.49	3 (3%)	51 23	111, 149, 165, 170	0
11	AN	119/129 (92%)	1.10	19 (15%)	2 1	64, 97, 128, 154	0
11	CN	119/129 (92%)	1.48	32 (26%)	1 0	79, 101, 134, 158	0
12	AO	125/132 (94%)	0.41	8 (6%)	20 7	63, 73, 105, 151	0
12	CO	125/132 (94%)	1.07	27 (21%)	1 0	75, 98, 124, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	116/126 (92%)	-0.15	4 (3%) 46 20	86, 117, 136, 145	0
13	CP	117/126 (92%)	0.44	11 (9%) 9 3	106, 146, 161, 164	0
14	AQ	60/61 (98%)	-0.12	0 100 100	86, 101, 115, 126	0
14	CQ	60/61 (98%)	0.93	11 (18%) 1 1	118, 132, 146, 153	0
15	AR	88/89 (98%)	0.04	2 (2%) 61 31	72, 93, 114, 117	0
15	CR	88/89 (98%)	0.02	2 (2%) 61 31	73, 104, 127, 133	0
16	AS	84/88 (95%)	-0.37	0 100 100	90, 107, 133, 165	0
16	CS	84/88 (95%)	-0.34	0 100 100	81, 96, 120, 153	0
17	AT	100/105 (95%)	-0.21	1 (1%) 82 58	82, 100, 118, 130	0
17	CT	100/105 (95%)	-0.24	1 (1%) 82 58	82, 102, 125, 137	0
18	AU	72/88 (81%)	1.10	12 (16%) 2 1	78, 99, 132, 159	0
18	CU	72/88 (81%)	1.08	11 (15%) 2 1	85, 106, 144, 157	0
19	AV	78/93 (83%)	0.20	2 (2%) 56 27	100, 122, 137, 144	0
19	CV	78/93 (83%)	0.78	12 (15%) 2 1	136, 154, 174, 177	0
20	AW	99/106 (93%)	-0.44	0 100 100	93, 115, 144, 155	0
20	CW	99/106 (93%)	-0.23	0 100 100	83, 109, 143, 157	0
21	AX	25/27 (92%)	-0.63	0 100 100	88, 109, 125, 147	0
21	CX	25/27 (92%)	0.03	1 (4%) 39 16	112, 133, 148, 160	0
22	AB	87/87 (100%)	1.67	29 (33%) 0 0	78, 145, 185, 196	0
22	CB	87/87 (100%)	4.01	55 (63%) 0 0	92, 148, 188, 200	0
23	AC	77/77 (100%)	-0.36	0 100 100	63, 100, 132, 147	0
23	AD	77/77 (100%)	0.15	3 (3%) 40 16	71, 218, 232, 234	0
23	CC	77/77 (100%)	-0.20	1 (1%) 77 51	73, 107, 141, 153	0
23	CD	77/77 (100%)	0.64	12 (15%) 2 1	77, 219, 231, 234	0
24	A1	10/10 (100%)	0.52	2 (20%) 1 1	67, 81, 112, 112	0
24	C1	10/10 (100%)	0.51	2 (20%) 1 1	81, 98, 118, 124	0
25	BA	2912/2912 (100%)	-0.30	37 (1%) 77 51	36, 66, 200, 234	0
25	DA	2907/2912 (99%)	-0.26	48 (1%) 70 42	45, 80, 220, 235	0
26	BB	122/122 (100%)	-0.60	1 (0%) 86 64	66, 91, 110, 169	0
26	DB	122/122 (100%)	-0.47	1 (0%) 86 64	84, 120, 141, 189	0
27	BD	272/276 (98%)	0.09	1 (0%) 92 77	35, 57, 79, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	272/276 (98%)	0.37	9 (3%)	47	21	42, 67, 88, 119	0
28	BE	205/206 (99%)	0.42	15 (7%)	16	6	43, 77, 123, 132	0
28	DE	205/206 (99%)	0.24	11 (5%)	26	11	52, 88, 137, 159	0
29	BF	202/210 (96%)	-0.13	1 (0%)	90	74	38, 70, 108, 123	0
29	DF	208/210 (99%)	0.59	20 (9%)	9	3	48, 94, 152, 175	0
30	BG	181/182 (99%)	0.69	17 (9%)	9	3	81, 101, 130, 142	0
30	DG	181/182 (99%)	1.21	44 (24%)	1	0	112, 135, 155, 162	0
31	BH	170/180 (94%)	0.45	11 (6%)	20	7	74, 104, 121, 146	0
31	DH	170/180 (94%)	1.06	38 (22%)	1	0	148, 188, 209, 218	0
32	BK	146/148 (98%)	0.22	4 (2%)	55	26	69, 121, 137, 142	0
32	DK	146/148 (98%)	0.38	10 (6%)	18	7	77, 120, 143, 150	0
33	BM	138/140 (98%)	0.09	2 (1%)	75	49	57, 81, 116, 129	0
33	DM	138/140 (98%)	0.11	4 (2%)	52	24	71, 102, 133, 143	0
34	BN	122/122 (100%)	0.35	1 (0%)	86	64	48, 67, 83, 97	0
34	DN	122/122 (100%)	0.42	2 (1%)	72	44	62, 82, 102, 118	0
35	BO	150/150 (100%)	-0.12	2 (1%)	77	51	42, 77, 106, 153	0
35	DO	150/150 (100%)	0.95	27 (18%)	2	1	44, 99, 135, 171	0
36	BP	141/141 (100%)	0.44	11 (7%)	14	5	52, 78, 99, 125	0
36	DP	141/141 (100%)	0.90	24 (17%)	2	1	58, 98, 129, 148	0
37	B0	118/118 (100%)	0.33	1 (0%)	86	64	50, 76, 94, 110	0
37	D0	117/118 (99%)	0.01	2 (1%)	70	42	50, 75, 97, 113	0
38	BQ	111/112 (99%)	0.36	4 (3%)	43	18	70, 88, 110, 127	0
38	DQ	111/112 (99%)	0.41	9 (8%)	13	5	83, 117, 139, 159	0
39	BR	137/146 (93%)	0.19	4 (2%)	52	24	60, 82, 134, 163	0
39	DR	137/146 (93%)	0.17	5 (3%)	43	18	69, 93, 154, 174	0
40	B1	117/118 (99%)	-0.19	2 (1%)	70	42	44, 70, 101, 132	0
40	D1	117/118 (99%)	0.23	2 (1%)	70	42	58, 89, 131, 152	0
41	B2	101/101 (100%)	0.08	3 (2%)	51	23	48, 92, 115, 132	0
41	D2	101/101 (100%)	0.78	13 (12%)	4	1	58, 115, 133, 142	0
42	BS	113/113 (100%)	0.05	4 (3%)	44	19	41, 65, 97, 147	0
42	DS	113/113 (100%)	0.06	2 (1%)	69	40	54, 69, 104, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BT	92/96 (95%)	0.10	2 (2%) 62 33	49, 63, 87, 104	0
43	DT	92/96 (95%)	0.22	5 (5%) 26 11	64, 80, 104, 121	0
44	BU	102/110 (92%)	0.37	7 (6%) 18 6	67, 92, 142, 159	0
44	DU	102/110 (92%)	1.12	24 (23%) 1 0	82, 109, 160, 176	0
45	BV	175/206 (84%)	1.67	58 (33%) 0 0	80, 117, 179, 183	0
45	DV	179/206 (86%)	2.69	96 (53%) 0 0	110, 151, 199, 206	0
46	B3	76/85 (89%)	-0.16	1 (1%) 77 51	52, 68, 83, 117	0
46	D3	77/85 (90%)	0.16	1 (1%) 77 51	65, 86, 108, 141	0
47	BZ	97/98 (98%)	0.27	9 (9%) 9 3	46, 64, 122, 151	0
47	DZ	97/98 (98%)	0.15	4 (4%) 38 15	54, 77, 126, 148	0
48	BW	66/72 (91%)	-0.00	1 (1%) 74 47	55, 73, 90, 120	0
48	DW	69/72 (95%)	0.27	4 (5%) 24 9	77, 100, 130, 167	0
49	BX	59/60 (98%)	0.11	2 (3%) 46 20	60, 75, 105, 120	0
49	DX	59/60 (98%)	0.62	2 (3%) 46 20	73, 98, 130, 153	0
50	B4	66/71 (92%)	1.49	18 (27%) 1 0	111, 146, 164, 173	0
50	D4	63/71 (88%)	3.03	43 (68%) 0 0	140, 176, 185, 191	0
51	B5	59/60 (98%)	0.93	11 (18%) 1 1	43, 80, 163, 168	0
51	D5	58/60 (96%)	0.43	6 (10%) 7 3	52, 78, 167, 178	0
52	B6	45/54 (83%)	2.85	27 (60%) 0 0	105, 134, 156, 160	0
52	D6	45/54 (83%)	3.12	30 (66%) 0 0	121, 156, 173, 176	0
53	B7	49/49 (100%)	-0.10	2 (4%) 38 15	35, 45, 88, 118	0
53	D7	49/49 (100%)	0.26	3 (6%) 22 8	44, 54, 112, 131	0
54	B8	61/65 (93%)	-0.04	1 (1%) 72 44	51, 64, 81, 102	0
54	D8	61/65 (93%)	0.60	4 (6%) 19 7	65, 79, 94, 123	0
All	All	21104/21634 (97%)	0.11	1257 (5%) 23 9	35, 96, 177, 235	0

The worst 5 of 1257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	CB	54	G	18.7
22	CB	53	A	15.6
22	CB	55	G	14.7
45	DV	147	GLY	14.6
22	CB	52	U	14.6



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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
55	MG	BA	3061	1/1	0.89	0.54	87.54	61,61,61,61	0
55	MG	BA	3032	1/1	0.93	0.52	57.32	49,49,49,49	0
55	MG	DA	3019	1/1	0.89	0.92	52.49	90,90,90,90	0
55	MG	BA	3027	1/1	0.99	0.54	43.66	36,36,36,36	0
55	MG	AA	1691	1/1	0.98	0.49	39.32	50,50,50,50	0
55	MG	BA	3173	1/1	0.99	0.59	37.75	52,52,52,52	0
55	MG	AA	1837	1/1	0.96	0.53	37.70	73,73,73,73	0
55	MG	DA	3081	1/1	0.93	0.51	36.95	64,64,64,64	0
55	MG	BA	3096	1/1	0.96	0.50	36.38	56,56,56,56	0
55	MG	DA	3165	1/1	0.95	0.59	35.71	65,65,65,65	0
55	MG	BA	3157	1/1	0.98	0.60	34.89	45,45,45,45	0
55	MG	DA	3174	1/1	0.96	0.57	34.71	44,44,44,44	0
55	MG	BA	3269	1/1	0.98	0.45	34.17	61,61,61,61	0
55	MG	DA	3156	1/1	0.96	0.69	33.92	48,48,48,48	0
55	MG	DA	3433	1/1	0.97	0.53	33.91	57,57,57,57	0
55	MG	DA	3227	1/1	0.97	0.72	33.84	50,50,50,50	0
55	MG	DA	3228	1/1	0.95	0.47	33.71	44,44,44,44	0
55	MG	BA	3095	1/1	0.97	0.47	33.41	37,37,37,37	0
55	MG	BA	3169	1/1	0.94	0.60	32.57	63,63,63,63	0
55	MG	DA	3221	1/1	0.97	0.70	32.54	63,63,63,63	0
55	MG	DA	3513	1/1	0.83	0.76	32.50	67,67,67,67	0
55	MG	DA	3188	1/1	0.91	0.60	32.36	56,56,56,56	0
55	MG	BA	3516	1/1	0.90	0.86	32.24	78,78,78,78	0
55	MG	BA	3521	1/1	0.82	0.60	32.24	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3385	1/1	0.90	0.70	32.18	62,62,62,62	0
55	MG	DA	3371	1/1	0.68	0.49	31.38	82,82,82,82	0
55	MG	BA	3163	1/1	0.98	0.58	31.22	50,50,50,50	0
55	MG	BA	3100	1/1	0.96	0.37	30.98	42,42,42,42	0
55	MG	DA	3260	1/1	0.99	0.62	30.40	41,41,41,41	0
55	MG	DA	3328	1/1	0.89	0.34	30.27	47,47,47,47	0
55	MG	DA	3204	1/1	0.97	0.39	29.83	51,51,51,51	0
55	MG	CA	1690	1/1	0.96	0.36	29.54	68,68,68,68	0
55	MG	CA	1668	1/1	0.89	0.42	29.08	79,79,79,79	0
55	MG	DA	3087	1/1	0.96	0.50	28.75	63,63,63,63	0
55	MG	DA	3113	1/1	0.97	0.55	28.54	43,43,43,43	0
55	MG	BA	3207	1/1	0.98	0.57	28.27	41,41,41,41	0
55	MG	BA	3393	1/1	0.90	0.51	27.71	81,81,81,81	0
55	MG	BA	3187	1/1	0.91	0.48	27.56	73,73,73,73	0
55	MG	DA	3264	1/1	0.97	0.65	27.30	59,59,59,59	0
55	MG	BA	3345	1/1	0.82	0.71	27.17	73,73,73,73	0
55	MG	AA	1610	1/1	0.95	0.49	26.99	51,51,51,51	0
55	MG	BA	3016	1/1	0.94	0.53	26.48	39,39,39,39	0
55	MG	BA	3172	1/1	0.98	0.36	26.42	34,34,34,34	0
55	MG	BA	3245	1/1	0.98	0.55	26.23	49,49,49,49	0
55	MG	DA	3355	1/1	0.91	0.50	25.97	77,77,77,77	0
55	MG	DA	3332	1/1	0.90	0.39	25.76	76,76,76,76	0
55	MG	BA	3262	1/1	0.99	0.57	25.69	33,33,33,33	0
55	MG	BA	3591	1/1	0.75	0.47	25.55	64,64,64,64	0
55	MG	BA	3001	1/1	0.97	0.48	25.34	47,47,47,47	0
55	MG	BA	3197	1/1	0.94	0.53	25.34	46,46,46,46	0
55	MG	BA	3314	1/1	0.89	0.58	25.21	64,64,64,64	0
55	MG	BA	3583	1/1	0.76	0.50	25.21	86,86,86,86	0
55	MG	BA	3361	1/1	0.81	0.41	24.46	64,64,64,64	0
55	MG	BA	3378	1/1	0.87	0.56	24.44	76,76,76,76	0
55	MG	DA	3114	1/1	0.99	0.56	24.41	54,54,54,54	0
55	MG	BA	3353	1/1	0.94	0.44	24.36	52,52,52,52	0
55	MG	DA	3063	1/1	0.92	0.53	24.22	75,75,75,75	0
55	MG	DA	3190	1/1	0.95	0.57	24.17	61,61,61,61	0
55	MG	DA	3080	1/1	0.73	0.55	23.86	75,75,75,75	0
55	MG	CC	102	1/1	0.97	0.52	23.78	73,73,73,73	0
55	MG	BA	3012	1/1	0.93	0.28	23.66	45,45,45,45	0
55	MG	BA	3153	1/1	0.95	0.44	23.42	52,52,52,52	0
55	MG	DA	3180	1/1	0.98	0.59	23.41	52,52,52,52	0
55	MG	CA	1739	1/1	0.93	0.56	23.25	75,75,75,75	0
55	MG	BA	3226	1/1	0.94	0.41	23.23	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3616	1/1	0.93	0.38	23.22	58,58,58,58	0
55	MG	DA	3145	1/1	0.97	0.51	23.00	60,60,60,60	0
55	MG	BA	3428	1/1	0.96	0.36	22.77	68,68,68,68	0
55	MG	BA	3610	1/1	0.98	0.43	22.33	61,61,61,61	0
55	MG	BA	3005	1/1	0.97	0.49	22.29	43,43,43,43	0
55	MG	DA	3254	1/1	0.97	0.55	22.11	50,50,50,50	0
55	MG	DA	3399	1/1	0.88	0.45	22.01	76,76,76,76	0
55	MG	CA	1750	1/1	0.97	0.48	21.97	79,79,79,79	0
55	MG	DA	3157	1/1	0.97	0.69	21.89	47,47,47,47	0
55	MG	AA	1712	1/1	0.89	0.38	21.88	78,78,78,78	0
55	MG	BA	3144	1/1	0.90	0.29	21.73	48,48,48,48	0
55	MG	BA	3091	1/1	0.98	0.52	21.72	35,35,35,35	0
55	MG	CA	1771	1/1	0.80	0.42	21.41	76,76,76,76	0
55	MG	AA	1717	1/1	0.92	0.40	21.37	74,74,74,74	0
55	MG	DA	3196	1/1	0.97	0.46	21.31	50,50,50,50	0
55	MG	DA	3245	1/1	0.97	0.51	21.27	60,60,60,60	0
55	MG	DA	3155	1/1	0.97	0.46	21.24	46,46,46,46	0
55	MG	BA	3289	1/1	0.89	0.56	21.21	60,60,60,60	0
55	MG	CA	1676	1/1	0.97	0.44	21.19	55,55,55,55	0
55	MG	BA	3344	1/1	0.91	0.36	21.15	55,55,55,55	0
55	MG	BA	3055	1/1	0.97	0.43	21.15	57,57,57,57	0
55	MG	BA	3399	1/1	0.72	0.58	21.00	90,90,90,90	0
55	MG	BA	3004	1/1	0.98	0.46	20.96	35,35,35,35	0
55	MG	BA	3125	1/1	0.95	0.53	20.49	52,52,52,52	0
55	MG	DA	3176	1/1	0.95	0.55	20.12	65,65,65,65	0
55	MG	BA	3033	1/1	0.97	0.38	20.02	38,38,38,38	0
55	MG	AA	1651	1/1	0.85	0.56	19.88	71,71,71,71	0
55	MG	DA	3263	1/1	0.88	0.86	19.78	82,82,82,82	0
55	MG	BA	3452	1/1	0.96	0.40	19.51	41,41,41,41	0
55	MG	AA	1678	1/1	0.90	0.35	19.44	74,74,74,74	0
55	MG	AA	1661	1/1	0.92	0.34	19.40	48,48,48,48	0
55	MG	DA	3400	1/1	0.85	0.40	19.30	89,89,89,89	0
55	MG	BA	3287	1/1	0.94	0.39	19.23	62,62,62,62	0
55	MG	BA	3137	1/1	0.96	0.37	19.23	47,47,47,47	0
55	MG	BA	3126	1/1	0.98	0.42	19.21	46,46,46,46	0
55	MG	CA	1691	1/1	0.87	0.33	19.20	78,78,78,78	0
55	MG	DA	3364	1/1	0.83	0.27	18.98	71,71,71,71	0
55	MG	BA	3304	1/1	0.81	0.28	18.95	56,56,56,56	0
55	MG	DA	3169	1/1	0.96	0.31	18.77	69,69,69,69	0
55	MG	DA	3283	1/1	0.84	0.44	18.72	61,61,61,61	0
55	MG	BA	3008	1/1	0.96	0.49	18.71	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3504	1/1	0.97	0.33	18.63	45,45,45,45	0
55	MG	CA	1634	1/1	0.88	0.46	18.59	77,77,77,77	0
55	MG	DA	3122	1/1	0.95	0.49	18.53	46,46,46,46	0
55	MG	DA	3104	1/1	0.98	0.40	18.51	43,43,43,43	0
55	MG	BA	3365	1/1	0.82	0.33	18.46	50,50,50,50	0
55	MG	BA	3162	1/1	0.97	0.52	18.23	45,45,45,45	0
55	MG	CA	1804	1/1	0.86	0.30	18.18	75,75,75,75	0
55	MG	BA	3308	1/1	0.94	0.32	18.15	61,61,61,61	0
55	MG	DA	3376	1/1	0.88	0.53	18.12	82,82,82,82	0
55	MG	DA	3129	1/1	0.83	0.25	18.09	82,82,82,82	0
55	MG	DA	3213	1/1	0.99	0.49	18.04	41,41,41,41	0
55	MG	AA	1679	1/1	0.79	0.28	18.02	86,86,86,86	0
55	MG	BA	3007	1/1	0.98	0.54	17.87	53,53,53,53	0
55	MG	BA	3108	1/1	0.93	0.36	17.76	86,86,86,86	0
55	MG	BA	3124	1/1	0.96	0.52	17.67	45,45,45,45	0
55	MG	BA	3528	1/1	0.95	0.44	17.67	76,76,76,76	0
55	MG	BA	3195	1/1	0.92	0.49	17.54	47,47,47,47	0
55	MG	DA	3426	1/1	0.93	0.42	17.42	58,58,58,58	0
55	MG	DA	3224	1/1	0.93	0.47	17.28	66,66,66,66	0
55	MG	BA	3092	1/1	0.96	0.46	17.16	32,32,32,32	0
55	MG	DA	3262	1/1	0.94	0.46	16.88	48,48,48,48	0
55	MG	DA	3319	1/1	0.87	0.40	16.78	74,74,74,74	0
55	MG	AA	1658	1/1	0.95	0.65	16.74	49,49,49,49	0
55	MG	DA	3047	1/1	0.89	0.42	16.71	76,76,76,76	0
55	MG	BA	3146	1/1	0.91	0.38	16.42	59,59,59,59	0
55	MG	DA	3150	1/1	0.89	0.34	16.35	68,68,68,68	0
55	MG	CA	1647	1/1	0.89	0.51	16.29	61,61,61,61	0
55	MG	DA	3412	1/1	0.89	0.33	16.23	89,89,89,89	0
55	MG	DA	3212	1/1	0.93	0.60	16.16	48,48,48,48	0
55	MG	BO	201	1/1	0.93	0.36	16.13	62,62,62,62	0
55	MG	DA	3128	1/1	0.91	0.35	16.11	77,77,77,77	0
55	MG	BA	3002	1/1	0.98	0.47	16.09	43,43,43,43	0
55	MG	DA	3374	1/1	0.94	0.41	16.07	62,62,62,62	0
55	MG	BA	3133	1/1	0.78	0.29	16.04	66,66,66,66	0
55	MG	BA	3090	1/1	0.87	0.47	15.81	49,49,49,49	0
55	MG	DA	3096	1/1	0.97	0.58	15.80	53,53,53,53	0
55	MG	DA	3125	1/1	0.88	0.43	15.77	45,45,45,45	0
55	MG	BA	3256	1/1	0.84	0.41	15.74	61,61,61,61	0
55	MG	CA	1766	1/1	0.79	0.30	15.72	85,85,85,85	0
55	MG	AC	101	1/1	0.97	0.48	15.69	53,53,53,53	0
55	MG	BA	3046	1/1	0.97	0.38	15.60	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1686	1/1	0.96	0.36	15.57	85,85,85,85	0
55	MG	DA	3456	1/1	0.95	0.36	15.41	83,83,83,83	0
55	MG	DA	3214	1/1	0.94	0.44	15.18	40,40,40,40	0
55	MG	BA	3206	1/1	0.85	0.38	15.12	75,75,75,75	0
55	MG	AA	1601	1/1	0.97	0.36	15.07	56,56,56,56	0
55	MG	BA	3130	1/1	0.92	0.43	15.05	44,44,44,44	0
55	MG	AA	1836	1/1	0.69	0.60	15.00	79,79,79,79	0
55	MG	DA	3164	1/1	0.86	0.45	14.97	47,47,47,47	0
55	MG	BA	3014	1/1	0.97	0.48	14.92	53,53,53,53	0
55	MG	DA	3337	1/1	0.82	0.46	14.41	89,89,89,89	0
55	MG	DA	3112	1/1	0.89	0.35	14.31	81,81,81,81	0
55	MG	DA	3135	1/1	0.97	0.42	14.30	49,49,49,49	0
55	MG	BA	3160	1/1	0.97	0.42	14.00	42,42,42,42	0
55	MG	CA	1755	1/1	0.81	0.49	13.91	92,92,92,92	0
55	MG	BA	3119	1/1	0.97	0.38	13.74	62,62,62,62	0
55	MG	DA	3310	1/1	0.93	0.49	13.70	71,71,71,71	0
55	MG	DA	3103	1/1	0.97	0.40	13.63	50,50,50,50	0
55	MG	BA	3154	1/1	0.85	0.30	13.63	55,55,55,55	0
55	MG	DA	3046	1/1	0.95	0.34	13.57	65,65,65,65	0
55	MG	DA	3522	1/1	0.64	0.48	13.56	78,78,78,78	0
55	MG	BA	3040	1/1	0.95	0.36	13.56	54,54,54,54	0
55	MG	BA	3020	1/1	0.97	0.47	13.53	41,41,41,41	0
55	MG	BA	3066	1/1	0.97	0.31	13.43	62,62,62,62	0
55	MG	AA	1639	1/1	0.87	0.31	13.25	91,91,91,91	0
55	MG	DA	3198	1/1	0.94	0.31	13.16	47,47,47,47	0
55	MG	BA	3302	1/1	0.91	0.41	13.16	26,26,26,26	0
55	MG	DA	3105	1/1	0.94	0.36	13.07	45,45,45,45	0
55	MG	DA	3275	1/1	0.95	0.36	13.07	76,76,76,76	0
55	MG	BA	3367	1/1	0.78	0.26	13.00	82,82,82,82	0
55	MG	BA	3401	1/1	0.84	0.45	12.82	62,62,62,62	0
55	MG	DA	3281	1/1	0.82	0.88	12.79	76,76,76,76	0
55	MG	BA	3442	1/1	0.77	0.37	12.66	76,76,76,76	0
55	MG	BA	3021	1/1	0.97	0.53	12.64	41,41,41,41	0
55	MG	DA	3261	1/1	0.94	0.49	12.61	58,58,58,58	0
55	MG	BA	3258	1/1	0.93	0.29	12.59	45,45,45,45	0
55	MG	BA	3109	1/1	0.96	0.32	12.55	70,70,70,70	0
55	MG	BA	3044	1/1	0.95	0.33	12.55	62,62,62,62	0
55	MG	DA	3094	1/1	0.85	0.95	12.47	94,94,94,94	0
55	MG	CA	1654	1/1	0.90	0.31	12.46	99,99,99,99	0
55	MG	DB	211	1/1	0.74	0.41	12.45	93,93,93,93	0
55	MG	BA	3082	1/1	0.95	0.36	12.41	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1686	1/1	0.88	0.42	12.35	73,73,73,73	0
55	MG	BA	3249	1/1	0.89	0.29	12.33	30,30,30,30	0
55	MG	DA	3450	1/1	0.94	0.33	12.28	88,88,88,88	0
55	MG	DA	3218	1/1	0.96	0.41	12.20	62,62,62,62	0
55	MG	DA	3278	1/1	0.96	0.51	12.15	42,42,42,42	0
55	MG	DA	3085	1/1	0.83	0.32	12.08	91,91,91,91	0
55	MG	BA	3600	1/1	0.93	0.34	12.08	66,66,66,66	0
55	MG	DA	3158	1/1	0.97	0.59	12.05	44,44,44,44	0
55	MG	DA	3210	1/1	0.97	0.42	12.00	63,63,63,63	0
55	MG	BE	301	1/1	0.92	0.39	11.89	59,59,59,59	0
55	MG	BA	3031	1/1	0.96	0.36	11.70	33,33,33,33	0
55	MG	BA	3102	1/1	0.97	0.28	11.64	66,66,66,66	0
55	MG	BB	215	1/1	0.95	0.26	11.59	82,82,82,82	0
55	MG	BA	3029	1/1	0.99	0.42	11.58	35,35,35,35	0
55	MG	DA	3127	1/1	0.94	0.40	11.55	74,74,74,74	0
55	MG	BA	3178	1/1	0.97	0.35	11.54	36,36,36,36	0
55	MG	CA	1646	1/1	0.95	0.37	11.53	76,76,76,76	0
55	MG	DA	3131	1/1	0.85	0.25	11.51	79,79,79,79	0
55	MG	CA	1606	1/1	0.90	0.35	11.40	87,87,87,87	0
55	MG	DA	3101	1/1	0.98	0.33	11.40	43,43,43,43	0
55	MG	BA	3211	1/1	0.88	0.46	11.37	39,39,39,39	0
55	MG	DA	3069	1/1	0.93	0.44	11.27	60,60,60,60	0
55	MG	BA	3138	1/1	0.96	0.47	11.23	46,46,46,46	0
55	MG	DA	3266	1/1	0.91	0.51	11.13	55,55,55,55	0
55	MG	DA	3187	1/1	0.80	0.45	11.10	42,42,42,42	0
55	MG	DA	3055	1/1	0.89	0.54	11.07	68,68,68,68	0
55	MG	CA	1648	1/1	0.88	0.42	10.92	65,65,65,65	0
55	MG	AA	1645	1/1	0.92	0.47	10.86	50,50,50,50	0
55	MG	CA	1754	1/1	0.98	0.32	10.82	86,86,86,86	0
55	MG	DA	3110	1/1	0.96	0.33	10.72	58,58,58,58	0
55	MG	AA	1663	1/1	0.91	0.27	10.71	47,47,47,47	0
55	MG	BA	3307	1/1	0.94	0.48	10.60	39,39,39,39	0
55	MG	BA	3183	1/1	0.97	0.30	10.49	47,47,47,47	0
55	MG	DB	207	1/1	0.55	0.33	10.48	115,115,115,115	0
55	MG	BA	3037	1/1	0.94	0.38	10.46	44,44,44,44	0
55	MG	BA	3186	1/1	0.97	0.42	10.42	36,36,36,36	0
55	MG	BA	3018	1/1	0.99	0.35	10.35	54,54,54,54	0
55	MG	DA	3331	1/1	0.95	0.55	10.24	50,50,50,50	0
55	MG	DA	3303	1/1	0.57	0.40	10.21	70,70,70,70	0
55	MG	BA	3389	1/1	0.93	0.23	10.20	59,59,59,59	0
55	MG	BA	3062	1/1	0.96	0.29	10.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3239	1/1	0.97	0.36	10.11	45,45,45,45	0
55	MG	CA	1803	1/1	0.88	0.30	10.06	96,96,96,96	0
55	MG	BA	3216	1/1	0.99	0.32	10.03	33,33,33,33	0
55	MG	DA	3420	1/1	0.97	0.31	9.86	67,67,67,67	0
55	MG	CA	1722	1/1	0.96	0.38	9.83	75,75,75,75	0
55	MG	BA	3319	1/1	0.87	0.28	9.83	65,65,65,65	0
55	MG	BA	3411	1/1	0.85	0.30	9.83	68,68,68,68	0
55	MG	AA	1602	1/1	0.97	0.33	9.68	79,79,79,79	0
55	MG	AA	1795	1/1	0.86	0.23	9.54	73,73,73,73	0
55	MG	BA	3064	1/1	0.95	0.29	9.50	49,49,49,49	0
55	MG	CA	1657	1/1	0.88	0.27	9.48	95,95,95,95	0
55	MG	BA	3375	1/1	0.87	0.25	9.45	50,50,50,50	0
55	MG	CA	1685	1/1	0.96	0.37	9.34	93,93,93,93	0
55	MG	DA	3274	1/1	0.78	0.30	9.33	87,87,87,87	0
55	MG	DA	3033	1/1	0.94	0.25	9.33	62,62,62,62	0
55	MG	BA	3025	1/1	0.94	0.36	9.13	42,42,42,42	0
55	MG	AA	1667	1/1	0.95	0.33	9.03	68,68,68,68	0
55	MG	AA	1783	1/1	0.98	0.60	8.83	67,67,67,67	0
55	MG	DA	3299	1/1	0.96	0.33	8.71	38,38,38,38	0
55	MG	CA	1650	1/1	0.98	0.26	8.67	102,102,102,102	0
55	MG	CA	1640	1/1	0.91	0.33	8.66	81,81,81,81	0
55	MG	DA	3326	1/1	0.93	0.36	8.62	70,70,70,70	0
55	MG	CA	1777	1/1	0.81	0.30	8.52	88,88,88,88	0
55	MG	DA	3162	1/1	0.97	0.38	8.51	66,66,66,66	0
55	MG	DA	3132	1/1	0.97	0.31	8.38	53,53,53,53	0
55	MG	BA	3619	1/1	0.89	0.33	8.38	69,69,69,69	0
55	MG	B1	201	1/1	0.93	0.30	8.23	47,47,47,47	0
55	MG	DA	3144	1/1	0.98	0.29	8.19	60,60,60,60	0
55	MG	BA	3158	1/1	0.98	0.32	8.19	41,41,41,41	0
55	MG	AA	1608	1/1	0.93	0.26	8.15	64,64,64,64	0
55	MG	DA	3335	1/1	0.70	0.21	8.09	61,61,61,61	0
55	MG	BA	3156	1/1	0.93	0.29	8.05	40,40,40,40	0
55	MG	BA	3346	1/1	0.93	0.33	7.92	51,51,51,51	0
55	MG	AA	1632	1/1	0.96	0.25	7.92	67,67,67,67	0
55	MG	CA	1678	1/1	0.92	0.23	7.81	70,70,70,70	0
55	MG	DA	3222	1/1	0.97	0.50	7.78	60,60,60,60	0
55	MG	BA	3076	1/1	0.94	0.33	7.72	68,68,68,68	0
55	MG	DA	3452	1/1	0.95	0.21	7.58	83,83,83,83	0
55	MG	BA	3184	1/1	0.96	0.23	7.55	39,39,39,39	0
55	MG	AA	1628	1/1	0.92	0.35	7.37	69,69,69,69	0
55	MG	DA	3284	1/1	0.97	0.33	7.34	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3237	1/1	0.85	0.27	7.24	83,83,83,83	0
55	MG	DA	3134	1/1	0.74	0.28	7.24	72,72,72,72	0
55	MG	DA	3285	1/1	0.91	0.25	7.19	50,50,50,50	0
55	MG	CA	1758	1/1	0.71	0.46	7.12	78,78,78,78	0
55	MG	BA	3024	1/1	0.98	0.38	7.09	27,27,27,27	0
55	MG	AC	107	1/1	0.86	0.28	7.03	94,94,94,94	0
55	MG	AA	1789	1/1	0.96	0.29	6.97	74,74,74,74	0
55	MG	DA	3427	1/1	0.84	0.28	6.92	76,76,76,76	0
55	MG	BA	3181	1/1	0.97	0.35	6.74	39,39,39,39	0
55	MG	CA	1610	1/1	0.92	0.27	6.69	97,97,97,97	0
55	MG	DA	3369	1/1	0.89	0.27	6.60	74,74,74,74	0
55	MG	CA	1622	1/1	0.95	0.33	6.53	95,95,95,95	0
55	MG	DA	3233	1/1	0.97	0.42	6.40	52,52,52,52	0
55	MG	BA	3049	1/1	0.95	0.40	6.31	68,68,68,68	0
55	MG	BA	3196	1/1	0.98	0.32	6.28	33,33,33,33	0
55	MG	BA	3190	1/1	0.98	0.33	6.24	63,63,63,63	0
55	MG	BA	3056	1/1	0.93	0.21	6.10	54,54,54,54	0
55	MG	D1	201	1/1	0.89	0.39	6.08	71,71,71,71	0
55	MG	BA	3259	1/1	0.97	0.25	6.07	40,40,40,40	0
55	MG	CA	1784	1/1	0.87	0.23	6.05	81,81,81,81	0
55	MG	CA	1802	1/1	0.84	0.45	6.01	74,74,74,74	0
55	MG	AA	1699	1/1	0.92	0.26	6.01	64,64,64,64	0
55	MG	BA	3436	1/1	0.95	0.23	6.00	59,59,59,59	0
55	MG	DA	3191	1/1	0.97	0.55	5.93	46,46,46,46	0
55	MG	DA	3438	1/1	0.87	0.25	5.82	87,87,87,87	0
55	MG	BA	3270	1/1	0.89	0.22	5.73	76,76,76,76	0
55	MG	D1	202	1/1	0.46	0.46	5.72	89,89,89,89	0
55	MG	DA	3086	1/1	0.93	0.20	5.66	114,114,114,114	0
55	MG	BA	3199	1/1	0.97	0.42	5.60	49,49,49,49	0
55	MG	DA	3143	1/1	0.93	0.28	5.55	58,58,58,58	0
55	MG	AA	1762	1/1	0.95	0.21	5.40	80,80,80,80	0
55	MG	AA	1605	1/1	0.93	0.40	5.38	82,82,82,82	0
55	MG	AA	1722	1/1	0.89	0.46	5.31	68,68,68,68	0
55	MG	AA	1825	1/1	0.92	0.24	5.12	93,93,93,93	0
55	MG	BA	3293	1/1	0.91	0.26	5.09	65,65,65,65	0
55	MG	DA	3161	1/1	0.97	0.44	4.99	45,45,45,45	0
55	MG	DA	3052	1/1	0.98	0.45	4.96	71,71,71,71	0
55	MG	BA	3104	1/1	0.80	0.20	4.91	57,57,57,57	0
55	MG	DA	3201	1/1	0.98	0.25	4.86	47,47,47,47	0
55	MG	BA	3052	1/1	0.83	0.20	4.85	64,64,64,64	0
55	MG	CA	1604	1/1	0.80	0.17	4.80	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3495	1/1	0.96	0.20	4.74	63,63,63,63	0
55	MG	BA	3275	1/1	0.95	0.21	4.68	73,73,73,73	0
55	MG	CA	1749	1/1	0.78	0.20	4.50	89,89,89,89	0
55	MG	BB	217	1/1	0.79	0.19	4.48	98,98,98,98	0
55	MG	BA	3484	1/1	0.67	0.23	4.31	117,117,117,117	0
55	MG	BA	3098	1/1	0.76	0.25	4.30	48,48,48,48	0
55	MG	CA	1719	1/1	0.81	0.23	4.05	129,129,129,129	0
55	MG	BA	3478	1/1	0.95	0.23	3.91	63,63,63,63	0
55	MG	DA	3397	1/1	0.92	0.29	3.83	60,60,60,60	0
55	MG	DA	3159	1/1	0.96	0.26	3.83	37,37,37,37	0
55	MG	B0	201	1/1	0.98	0.32	3.82	51,51,51,51	0
55	MG	DA	3295	1/1	0.96	0.37	3.81	50,50,50,50	0
55	MG	DA	3317	1/1	0.95	0.22	3.80	81,81,81,81	0
55	MG	AA	1711	1/1	0.84	0.28	3.68	89,89,89,89	0
55	MG	AA	1636	1/1	0.93	0.28	3.68	87,87,87,87	0
55	MG	BA	3524	1/1	0.91	0.19	3.66	66,66,66,66	0
55	MG	BA	3093	1/1	0.93	0.27	3.54	57,57,57,57	0
55	MG	BA	3067	1/1	0.93	0.23	3.52	48,48,48,48	0
55	MG	DA	3215	1/1	0.97	0.42	3.52	42,42,42,42	0
55	MG	CA	1716	1/1	0.93	0.25	3.46	79,79,79,79	0
55	MG	CA	1798	1/1	0.82	0.21	3.35	85,85,85,85	0
55	MG	CS	101	1/1	0.61	0.30	3.32	87,87,87,87	0
55	MG	AA	1635	1/1	0.72	0.24	3.19	86,86,86,86	0
55	MG	BA	3514	1/1	0.85	0.31	3.16	71,71,71,71	0
55	MG	AA	1619	1/1	0.98	0.40	3.11	63,63,63,63	0
55	MG	BA	3297	1/1	0.94	0.22	3.04	58,58,58,58	0
55	MG	BA	3274	1/1	0.95	0.17	3.02	46,46,46,46	0
55	MG	BA	3532	1/1	0.88	0.22	2.83	85,85,85,85	0
55	MG	BA	3080	1/1	0.79	0.17	2.81	91,91,91,91	0
55	MG	DA	3230	1/1	0.90	0.16	2.78	59,59,59,59	0
55	MG	CA	1785	1/1	0.90	0.24	2.58	105,105,105,105	0
55	MG	AA	1682	1/1	0.86	0.16	2.39	91,91,91,91	0
55	MG	AA	1822	1/1	0.76	0.14	2.29	107,107,107,107	0
55	MG	BA	3584	1/1	0.86	0.18	2.14	72,72,72,72	0
55	MG	DE	303	1/1	0.96	0.35	2.14	56,56,56,56	0
55	MG	DA	3130	1/1	0.92	0.18	2.13	60,60,60,60	0
55	MG	DA	3121	1/1	0.96	0.17	2.12	64,64,64,64	0
55	MG	AA	1700	1/1	0.51	0.21	1.81	99,99,99,99	0
55	MG	AA	1701	1/1	0.92	0.19	1.77	70,70,70,70	0
55	MG	DA	3074	1/1	0.92	0.19	1.75	70,70,70,70	0
55	MG	BA	3380	1/1	0.96	0.17	1.70	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1625	1/1	0.83	0.22	1.69	90,90,90,90	0
55	MG	CA	1653	1/1	0.93	0.17	1.69	77,77,77,77	0
55	MG	CA	1617	1/1	0.95	0.24	1.64	93,93,93,93	0
55	MG	DA	3037	1/1	0.89	0.34	1.63	98,98,98,98	0
55	MG	AA	1729	1/1	0.84	0.36	1.61	113,113,113,113	0
55	MG	DE	302	1/1	0.88	0.27	1.59	65,65,65,65	0
55	MG	CA	1629	1/1	0.84	0.16	1.51	98,98,98,98	0
55	MG	BA	3510	1/1	0.88	0.15	1.38	108,108,108,108	0
55	MG	DA	3401	1/1	0.68	0.16	1.17	71,71,71,71	0
55	MG	BB	202	1/1	0.90	0.14	1.10	79,79,79,79	0
55	MG	CA	1669	1/1	0.80	0.19	0.96	60,60,60,60	0
55	MG	BE	302	1/1	0.97	0.23	0.95	56,56,56,56	0
55	MG	DA	3324	1/1	0.92	0.20	0.77	78,78,78,78	0
56	ZN	AG	302	1/1	0.97	0.34	0.70	95,95,95,95	0
55	MG	A1	101	1/1	0.95	0.17	0.69	66,66,66,66	0
55	MG	AA	1744	1/1	0.88	0.13	0.65	117,117,117,117	0
55	MG	BA	3614	1/1	0.81	0.17	0.56	69,69,69,69	0
55	MG	AA	1644	1/1	0.91	0.16	0.47	62,62,62,62	0
55	MG	DB	202	1/1	0.90	0.18	0.45	98,98,98,98	0
55	MG	AA	1764	1/1	0.91	0.17	0.26	79,79,79,79	0
55	MG	CA	1609	1/1	0.88	0.17	0.18	115,115,115,115	0
55	MG	BA	3136	1/1	0.94	0.16	0.11	74,74,74,74	0
55	MG	BA	3342	1/1	0.75	0.30	0.10	66,66,66,66	0
55	MG	DA	3489	1/1	0.91	0.16	-0.09	71,71,71,71	0
55	MG	BA	3060	1/1	0.89	0.17	-0.12	64,64,64,64	0
55	MG	BA	3191	1/1	0.84	0.21	-0.21	81,81,81,81	0
56	ZN	CG	303	1/1	0.98	0.31	-0.33	118,118,118,118	0
55	MG	AN	201	1/1	0.96	0.18	-0.38	68,68,68,68	0
55	MG	BA	3198	1/1	0.93	0.17	-0.41	45,45,45,45	0
55	MG	BA	3229	1/1	0.98	0.12	-0.84	50,50,50,50	0
55	MG	B8	101	1/1	0.85	0.19	-0.85	97,97,97,97	0
56	ZN	CQ	101	1/1	0.94	0.14	-0.97	120,120,120,120	0
55	MG	BA	3083	1/1	0.86	0.12	-0.97	62,62,62,62	0
56	ZN	AQ	102	1/1	0.98	0.09	-1.11	122,122,122,122	0
55	MG	CN	201	1/1	0.96	0.15	-1.14	74,74,74,74	0
55	MG	CA	1623	1/1	0.80	0.10	-1.19	90,90,90,90	0
55	MG	BA	3558	1/1	0.93	0.14	-1.21	63,63,63,63	0
55	MG	DA	3286	1/1	0.97	0.14	-1.24	47,47,47,47	0
55	MG	CG	302	1/1	0.86	0.14	-1.38	101,101,101,101	0
55	MG	BA	3250	1/1	0.82	0.15	-1.59	60,60,60,60	0
55	MG	BA	3224	1/1	0.94	0.11	-1.65	55,55,55,55	0
55	MG	BA	3490	1/1	0.28	0.08	-1.70	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BF	301	1/1	0.95	0.07	-2.03	73,73,73,73	0
55	MG	CA	1631	1/1	0.91	0.11	-2.14	81,81,81,81	0
55	MG	DA	3077	1/1	0.86	0.11	-2.39	64,64,64,64	0
55	MG	CA	1698	1/1	0.86	0.09	-2.48	107,107,107,107	0
55	MG	DA	3323	1/1	0.94	0.14	-3.01	42,42,42,42	0
55	MG	AA	1797	1/1	0.83	0.11	-3.05	99,99,99,99	0
55	MG	CA	1674	1/1	0.96	0.12	-3.38	70,70,70,70	0
55	MG	BA	3063	1/1	0.97	0.13	-3.58	43,43,43,43	0
55	MG	AA	1606	1/1	0.96	0.07	-5.21	91,91,91,91	0
55	MG	BA	3208	1/1	0.92	0.10	-5.66	45,45,45,45	0
55	MG	DA	3152	1/1	0.91	0.07	-7.21	67,67,67,67	0
55	MG	AA	1692	1/1	0.90	0.13	-	115,115,115,115	0
55	MG	BB	207	1/1	0.96	0.18	-	83,83,83,83	0
55	MG	BA	3474	1/1	0.91	0.43	-	80,80,80,80	0
55	MG	BA	3493	1/1	0.94	0.37	-	63,63,63,63	0
55	MG	AA	1642	1/1	0.95	0.68	-	72,72,72,72	0
55	MG	BA	3019	1/1	0.99	0.44	-	66,66,66,66	0
55	MG	BA	3491	1/1	0.95	0.53	-	42,42,42,42	0
55	MG	CA	1775	1/1	0.93	0.40	-	72,72,72,72	0
55	MG	BA	3151	1/1	0.56	0.27	-	83,83,83,83	0
55	MG	BA	3549	1/1	0.92	0.34	-	68,68,68,68	0
55	MG	BA	3527	1/1	0.70	0.55	-	93,93,93,93	0
55	MG	BA	3485	1/1	0.85	0.26	-	80,80,80,80	0
55	MG	AA	1634	1/1	0.97	0.29	-	62,62,62,62	0
55	MG	BA	3086	1/1	0.68	0.31	-	95,95,95,95	0
55	MG	CA	1725	1/1	0.87	0.24	-	86,86,86,86	0
55	MG	AA	1676	1/1	0.94	0.38	-	70,70,70,70	0
55	MG	DA	3279	1/1	0.90	0.24	-	84,84,84,84	0
55	MG	BA	3567	1/1	0.97	0.23	-	80,80,80,80	0
55	MG	BA	3568	1/1	0.94	0.39	-	83,83,83,83	0
55	MG	DA	3363	1/1	0.86	0.79	-	79,79,79,79	0
55	MG	CA	1656	1/1	0.84	0.30	-	92,92,92,92	0
55	MG	BA	3414	1/1	0.92	0.13	-	72,72,72,72	0
55	MG	BA	3489	1/1	0.88	0.24	-	70,70,70,70	0
55	MG	AA	1777	1/1	0.62	0.38	-	90,90,90,90	0
55	MG	DA	3089	1/1	0.93	0.54	-	82,82,82,82	0
55	MG	DA	3461	1/1	0.66	0.23	-	84,84,84,84	0
55	MG	DA	3357	1/1	0.51	0.29	-	96,96,96,96	0
55	MG	DA	3220	1/1	0.89	0.36	-	66,66,66,66	0
55	MG	AA	1820	1/1	0.77	0.30	-	75,75,75,75	0
55	MG	CA	1692	1/1	0.96	0.49	-	82,82,82,82	0
55	MG	DA	3182	1/1	0.99	0.81	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3469	1/1	0.93	0.60	-	80,80,80,80	0
55	MG	DA	3273	1/1	0.66	0.19	-	99,99,99,99	0
55	MG	BA	3212	1/1	0.98	0.61	-	43,43,43,43	0
55	MG	BA	3045	1/1	0.98	0.41	-	45,45,45,45	0
55	MG	BA	3457	1/1	0.81	0.91	-	88,88,88,88	0
55	MG	DA	3141	1/1	0.97	0.52	-	38,38,38,38	0
55	MG	BA	3481	1/1	0.73	0.55	-	69,69,69,69	0
55	MG	DA	3045	1/1	0.78	0.54	-	94,94,94,94	0
55	MG	DA	3439	1/1	0.88	0.33	-	62,62,62,62	0
55	MG	BA	3466	1/1	0.75	0.44	-	97,97,97,97	0
55	MG	DA	3202	1/1	0.97	0.43	-	47,47,47,47	0
55	MG	AA	1821	1/1	0.88	0.23	-	75,75,75,75	0
55	MG	DA	3480	1/1	0.69	0.41	-	63,63,63,63	0
55	MG	BA	3278	1/1	0.91	0.42	-	81,81,81,81	0
55	MG	BE	305	1/1	0.88	0.42	-	71,71,71,71	0
55	MG	DA	3493	1/1	0.76	0.55	-	82,82,82,82	0
55	MG	DA	3334	1/1	0.94	0.56	-	68,68,68,68	0
55	MG	DA	3409	1/1	0.78	0.50	-	76,76,76,76	0
55	MG	AA	1719	1/1	0.81	0.60	-	79,79,79,79	0
55	MG	AA	1728	1/1	0.82	0.12	-	108,108,108,108	0
55	MG	DA	3377	1/1	0.88	0.22	-	98,98,98,98	0
55	MG	DA	3036	1/1	0.95	0.21	-	99,99,99,99	0
55	MG	AA	1826	1/1	0.73	0.12	-	101,101,101,101	0
55	MG	DA	3443	1/1	0.94	0.35	-	80,80,80,80	0
55	MG	AA	1799	1/1	0.94	0.33	-	78,78,78,78	0
55	MG	BA	3325	1/1	0.52	0.43	-	76,76,76,76	0
55	MG	DA	3123	1/1	0.79	0.25	-	83,83,83,83	0
55	MG	DA	3246	1/1	0.97	0.43	-	53,53,53,53	0
55	MG	CA	1660	1/1	0.69	0.17	-	85,85,85,85	0
55	MG	BA	3594	1/1	0.97	0.55	-	79,79,79,79	0
55	MG	BA	3366	1/1	0.80	1.04	-	94,94,94,94	0
55	MG	BA	3382	1/1	0.98	0.39	-	43,43,43,43	0
55	MG	CA	1641	1/1	0.74	0.29	-	66,66,66,66	0
55	MG	DA	3416	1/1	0.92	0.49	-	59,59,59,59	0
55	MG	DA	3002	1/1	0.83	0.33	-	93,93,93,93	0
55	MG	DA	3498	1/1	0.90	0.24	-	85,85,85,85	0
55	MG	DA	3434	1/1	0.87	0.15	-	74,74,74,74	0
55	MG	DA	3474	1/1	0.99	0.60	-	83,83,83,83	0
55	MG	DA	3368	1/1	0.88	0.72	-	73,73,73,73	0
55	MG	DA	3428	1/1	0.88	0.58	-	84,84,84,84	0
55	MG	BA	3280	1/1	0.94	0.52	-	50,50,50,50	0
55	MG	AA	1708	1/1	0.79	0.40	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3240	1/1	0.98	0.55	-	42,42,42,42	0
55	MG	AA	1706	1/1	0.77	0.46	-	74,74,74,74	0
55	MG	DA	3338	1/1	0.70	0.32	-	86,86,86,86	0
55	MG	DA	3325	1/1	0.93	0.54	-	73,73,73,73	0
55	MG	CA	1772	1/1	0.84	0.29	-	72,72,72,72	0
55	MG	AA	1775	1/1	0.93	0.12	-	79,79,79,79	0
55	MG	DA	3030	1/1	0.92	0.40	-	74,74,74,74	0
55	MG	CA	1612	1/1	0.78	0.51	-	82,82,82,82	0
55	MG	BA	3577	1/1	0.94	0.18	-	73,73,73,73	0
55	MG	DA	3108	1/1	0.96	0.33	-	54,54,54,54	0
55	MG	BA	3246	1/1	0.91	0.40	-	68,68,68,68	0
55	MG	AA	1773	1/1	0.89	0.26	-	87,87,87,87	0
55	MG	CA	1687	1/1	0.89	0.17	-	89,89,89,89	0
55	MG	DA	3022	1/1	0.95	0.55	-	60,60,60,60	0
55	MG	AA	1778	1/1	0.87	0.14	-	106,106,106,106	0
55	MG	BA	3017	1/1	0.98	0.46	-	25,25,25,25	0
55	MG	BA	3010	1/1	0.96	0.41	-	46,46,46,46	0
55	MG	BA	3494	1/1	0.89	0.77	-	76,76,76,76	0
55	MG	BA	3188	1/1	0.97	0.37	-	60,60,60,60	0
55	MG	BA	3589	1/1	0.89	0.31	-	41,41,41,41	0
55	MG	AA	1782	1/1	0.73	0.19	-	96,96,96,96	0
55	MG	BA	3312	1/1	0.94	0.48	-	57,57,57,57	0
55	MG	DA	3088	1/1	0.74	0.24	-	96,96,96,96	0
55	MG	CA	1787	1/1	0.82	0.13	-	87,87,87,87	0
55	MG	AA	1616	1/1	0.77	0.18	-	94,94,94,94	0
55	MG	BA	3400	1/1	0.84	0.52	-	80,80,80,80	0
55	MG	BA	3587	1/1	0.90	0.32	-	64,64,64,64	0
55	MG	BA	3448	1/1	0.88	0.43	-	100,100,100,100	0
55	MG	AA	1657	1/1	0.97	0.45	-	50,50,50,50	0
55	MG	BA	3435	1/1	0.89	0.28	-	65,65,65,65	0
55	MG	AA	1801	1/1	0.91	0.50	-	84,84,84,84	0
55	MG	DA	3313	1/1	0.92	0.29	-	85,85,85,85	0
55	MG	AA	1684	1/1	0.84	0.18	-	90,90,90,90	0
55	MG	BA	3605	1/1	0.96	0.51	-	47,47,47,47	0
55	MG	BA	3131	1/1	0.99	0.32	-	59,59,59,59	0
55	MG	AA	1823	1/1	0.83	0.44	-	77,77,77,77	0
55	MG	DA	3042	1/1	0.62	0.50	-	81,81,81,81	0
55	MG	CA	1608	1/1	0.84	0.30	-	81,81,81,81	0
55	MG	AA	1780	1/1	0.95	0.26	-	86,86,86,86	0
55	MG	AA	1714	1/1	0.95	0.32	-	107,107,107,107	0
55	MG	BA	3445	1/1	0.88	0.35	-	79,79,79,79	0
55	MG	CA	1760	1/1	0.88	0.27	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3252	1/1	0.83	0.43	-	67,67,67,67	0
55	MG	DA	3244	1/1	0.96	0.46	-	71,71,71,71	0
55	MG	BA	3327	1/1	0.74	0.20	-	70,70,70,70	0
55	MG	AA	1741	1/1	0.96	0.31	-	67,67,67,67	0
55	MG	AA	1654	1/1	0.92	0.44	-	75,75,75,75	0
55	MG	BA	3597	1/1	0.82	0.23	-	79,79,79,79	0
55	MG	BA	3189	1/1	0.98	0.39	-	49,49,49,49	0
55	MG	DA	3485	1/1	0.74	0.20	-	81,81,81,81	0
55	MG	CC	104	1/1	0.75	0.59	-	89,89,89,89	0
55	MG	DA	3072	1/1	0.81	0.44	-	112,112,112,112	0
55	MG	AA	1695	1/1	0.94	0.23	-	90,90,90,90	0
55	MG	AA	1737	1/1	0.88	0.55	-	83,83,83,83	0
55	MG	CC	103	1/1	0.95	1.01	-	72,72,72,72	0
55	MG	BA	3391	1/1	0.85	0.46	-	86,86,86,86	0
55	MG	AA	1839	1/1	0.85	0.37	-	74,74,74,74	0
55	MG	AA	1707	1/1	0.98	0.58	-	50,50,50,50	0
55	MG	AA	1731	1/1	0.63	0.30	-	103,103,103,103	0
55	MG	AA	1620	1/1	0.95	0.28	-	66,66,66,66	0
55	MG	DA	3422	1/1	0.68	0.39	-	84,84,84,84	0
55	MG	BA	3057	1/1	0.70	0.14	-	70,70,70,70	0
55	MG	BA	3379	1/1	0.59	0.45	-	82,82,82,82	0
55	MG	AA	1781	1/1	0.71	0.44	-	94,94,94,94	0
55	MG	DA	3229	1/1	0.92	0.50	-	62,62,62,62	0
55	MG	CA	1723	1/1	0.86	0.07	-	86,86,86,86	0
55	MG	BA	3288	1/1	0.92	0.46	-	76,76,76,76	0
55	MG	BA	3165	1/1	0.94	0.56	-	61,61,61,61	0
55	MG	BA	3607	1/1	0.84	0.34	-	96,96,96,96	0
55	MG	BA	3277	1/1	0.81	0.30	-	86,86,86,86	0
55	MG	BA	3450	1/1	0.94	0.18	-	54,54,54,54	0
55	MG	DA	3437	1/1	0.90	0.20	-	87,87,87,87	0
55	MG	BA	3585	1/1	0.97	0.38	-	60,60,60,60	0
55	MG	CA	1639	1/1	0.89	0.36	-	95,95,95,95	0
55	MG	BA	3225	1/1	0.89	0.17	-	65,65,65,65	0
55	MG	BA	3336	1/1	0.90	0.47	-	66,66,66,66	0
55	MG	BA	3368	1/1	0.75	0.30	-	88,88,88,88	0
55	MG	BA	3339	1/1	0.77	0.58	-	88,88,88,88	0
55	MG	CA	1732	1/1	0.80	0.21	-	109,109,109,109	0
55	MG	BA	3612	1/1	0.94	0.44	-	66,66,66,66	0
55	MG	DA	3382	1/1	0.96	0.52	-	78,78,78,78	0
55	MG	CA	1795	1/1	0.96	0.29	-	76,76,76,76	0
55	MG	BA	3536	1/1	0.78	0.68	-	73,73,73,73	0
55	MG	DA	3028	1/1	0.68	0.22	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1750	1/1	0.97	0.54	-	62,62,62,62	0
55	MG	DA	3171	1/1	0.98	0.34	-	63,63,63,63	0
55	MG	DA	3342	1/1	0.84	0.42	-	82,82,82,82	0
55	MG	DA	3347	1/1	0.84	0.12	-	75,75,75,75	0
55	MG	BA	3569	1/1	0.88	0.54	-	85,85,85,85	0
55	MG	DA	3448	1/1	0.81	0.71	-	79,79,79,79	0
55	MG	AA	1726	1/1	0.95	0.48	-	81,81,81,81	0
55	MG	DA	3238	1/1	0.95	0.42	-	60,60,60,60	0
55	MG	DA	3526	1/1	0.88	0.31	-	68,68,68,68	0
55	MG	DA	3035	1/1	0.94	0.26	-	62,62,62,62	0
55	MG	CA	1742	1/1	0.88	0.15	-	97,97,97,97	0
55	MG	AA	1669	1/1	0.95	0.43	-	68,68,68,68	0
55	MG	BA	3350	1/1	0.84	0.32	-	55,55,55,55	0
55	MG	BA	3026	1/1	0.96	0.31	-	47,47,47,47	0
55	MG	BU	201	1/1	0.96	0.25	-	81,81,81,81	0
55	MG	CA	1677	1/1	0.81	0.42	-	73,73,73,73	0
55	MG	BA	3561	1/1	0.97	0.31	-	74,74,74,74	0
55	MG	BA	3476	1/1	0.82	0.26	-	81,81,81,81	0
55	MG	BA	3255	1/1	0.98	0.38	-	46,46,46,46	0
55	MG	CA	1670	1/1	0.94	0.49	-	56,56,56,56	0
55	MG	BA	3438	1/1	0.81	0.41	-	91,91,91,91	0
55	MG	CA	1703	1/1	0.93	0.27	-	94,94,94,94	0
55	MG	BA	3243	1/1	0.96	0.48	-	48,48,48,48	0
55	MG	DU	201	1/1	0.81	0.15	-	72,72,72,72	0
55	MG	DA	3402	1/1	0.68	0.32	-	101,101,101,101	0
55	MG	CA	1779	1/1	0.94	0.33	-	72,72,72,72	0
55	MG	DA	3391	1/1	0.89	0.23	-	78,78,78,78	0
55	MG	DA	3370	1/1	0.86	0.10	-	67,67,67,67	0
55	MG	B2	201	1/1	0.86	0.42	-	85,85,85,85	0
55	MG	BA	3254	1/1	0.96	0.34	-	43,43,43,43	0
55	MG	DA	3117	1/1	0.85	0.38	-	78,78,78,78	0
55	MG	DA	3252	1/1	0.97	0.32	-	64,64,64,64	0
55	MG	BA	3395	1/1	0.88	0.31	-	72,72,72,72	0
55	MG	AA	1687	1/1	0.93	0.32	-	72,72,72,72	0
55	MG	BA	3451	1/1	0.90	0.48	-	65,65,65,65	0
55	MG	CA	1602	1/1	0.92	0.28	-	80,80,80,80	0
55	MG	BA	3447	1/1	0.89	0.49	-	71,71,71,71	0
55	MG	BF	302	1/1	0.88	0.22	-	72,72,72,72	0
55	MG	DA	3463	1/1	0.99	0.20	-	73,73,73,73	0
55	MG	BA	3123	1/1	0.98	0.21	-	51,51,51,51	0
55	MG	CA	1759	1/1	0.67	0.37	-	103,103,103,103	0
55	MG	BA	3506	1/1	0.87	0.37	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1780	1/1	0.85	0.32	-	88,88,88,88	0
55	MG	DA	3356	1/1	0.84	0.29	-	67,67,67,67	0
55	MG	DA	3091	1/1	0.79	0.31	-	92,92,92,92	0
55	MG	BA	3285	1/1	0.86	0.35	-	72,72,72,72	0
55	MG	BA	3143	1/1	0.94	0.68	-	72,72,72,72	0
55	MG	BA	3534	1/1	0.75	0.30	-	79,79,79,79	0
55	MG	CA	1636	1/1	0.83	0.27	-	78,78,78,78	0
55	MG	BA	3175	1/1	0.81	0.52	-	69,69,69,69	0
55	MG	DA	3477	1/1	0.84	0.60	-	89,89,89,89	0
55	MG	AA	1740	1/1	0.93	0.18	-	75,75,75,75	0
55	MG	DA	3151	1/1	0.61	0.25	-	85,85,85,85	0
55	MG	AA	1723	1/1	0.84	0.32	-	84,84,84,84	0
55	MG	DA	3025	1/1	0.82	1.38	-	84,84,84,84	0
55	MG	DA	3424	1/1	0.72	0.73	-	70,70,70,70	0
55	MG	BA	3147	1/1	0.95	0.15	-	55,55,55,55	0
55	MG	BA	3408	1/1	0.76	0.45	-	87,87,87,87	0
55	MG	CA	1626	1/1	0.81	0.18	-	93,93,93,93	0
55	MG	DA	3078	1/1	0.77	0.37	-	89,89,89,89	0
55	MG	DA	3312	1/1	0.77	0.29	-	85,85,85,85	0
55	MG	DA	3483	1/1	0.84	0.15	-	90,90,90,90	0
55	MG	BA	3301	1/1	0.81	0.32	-	76,76,76,76	0
55	MG	DA	3475	1/1	0.84	0.35	-	88,88,88,88	0
55	MG	DA	3211	1/1	0.98	0.49	-	42,42,42,42	0
55	MG	DA	3142	1/1	0.99	0.52	-	40,40,40,40	0
55	MG	BA	3236	1/1	0.93	0.44	-	52,52,52,52	0
55	MG	CA	1763	1/1	0.59	0.47	-	91,91,91,91	0
55	MG	CA	1615	1/1	0.88	0.22	-	81,81,81,81	0
55	MG	BA	3149	1/1	0.93	0.20	-	80,80,80,80	0
55	MG	DA	3518	1/1	0.91	0.41	-	83,83,83,83	0
55	MG	BA	3593	1/1	0.90	0.26	-	80,80,80,80	0
55	MG	DA	3417	1/1	0.81	0.22	-	81,81,81,81	0
55	MG	DA	3516	1/1	0.92	0.33	-	105,105,105,105	0
55	MG	DA	3306	1/1	0.86	0.54	-	65,65,65,65	0
55	MG	DA	3304	1/1	0.55	0.37	-	85,85,85,85	0
55	MG	DA	3511	1/1	0.89	0.43	-	76,76,76,76	0
55	MG	BA	3437	1/1	0.90	0.42	-	67,67,67,67	0
55	MG	CA	1671	1/1	0.96	0.56	-	49,49,49,49	0
55	MG	DA	3249	1/1	0.95	0.40	-	72,72,72,72	0
55	MG	BA	3292	1/1	0.90	0.40	-	85,85,85,85	0
55	MG	DA	3329	1/1	0.96	0.35	-	44,44,44,44	0
55	MG	CA	1638	1/1	0.71	0.34	-	101,101,101,101	0
55	MG	AA	1622	1/1	0.94	0.23	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3464	1/1	0.50	0.49	-	98,98,98,98	0
55	MG	CA	1720	1/1	0.83	0.49	-	102,102,102,102	0
55	MG	BA	3218	1/1	0.94	0.54	-	48,48,48,48	0
55	MG	DA	3327	1/1	0.82	0.34	-	61,61,61,61	0
55	MG	BA	3351	1/1	0.92	0.96	-	78,78,78,78	0
55	MG	AA	1841	1/1	0.98	0.38	-	59,59,59,59	0
55	MG	AA	1607	1/1	0.91	0.22	-	89,89,89,89	0
55	MG	CA	1614	1/1	0.73	0.38	-	86,86,86,86	0
55	MG	BA	3618	1/1	0.91	0.47	-	73,73,73,73	0
55	MG	DA	3216	1/1	0.95	0.30	-	49,49,49,49	0
55	MG	DA	3431	1/1	0.80	0.43	-	91,91,91,91	0
55	MG	DA	3484	1/1	0.83	0.40	-	83,83,83,83	0
55	MG	AA	1630	1/1	0.68	0.16	-	101,101,101,101	0
55	MG	DA	3419	1/1	0.78	0.45	-	84,84,84,84	0
55	MG	BA	3432	1/1	0.78	0.32	-	80,80,80,80	0
55	MG	CA	1696	1/1	0.67	0.37	-	91,91,91,91	0
55	MG	CA	1740	1/1	0.80	0.33	-	68,68,68,68	0
55	MG	AA	1734	1/1	0.89	0.19	-	96,96,96,96	0
55	MG	DA	3060	1/1	0.90	0.86	-	73,73,73,73	0
55	MG	BA	3041	1/1	0.99	0.31	-	46,46,46,46	0
55	MG	BA	3601	1/1	0.91	0.20	-	85,85,85,85	0
55	MG	BA	3364	1/1	0.87	0.45	-	82,82,82,82	0
55	MG	AA	1670	1/1	0.95	0.38	-	63,63,63,63	0
55	MG	DB	213	1/1	0.45	0.16	-	94,94,94,94	0
55	MG	BA	3213	1/1	0.97	0.56	-	49,49,49,49	0
55	MG	AA	1816	1/1	0.84	0.24	-	81,81,81,81	0
55	MG	CA	1645	1/1	0.74	0.22	-	86,86,86,86	0
55	MG	DA	3521	1/1	0.95	0.58	-	69,69,69,69	0
55	MG	BA	3576	1/1	0.95	0.41	-	74,74,74,74	0
55	MG	DA	3300	1/1	0.92	0.27	-	81,81,81,81	0
55	MG	BA	3413	1/1	0.93	0.52	-	78,78,78,78	0
55	MG	DA	3298	1/1	0.76	0.33	-	77,77,77,77	0
55	MG	BA	3338	1/1	0.92	0.21	-	71,71,71,71	0
55	MG	BA	3458	1/1	0.92	0.12	-	82,82,82,82	0
55	MG	DA	3208	1/1	0.93	0.47	-	74,74,74,74	0
55	MG	DA	3020	1/1	0.69	0.32	-	85,85,85,85	0
55	MG	AA	1611	1/1	0.79	0.18	-	92,92,92,92	0
55	MG	BA	3105	1/1	0.92	0.32	-	75,75,75,75	0
55	MG	DA	3013	1/1	0.95	0.53	-	56,56,56,56	0
55	MG	BA	3101	1/1	0.92	0.64	-	63,63,63,63	0
55	MG	AA	1612	1/1	0.71	0.14	-	91,91,91,91	0
55	MG	AA	1756	1/1	0.92	0.22	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3015	1/1	0.98	0.34	-	38,38,38,38	0
55	MG	DA	3515	1/1	0.87	0.63	-	82,82,82,82	0
55	MG	DA	3496	1/1	0.90	0.24	-	83,83,83,83	0
55	MG	BA	3434	1/1	0.92	0.51	-	75,75,75,75	0
55	MG	DA	3346	1/1	0.79	0.58	-	75,75,75,75	0
55	MG	DA	3386	1/1	0.94	0.48	-	61,61,61,61	0
55	MG	DB	210	1/1	0.82	0.38	-	71,71,71,71	0
55	MG	AA	1838	1/1	0.94	0.41	-	61,61,61,61	0
55	MG	DA	3017	1/1	0.91	0.37	-	75,75,75,75	0
55	MG	BA	3265	1/1	0.82	0.74	-	60,60,60,60	0
55	MG	DA	3243	1/1	0.95	0.51	-	79,79,79,79	0
55	MG	DA	3414	1/1	0.92	0.31	-	85,85,85,85	0
55	MG	DA	3491	1/1	0.46	0.61	-	103,103,103,103	0
55	MG	BA	3117	1/1	0.96	0.49	-	60,60,60,60	0
55	MG	AA	1627	1/1	0.98	0.32	-	53,53,53,53	0
55	MG	DA	3064	1/1	0.59	0.43	-	101,101,101,101	0
55	MG	DA	3487	1/1	0.37	0.39	-	95,95,95,95	0
55	MG	CA	1652	1/1	0.91	0.33	-	71,71,71,71	0
55	MG	AA	1798	1/1	0.95	0.25	-	58,58,58,58	0
55	MG	DA	3027	1/1	0.89	0.23	-	77,77,77,77	0
55	MG	BA	3200	1/1	0.93	0.39	-	62,62,62,62	0
55	MG	BA	3030	1/1	0.97	0.54	-	44,44,44,44	0
55	MG	BA	3545	1/1	0.92	0.38	-	69,69,69,69	0
55	MG	CA	1709	1/1	0.72	0.50	-	108,108,108,108	0
55	MG	BA	3337	1/1	0.94	0.30	-	72,72,72,72	0
55	MG	BA	3038	1/1	0.90	0.40	-	56,56,56,56	0
55	MG	BA	3215	1/1	0.85	0.48	-	74,74,74,74	0
55	MG	AC	105	1/1	0.85	0.50	-	93,93,93,93	0
55	MG	DA	3407	1/1	0.91	0.42	-	73,73,73,73	0
55	MG	DA	3044	1/1	0.91	0.29	-	73,73,73,73	0
55	MG	BA	3182	1/1	0.97	0.33	-	43,43,43,43	0
55	MG	BA	3107	1/1	0.95	0.43	-	36,36,36,36	0
55	MG	BA	3453	1/1	0.97	0.57	-	60,60,60,60	0
55	MG	AA	1748	1/1	0.92	0.42	-	84,84,84,84	0
55	MG	DA	3352	1/1	0.89	0.65	-	64,64,64,64	0
55	MG	AA	1818	1/1	0.95	0.60	-	76,76,76,76	0
55	MG	BA	3299	1/1	0.92	0.49	-	89,89,89,89	0
55	MG	BA	3205	1/1	0.91	0.33	-	80,80,80,80	0
55	MG	BA	3237	1/1	0.95	0.49	-	57,57,57,57	0
55	MG	AA	1827	1/1	0.95	0.28	-	87,87,87,87	0
55	MG	CA	1721	1/1	0.93	0.20	-	80,80,80,80	0
55	MG	DA	3384	1/1	0.85	0.42	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1680	1/1	0.68	0.29	-	80,80,80,80	0
55	MG	BA	3454	1/1	0.94	0.36	-	92,92,92,92	0
55	MG	BA	3425	1/1	0.89	0.51	-	91,91,91,91	0
55	MG	BA	3467	1/1	0.74	0.32	-	78,78,78,78	0
55	MG	CC	106	1/1	0.96	0.60	-	96,96,96,96	0
55	MG	DA	3309	1/1	0.84	0.21	-	94,94,94,94	0
55	MG	BA	3333	1/1	0.92	0.47	-	80,80,80,80	0
55	MG	BA	3517	1/1	0.84	0.54	-	70,70,70,70	0
55	MG	DA	3509	1/1	0.85	0.41	-	64,64,64,64	0
55	MG	AA	1617	1/1	0.80	0.50	-	69,69,69,69	0
55	MG	BB	213	1/1	0.94	0.45	-	66,66,66,66	0
55	MG	BA	3112	1/1	0.85	0.28	-	77,77,77,77	0
55	MG	BA	3177	1/1	0.95	0.51	-	57,57,57,57	0
55	MG	BB	211	1/1	0.94	0.28	-	92,92,92,92	0
55	MG	AA	1664	1/1	0.90	0.20	-	45,45,45,45	0
55	MG	AA	1743	1/1	0.88	0.11	-	107,107,107,107	0
55	MG	BA	3282	1/1	0.74	0.09	-	83,83,83,83	0
55	MG	BA	3209	1/1	0.96	0.47	-	39,39,39,39	0
55	MG	BA	3242	1/1	0.94	0.44	-	50,50,50,50	0
55	MG	BA	3071	1/1	0.91	0.23	-	70,70,70,70	0
55	MG	BA	3318	1/1	0.91	0.53	-	75,75,75,75	0
55	MG	CA	1601	1/1	0.87	0.31	-	96,96,96,96	0
55	MG	AC	109	1/1	0.88	0.41	-	82,82,82,82	0
55	MG	DA	3106	1/1	0.98	0.41	-	48,48,48,48	0
55	MG	AA	1615	1/1	0.89	0.55	-	105,105,105,105	0
55	MG	AA	1751	1/1	0.54	0.29	-	98,98,98,98	0
55	MG	DA	3041	1/1	0.86	0.41	-	86,86,86,86	0
55	MG	BA	3421	1/1	0.90	0.35	-	62,62,62,62	0
55	MG	CA	1799	1/1	0.97	0.31	-	96,96,96,96	0
55	MG	BA	3479	1/1	0.87	0.46	-	82,82,82,82	0
55	MG	CC	108	1/1	0.91	0.56	-	106,106,106,106	0
55	MG	BA	3048	1/1	0.92	0.54	-	77,77,77,77	0
55	MG	CA	1689	1/1	0.48	0.29	-	89,89,89,89	0
55	MG	AA	1715	1/1	0.57	0.27	-	115,115,115,115	0
55	MG	CA	1701	1/1	0.92	0.42	-	88,88,88,88	0
55	MG	AA	1730	1/1	0.81	0.42	-	78,78,78,78	0
55	MG	BA	3503	1/1	0.88	0.20	-	65,65,65,65	0
55	MG	BA	3424	1/1	0.88	0.65	-	72,72,72,72	0
55	MG	BA	3497	1/1	0.87	0.21	-	71,71,71,71	0
55	MG	CA	1733	1/1	0.91	0.43	-	69,69,69,69	0
55	MG	DA	3209	1/1	0.97	0.50	-	66,66,66,66	0
55	MG	AA	1746	1/1	0.95	0.41	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1655	1/1	0.90	0.37	-	87,87,87,87	0
55	MG	BA	3495	1/1	0.85	0.25	-	123,123,123,123	0
55	MG	AA	1694	1/1	0.88	0.12	-	91,91,91,91	0
55	MG	BA	3525	1/1	0.95	0.28	-	77,77,77,77	0
55	MG	BA	3359	1/1	0.83	0.43	-	79,79,79,79	0
55	MG	BA	3116	1/1	0.76	0.33	-	73,73,73,73	0
55	MG	DA	3004	1/1	0.83	0.48	-	99,99,99,99	0
55	MG	BA	3161	1/1	0.82	0.22	-	56,56,56,56	0
55	MG	DA	3296	1/1	0.99	0.66	-	51,51,51,51	0
55	MG	BA	3272	1/1	0.67	0.16	-	94,94,94,94	0
55	MG	DA	3341	1/1	0.81	0.52	-	84,84,84,84	0
55	MG	BA	3330	1/1	0.81	0.29	-	79,79,79,79	0
55	MG	DA	3120	1/1	0.67	0.26	-	90,90,90,90	0
55	MG	BA	3540	1/1	0.91	0.30	-	61,61,61,61	0
55	MG	DA	3205	1/1	0.95	0.54	-	67,67,67,67	0
55	MG	B3	101	1/1	0.81	0.55	-	71,71,71,71	0
55	MG	DA	3154	1/1	0.89	0.32	-	69,69,69,69	0
55	MG	BA	3352	1/1	0.95	0.35	-	76,76,76,76	0
55	MG	BA	3228	1/1	0.94	0.62	-	72,72,72,72	0
55	MG	DA	3272	1/1	0.94	0.28	-	64,64,64,64	0
55	MG	BA	3251	1/1	0.96	0.39	-	68,68,68,68	0
55	MG	DA	3353	1/1	0.72	0.75	-	93,93,93,93	0
55	MG	BA	3127	1/1	0.91	0.59	-	53,53,53,53	0
55	MG	BA	3523	1/1	0.86	0.60	-	70,70,70,70	0
55	MG	DA	3116	1/1	0.98	0.40	-	74,74,74,74	0
55	MG	BA	3455	1/1	0.87	0.24	-	76,76,76,76	0
55	MG	AA	1791	1/1	0.82	0.11	-	109,109,109,109	0
55	MG	BA	3553	1/1	0.91	0.22	-	78,78,78,78	0
55	MG	BA	3194	1/1	0.92	0.42	-	68,68,68,68	0
55	MG	BA	3283	1/1	0.98	0.38	-	49,49,49,49	0
55	MG	CA	1764	1/1	0.96	0.54	-	72,72,72,72	0
55	MG	DA	3148	1/1	0.94	0.48	-	75,75,75,75	0
55	MG	BA	3311	1/1	0.92	0.30	-	83,83,83,83	0
55	MG	BA	3324	1/1	0.72	0.50	-	73,73,73,73	0
55	MG	BA	3498	1/1	0.94	0.33	-	85,85,85,85	0
55	MG	DA	3478	1/1	0.81	0.32	-	80,80,80,80	0
55	MG	D3	101	1/1	0.97	0.43	-	66,66,66,66	0
55	MG	AA	1696	1/1	0.79	0.29	-	88,88,88,88	0
55	MG	DA	3436	1/1	0.88	0.30	-	98,98,98,98	0
55	MG	DA	3405	1/1	0.88	0.47	-	79,79,79,79	0
55	MG	AA	1771	1/1	0.91	0.11	-	70,70,70,70	0
55	MG	BA	3502	1/1	0.88	0.26	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1796	1/1	0.86	0.40	-	102,102,102,102	0
55	MG	CA	1681	1/1	0.81	0.52	-	72,72,72,72	0
55	MG	CA	1642	1/1	0.94	0.20	-	91,91,91,91	0
55	MG	CA	1753	1/1	0.85	0.26	-	123,123,123,123	0
55	MG	DA	3186	1/1	0.78	0.31	-	60,60,60,60	0
55	MG	BA	3316	1/1	0.93	0.50	-	69,69,69,69	0
55	MG	DA	3514	1/1	0.90	0.68	-	59,59,59,59	0
55	MG	DA	3503	1/1	0.83	0.65	-	80,80,80,80	0
55	MG	BA	3468	1/1	0.92	0.32	-	77,77,77,77	0
55	MG	CA	1743	1/1	0.94	0.49	-	80,80,80,80	0
55	MG	BA	3606	1/1	0.68	0.35	-	77,77,77,77	0
55	MG	AA	1769	1/1	0.68	0.14	-	104,104,104,104	0
55	MG	CA	1632	1/1	0.72	0.30	-	95,95,95,95	0
55	MG	DA	3476	1/1	0.80	0.33	-	107,107,107,107	0
55	MG	DB	205	1/1	0.83	0.36	-	69,69,69,69	0
55	MG	DA	3056	1/1	0.91	0.44	-	81,81,81,81	0
55	MG	BA	3358	1/1	0.86	0.37	-	74,74,74,74	0
55	MG	CA	1715	1/1	0.89	0.25	-	104,104,104,104	0
55	MG	DA	3396	1/1	0.74	0.25	-	82,82,82,82	0
55	MG	DA	3048	1/1	0.89	0.49	-	75,75,75,75	0
55	MG	DA	3308	1/1	0.93	0.38	-	97,97,97,97	0
55	MG	DA	3361	1/1	0.85	0.71	-	79,79,79,79	0
55	MG	BA	3320	1/1	0.97	0.27	-	62,62,62,62	0
55	MG	BA	3073	1/1	0.76	0.42	-	82,82,82,82	0
55	MG	BA	3480	1/1	0.96	0.51	-	50,50,50,50	0
55	MG	BF	303	1/1	0.89	0.48	-	66,66,66,66	0
55	MG	BA	3586	1/1	0.82	0.35	-	63,63,63,63	0
55	MG	CA	1768	1/1	0.87	0.41	-	84,84,84,84	0
55	MG	DA	3267	1/1	0.93	0.36	-	64,64,64,64	0
55	MG	BA	3385	1/1	0.78	0.16	-	87,87,87,87	0
55	MG	CA	1707	1/1	0.88	0.57	-	98,98,98,98	0
55	MG	DA	3172	1/1	0.93	0.10	-	88,88,88,88	0
55	MG	CA	1736	1/1	0.95	0.73	-	79,79,79,79	0
55	MG	AA	1641	1/1	0.94	0.37	-	57,57,57,57	0
55	MG	DA	3012	1/1	0.94	0.50	-	66,66,66,66	0
55	MG	AA	1716	1/1	0.86	0.22	-	92,92,92,92	0
55	MG	DA	3007	1/1	0.81	0.25	-	74,74,74,74	0
55	MG	DB	214	1/1	0.88	0.19	-	96,96,96,96	0
55	MG	AA	1662	1/1	0.72	0.64	-	81,81,81,81	0
55	MG	CA	1662	1/1	0.83	0.24	-	90,90,90,90	0
55	MG	BA	3500	1/1	0.58	0.28	-	97,97,97,97	0
55	MG	DA	3343	1/1	0.91	0.36	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1785	1/1	0.80	0.40	-	96,96,96,96	0
55	MG	BA	3486	1/1	0.93	0.41	-	80,80,80,80	0
55	MG	BA	3440	1/1	0.94	0.44	-	74,74,74,74	0
55	MG	CA	1710	1/1	0.98	0.28	-	106,106,106,106	0
55	MG	AA	1681	1/1	0.72	0.33	-	80,80,80,80	0
55	MG	BA	3373	1/1	0.95	0.44	-	64,64,64,64	0
55	MG	AB	105	1/1	0.76	0.19	-	110,110,110,110	0
55	MG	BA	3369	1/1	0.93	0.30	-	73,73,73,73	0
55	MG	CA	1734	1/1	0.79	0.25	-	93,93,93,93	0
55	MG	DA	3333	1/1	0.81	0.52	-	87,87,87,87	0
55	MG	BA	3513	1/1	0.91	0.41	-	90,90,90,90	0
55	MG	BA	3349	1/1	0.68	0.43	-	97,97,97,97	0
55	MG	BA	3170	1/1	0.95	0.48	-	55,55,55,55	0
55	MG	BA	3371	1/1	0.86	0.31	-	70,70,70,70	0
55	MG	BA	3397	1/1	0.71	0.24	-	81,81,81,81	0
55	MG	DA	3289	1/1	0.94	0.43	-	90,90,90,90	0
55	MG	BA	3331	1/1	0.89	0.42	-	65,65,65,65	0
55	MG	AA	1808	1/1	0.90	0.53	-	76,76,76,76	0
55	MG	DA	3291	1/1	0.87	0.59	-	65,65,65,65	0
55	MG	BA	3023	1/1	0.99	0.36	-	45,45,45,45	0
55	MG	BA	3531	1/1	0.88	0.36	-	53,53,53,53	0
55	MG	AA	1677	1/1	0.82	0.32	-	87,87,87,87	0
55	MG	BA	3522	1/1	0.95	0.48	-	82,82,82,82	0
55	MG	AA	1690	1/1	0.71	0.17	-	96,96,96,96	0
55	MG	AA	1805	1/1	0.92	0.35	-	65,65,65,65	0
55	MG	DA	3179	1/1	0.90	0.32	-	70,70,70,70	0
55	MG	DA	3350	1/1	0.67	0.25	-	91,91,91,91	0
55	MG	DA	3001	1/1	0.96	0.46	-	67,67,67,67	0
55	MG	BA	3383	1/1	0.98	0.22	-	71,71,71,71	0
55	MG	BA	3469	1/1	0.91	0.30	-	60,60,60,60	0
55	MG	DA	3082	1/1	0.92	0.38	-	91,91,91,91	0
55	MG	BA	3390	1/1	0.98	0.31	-	60,60,60,60	0
55	MG	AA	1693	1/1	0.88	0.16	-	87,87,87,87	0
55	MG	CA	1712	1/1	0.83	0.53	-	86,86,86,86	0
55	MG	DA	3259	1/1	0.91	0.26	-	72,72,72,72	0
55	MG	BA	3150	1/1	0.94	0.44	-	36,36,36,36	0
55	MG	CA	1724	1/1	0.94	0.51	-	84,84,84,84	0
55	MG	CA	1699	1/1	0.76	0.27	-	97,97,97,97	0
55	MG	BA	3449	1/1	0.90	0.36	-	80,80,80,80	0
55	MG	DA	3362	1/1	0.93	0.61	-	53,53,53,53	0
55	MG	DA	3153	1/1	0.95	0.31	-	70,70,70,70	0
55	MG	AA	1800	1/1	0.96	0.31	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3217	1/1	0.90	0.31	-	52,52,52,52	0
55	MG	BA	3604	1/1	0.96	0.11	-	61,61,61,61	0
55	MG	BA	3291	1/1	0.86	0.39	-	72,72,72,72	0
55	MG	BA	3515	1/1	0.94	0.21	-	72,72,72,72	0
55	MG	DA	3058	1/1	0.79	0.31	-	76,76,76,76	0
55	MG	BA	3084	1/1	0.80	0.53	-	82,82,82,82	0
55	MG	DA	3423	1/1	0.94	0.89	-	75,75,75,75	0
55	MG	DA	3071	1/1	0.93	0.24	-	81,81,81,81	0
55	MG	BA	3079	1/1	0.98	0.41	-	55,55,55,55	0
55	MG	BA	3370	1/1	0.82	0.46	-	56,56,56,56	0
55	MG	AA	1811	1/1	0.96	0.50	-	67,67,67,67	0
55	MG	CA	1705	1/1	0.94	0.47	-	80,80,80,80	0
55	MG	BA	3214	1/1	0.92	0.55	-	67,67,67,67	0
55	MG	DA	3425	1/1	0.74	0.25	-	81,81,81,81	0
55	MG	AA	1784	1/1	0.97	0.47	-	66,66,66,66	0
55	MG	AA	1637	1/1	0.82	0.18	-	98,98,98,98	0
55	MG	AA	1831	1/1	0.91	0.45	-	90,90,90,90	0
55	MG	DB	209	1/1	0.85	0.20	-	92,92,92,92	0
55	MG	DA	3207	1/1	0.93	0.57	-	66,66,66,66	0
55	MG	BA	3072	1/1	0.76	0.29	-	77,77,77,77	0
55	MG	DA	3282	1/1	0.94	0.44	-	69,69,69,69	0
55	MG	CA	1704	1/1	0.89	0.28	-	99,99,99,99	0
55	MG	CA	1790	1/1	0.84	0.19	-	110,110,110,110	0
55	MG	DA	3039	1/1	0.94	0.33	-	85,85,85,85	0
55	MG	BA	3166	1/1	0.84	0.62	-	72,72,72,72	0
55	MG	DA	3189	1/1	0.95	0.50	-	41,41,41,41	0
55	MG	BA	3566	1/1	0.91	0.29	-	88,88,88,88	0
55	MG	CA	1683	1/1	0.79	0.41	-	87,87,87,87	0
55	MG	BA	3461	1/1	0.39	0.27	-	91,91,91,91	0
55	MG	AA	1759	1/1	0.84	0.36	-	77,77,77,77	0
55	MG	DA	3345	1/1	0.95	0.39	-	64,64,64,64	0
55	MG	BA	3142	1/1	0.96	0.37	-	51,51,51,51	0
55	MG	CA	1611	1/1	0.87	0.89	-	93,93,93,93	0
55	MG	AA	1788	1/1	0.92	0.52	-	77,77,77,77	0
55	MG	AA	1646	1/1	0.96	0.41	-	67,67,67,67	0
55	MG	BA	3239	1/1	0.93	0.27	-	74,74,74,74	0
55	MG	BA	3431	1/1	0.74	0.71	-	88,88,88,88	0
55	MG	B5	101	1/1	0.94	0.35	-	45,45,45,45	0
55	MG	DA	3315	1/1	0.23	0.28	-	108,108,108,108	0
55	MG	DA	3075	1/1	0.82	0.35	-	79,79,79,79	0
55	MG	AA	1817	1/1	0.87	0.21	-	85,85,85,85	0
55	MG	DA	3512	1/1	0.80	0.48	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3016	1/1	0.95	0.43	-	78,78,78,78	0
55	MG	CA	1735	1/1	0.94	0.20	-	89,89,89,89	0
55	MG	DA	3003	1/1	0.90	0.29	-	64,64,64,64	0
55	MG	BA	3013	1/1	0.98	0.43	-	34,34,34,34	0
55	MG	DA	3294	1/1	0.91	0.23	-	64,64,64,64	0
55	MG	CA	1637	1/1	0.75	0.34	-	79,79,79,79	0
55	MG	AA	1618	1/1	0.84	0.27	-	82,82,82,82	0
55	MG	BA	3419	1/1	0.92	0.53	-	85,85,85,85	0
55	MG	BA	3221	1/1	0.96	0.37	-	60,60,60,60	0
55	MG	BA	3396	1/1	0.86	0.19	-	82,82,82,82	0
55	MG	BA	3535	1/1	0.90	0.44	-	80,80,80,80	0
55	MG	BA	3533	1/1	0.79	0.57	-	72,72,72,72	0
55	MG	DA	3093	1/1	0.91	0.20	-	80,80,80,80	0
55	MG	DA	3008	1/1	0.96	0.38	-	70,70,70,70	0
55	MG	DA	3051	1/1	0.84	0.27	-	85,85,85,85	0
55	MG	CA	1643	1/1	0.89	0.49	-	82,82,82,82	0
55	MG	CA	1800	1/1	0.87	0.32	-	78,78,78,78	0
55	MG	BA	3009	1/1	0.98	0.33	-	36,36,36,36	0
55	MG	BA	3571	1/1	0.80	0.36	-	92,92,92,92	0
55	MG	CA	1620	1/1	0.93	0.46	-	64,64,64,64	0
55	MG	DA	3322	1/1	0.92	0.54	-	70,70,70,70	0
55	MG	BA	3222	1/1	0.84	0.33	-	89,89,89,89	0
55	MG	CA	1793	1/1	0.95	0.34	-	91,91,91,91	0
55	MG	DA	3408	1/1	0.89	0.11	-	73,73,73,73	0
55	MG	BA	3356	1/1	0.86	0.51	-	70,70,70,70	0
55	MG	AA	1772	1/1	0.52	0.55	-	85,85,85,85	0
55	MG	BA	3281	1/1	0.90	0.54	-	72,72,72,72	0
55	MG	CA	1702	1/1	0.78	0.41	-	78,78,78,78	0
55	MG	DA	3441	1/1	0.53	0.10	-	137,137,137,137	0
55	MG	DA	3468	1/1	0.84	0.42	-	92,92,92,92	0
55	MG	DA	3268	1/1	0.93	0.48	-	69,69,69,69	0
55	MG	AA	1833	1/1	0.93	0.44	-	88,88,88,88	0
55	MG	DA	3241	1/1	0.96	0.47	-	46,46,46,46	0
55	MG	AB	101	1/1	0.84	0.28	-	90,90,90,90	0
55	MG	BO	202	1/1	0.89	0.23	-	37,37,37,37	0
55	MG	BA	3070	1/1	0.92	0.13	-	63,63,63,63	0
55	MG	CA	1738	1/1	0.96	0.41	-	63,63,63,63	0
55	MG	AA	1609	1/1	0.99	0.41	-	78,78,78,78	0
55	MG	BA	3599	1/1	0.94	0.47	-	69,69,69,69	0
55	MG	DA	3465	1/1	0.71	0.34	-	74,74,74,74	0
55	MG	DA	3293	1/1	0.91	0.47	-	75,75,75,75	0
55	MG	DA	3429	1/1	0.55	0.33	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3348	1/1	0.90	0.60	-	73,73,73,73	0
55	MG	DA	3517	1/1	0.66	0.40	-	84,84,84,84	0
55	MG	BA	3488	1/1	0.91	0.36	-	80,80,80,80	0
55	MG	BA	3317	1/1	0.77	0.73	-	89,89,89,89	0
55	MG	BA	3266	1/1	0.87	0.41	-	77,77,77,77	0
55	MG	BA	3417	1/1	0.73	0.27	-	99,99,99,99	0
55	MG	DA	3379	1/1	0.94	0.44	-	85,85,85,85	0
55	MG	CA	1718	1/1	0.91	0.07	-	92,92,92,92	0
55	MG	AC	102	1/1	0.88	0.67	-	93,93,93,93	0
55	MG	BB	210	1/1	0.79	0.40	-	64,64,64,64	0
55	MG	BA	3099	1/1	0.93	0.58	-	67,67,67,67	0
55	MG	AA	1803	1/1	0.84	0.29	-	91,91,91,91	0
55	MG	BA	3551	1/1	0.86	0.40	-	87,87,87,87	0
55	MG	DA	3482	1/1	0.87	0.45	-	81,81,81,81	0
55	MG	AB	103	1/1	0.69	0.30	-	111,111,111,111	0
55	MG	BA	3357	1/1	0.86	0.56	-	81,81,81,81	0
55	MG	BA	3578	1/1	0.87	0.35	-	81,81,81,81	0
55	MG	BA	3422	1/1	0.94	0.26	-	78,78,78,78	0
55	MG	AA	1666	1/1	0.94	0.52	-	62,62,62,62	0
55	MG	DA	3010	1/1	0.61	0.40	-	97,97,97,97	0
55	MG	BA	3118	1/1	0.88	0.42	-	61,61,61,61	0
55	MG	DA	3403	1/1	0.80	0.47	-	76,76,76,76	0
55	MG	BA	3402	1/1	0.72	0.27	-	91,91,91,91	0
55	MG	AA	1629	1/1	0.93	0.12	-	86,86,86,86	0
55	MG	BA	3544	1/1	0.90	0.41	-	72,72,72,72	0
55	MG	BA	3520	1/1	0.92	0.46	-	44,44,44,44	0
55	MG	DA	3455	1/1	0.87	0.29	-	69,69,69,69	0
55	MG	DA	3520	1/1	0.87	0.83	-	76,76,76,76	0
55	MG	BA	3047	1/1	0.94	0.41	-	74,74,74,74	0
55	MG	AB	104	1/1	0.89	0.35	-	82,82,82,82	0
55	MG	DA	3098	1/1	0.86	0.46	-	68,68,68,68	0
55	MG	CA	1801	1/1	0.83	0.28	-	89,89,89,89	0
55	MG	AC	106	1/1	0.83	0.56	-	89,89,89,89	0
55	MG	CA	1782	1/1	0.92	0.38	-	93,93,93,93	0
55	MG	CA	1783	1/1	0.85	0.47	-	100,100,100,100	0
55	MG	BA	3128	1/1	0.98	0.50	-	46,46,46,46	0
55	MG	DA	3292	1/1	0.85	0.24	-	89,89,89,89	0
55	MG	DA	3471	1/1	0.88	0.43	-	80,80,80,80	0
55	MG	AA	1757	1/1	0.84	0.06	-	110,110,110,110	0
55	MG	DA	3026	1/1	0.87	0.43	-	95,95,95,95	0
55	MG	BA	3167	1/1	0.89	0.38	-	73,73,73,73	0
55	MG	CA	1713	1/1	0.88	0.57	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1793	1/1	0.85	0.39	-	73,73,73,73	0
55	MG	BA	3087	1/1	0.71	0.38	-	77,77,77,77	0
55	MG	AA	1647	1/1	0.77	0.36	-	88,88,88,88	0
55	MG	AA	1672	1/1	0.94	0.33	-	87,87,87,87	0
55	MG	AA	1668	1/1	0.90	0.63	-	76,76,76,76	0
55	MG	AA	1626	1/1	0.86	0.46	-	69,69,69,69	0
55	MG	BA	3596	1/1	0.91	0.46	-	55,55,55,55	0
55	MG	DA	3040	1/1	0.88	0.14	-	81,81,81,81	0
55	MG	CA	1603	1/1	0.97	0.35	-	77,77,77,77	0
55	MG	DA	3344	1/1	0.73	0.33	-	95,95,95,95	0
55	MG	BA	3546	1/1	0.81	0.16	-	87,87,87,87	0
55	MG	DA	3288	1/1	0.97	0.37	-	47,47,47,47	0
55	MG	DA	3389	1/1	0.84	0.79	-	64,64,64,64	0
55	MG	BA	3573	1/1	0.73	0.46	-	83,83,83,83	0
55	MG	BD	301	1/1	0.59	0.62	-	85,85,85,85	0
55	MG	DA	3248	1/1	0.92	0.48	-	75,75,75,75	0
55	MG	DA	3440	1/1	0.81	0.36	-	86,86,86,86	0
55	MG	BA	3386	1/1	0.94	0.50	-	59,59,59,59	0
55	MG	DB	206	1/1	0.83	0.28	-	90,90,90,90	0
55	MG	DA	3090	1/1	0.88	0.33	-	86,86,86,86	0
55	MG	BA	3094	1/1	0.88	0.56	-	78,78,78,78	0
55	MG	BA	3114	1/1	0.88	0.20	-	74,74,74,74	0
55	MG	BA	3588	1/1	0.82	0.34	-	83,83,83,83	0
55	MG	AA	1698	1/1	0.81	0.33	-	72,72,72,72	0
55	MG	BA	3427	1/1	0.94	0.41	-	65,65,65,65	0
55	MG	BA	3465	1/1	0.55	0.46	-	93,93,93,93	0
55	MG	DA	3043	1/1	0.80	0.23	-	82,82,82,82	0
55	MG	CA	1695	1/1	0.96	0.50	-	87,87,87,87	0
55	MG	BA	3563	1/1	0.79	0.19	-	82,82,82,82	0
55	MG	BA	3129	1/1	0.97	0.44	-	52,52,52,52	0
55	MG	BA	3036	1/1	0.98	0.54	-	44,44,44,44	0
55	MG	BA	3219	1/1	0.91	0.43	-	76,76,76,76	0
55	MG	AA	1625	1/1	0.78	0.45	-	57,57,57,57	0
55	MG	AA	1830	1/1	0.87	0.30	-	73,73,73,73	0
55	MG	DA	3276	1/1	0.94	0.52	-	68,68,68,68	0
55	MG	BA	3459	1/1	0.91	0.42	-	70,70,70,70	0
55	MG	BA	3623	1/1	0.88	0.40	-	60,60,60,60	0
55	MG	AA	1787	1/1	0.89	0.47	-	96,96,96,96	0
55	MG	BA	3557	1/1	0.97	0.47	-	77,77,77,77	0
55	MG	CA	1675	1/1	0.95	0.48	-	62,62,62,62	0
55	MG	CA	1746	1/1	0.96	0.61	-	57,57,57,57	0
55	MG	BA	3562	1/1	0.94	0.30	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3441	1/1	0.82	0.20	-	86,86,86,86	0
55	MG	DB	204	1/1	0.87	0.28	-	82,82,82,82	0
55	MG	BA	3305	1/1	0.91	0.42	-	70,70,70,70	0
55	MG	AA	1705	1/1	0.81	0.31	-	83,83,83,83	0
55	MG	DA	3432	1/1	0.83	0.29	-	69,69,69,69	0
55	MG	BA	3069	1/1	0.77	0.45	-	77,77,77,77	0
55	MG	BA	3264	1/1	0.94	0.21	-	30,30,30,30	0
55	MG	BA	3286	1/1	0.94	0.28	-	66,66,66,66	0
55	MG	DA	3406	1/1	0.78	0.73	-	86,86,86,86	0
55	MG	BB	201	1/1	0.85	0.43	-	92,92,92,92	0
55	MG	BA	3227	1/1	0.69	0.40	-	91,91,91,91	0
55	MG	DA	3038	1/1	0.77	0.47	-	97,97,97,97	0
55	MG	DA	3076	1/1	0.90	0.37	-	86,86,86,86	0
55	MG	DA	3163	1/1	0.95	0.59	-	62,62,62,62	0
55	MG	DA	3494	1/1	0.67	0.21	-	75,75,75,75	0
55	MG	DA	3378	1/1	0.93	0.50	-	63,63,63,63	0
55	MG	BA	3276	1/1	0.97	0.23	-	74,74,74,74	0
55	MG	DE	301	1/1	0.99	0.38	-	41,41,41,41	0
55	MG	DA	3206	1/1	0.95	0.53	-	65,65,65,65	0
55	MG	AA	1770	1/1	0.70	0.25	-	102,102,102,102	0
55	MG	DB	203	1/1	0.88	0.33	-	66,66,66,66	0
55	MG	DA	3305	1/1	0.94	0.36	-	77,77,77,77	0
55	MG	BA	3326	1/1	0.95	0.34	-	52,52,52,52	0
55	MG	DA	3192	1/1	0.92	0.48	-	62,62,62,62	0
55	MG	DA	3251	1/1	0.79	0.27	-	74,74,74,74	0
55	MG	DA	3447	1/1	0.64	0.46	-	82,82,82,82	0
55	MG	BA	3471	1/1	0.87	0.31	-	72,72,72,72	0
55	MG	CA	1684	1/1	0.89	0.61	-	85,85,85,85	0
55	MG	BA	3621	1/1	0.88	0.15	-	63,63,63,63	0
55	MG	AA	1727	1/1	0.62	0.86	-	87,87,87,87	0
55	MG	DA	3170	1/1	0.95	0.44	-	68,68,68,68	0
55	MG	DA	3137	1/1	0.77	0.18	-	82,82,82,82	0
55	MG	AA	1819	1/1	0.83	0.35	-	87,87,87,87	0
55	MG	BA	3309	1/1	0.83	0.19	-	68,68,68,68	0
55	MG	DA	3140	1/1	0.85	0.28	-	78,78,78,78	0
55	MG	BA	3176	1/1	0.96	0.51	-	48,48,48,48	0
55	MG	BA	3496	1/1	0.82	0.26	-	96,96,96,96	0
55	MG	BA	3050	1/1	0.95	0.48	-	39,39,39,39	0
55	MG	BA	3121	1/1	0.74	0.48	-	57,57,57,57	0
55	MG	AA	1653	1/1	0.90	0.54	-	81,81,81,81	0
55	MG	DA	3079	1/1	0.98	0.38	-	54,54,54,54	0
55	MG	BA	3321	1/1	0.90	0.41	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1694	1/1	0.92	0.47	-	97,97,97,97	0
55	MG	AA	1776	1/1	0.83	0.18	-	82,82,82,82	0
55	MG	AA	1660	1/1	0.98	0.62	-	53,53,53,53	0
55	MG	AA	1832	1/1	0.81	0.35	-	94,94,94,94	0
55	MG	AA	1631	1/1	0.89	0.21	-	66,66,66,66	0
55	MG	DA	3247	1/1	0.83	0.20	-	87,87,87,87	0
55	MG	CA	1791	1/1	0.84	0.30	-	79,79,79,79	0
55	MG	AA	1834	1/1	0.86	0.48	-	97,97,97,97	0
55	MG	BA	3279	1/1	0.93	0.09	-	70,70,70,70	0
55	MG	DA	3479	1/1	0.80	0.11	-	99,99,99,99	0
55	MG	CB	101	1/1	0.81	0.20	-	101,101,101,101	0
55	MG	AA	1824	1/1	0.83	0.56	-	86,86,86,86	0
55	MG	CA	1778	1/1	0.90	0.40	-	96,96,96,96	0
55	MG	BA	3294	1/1	0.98	0.35	-	72,72,72,72	0
55	MG	BA	3085	1/1	0.92	0.17	-	73,73,73,73	0
55	MG	AA	1604	1/1	0.99	0.33	-	67,67,67,67	0
55	MG	BA	3155	1/1	0.98	0.18	-	45,45,45,45	0
55	MG	BA	3122	1/1	0.91	0.30	-	37,37,37,37	0
55	MG	CA	1756	1/1	0.79	0.40	-	81,81,81,81	0
55	MG	BA	3477	1/1	0.92	0.46	-	95,95,95,95	0
55	MG	AA	1650	1/1	0.92	0.49	-	71,71,71,71	0
55	MG	DA	3126	1/1	0.97	0.26	-	41,41,41,41	0
55	MG	CA	1605	1/1	0.92	0.38	-	76,76,76,76	0
55	MG	CA	1792	1/1	0.99	0.62	-	70,70,70,70	0
55	MG	AA	1683	1/1	0.84	0.20	-	87,87,87,87	0
55	MG	AA	1806	1/1	0.81	0.28	-	81,81,81,81	0
55	MG	BA	3347	1/1	0.92	0.43	-	68,68,68,68	0
55	MG	DA	3490	1/1	0.42	0.14	-	126,126,126,126	0
55	MG	DB	201	1/1	0.89	0.37	-	81,81,81,81	0
55	MG	BA	3381	1/1	0.89	0.44	-	90,90,90,90	0
55	MG	BA	3171	1/1	0.99	0.54	-	61,61,61,61	0
55	MG	BA	3003	1/1	0.95	0.44	-	47,47,47,47	0
55	MG	BA	3377	1/1	0.93	0.74	-	62,62,62,62	0
55	MG	DA	3365	1/1	0.93	0.53	-	58,58,58,58	0
55	MG	DA	3481	1/1	0.88	0.41	-	96,96,96,96	0
55	MG	CA	1781	1/1	0.89	0.05	-	117,117,117,117	0
55	MG	BA	3120	1/1	0.84	0.42	-	56,56,56,56	0
55	MG	BB	205	1/1	0.93	0.35	-	74,74,74,74	0
55	MG	BA	3501	1/1	0.92	0.24	-	55,55,55,55	0
55	MG	AA	1738	1/1	0.93	0.54	-	79,79,79,79	0
55	MG	DA	3232	1/1	0.96	0.42	-	44,44,44,44	0
55	MG	AA	1735	1/1	0.79	0.46	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3223	1/1	0.89	0.27	-	92,92,92,92	0
55	MG	DA	3394	1/1	0.76	0.20	-	90,90,90,90	0
55	MG	AA	1767	1/1	0.91	0.22	-	96,96,96,96	0
55	MG	DA	3415	1/1	0.75	0.54	-	96,96,96,96	0
55	MG	AA	1796	1/1	0.95	0.14	-	75,75,75,75	0
55	MG	BA	3322	1/1	0.90	0.63	-	64,64,64,64	0
55	MG	DP	201	1/1	0.97	0.35	-	65,65,65,65	0
55	MG	CA	1679	1/1	0.88	0.37	-	85,85,85,85	0
55	MG	BA	3077	1/1	0.97	0.45	-	54,54,54,54	0
55	MG	DA	3318	1/1	0.91	0.22	-	63,63,63,63	0
55	MG	BA	3141	1/1	0.94	0.48	-	35,35,35,35	0
55	MG	CA	1667	1/1	0.80	0.16	-	102,102,102,102	0
55	MG	CA	1682	1/1	0.92	0.38	-	86,86,86,86	0
55	MG	DA	3109	1/1	0.96	0.23	-	65,65,65,65	0
55	MG	DA	3168	1/1	0.87	0.29	-	49,49,49,49	0
55	MG	AA	1652	1/1	0.80	0.44	-	81,81,81,81	0
55	MG	DA	3092	1/1	0.81	0.30	-	68,68,68,68	0
55	MG	BA	3248	1/1	0.95	0.35	-	53,53,53,53	0
55	MG	BB	203	1/1	0.93	0.42	-	65,65,65,65	0
55	MG	AA	1829	1/1	0.91	0.55	-	77,77,77,77	0
55	MG	CA	1635	1/1	0.90	0.78	-	86,86,86,86	0
55	MG	DA	3373	1/1	0.90	0.43	-	79,79,79,79	0
55	MG	DA	3470	1/1	0.95	0.11	-	80,80,80,80	0
55	MG	AA	1774	1/1	0.90	0.12	-	91,91,91,91	0
55	MG	BA	3247	1/1	0.77	0.48	-	70,70,70,70	0
55	MG	DA	3297	1/1	0.80	0.23	-	83,83,83,83	0
55	MG	BA	3398	1/1	0.82	0.44	-	70,70,70,70	0
55	MG	AA	1842	1/1	0.98	0.46	-	59,59,59,59	0
55	MG	DA	3029	1/1	0.78	0.27	-	79,79,79,79	0
55	MG	DA	3430	1/1	0.86	0.58	-	62,62,62,62	0
55	MG	DA	3435	1/1	0.88	0.11	-	72,72,72,72	0
55	MG	BA	3412	1/1	0.78	0.35	-	78,78,78,78	0
55	MG	DA	3253	1/1	0.90	0.17	-	87,87,87,87	0
55	MG	DA	3459	1/1	0.68	0.28	-	86,86,86,86	0
55	MG	BA	3615	1/1	0.92	0.41	-	81,81,81,81	0
55	MG	CA	1607	1/1	0.92	0.43	-	85,85,85,85	0
55	MG	DA	3054	1/1	0.95	0.61	-	58,58,58,58	0
55	MG	CA	1680	1/1	0.93	0.55	-	68,68,68,68	0
55	MG	DA	3388	1/1	0.94	0.28	-	74,74,74,74	0
55	MG	AA	1815	1/1	0.83	0.46	-	84,84,84,84	0
55	MG	DA	3393	1/1	0.78	0.52	-	69,69,69,69	0
55	MG	BA	3487	1/1	0.91	0.10	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3242	1/1	0.91	0.58	-	63,63,63,63	0
55	MG	BA	3548	1/1	0.89	0.48	-	76,76,76,76	0
55	MG	AA	1673	1/1	0.89	0.47	-	78,78,78,78	0
55	MG	AA	1755	1/1	0.53	0.55	-	104,104,104,104	0
55	MG	DA	3360	1/1	0.93	0.39	-	65,65,65,65	0
55	MG	BA	3622	1/1	0.86	0.47	-	59,59,59,59	0
55	MG	AC	103	1/1	0.81	0.38	-	66,66,66,66	0
55	MG	BA	3384	1/1	0.92	0.24	-	73,73,73,73	0
55	MG	DA	3031	1/1	0.93	0.22	-	72,72,72,72	0
55	MG	AA	1814	1/1	0.94	0.32	-	83,83,83,83	0
55	MG	BA	3006	1/1	0.94	0.43	-	38,38,38,38	0
55	MG	BA	3470	1/1	0.91	0.31	-	88,88,88,88	0
55	MG	AA	1813	1/1	0.75	0.29	-	107,107,107,107	0
55	MG	CA	1794	1/1	0.91	0.34	-	74,74,74,74	0
55	MG	BA	3538	1/1	0.98	0.55	-	66,66,66,66	0
55	MG	CA	1630	1/1	0.71	0.45	-	91,91,91,91	0
55	MG	AA	1768	1/1	0.82	0.36	-	101,101,101,101	0
55	MG	DA	3508	1/1	0.73	0.70	-	80,80,80,80	0
55	MG	DA	3178	1/1	0.97	0.75	-	59,59,59,59	0
55	MG	DA	3442	1/1	0.88	0.22	-	91,91,91,91	0
55	MG	CC	101	1/1	0.66	0.36	-	92,92,92,92	0
55	MG	BB	209	1/1	0.79	0.40	-	102,102,102,102	0
55	MG	CA	1727	1/1	0.80	0.45	-	94,94,94,94	0
55	MG	BU	202	1/1	0.91	0.12	-	55,55,55,55	0
55	MG	BA	3164	1/1	0.85	0.68	-	86,86,86,86	0
55	MG	BA	3404	1/1	0.79	0.17	-	60,60,60,60	0
55	MG	BA	3418	1/1	0.76	0.41	-	78,78,78,78	0
55	MG	AA	1623	1/1	0.95	0.74	-	65,65,65,65	0
55	MG	DA	3219	1/1	0.97	0.24	-	70,70,70,70	0
55	MG	DA	3257	1/1	0.97	0.33	-	49,49,49,49	0
55	MG	BA	3132	1/1	0.90	0.41	-	71,71,71,71	0
55	MG	BA	3603	1/1	0.64	0.61	-	63,63,63,63	0
55	MG	AD	101	1/1	0.45	0.39	-	101,101,101,101	0
55	MG	BA	3555	1/1	0.97	0.23	-	38,38,38,38	0
55	MG	DA	3492	1/1	0.61	0.34	-	88,88,88,88	0
55	MG	DA	3160	1/1	0.97	0.40	-	49,49,49,49	0
55	MG	DA	3223	1/1	0.98	0.48	-	52,52,52,52	0
55	MG	BA	3295	1/1	0.84	0.44	-	81,81,81,81	0
55	MG	CA	1770	1/1	0.74	0.23	-	102,102,102,102	0
55	MG	DA	3488	1/1	0.89	0.58	-	86,86,86,86	0
55	MG	DA	3453	1/1	0.94	0.24	-	66,66,66,66	0
55	MG	AA	1763	1/1	0.95	0.58	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3387	1/1	0.79	0.29	-	92,92,92,92	0
55	MG	CA	1717	1/1	0.93	0.18	-	106,106,106,106	0
55	MG	BA	3348	1/1	0.86	0.29	-	61,61,61,61	0
55	MG	AA	1804	1/1	0.69	0.11	-	74,74,74,74	0
55	MG	BA	3303	1/1	0.91	0.38	-	72,72,72,72	0
55	MG	DA	3133	1/1	0.98	0.38	-	42,42,42,42	0
55	MG	DA	3287	1/1	0.84	0.64	-	65,65,65,65	0
55	MG	BA	3028	1/1	0.97	0.41	-	46,46,46,46	0
55	MG	BA	3230	1/1	0.98	0.59	-	56,56,56,56	0
55	MG	DA	3173	1/1	0.89	0.22	-	60,60,60,60	0
55	MG	BA	3341	1/1	0.76	0.25	-	81,81,81,81	0
55	MG	BA	3405	1/1	0.94	0.47	-	56,56,56,56	0
55	MG	CA	1621	1/1	0.95	0.36	-	66,66,66,66	0
55	MG	DA	3457	1/1	0.96	0.76	-	65,65,65,65	0
55	MG	BA	3078	1/1	0.96	0.37	-	65,65,65,65	0
55	MG	BA	3159	1/1	0.92	0.51	-	58,58,58,58	0
55	MG	BA	3392	1/1	0.85	0.39	-	70,70,70,70	0
55	MG	BB	214	1/1	0.79	0.24	-	86,86,86,86	0
55	MG	BA	3220	1/1	0.97	0.45	-	44,44,44,44	0
55	MG	AA	1745	1/1	0.88	0.56	-	67,67,67,67	0
55	MG	BA	3323	1/1	0.89	0.32	-	66,66,66,66	0
55	MG	BA	3148	1/1	0.94	0.41	-	32,32,32,32	0
55	MG	BA	3313	1/1	0.80	0.18	-	88,88,88,88	0
55	MG	CA	1737	1/1	0.84	0.28	-	99,99,99,99	0
55	MG	BA	3554	1/1	0.98	0.47	-	45,45,45,45	0
55	MG	DA	3059	1/1	0.70	0.77	-	106,106,106,106	0
55	MG	DA	3023	1/1	0.87	0.44	-	57,57,57,57	0
55	MG	BA	3241	1/1	0.96	0.49	-	60,60,60,60	0
55	MG	DA	3375	1/1	0.94	0.69	-	88,88,88,88	0
55	MG	D5	2001	1/1	0.98	0.41	-	46,46,46,46	0
55	MG	AA	1749	1/1	0.83	0.21	-	81,81,81,81	0
55	MG	BA	3168	1/1	0.96	0.36	-	49,49,49,49	0
55	MG	BA	3416	1/1	0.89	0.18	-	87,87,87,87	0
55	MG	DA	3418	1/1	0.93	0.41	-	78,78,78,78	0
55	MG	DA	3506	1/1	0.91	0.40	-	78,78,78,78	0
55	MG	CA	1658	1/1	0.93	0.45	-	91,91,91,91	0
55	MG	AA	1633	1/1	0.87	0.25	-	74,74,74,74	0
55	MG	CA	1773	1/1	0.83	0.73	-	92,92,92,92	0
55	MG	BA	3340	1/1	0.93	0.31	-	77,77,77,77	0
55	MG	CA	1708	1/1	0.92	0.09	-	97,97,97,97	0
55	MG	BA	3443	1/1	0.95	0.14	-	77,77,77,77	0
55	MG	DA	3084	1/1	0.83	0.29	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3349	1/1	0.91	0.29	-	63,63,63,63	0
55	MG	BA	3403	1/1	0.80	0.66	-	93,93,93,93	0
55	MG	DA	3197	1/1	0.83	0.70	-	70,70,70,70	0
55	MG	DA	3005	1/1	0.86	0.48	-	77,77,77,77	0
55	MG	CA	1627	1/1	0.91	0.31	-	88,88,88,88	0
55	MG	BA	3509	1/1	0.77	0.29	-	83,83,83,83	0
55	MG	DA	3340	1/1	0.76	0.20	-	85,85,85,85	0
55	MG	AC	104	1/1	0.95	0.47	-	56,56,56,56	0
55	MG	CA	1807	1/1	0.66	0.24	-	126,126,126,126	0
55	MG	DB	212	1/1	0.86	0.26	-	88,88,88,88	0
55	MG	DA	3053	1/1	0.89	0.62	-	62,62,62,62	0
55	MG	AA	1643	1/1	0.89	0.62	-	85,85,85,85	0
55	MG	DA	3413	1/1	0.86	0.30	-	94,94,94,94	0
55	MG	DA	3339	1/1	0.94	0.32	-	66,66,66,66	0
55	MG	DA	3097	1/1	0.98	0.29	-	52,52,52,52	0
55	MG	DA	3061	1/1	0.85	0.56	-	74,74,74,74	0
55	MG	BA	3232	1/1	0.72	0.31	-	72,72,72,72	0
55	MG	BA	3410	1/1	0.95	0.72	-	62,62,62,62	0
55	MG	CA	1767	1/1	0.88	0.46	-	77,77,77,77	0
55	MG	A1	102	1/1	0.89	0.42	-	86,86,86,86	0
55	MG	CA	1751	1/1	0.46	0.27	-	94,94,94,94	0
55	MG	CA	1761	1/1	0.86	0.40	-	92,92,92,92	0
55	MG	AA	1621	1/1	0.70	0.19	-	108,108,108,108	0
55	MG	BA	3261	1/1	0.98	0.62	-	52,52,52,52	0
55	MG	AA	1659	1/1	0.95	0.75	-	69,69,69,69	0
55	MG	AA	1794	1/1	0.97	0.21	-	84,84,84,84	0
55	MG	AA	1732	1/1	0.92	0.33	-	92,92,92,92	0
55	MG	AA	1624	1/1	0.90	0.28	-	79,79,79,79	0
55	MG	DA	3006	1/1	0.97	0.48	-	71,71,71,71	0
55	MG	DA	3316	1/1	0.93	0.33	-	61,61,61,61	0
55	MG	AA	1753	1/1	0.61	0.10	-	108,108,108,108	0
55	MG	CB	103	1/1	0.82	0.46	-	103,103,103,103	0
55	MG	BA	3334	1/1	0.44	0.56	-	96,96,96,96	0
55	MG	BA	3042	1/1	0.98	0.34	-	41,41,41,41	0
55	MG	BA	3530	1/1	0.78	0.30	-	81,81,81,81	0
55	MG	BA	3529	1/1	0.95	0.38	-	68,68,68,68	0
55	MG	BA	3613	1/1	0.82	0.28	-	93,93,93,93	0
55	MG	AA	1640	1/1	0.85	0.33	-	90,90,90,90	0
55	MG	DA	3505	1/1	0.82	0.48	-	81,81,81,81	0
55	MG	BA	3253	1/1	0.96	0.26	-	51,51,51,51	0
55	MG	AA	1665	1/1	0.97	0.75	-	70,70,70,70	0
55	MG	CA	1697	1/1	0.88	0.30	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1741	1/1	0.63	0.14	-	106,106,106,106	0
55	MG	DA	3067	1/1	0.73	0.35	-	94,94,94,94	0
55	MG	DA	3277	1/1	0.73	0.28	-	89,89,89,89	0
55	MG	BA	3234	1/1	0.91	0.43	-	86,86,86,86	0
55	MG	BA	3552	1/1	0.89	0.30	-	102,102,102,102	0
55	MG	DA	3024	1/1	0.94	0.32	-	108,108,108,108	0
55	MG	DA	3146	1/1	0.59	0.53	-	92,92,92,92	0
55	MG	BA	3376	1/1	0.97	0.44	-	73,73,73,73	0
55	MG	AA	1725	1/1	0.53	0.19	-	82,82,82,82	0
55	MG	DA	3193	1/1	0.96	0.68	-	63,63,63,63	0
55	MG	DA	3445	1/1	0.93	0.33	-	78,78,78,78	0
55	MG	BA	3374	1/1	0.93	0.40	-	71,71,71,71	0
55	MG	AA	1709	1/1	0.85	0.19	-	70,70,70,70	0
55	MG	DA	3166	1/1	0.97	0.45	-	58,58,58,58	0
55	MG	DA	3499	1/1	0.95	0.21	-	61,61,61,61	0
55	MG	BA	3267	1/1	0.88	0.30	-	61,61,61,61	0
55	MG	DA	3234	1/1	0.96	0.43	-	52,52,52,52	0
55	MG	BA	3542	1/1	0.91	0.48	-	72,72,72,72	0
55	MG	DA	3083	1/1	0.94	0.49	-	85,85,85,85	0
55	MG	BA	3602	1/1	0.92	0.25	-	67,67,67,67	0
55	MG	BA	3068	1/1	0.98	0.34	-	75,75,75,75	0
55	MG	AA	1702	1/1	0.81	0.19	-	93,93,93,93	0
55	MG	BA	3473	1/1	0.80	0.49	-	76,76,76,76	0
55	MG	DA	3183	1/1	0.86	0.51	-	57,57,57,57	0
55	MG	BA	3582	1/1	0.91	0.42	-	86,86,86,86	0
55	MG	BA	3460	1/1	0.91	0.13	-	83,83,83,83	0
55	MG	DA	3462	1/1	0.79	0.78	-	107,107,107,107	0
55	MG	BA	3415	1/1	0.70	0.37	-	84,84,84,84	0
55	MG	CA	1748	1/1	0.94	0.16	-	87,87,87,87	0
55	MG	DA	3524	1/1	0.78	0.28	-	105,105,105,105	0
55	MG	AN	202	1/1	0.89	0.32	-	82,82,82,82	0
55	MG	DA	3525	1/1	0.84	0.78	-	79,79,79,79	0
55	MG	BA	3335	1/1	0.91	0.35	-	58,58,58,58	0
55	MG	AA	1655	1/1	0.94	0.47	-	88,88,88,88	0
55	MG	CA	1700	1/1	0.88	0.47	-	77,77,77,77	0
55	MG	DA	3358	1/1	0.90	0.53	-	88,88,88,88	0
55	MG	BA	3426	1/1	0.92	0.49	-	85,85,85,85	0
55	MG	DA	3050	1/1	0.91	0.68	-	66,66,66,66	0
55	MG	BA	3462	1/1	0.76	0.27	-	87,87,87,87	0
55	MG	BA	3290	1/1	0.74	0.39	-	97,97,97,97	0
55	MG	BA	3306	1/1	0.94	0.25	-	67,67,67,67	0
55	MG	CA	1711	1/1	0.85	0.38	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3135	1/1	0.93	0.49	-	72,72,72,72	0
55	MG	BA	3407	1/1	0.97	0.26	-	59,59,59,59	0
55	MG	DA	3099	1/1	0.94	0.27	-	40,40,40,40	0
55	MG	BA	3430	1/1	0.94	0.27	-	57,57,57,57	0
55	MG	AA	1638	1/1	0.86	0.31	-	104,104,104,104	0
55	MG	AA	1810	1/1	0.91	0.45	-	67,67,67,67	0
55	MG	BB	208	1/1	0.74	0.25	-	74,74,74,74	0
55	MG	BA	3608	1/1	0.99	0.37	-	39,39,39,39	0
55	MG	AA	1710	1/1	0.79	0.29	-	92,92,92,92	0
55	MG	BA	3043	1/1	0.95	0.25	-	32,32,32,32	0
55	MG	BA	3360	1/1	0.90	0.14	-	84,84,84,84	0
55	MG	DA	3194	1/1	0.98	0.43	-	73,73,73,73	0
55	MG	BA	3519	1/1	0.93	0.31	-	80,80,80,80	0
55	MG	CA	1730	1/1	0.94	0.19	-	106,106,106,106	0
55	MG	AA	1809	1/1	0.90	0.36	-	63,63,63,63	0
55	MG	AH	201	1/1	0.49	0.39	-	99,99,99,99	0
55	MG	AA	1840	1/1	0.81	0.47	-	87,87,87,87	0
55	MG	CA	1789	1/1	0.92	0.58	-	71,71,71,71	0
55	MG	AA	1704	1/1	0.91	0.11	-	83,83,83,83	0
55	MG	BA	3174	1/1	0.92	0.81	-	71,71,71,71	0
55	MG	BA	3180	1/1	0.95	0.40	-	37,37,37,37	0
55	MG	DA	3065	1/1	0.98	0.41	-	74,74,74,74	0
55	MG	BA	3035	1/1	0.97	0.27	-	37,37,37,37	0
55	MG	CA	1714	1/1	0.18	0.60	-	92,92,92,92	0
55	MG	DA	3381	1/1	0.77	0.47	-	99,99,99,99	0
55	MG	DA	3184	1/1	0.96	0.65	-	61,61,61,61	0
55	MG	AA	1747	1/1	0.94	0.40	-	88,88,88,88	0
55	MG	BA	3240	1/1	0.86	0.54	-	88,88,88,88	0
55	MG	BA	3298	1/1	0.93	0.27	-	65,65,65,65	0
55	MG	DA	3367	1/1	0.86	0.43	-	82,82,82,82	0
55	MG	DA	3167	1/1	0.95	0.40	-	70,70,70,70	0
55	MG	BA	3203	1/1	0.87	0.34	-	85,85,85,85	0
55	MG	CA	1752	1/1	0.93	0.18	-	70,70,70,70	0
55	MG	BA	3231	1/1	0.88	0.50	-	73,73,73,73	0
55	MG	CA	1706	1/1	0.99	0.42	-	87,87,87,87	0
55	MG	AA	1752	1/1	0.87	0.27	-	78,78,78,78	0
55	MG	BA	3022	1/1	0.97	0.45	-	30,30,30,30	0
55	MG	CA	1644	1/1	0.72	0.29	-	120,120,120,120	0
55	MG	BA	3609	1/1	0.91	0.65	-	70,70,70,70	0
55	MG	BA	3134	1/1	0.86	0.18	-	81,81,81,81	0
55	MG	CA	1769	1/1	0.59	0.33	-	105,105,105,105	0
55	MG	CA	1728	1/1	0.95	0.66	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	BA	3244	1/1	0.97	0.33	-	58,58,58,58	0
55	MG	BA	3617	1/1	0.91	0.72	-	71,71,71,71	0
55	MG	DA	3410	1/1	0.92	0.39	-	78,78,78,78	0
55	MG	DA	3068	1/1	0.67	0.18	-	91,91,91,91	0
55	MG	DA	3454	1/1	0.88	0.37	-	92,92,92,92	0
55	MG	BA	3420	1/1	0.66	0.34	-	94,94,94,94	0
55	MG	AA	1802	1/1	0.85	0.45	-	85,85,85,85	0
55	MG	AA	1713	1/1	0.82	0.31	-	115,115,115,115	0
55	MG	BA	3296	1/1	0.92	0.40	-	53,53,53,53	0
55	MG	AA	1703	1/1	0.62	0.23	-	92,92,92,92	0
55	MG	BA	3518	1/1	0.92	0.23	-	70,70,70,70	0
55	MG	BA	3394	1/1	0.86	0.19	-	81,81,81,81	0
55	MG	BA	3564	1/1	0.95	0.61	-	84,84,84,84	0
55	MG	DA	3177	1/1	0.97	0.34	-	74,74,74,74	0
55	MG	DA	3519	1/1	0.83	0.47	-	85,85,85,85	0
55	MG	DA	3107	1/1	0.97	0.36	-	53,53,53,53	0
55	MG	BA	3559	1/1	0.92	0.17	-	81,81,81,81	0
55	MG	CA	1765	1/1	0.92	0.25	-	101,101,101,101	0
55	MG	AA	1685	1/1	0.93	0.29	-	88,88,88,88	0
55	MG	BA	3065	1/1	0.91	0.34	-	91,91,91,91	0
55	MG	DA	3111	1/1	0.93	0.26	-	52,52,52,52	0
55	MG	BA	3423	1/1	0.90	0.56	-	61,61,61,61	0
55	MG	CA	1666	1/1	0.96	0.29	-	71,71,71,71	0
55	MG	BA	3492	1/1	0.95	0.43	-	77,77,77,77	0
55	MG	AA	1736	1/1	0.94	0.46	-	90,90,90,90	0
55	MG	CA	1774	1/1	0.87	0.13	-	104,104,104,104	0
55	MG	DA	3351	1/1	0.89	0.28	-	79,79,79,79	0
55	MG	DA	3009	1/1	0.92	0.53	-	68,68,68,68	0
55	MG	DA	3070	1/1	0.80	0.28	-	78,78,78,78	0
55	MG	AA	1689	1/1	0.82	0.26	-	115,115,115,115	0
55	MG	DA	3231	1/1	0.92	0.43	-	72,72,72,72	0
55	MG	DA	3015	1/1	0.88	0.69	-	89,89,89,89	0
55	MG	BA	3512	1/1	0.92	0.27	-	69,69,69,69	0
55	MG	DA	3354	1/1	0.97	0.41	-	73,73,73,73	0
55	MG	DA	3203	1/1	0.99	0.27	-	48,48,48,48	0
55	MG	DA	3473	1/1	0.82	0.48	-	96,96,96,96	0
55	MG	AA	1721	1/1	0.94	0.29	-	77,77,77,77	0
55	MG	DA	3380	1/1	0.59	0.18	-	139,139,139,139	0
55	MG	BA	3433	1/1	0.97	0.15	-	70,70,70,70	0
55	MG	BA	3483	1/1	0.92	0.34	-	68,68,68,68	0
55	MG	BE	303	1/1	0.97	0.40	-	44,44,44,44	0
55	MG	DA	3032	1/1	0.90	0.11	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1688	1/1	0.90	0.34	-	71,71,71,71	0
55	MG	BA	3464	1/1	0.94	0.51	-	77,77,77,77	0
55	MG	BA	3499	1/1	0.93	0.39	-	68,68,68,68	0
55	MG	DA	3411	1/1	0.95	0.19	-	70,70,70,70	0
55	MG	BA	3598	1/1	0.73	0.38	-	77,77,77,77	0
55	MG	DA	3199	1/1	0.95	0.48	-	61,61,61,61	0
55	MG	DA	3451	1/1	0.91	0.47	-	75,75,75,75	0
55	MG	BA	3263	1/1	0.94	0.64	-	54,54,54,54	0
55	MG	AA	1761	1/1	0.79	0.41	-	113,113,113,113	0
55	MG	BA	3363	1/1	0.92	0.56	-	67,67,67,67	0
55	MG	BA	3081	1/1	0.92	0.30	-	75,75,75,75	0
55	MG	DA	3458	1/1	0.92	0.60	-	92,92,92,92	0
55	MG	DA	3256	1/1	0.97	0.44	-	49,49,49,49	0
55	MG	BA	3526	1/1	0.81	0.39	-	86,86,86,86	0
55	MG	BA	3201	1/1	0.96	0.64	-	66,66,66,66	0
55	MG	AA	1656	1/1	0.87	0.43	-	87,87,87,87	0
55	MG	CA	1731	1/1	0.95	0.58	-	72,72,72,72	0
55	MG	DA	3095	1/1	0.98	0.44	-	49,49,49,49	0
55	MG	CA	1797	1/1	0.78	0.32	-	87,87,87,87	0
55	MG	DA	3066	1/1	0.93	0.53	-	65,65,65,65	0
55	MG	AA	1671	1/1	0.95	0.12	-	67,67,67,67	0
55	MG	DA	3500	1/1	0.49	0.33	-	92,92,92,92	0
55	MG	DA	3510	1/1	0.92	0.31	-	85,85,85,85	0
55	MG	BA	3387	1/1	0.87	0.40	-	73,73,73,73	0
55	MG	BA	3355	1/1	0.97	0.57	-	46,46,46,46	0
55	MG	DA	3014	1/1	0.92	0.56	-	74,74,74,74	0
55	MG	BE	304	1/1	0.76	0.37	-	80,80,80,80	0
55	MG	BA	3145	1/1	0.91	0.35	-	74,74,74,74	0
55	MG	BA	3620	1/1	0.94	0.28	-	68,68,68,68	0
55	MG	CA	1672	1/1	0.86	0.75	-	75,75,75,75	0
55	MG	DA	3321	1/1	0.93	0.57	-	66,66,66,66	0
55	MG	AA	1739	1/1	0.88	0.07	-	93,93,93,93	0
55	MG	DA	3021	1/1	0.96	0.48	-	51,51,51,51	0
55	MG	BA	3139	1/1	0.98	0.39	-	35,35,35,35	0
55	MG	BA	3372	1/1	0.92	0.27	-	73,73,73,73	0
55	MG	BA	3152	1/1	0.96	0.51	-	40,40,40,40	0
55	MG	DA	3404	1/1	0.75	0.30	-	61,61,61,61	0
55	MG	DA	3018	1/1	0.89	0.28	-	77,77,77,77	0
55	MG	BA	3595	1/1	0.83	0.18	-	65,65,65,65	0
55	MG	DA	3390	1/1	0.97	0.35	-	75,75,75,75	0
55	MG	BA	3300	1/1	0.84	0.35	-	88,88,88,88	0
55	MG	BA	3328	1/1	0.79	0.71	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3446	1/1	0.97	0.50	-	75,75,75,75	0
55	MG	BA	3058	1/1	0.97	0.32	-	62,62,62,62	0
55	MG	CA	1649	1/1	0.92	0.29	-	64,64,64,64	0
55	MG	BA	3110	1/1	0.84	0.52	-	59,59,59,59	0
55	MG	AA	1807	1/1	0.74	0.60	-	98,98,98,98	0
55	MG	BA	3193	1/1	0.83	0.51	-	85,85,85,85	0
55	MG	DA	3258	1/1	0.95	0.32	-	37,37,37,37	0
55	MG	BA	3051	1/1	0.97	0.23	-	74,74,74,74	0
55	MG	BA	3088	1/1	0.81	0.17	-	77,77,77,77	0
55	MG	DA	3280	1/1	0.97	0.57	-	46,46,46,46	0
55	MG	AA	1812	1/1	0.80	0.59	-	73,73,73,73	0
55	MG	BA	3074	1/1	0.99	0.47	-	49,49,49,49	0
55	MG	DA	3102	1/1	0.98	0.37	-	51,51,51,51	0
55	MG	AA	1720	1/1	0.68	0.19	-	93,93,93,93	0
55	MG	CA	1651	1/1	0.93	0.35	-	90,90,90,90	0
55	MG	BA	3409	1/1	0.81	0.20	-	68,68,68,68	0
55	MG	CA	1693	1/1	0.81	0.54	-	76,76,76,76	0
55	MG	BA	3547	1/1	0.41	0.41	-	77,77,77,77	0
55	MG	DA	3136	1/1	0.82	0.34	-	76,76,76,76	0
55	MG	BA	3511	1/1	0.88	0.15	-	89,89,89,89	0
55	MG	DA	3200	1/1	0.96	0.45	-	44,44,44,44	0
55	MG	CA	1776	1/1	0.92	0.50	-	71,71,71,71	0
55	MG	DA	3250	1/1	0.95	0.39	-	63,63,63,63	0
55	MG	BA	3257	1/1	0.90	0.25	-	64,64,64,64	0
55	MG	BB	204	1/1	0.88	0.31	-	78,78,78,78	0
55	MG	BA	3235	1/1	0.95	0.39	-	54,54,54,54	0
55	MG	DA	3226	1/1	0.91	0.41	-	62,62,62,62	0
55	MG	AA	1674	1/1	0.86	0.33	-	98,98,98,98	0
55	MG	DA	3501	1/1	0.84	0.92	-	88,88,88,88	0
55	MG	BA	3310	1/1	0.86	0.37	-	57,57,57,57	0
55	MG	BA	3579	1/1	0.81	0.13	-	92,92,92,92	0
55	MG	BA	3011	1/1	0.93	0.29	-	42,42,42,42	0
55	MG	BA	3054	1/1	0.77	0.25	-	80,80,80,80	0
55	MG	BA	3362	1/1	0.86	0.24	-	48,48,48,48	0
55	MG	DA	3311	1/1	0.96	0.41	-	73,73,73,73	0
55	MG	BA	3406	1/1	0.96	0.50	-	82,82,82,82	0
55	MG	AA	1675	1/1	0.88	0.45	-	80,80,80,80	0
55	MG	AA	1742	1/1	0.87	0.17	-	78,78,78,78	0
55	MG	B7	101	1/1	0.82	0.46	-	67,67,67,67	0
55	MG	AA	1754	1/1	0.79	0.19	-	95,95,95,95	0
55	MG	BA	3233	1/1	0.99	0.41	-	48,48,48,48	0
55	MG	CA	1805	1/1	0.18	0.28	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3502	1/1	0.81	0.50	-	97,97,97,97	0
55	MG	DA	3139	1/1	0.81	0.44	-	80,80,80,80	0
55	MG	DA	3185	1/1	0.92	0.35	-	74,74,74,74	0
55	MG	BA	3034	1/1	0.89	0.34	-	41,41,41,41	0
55	MG	BA	3592	1/1	0.81	0.36	-	89,89,89,89	0
55	MG	CA	1747	1/1	0.88	0.26	-	94,94,94,94	0
55	MG	BA	3444	1/1	0.88	0.50	-	78,78,78,78	0
55	MG	CA	1619	1/1	0.98	0.49	-	61,61,61,61	0
55	MG	DA	3062	1/1	0.86	0.27	-	72,72,72,72	0
55	MG	DA	3011	1/1	0.77	0.21	-	65,65,65,65	0
55	MG	BA	3446	1/1	0.75	0.19	-	92,92,92,92	0
55	MG	BA	3103	1/1	0.89	0.49	-	52,52,52,52	0
55	MG	DA	3236	1/1	0.76	0.32	-	55,55,55,55	0
55	MG	BA	3329	1/1	0.97	0.40	-	65,65,65,65	0
55	MG	DA	3270	1/1	0.94	0.28	-	83,83,83,83	0
55	MG	CA	1628	1/1	0.90	0.21	-	101,101,101,101	0
55	MG	CA	1661	1/1	0.81	0.22	-	87,87,87,87	0
55	MG	BA	3075	1/1	0.58	0.27	-	110,110,110,110	0
55	MG	CC	105	1/1	0.88	0.59	-	82,82,82,82	0
55	MG	CA	1616	1/1	0.77	0.28	-	88,88,88,88	0
55	MG	AA	1724	1/1	0.84	0.20	-	84,84,84,84	0
55	MG	DA	3449	1/1	0.83	0.38	-	87,87,87,87	0
55	MG	BA	3343	1/1	0.92	0.30	-	60,60,60,60	0
55	MG	BA	3059	1/1	0.75	0.38	-	91,91,91,91	0
55	MG	BA	3580	1/1	0.50	0.21	-	71,71,71,71	0
55	MG	DA	3235	1/1	0.98	0.42	-	48,48,48,48	0
55	MG	BA	3238	1/1	0.96	0.56	-	41,41,41,41	0
55	MG	AA	1766	1/1	0.83	0.16	-	79,79,79,79	0
55	MG	BA	3140	1/1	0.86	0.25	-	58,58,58,58	0
55	MG	DA	3467	1/1	0.85	0.40	-	61,61,61,61	0
55	MG	DA	3073	1/1	0.91	0.52	-	80,80,80,80	0
55	MG	DA	3504	1/1	0.88	0.34	-	65,65,65,65	0
55	MG	DR	201	1/1	0.79	0.22	-	71,71,71,71	0
55	MG	DA	3195	1/1	0.97	0.76	-	70,70,70,70	0
55	MG	BA	3111	1/1	0.97	0.33	-	59,59,59,59	0
55	MG	DA	3507	1/1	0.67	0.44	-	91,91,91,91	0
55	MG	BA	3505	1/1	0.73	0.48	-	96,96,96,96	0
55	MG	DA	3497	1/1	0.84	0.35	-	74,74,74,74	0
55	MG	BA	3113	1/1	0.96	0.53	-	57,57,57,57	0
55	MG	AA	1779	1/1	0.93	0.36	-	72,72,72,72	0
55	MG	AA	1613	1/1	0.88	0.07	-	85,85,85,85	0
55	MG	CA	1613	1/1	0.93	0.28	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AB	102	1/1	0.79	0.26	-	86,86,86,86	0
55	MG	DA	3149	1/1	0.97	0.62	-	57,57,57,57	0
55	MG	BA	3508	1/1	0.95	0.41	-	59,59,59,59	0
55	MG	CB	102	1/1	0.84	0.28	-	87,87,87,87	0
55	MG	DA	3265	1/1	0.97	0.41	-	50,50,50,50	0
55	MG	BB	206	1/1	0.93	0.34	-	86,86,86,86	0
55	MG	BA	3429	1/1	0.93	0.12	-	75,75,75,75	0
55	MG	AQ	101	1/1	0.52	0.15	-	88,88,88,88	0
55	MG	BA	3543	1/1	0.89	0.41	-	80,80,80,80	0
55	MG	DA	3217	1/1	0.96	0.40	-	55,55,55,55	0
55	MG	DA	3466	1/1	0.86	0.63	-	78,78,78,78	0
55	MG	CG	301	1/1	0.66	0.36	-	83,83,83,83	0
55	MG	BA	3550	1/1	0.94	0.24	-	93,93,93,93	0
55	MG	CA	1757	1/1	0.64	0.21	-	97,97,97,97	0
55	MG	DA	3421	1/1	0.93	0.32	-	62,62,62,62	0
55	MG	DA	3175	1/1	0.88	0.34	-	83,83,83,83	0
55	MG	BA	3456	1/1	0.97	0.50	-	78,78,78,78	0
55	MG	AA	1835	1/1	0.87	0.29	-	87,87,87,87	0
55	MG	CC	107	1/1	0.31	0.63	-	99,99,99,99	0
55	MG	AA	1760	1/1	0.92	0.69	-	78,78,78,78	0
55	MG	AC	108	1/1	0.95	0.40	-	85,85,85,85	0
55	MG	BA	3106	1/1	0.74	0.36	-	75,75,75,75	0
55	MG	CA	1659	1/1	0.85	0.20	-	110,110,110,110	0
55	MG	BA	3284	1/1	0.95	0.45	-	56,56,56,56	0
55	MG	BA	3097	1/1	0.96	0.36	-	59,59,59,59	0
55	MG	BA	3210	1/1	0.89	0.20	-	74,74,74,74	0
55	MG	CA	1673	1/1	0.87	0.53	-	64,64,64,64	0
55	MG	DA	3359	1/1	0.91	0.36	-	76,76,76,76	0
55	MG	BA	3039	1/1	0.98	0.30	-	42,42,42,42	0
55	MG	DA	3472	1/1	0.98	0.69	-	71,71,71,71	0
55	MG	BA	3575	1/1	0.88	0.35	-	71,71,71,71	0
55	MG	BA	3574	1/1	0.88	0.53	-	78,78,78,78	0
55	MG	AA	1697	1/1	0.91	0.41	-	84,84,84,84	0
55	MG	BA	3570	1/1	0.68	0.41	-	87,87,87,87	0
55	MG	BA	3268	1/1	0.93	0.58	-	67,67,67,67	0
55	MG	CA	1762	1/1	0.67	0.31	-	96,96,96,96	0
55	MG	BA	3179	1/1	0.91	0.44	-	64,64,64,64	0
55	MG	BA	3556	1/1	0.91	0.51	-	58,58,58,58	0
55	MG	BA	3482	1/1	0.88	0.39	-	57,57,57,57	0
55	MG	DA	3330	1/1	0.81	0.15	-	81,81,81,81	0
55	MG	AG	301	1/1	0.98	0.57	-	81,81,81,81	0
55	MG	BA	3089	1/1	0.85	0.33	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	1618	1/1	0.80	0.17	-	93,93,93,93	0
55	MG	AA	1786	1/1	0.79	0.19	-	86,86,86,86	0
55	MG	CA	1806	1/1	0.94	0.48	-	96,96,96,96	0
55	MG	DA	3383	1/1	0.88	0.47	-	87,87,87,87	0
55	MG	DA	3314	1/1	0.91	0.47	-	76,76,76,76	0
55	MG	DA	3271	1/1	0.96	0.47	-	58,58,58,58	0
55	MG	BA	3332	1/1	0.78	0.32	-	61,61,61,61	0
55	MG	DA	3255	1/1	0.92	0.28	-	75,75,75,75	0
55	MG	BA	3539	1/1	0.89	0.26	-	74,74,74,74	0
55	MG	DA	3486	1/1	0.87	0.33	-	68,68,68,68	0
55	MG	DA	3302	1/1	0.81	0.57	-	95,95,95,95	0
55	MG	BA	3463	1/1	0.47	0.30	-	72,72,72,72	0
55	MG	BA	3541	1/1	0.64	0.20	-	96,96,96,96	0
55	MG	DA	3395	1/1	0.88	0.47	-	69,69,69,69	0
55	MG	CA	1786	1/1	0.91	0.26	-	73,73,73,73	0
55	MG	DA	3269	1/1	0.90	0.42	-	84,84,84,84	0
55	MG	CA	1624	1/1	0.82	0.36	-	88,88,88,88	0
55	MG	DA	3118	1/1	0.98	0.35	-	71,71,71,71	0
55	MG	AA	1790	1/1	0.81	0.23	-	98,98,98,98	0
55	MG	BA	3204	1/1	0.88	0.34	-	78,78,78,78	0
55	MG	CA	1744	1/1	0.95	0.27	-	79,79,79,79	0
55	MG	BA	3590	1/1	0.94	0.34	-	63,63,63,63	0
55	MG	DA	3119	1/1	0.65	0.44	-	98,98,98,98	0
55	MG	DA	3225	1/1	0.90	0.59	-	73,73,73,73	0
55	MG	CA	1665	1/1	0.89	0.17	-	83,83,83,83	0
55	MG	BA	3439	1/1	0.90	0.36	-	71,71,71,71	0
55	MG	BA	3271	1/1	0.92	0.20	-	35,35,35,35	0
55	MG	BA	3537	1/1	0.84	0.41	-	89,89,89,89	0
55	MG	CA	1663	1/1	0.89	0.35	-	81,81,81,81	0
55	MG	AA	1688	1/1	0.82	0.21	-	72,72,72,72	0
55	MG	BA	3611	1/1	0.91	0.52	-	87,87,87,87	0
55	MG	DA	3523	1/1	0.87	0.91	-	81,81,81,81	0
55	MG	BA	3354	1/1	0.73	0.21	-	72,72,72,72	0
55	MG	AA	1718	1/1	0.89	0.58	-	82,82,82,82	0
55	MG	BA	3185	1/1	0.83	0.36	-	76,76,76,76	0
55	MG	AA	1603	1/1	0.94	0.33	-	63,63,63,63	0
55	MG	BA	3388	1/1	0.79	0.49	-	88,88,88,88	0
55	MG	CA	1729	1/1	0.75	0.84	-	77,77,77,77	0
55	MG	BA	3507	1/1	0.88	0.30	-	89,89,89,89	0
55	MG	BA	3192	1/1	0.97	0.33	-	34,34,34,34	0
55	MG	DB	208	1/1	0.73	0.22	-	90,90,90,90	0
55	MG	DA	3057	1/1	0.79	0.35	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3100	1/1	0.95	0.44	-	44,44,44,44	0
55	MG	AA	1765	1/1	0.95	0.51	-	84,84,84,84	0
55	MG	BA	3053	1/1	0.89	0.28	-	95,95,95,95	0
55	MG	AA	1792	1/1	0.96	0.21	-	55,55,55,55	0
55	MG	CA	1726	1/1	0.99	0.62	-	75,75,75,75	0
55	MG	DA	3290	1/1	0.72	0.31	-	79,79,79,79	0
55	MG	CA	1633	1/1	0.90	0.28	-	91,91,91,91	0
55	MG	CA	1664	1/1	0.66	0.29	-	99,99,99,99	0
55	MG	DA	3444	1/1	0.92	0.17	-	73,73,73,73	0
55	MG	BA	3560	1/1	0.94	0.56	-	78,78,78,78	0
55	MG	BA	3115	1/1	0.94	0.27	-	87,87,87,87	0
55	MG	BA	3565	1/1	0.86	0.28	-	77,77,77,77	0
55	MG	DA	3307	1/1	0.89	0.26	-	77,77,77,77	0
55	MG	DA	3366	1/1	0.76	0.43	-	83,83,83,83	0
55	MG	DA	3124	1/1	0.93	0.57	-	54,54,54,54	0
55	MG	DA	3181	1/1	0.96	0.49	-	50,50,50,50	0
55	MG	DA	3301	1/1	0.96	0.34	-	63,63,63,63	0
55	MG	BA	3202	1/1	0.97	0.39	-	51,51,51,51	0
55	MG	BA	3581	1/1	0.90	0.33	-	69,69,69,69	0
55	MG	BB	212	1/1	0.83	0.50	-	81,81,81,81	0
55	MG	DA	3392	1/1	0.92	0.42	-	68,68,68,68	0
55	MG	AA	1733	1/1	0.96	0.60	-	71,71,71,71	0
55	MG	DA	3320	1/1	0.71	0.15	-	76,76,76,76	0
55	MG	DA	3460	1/1	0.85	0.46	-	72,72,72,72	0
55	MG	AA	1649	1/1	0.96	0.37	-	79,79,79,79	0
55	MG	AA	1614	1/1	0.75	0.26	-	91,91,91,91	0
55	MG	CA	1788	1/1	0.92	0.33	-	84,84,84,84	0
55	MG	DA	3034	1/1	0.88	0.33	-	62,62,62,62	0
55	MG	DA	3372	1/1	0.93	0.36	-	65,65,65,65	0
55	MG	BA	3475	1/1	0.87	0.31	-	83,83,83,83	0
55	MG	AA	1758	1/1	0.49	0.35	-	85,85,85,85	0
55	MG	AA	1648	1/1	0.94	0.52	-	78,78,78,78	0
55	MG	DA	3115	1/1	0.99	0.53	-	49,49,49,49	0
55	MG	BA	3273	1/1	0.89	0.41	-	94,94,94,94	0
55	MG	CA	1745	1/1	0.86	0.12	-	91,91,91,91	0
55	MG	BB	216	1/1	0.75	0.15	-	94,94,94,94	0
55	MG	DA	3147	1/1	0.98	0.38	-	53,53,53,53	0
55	MG	BA	3472	1/1	0.69	0.61	-	89,89,89,89	0
55	MG	DA	3138	1/1	0.93	0.20	-	70,70,70,70	0
55	MG	BA	3260	1/1	0.89	0.42	-	47,47,47,47	0
55	MG	DA	3336	1/1	0.90	0.41	-	87,87,87,87	0
55	MG	DA	3398	1/1	0.90	0.40	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3049	1/1	0.86	0.28	-	74,74,74,74	0
55	MG	BA	3572	1/1	0.82	0.30	-	87,87,87,87	0
55	MG	AA	1828	1/1	0.83	0.11	-	105,105,105,105	0
55	MG	BA	3315	1/1	0.92	0.34	-	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.