



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:59 PM GMT

PDB ID : 4V5K  
Title : Structure of cytotoxic domain of colicin E3 bound to the 70S ribosome  
Authors : Ng, C.L.; Lang, K.; Meenan, N.A.G.; Sharma, A.; Kelley, A.C.; Kleanthous, C.; Ramakrishnan, V.  
Deposited on : 2010-05-29  
Resolution : 3.20 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

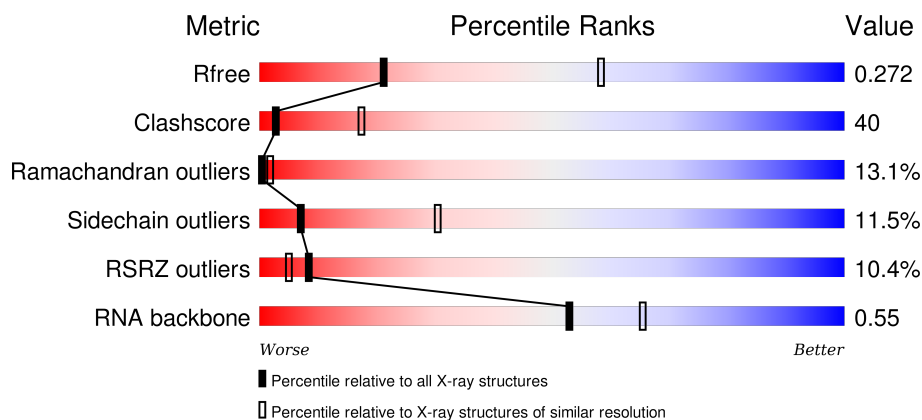
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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	1522	<div> <div>3%</div> <div>29%</div> <div>61%</div> <div>9%</div> <div>.</div> </div>
1	CA	1522	<div> <div>13%</div> <div>23%</div> <div>63%</div> <div>13%</div> <div>.</div> </div>
2	AB	256	<div> <div>7%</div> <div>17%</div> <div>61%</div> <div>13%</div> <div>8%</div> <div>.</div> </div>
2	CB	256	<div> <div>18%</div> <div>18%</div> <div>61%</div> <div>13%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	AW	77	
22	CV	77	
22	CW	77	
23	AX	25	
24	AY	97	
24	CY	97	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	
27	B2	72	

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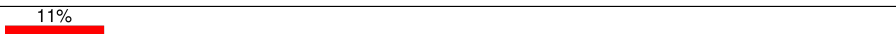
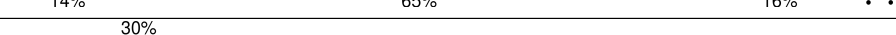
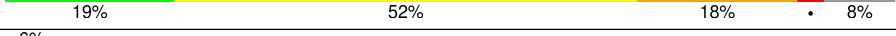
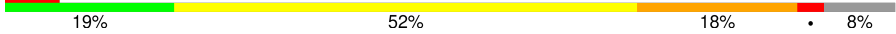
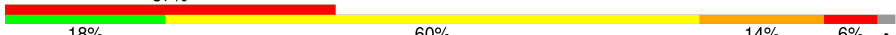

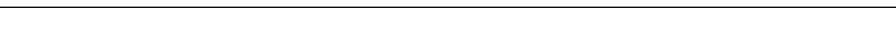
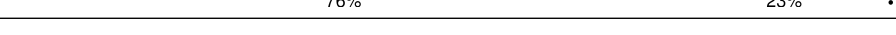


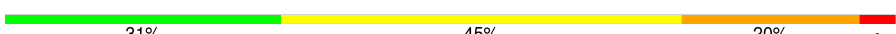

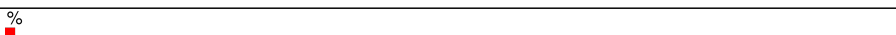


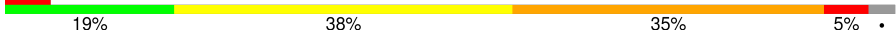
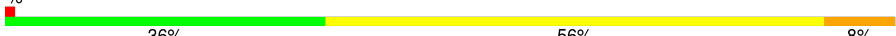


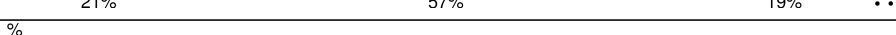
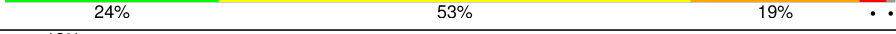



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Mol	Chain	Length	Quality of chain
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2848	
35	DA	2848	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	
39	DE	206	


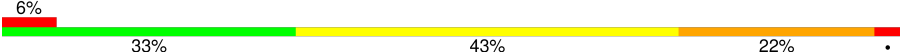

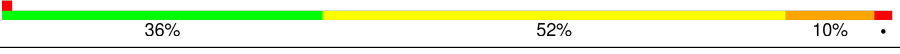
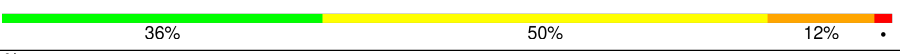
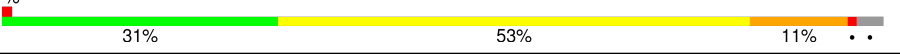



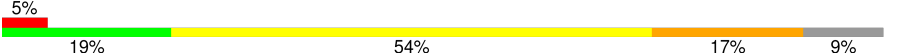
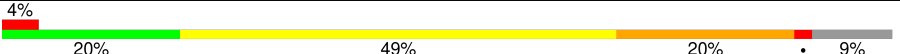

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Mol	Chain	Length	Quality of chain
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	131	
44	DJ	131	
45	BN	140	
45	DN	140	
46	BO	122	
46	DO	122	
47	BP	150	
47	DP	150	
48	BQ	141	
48	DQ	141	
49	BR	118	
49	DR	118	
50	BS	112	
50	DS	112	
51	BT	146	
51	DT	146	
52	BU	118	

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Mol	Chain	Length	Quality of chain
52	DU	118	
53	BV	101	
53	DV	101	
54	BW	113	
54	DW	113	
55	BX	96	
55	DX	96	
56	BY	110	
56	DY	110	
57	BZ	206	
57	DZ	206	
58	CX	25	

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
1	A3P	AA	1493	-	-	X	-
59	MG	AA	1616	-	-	-	X
59	MG	AA	1630	-	-	-	X
59	MG	AA	1650	-	-	-	X
59	MG	AA	1662	-	-	-	X
59	MG	AA	1669	-	-	-	X
59	MG	AA	1691	-	-	-	X
59	MG	AA	1692	-	-	-	X
59	MG	AA	1694	-	-	-	X
59	MG	AA	1697	-	-	-	X
59	MG	AA	1726	-	-	-	X
59	MG	AA	1729	-	-	-	X
59	MG	AA	1737	-	-	-	X
59	MG	AA	1760	-	-	-	X
59	MG	AA	1790	-	-	-	X
59	MG	AA	1812	-	-	-	X
59	MG	AA	1820	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1829	-	-	-	X
59	MG	AA	1845	-	-	-	X
59	MG	AA	1848	-	-	-	X
59	MG	AA	1857	-	-	-	X
59	MG	AA	1858	-	-	-	X
59	MG	AA	1862	-	-	-	X
59	MG	AA	1872	-	-	-	X
59	MG	AA	1888	-	-	-	X
59	MG	AA	1893	-	-	-	X
59	MG	AA	1899	-	-	-	X
59	MG	AA	1905	-	-	-	X
59	MG	AA	1915	-	-	-	X
59	MG	AA	1932	-	-	-	X
59	MG	AA	1938	-	-	-	X
59	MG	AA	1948	-	-	-	X
59	MG	AA	1968	-	-	-	X
59	MG	AV	102	-	-	-	X
59	MG	B6	101	-	-	-	X
59	MG	BA	2920	-	-	-	X
59	MG	BA	2925	-	-	-	X
59	MG	BA	2927	-	-	-	X
59	MG	BA	2937	-	-	-	X
59	MG	BA	2940	-	-	-	X
59	MG	BA	2947	-	-	-	X
59	MG	BA	2953	-	-	-	X
59	MG	BA	2954	-	-	-	X
59	MG	BA	2969	-	-	-	X
59	MG	BA	2974	-	-	-	X
59	MG	BA	2975	-	-	-	X
59	MG	BA	2979	-	-	-	X
59	MG	BA	2980	-	-	-	X
59	MG	BA	2985	-	-	-	X
59	MG	BA	2989	-	-	-	X
59	MG	BA	2992	-	-	-	X
59	MG	BA	2993	-	-	-	X
59	MG	BA	2997	-	-	-	X
59	MG	BA	3003	-	-	-	X
59	MG	BA	3010	-	-	-	X
59	MG	BA	3012	-	-	-	X
59	MG	BA	3019	-	-	-	X
59	MG	BA	3028	-	-	-	X
59	MG	BA	3031	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3032	-	-	-	X
59	MG	BA	3035	-	-	-	X
59	MG	BA	3037	-	-	-	X
59	MG	BA	3039	-	-	-	X
59	MG	BA	3040	-	-	-	X
59	MG	BA	3043	-	-	-	X
59	MG	BA	3052	-	-	-	X
59	MG	BA	3053	-	-	-	X
59	MG	BA	3055	-	-	-	X
59	MG	BA	3058	-	-	-	X
59	MG	BA	3063	-	-	-	X
59	MG	BA	3064	-	-	-	X
59	MG	BA	3066	-	-	-	X
59	MG	BA	3068	-	-	-	X
59	MG	BA	3074	-	-	-	X
59	MG	BA	3081	-	-	-	X
59	MG	BA	3094	-	-	-	X
59	MG	BA	3099	-	-	-	X
59	MG	BA	3119	-	-	-	X
59	MG	BA	3137	-	-	-	X
59	MG	BA	3155	-	-	-	X
59	MG	BA	3161	-	-	-	X
59	MG	BA	3162	-	-	-	X
59	MG	BA	3167	-	-	-	X
59	MG	BA	3168	-	-	-	X
59	MG	BA	3169	-	-	-	X
59	MG	BA	3171	-	-	-	X
59	MG	BA	3172	-	-	-	X
59	MG	BA	3176	-	-	-	X
59	MG	BA	3177	-	-	-	X
59	MG	BA	3184	-	-	-	X
59	MG	BA	3187	-	-	-	X
59	MG	BA	3191	-	-	-	X
59	MG	BA	3197	-	-	-	X
59	MG	BA	3204	-	-	-	X
59	MG	BA	3206	-	-	-	X
59	MG	BA	3210	-	-	-	X
59	MG	BA	3211	-	-	-	X
59	MG	BA	3213	-	-	-	X
59	MG	BA	3214	-	-	-	X
59	MG	BA	3221	-	-	-	X
59	MG	BA	3243	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3246	-	-	-	X
59	MG	BA	3247	-	-	-	X
59	MG	BA	3248	-	-	-	X
59	MG	BA	3249	-	-	-	X
59	MG	BA	3255	-	-	-	X
59	MG	BA	3256	-	-	-	X
59	MG	BA	3257	-	-	-	X
59	MG	BA	3261	-	-	-	X
59	MG	BA	3265	-	-	-	X
59	MG	BA	3271	-	-	-	X
59	MG	BA	3273	-	-	-	X
59	MG	BA	3286	-	-	-	X
59	MG	BA	3292	-	-	-	X
59	MG	BA	3305	-	-	-	X
59	MG	BA	3309	-	-	-	X
59	MG	BA	3312	-	-	-	X
59	MG	BA	3323	-	-	-	X
59	MG	BA	3327	-	-	-	X
59	MG	BA	3329	-	-	-	X
59	MG	BA	3330	-	-	-	X
59	MG	BA	3337	-	-	-	X
59	MG	BA	3351	-	-	-	X
59	MG	BA	3352	-	-	-	X
59	MG	BA	3368	-	-	-	X
59	MG	BA	3373	-	-	-	X
59	MG	BA	3381	-	-	-	X
59	MG	BA	3395	-	-	-	X
59	MG	BA	3397	-	-	-	X
59	MG	BA	3402	-	-	-	X
59	MG	BA	3405	-	-	-	X
59	MG	BA	3410	-	-	-	X
59	MG	BA	3412	-	-	-	X
59	MG	BA	3413	-	-	-	X
59	MG	BA	3414	-	-	-	X
59	MG	BA	3419	-	-	-	X
59	MG	BA	3428	-	-	-	X
59	MG	BA	3438	-	-	-	X
59	MG	BA	3439	-	-	-	X
59	MG	BA	3445	-	-	-	X
59	MG	BA	3446	-	-	-	X
59	MG	BA	3448	-	-	-	X
59	MG	BA	3450	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3452	-	-	-	X
59	MG	BA	3456	-	-	-	X
59	MG	BA	3460	-	-	-	X
59	MG	BA	3462	-	-	-	X
59	MG	BA	3463	-	-	-	X
59	MG	BA	3465	-	-	-	X
59	MG	BA	3468	-	-	-	X
59	MG	BA	3484	-	-	-	X
59	MG	BA	3488	-	-	-	X
59	MG	BA	3490	-	-	-	X
59	MG	BA	3496	-	-	-	X
59	MG	BA	3509	-	-	-	X
59	MG	BA	3510	-	-	-	X
59	MG	BA	3512	-	-	-	X
59	MG	BA	3514	-	-	-	X
59	MG	BA	3517	-	-	-	X
59	MG	BA	3521	-	-	-	X
59	MG	BA	3525	-	-	-	X
59	MG	BA	3527	-	-	-	X
59	MG	BA	3558	-	-	-	X
59	MG	BA	3559	-	-	-	X
59	MG	BA	3574	-	-	-	X
59	MG	BA	3582	-	-	-	X
59	MG	BA	3583	-	-	-	X
59	MG	BA	3584	-	-	-	X
59	MG	BA	3594	-	-	-	X
59	MG	BA	3603	-	-	-	X
59	MG	BD	301	-	-	-	X
59	MG	BD	302	-	-	-	X
59	MG	BE	304	-	-	-	X
59	MG	BF	301	-	-	-	X
59	MG	BN	201	-	-	-	X
59	MG	BP	202	-	-	X	-
59	MG	BP	203	-	-	X	-
59	MG	BR	203	-	-	-	X
59	MG	BU	201	-	-	-	X
59	MG	BU	202	-	-	-	X
59	MG	CA	1611	-	-	-	X
59	MG	CA	1626	-	-	-	X
59	MG	CA	1631	-	-	-	X
59	MG	CA	1668	-	-	-	X
59	MG	CA	1680	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	1700	-	-	-	X
59	MG	CA	1752	-	-	-	X
59	MG	CA	1765	-	-	-	X
59	MG	CH	201	-	-	-	X
59	MG	D6	102	-	-	-	X
59	MG	D7	102	-	-	-	X
59	MG	D7	103	-	-	-	X
59	MG	DA	2901	-	-	-	X
59	MG	DA	2904	-	-	-	X
59	MG	DA	2908	-	-	-	X
59	MG	DA	2913	-	-	-	X
59	MG	DA	2918	-	-	-	X
59	MG	DA	2919	-	-	-	X
59	MG	DA	2924	-	-	-	X
59	MG	DA	2927	-	-	-	X
59	MG	DA	2930	-	-	-	X
59	MG	DA	2935	-	-	-	X
59	MG	DA	2939	-	-	-	X
59	MG	DA	2942	-	-	-	X
59	MG	DA	2946	-	-	-	X
59	MG	DA	2953	-	-	-	X
59	MG	DA	2959	-	-	-	X
59	MG	DA	2964	-	-	-	X
59	MG	DA	2967	-	-	-	X
59	MG	DA	2990	-	-	-	X
59	MG	DA	2997	-	-	-	X
59	MG	DA	3003	-	-	-	X
59	MG	DA	3012	-	-	-	X
59	MG	DA	3013	-	-	-	X
59	MG	DA	3015	-	-	-	X
59	MG	DA	3017	-	-	-	X
59	MG	DA	3019	-	-	-	X
59	MG	DA	3022	-	-	-	X
59	MG	DA	3025	-	-	-	X
59	MG	DA	3026	-	-	-	X
59	MG	DA	3028	-	-	-	X
59	MG	DA	3031	-	-	-	X
59	MG	DA	3032	-	-	-	X
59	MG	DA	3037	-	-	-	X
59	MG	DA	3042	-	-	-	X
59	MG	DA	3050	-	-	-	X
59	MG	DA	3060	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3068	-	-	-	X
59	MG	DA	3071	-	-	-	X
59	MG	DA	3072	-	-	-	X
59	MG	DA	3080	-	-	-	X
59	MG	DA	3084	-	-	-	X
59	MG	DA	3086	-	-	-	X
59	MG	DA	3087	-	-	-	X
59	MG	DA	3090	-	-	-	X
59	MG	DA	3122	-	-	-	X
59	MG	DA	3126	-	-	-	X
59	MG	DA	3137	-	-	-	X
59	MG	DA	3140	-	-	-	X
59	MG	DA	3141	-	-	-	X
59	MG	DA	3157	-	-	-	X
59	MG	DA	3169	-	-	-	X
59	MG	DA	3176	-	-	-	X
59	MG	DA	3178	-	-	-	X
59	MG	DA	3180	-	-	-	X
59	MG	DA	3187	-	-	-	X
59	MG	DA	3197	-	-	-	X
59	MG	DA	3199	-	-	-	X
59	MG	DA	3211	-	-	-	X
59	MG	DA	3215	-	-	-	X
59	MG	DA	3217	-	-	-	X
59	MG	DA	3219	-	-	-	X
59	MG	DA	3224	-	-	-	X
59	MG	DA	3232	-	-	-	X
59	MG	DA	3236	-	-	-	X
59	MG	DA	3244	-	-	-	X
59	MG	DA	3247	-	-	-	X
59	MG	DA	3251	-	-	-	X
59	MG	DA	3255	-	-	-	X
59	MG	DA	3257	-	-	-	X
59	MG	DA	3262	-	-	-	X
59	MG	DA	3264	-	-	-	X
59	MG	DA	3266	-	-	-	X
59	MG	DA	3268	-	-	-	X
59	MG	DA	3271	-	-	-	X
59	MG	DA	3276	-	-	-	X
59	MG	DA	3277	-	-	-	X
59	MG	DA	3278	-	-	-	X
59	MG	DA	3281	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3282	-	-	-	X
59	MG	DA	3284	-	-	-	X
59	MG	DA	3290	-	-	-	X
59	MG	DA	3292	-	-	-	X
59	MG	DA	3298	-	-	-	X
59	MG	DA	3300	-	-	-	X
59	MG	DA	3301	-	-	-	X
59	MG	DA	3303	-	-	-	X
59	MG	DA	3305	-	-	-	X
59	MG	DA	3333	-	-	-	X
59	MG	DA	3335	-	-	-	X
59	MG	DA	3339	-	-	-	X
59	MG	DA	3341	-	-	-	X
59	MG	DA	3342	-	-	-	X
59	MG	DA	3343	-	-	-	X
59	MG	DA	3344	-	-	-	X
59	MG	DA	3345	-	-	-	X
59	MG	DA	3346	-	-	-	X
59	MG	DA	3349	-	-	-	X
59	MG	DA	3350	-	-	-	X
59	MG	DA	3356	-	-	-	X
59	MG	DA	3363	-	-	-	X
59	MG	DA	3364	-	-	-	X
59	MG	DA	3365	-	-	-	X
59	MG	DA	3366	-	-	-	X
59	MG	DA	3372	-	-	-	X
59	MG	DA	3381	-	-	-	X
59	MG	DA	3390	-	-	-	X
59	MG	DA	3394	-	-	-	X
59	MG	DA	3396	-	-	-	X
59	MG	DA	3397	-	-	-	X
59	MG	DA	3398	-	-	-	X
59	MG	DA	3401	-	-	-	X
59	MG	DA	3402	-	-	-	X
59	MG	DA	3406	-	-	-	X
59	MG	DA	3408	-	-	-	X
59	MG	DA	3412	-	-	-	X
59	MG	DA	3416	-	-	-	X
59	MG	DA	3426	-	-	-	X
59	MG	DA	3444	-	-	-	X
59	MG	DA	3452	-	-	-	X
59	MG	DA	3454	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3458	-	-	-	X
59	MG	DA	3459	-	-	-	X
59	MG	DA	3462	-	-	-	X
59	MG	DA	3468	-	-	-	X
59	MG	DA	3473	-	-	-	X
59	MG	DA	3477	-	-	-	X
59	MG	DA	3488	-	-	-	X
59	MG	DA	3489	-	-	-	X
59	MG	DA	3494	-	-	-	X
59	MG	DA	3500	-	-	-	X
59	MG	DA	3502	-	-	-	X
59	MG	DA	3503	-	-	-	X
59	MG	DA	3522	-	-	-	X
59	MG	DA	3535	-	-	-	X
59	MG	DA	3536	-	-	-	X
59	MG	DA	3543	-	-	-	X
59	MG	DA	3553	-	-	-	X
59	MG	DA	3579	-	-	-	X
59	MG	DA	3589	-	-	-	X
59	MG	DA	3600	-	-	-	X
59	MG	DA	3604	-	-	-	X
59	MG	DA	3608	-	-	-	X
59	MG	DA	3611	-	-	-	X
59	MG	DA	3624	-	-	-	X
59	MG	DA	3625	-	-	-	X
59	MG	DA	3631	-	-	-	X
59	MG	DA	3635	-	-	-	X
59	MG	DA	3638	-	-	-	X
59	MG	DA	3641	-	-	-	X
59	MG	DA	3649	-	-	-	X
59	MG	DA	3662	-	-	-	X
59	MG	DA	3669	-	-	-	X
59	MG	DA	3677	-	-	-	X
59	MG	DA	3679	-	-	-	X
59	MG	DA	3696	-	-	-	X
59	MG	DA	3705	-	-	-	X
59	MG	DA	3717	-	-	-	X
59	MG	DA	3722	-	-	-	X
59	MG	DA	3729	-	-	-	X
59	MG	DA	3741	-	-	-	X
59	MG	DA	3759	-	-	-	X
59	MG	DA	3763	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3771	-	-	-	X
59	MG	DA	3782	-	-	-	X
59	MG	DA	3788	-	-	-	X
59	MG	DA	3795	-	-	-	X
59	MG	DD	303	-	-	-	X
59	MG	DE	301	-	-	-	X
59	MG	DP	202	-	-	-	X
59	MG	DP	203	-	-	-	X
59	MG	DP	205	-	-	-	X
59	MG	DU	202	-	-	-	X
59	MG	DU	203	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296762 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1508	Total	C	N	O	P	0	0	0
			32412	14427	6003	10475	1507			
1	CA	1508	Total	C	N	O	P	0	0	0
			32413	14427	6004	10475	1507			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	1
			1692	1060	336	289	7			
4	CD	208	Total	C	N	O	S	0	0	1
			1692	1060	336	289	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

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

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	118	Total	C	N	O	S	0	0	1
			934	577	193	162	2			
13	CM	118	Total	C	N	O	S	0	0	1
			934	577	193	162	2			

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

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	85	Total	C	N	O	S	0	0	1
			671	427	124	118	2			
19	CS	85	Total	C	N	O	S	0	0	1
			671	427	124	118	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	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	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	16	Total	C	N	O	P	0	0	0
			341	155	66	105	15			

- Molecule 24 is a protein called COLICIN-E3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AY	97	Total	C	N	O	0	0	0
			769	483	144	142			
24	CY	16	Total	C	N	O	0	0	1
			126	82	23	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	58	ALA	HIS	ENGINEERED MUTATION	UNP P06646
CY	58	ALA	HIS	ENGINEERED MUTATION	UNP P00646

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			
26	D1	94	Total	C	N	O	S	0	0	1
			734	460	148	125	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	CONFLICT	UNP P60494
D1	81	ARG	LYS	CONFLICT	UNP P60494

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
27	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
28	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	56	Total	C	N	O	S	0	0	1
			434	274	75	81	4			
29	D4	56	Total	C	N	O	S	0	0	1
			434	274	75	81	4			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
31	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
32	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
33	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
34	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 35 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

- Molecule 36 is a RNA chain called RNA (119-MER).

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
37	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
38	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
39	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
40	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
42	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	145	Total	C	N	O	S	0	0	1
			1125	718	200	206	1			
43	DI	145	Total	C	N	O	S	0	0	1
			1125	718	200	206	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			
44	DJ	131	Total	C	N	O	0	0	1
			651	390	131	130			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
45	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
46	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
48	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
50	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
52	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
54	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
55	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
56	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BZ	187	Total	C	N	O	S	0	0	1
			1482	944	264	272	2			
57	DZ	187	Total	C	N	O	S	0	0	1
			1482	944	264	272	2			

- Molecule 58 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	CX	8	Total	C	N	O	P	0	0	0
			173	79	37	50	7			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AP	1	Total	Mg	0	0
			1	1		
59	BA	709	Total	Mg	0	0
			709	709		
59	CA	184	Total	Mg	0	0
			184	184		
59	DN	3	Total	Mg	0	0
			3	3		
59	CH	1	Total	Mg	0	0
			1	1		
59	DF	3	Total	Mg	0	0
			3	3		
59	CV	12	Total	Mg	0	0
			12	12		
59	D2	1	Total	Mg	0	0
			1	1		
59	BE	4	Total	Mg	0	0
			4	4		
59	DU	4	Total	Mg	0	0
			4	4		
59	B1	1	Total	Mg	0	0
			1	1		
59	AN	2	Total	Mg	0	0
			2	2		
59	BP	4	Total	Mg	0	0
			4	4		
59	AX	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D6	2	Total 2	Mg 2	0	0
59	CY	1	Total 1	Mg 1	0	0
59	DD	6	Total 6	Mg 6	0	0
59	B5	3	Total 3	Mg 3	0	0
59	BB	6	Total 6	Mg 6	0	0
59	BT	1	Total 1	Mg 1	0	0
59	DO	1	Total 1	Mg 1	0	0
59	D3	1	Total 1	Mg 1	0	0
59	BF	1	Total 1	Mg 1	0	0
59	AV	7	Total 7	Mg 7	0	0
59	DR	2	Total 2	Mg 2	0	0
59	D8	1	Total 1	Mg 1	0	0
59	AA	373	Total 373	Mg 373	0	0
59	BQ	1	Total 1	Mg 1	0	0
59	CQ	1	Total 1	Mg 1	0	0
59	D7	4	Total 4	Mg 4	0	0
59	B6	1	Total 1	Mg 1	0	0
59	BU	2	Total 2	Mg 2	0	0
59	CC	3	Total 3	Mg 3	0	0
59	AD	3	Total 3	Mg 3	0	0
59	BN	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D0	4	Total 4	Mg 4	0	0
59	AI	3	Total 3	Mg 3	0	0
59	BY	1	Total 1	Mg 1	0	0
59	DE	4	Total 4	Mg 4	0	0
59	D9	1	Total 1	Mg 1	0	0
59	CJ	2	Total 2	Mg 2	0	0
59	BR	5	Total 5	Mg 5	0	0
59	CP	1	Total 1	Mg 1	0	0
59	DA	897	Total 897	Mg 897	0	0
59	DW	1	Total 1	Mg 1	0	0
59	D5	3	Total 3	Mg 3	0	0
59	B7	1	Total 1	Mg 1	0	0
59	AL	6	Total 6	Mg 6	0	0
59	CM	3	Total 3	Mg 3	0	0
59	BO	1	Total 1	Mg 1	0	0
59	AQ	3	Total 3	Mg 3	0	0
59	D1	2	Total 2	Mg 2	0	0
59	AH	1	Total 1	Mg 1	0	0
59	DP	6	Total 6	Mg 6	0	0
59	AC	2	Total 2	Mg 2	0	0
59	DY	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	11	Total 11	Mg 11	0	0
59	CS	2	Total 2	Mg 2	0	0
59	CD	1	Total 1	Mg 1	0	0
59	BD	5	Total 5	Mg 5	0	0
59	AT	1	Total 1	Mg 1	0	0
59	DT	1	Total 1	Mg 1	0	0
59	B0	2	Total 2	Mg 2	0	0
59	AO	2	Total 2	Mg 2	0	0
59	AY	3	Total 3	Mg 3	0	0
59	BH	4	Total 4	Mg 4	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AD	2	Total 2	Zn 2	0	0
60	CD	1	Total 1	Zn 1	0	0
60	AN	1	Total 1	Zn 1	0	0

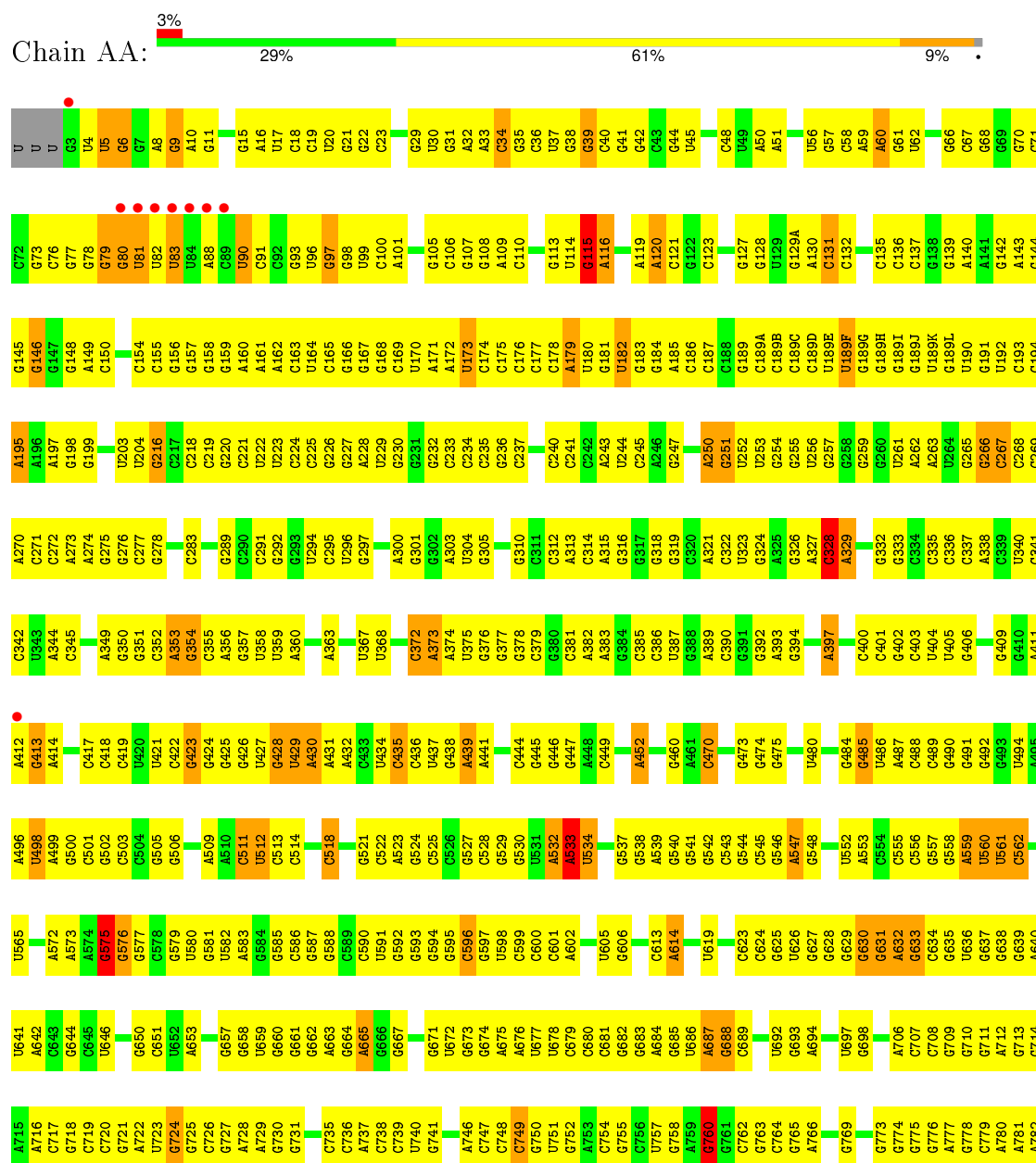
- Molecule 61 is water.

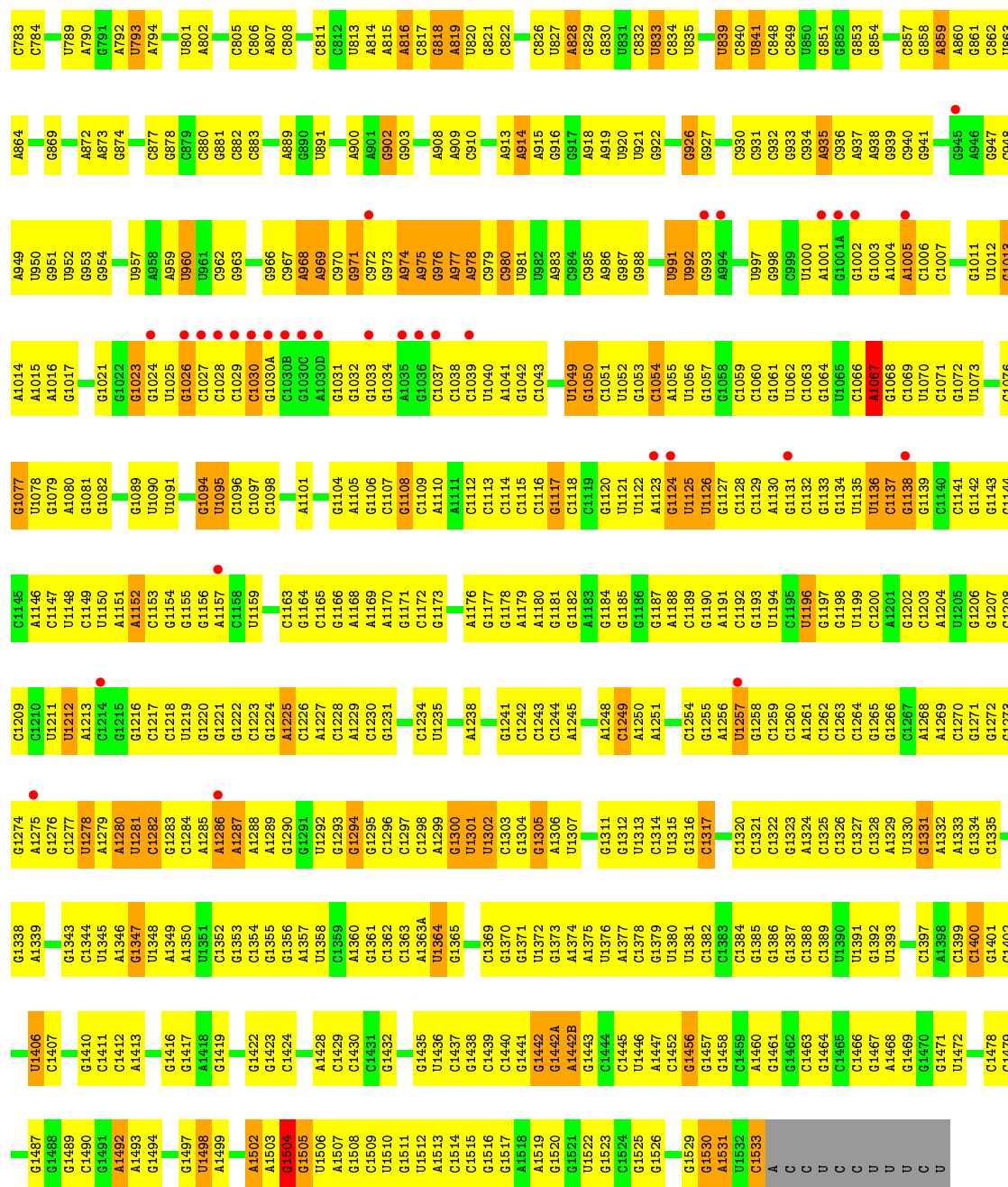
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	2	Total 2	O 2	0	0

### 3 Residue-property plots

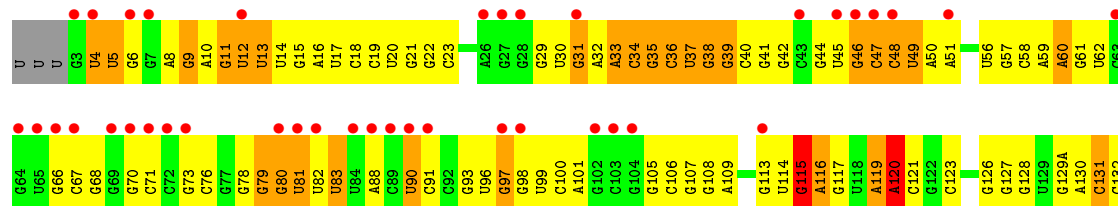
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

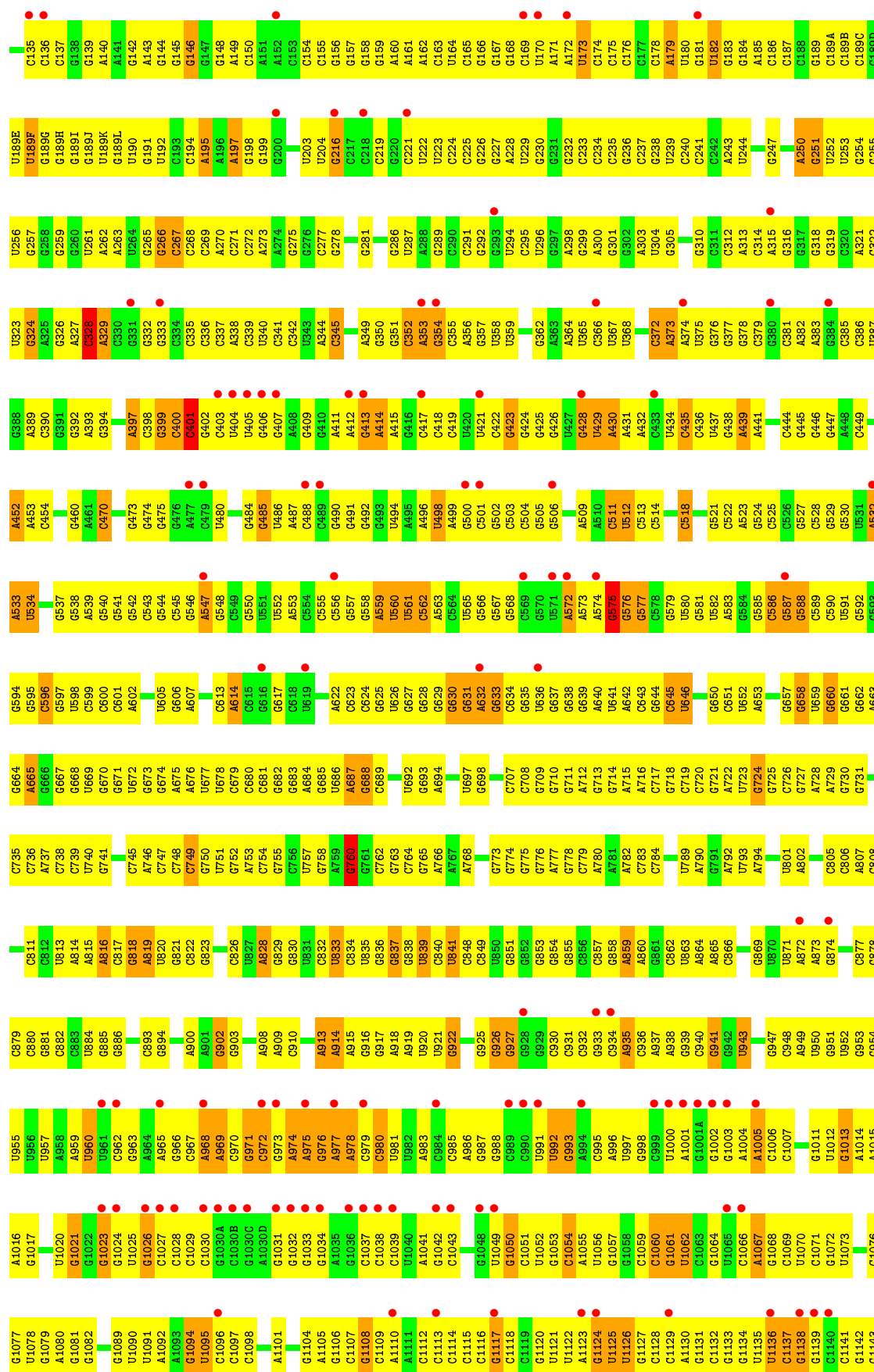
#### • Molecule 1: 16S rRNA

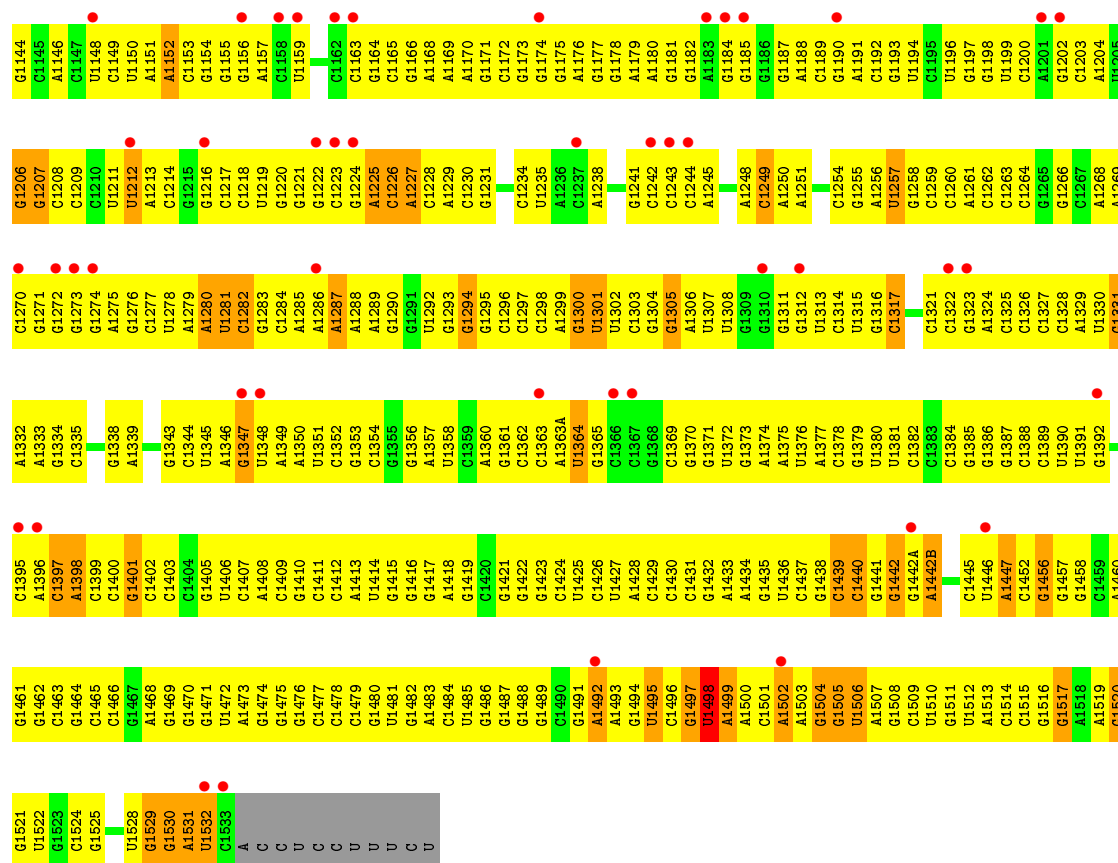




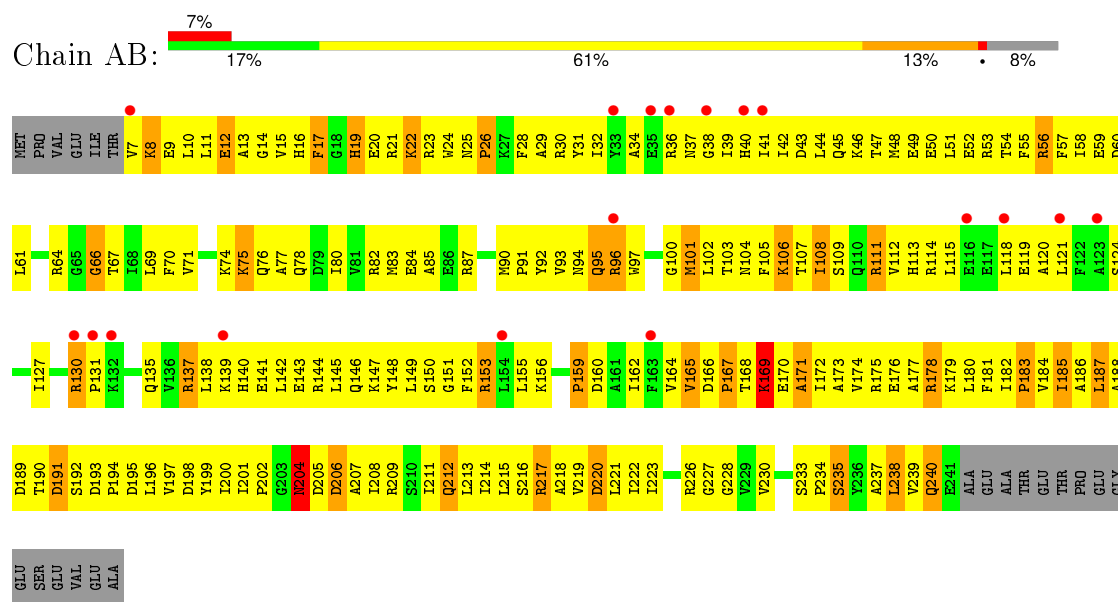
• Molecule 1: 16S rRNA



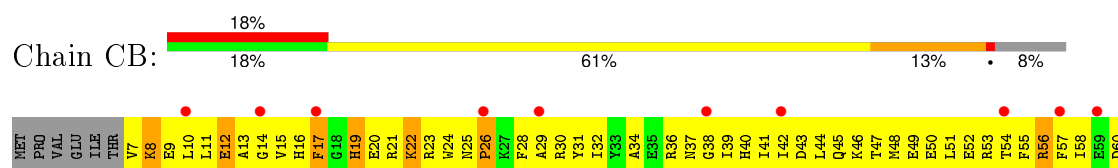


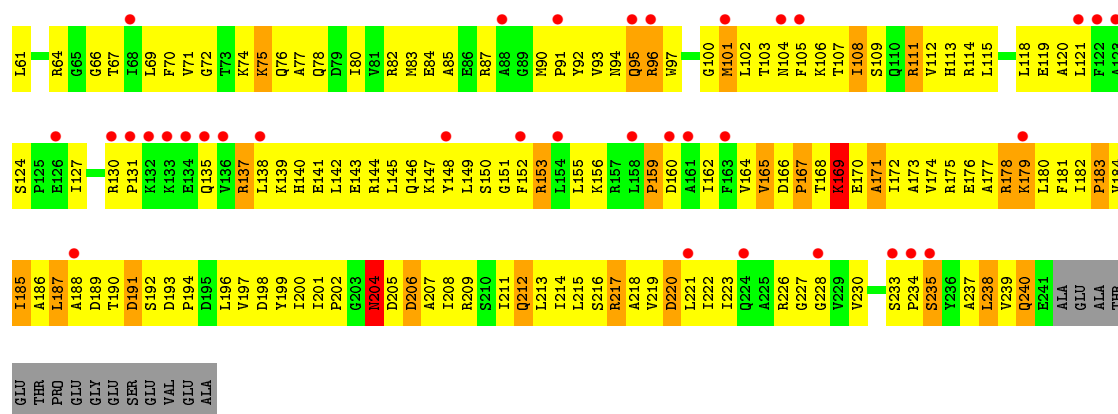


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

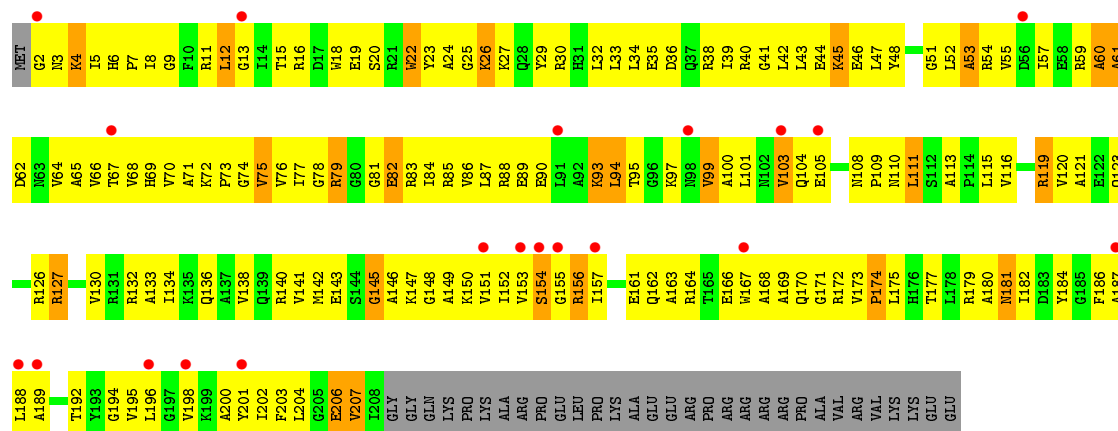


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

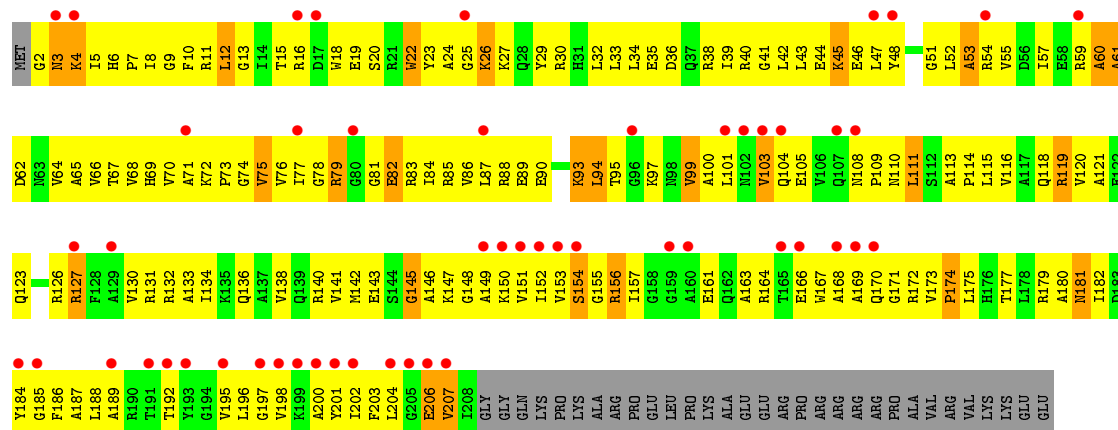




### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



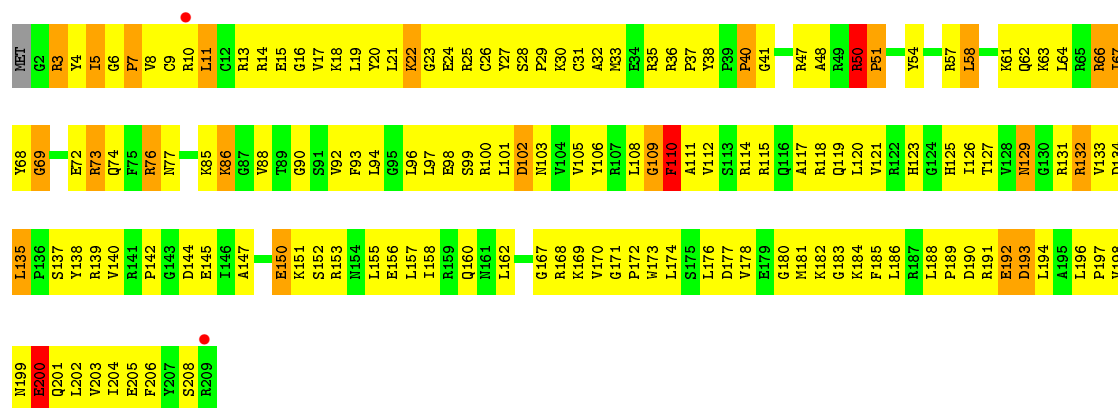
### • Molecule 3: 30S RIBOSOMAL PROTEIN S3



### • Molecule 4: 30S RIBOSOMAL PROTEIN S4



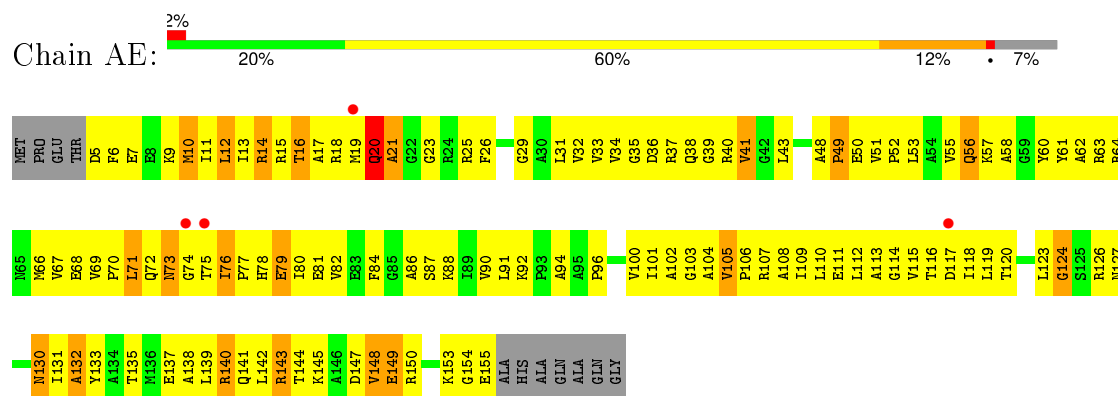




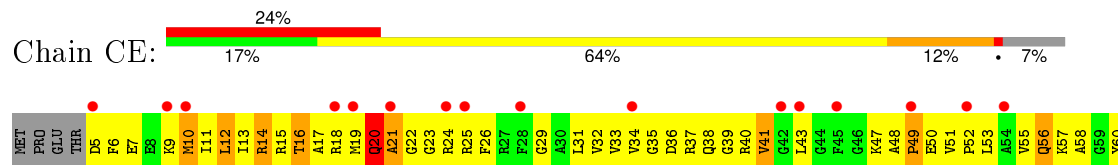
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

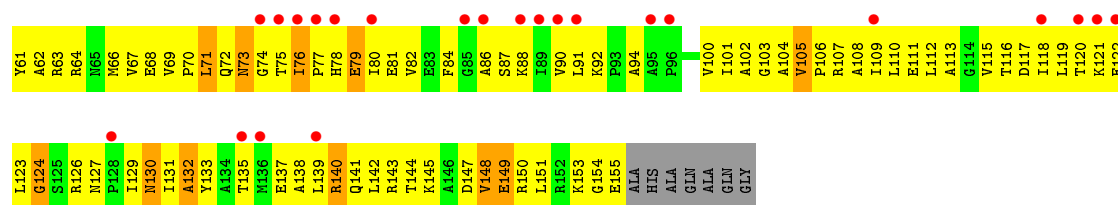


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

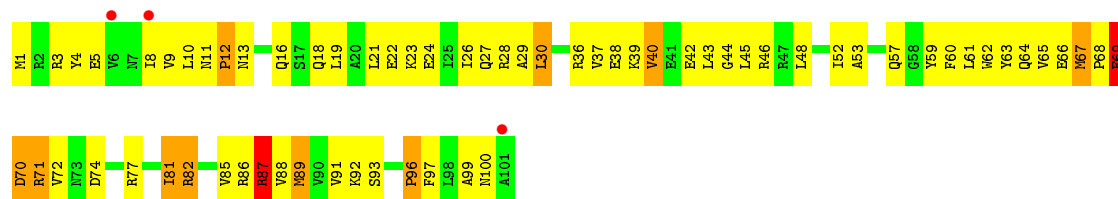


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

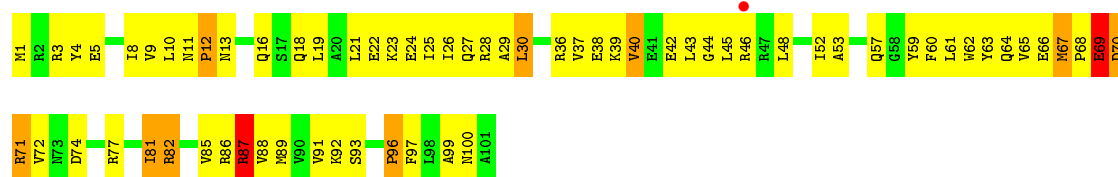




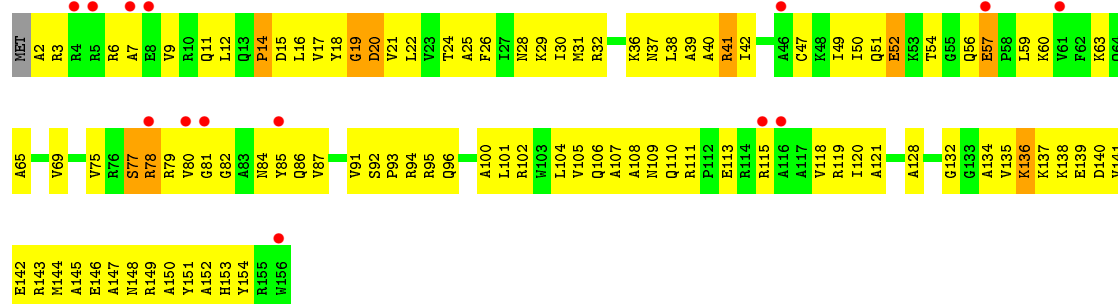
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



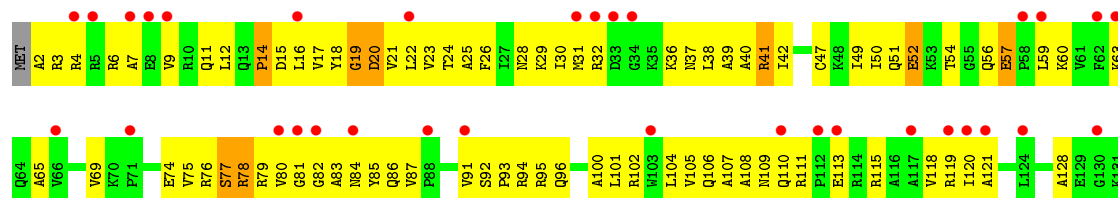
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

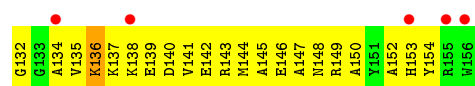


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

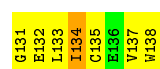
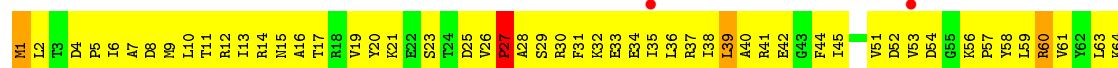


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

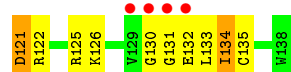
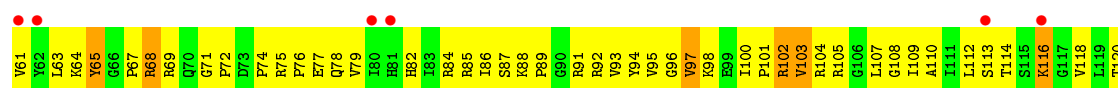
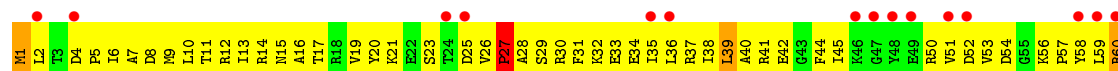




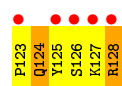
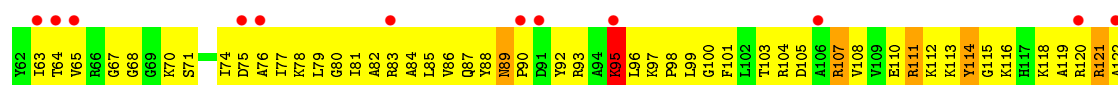
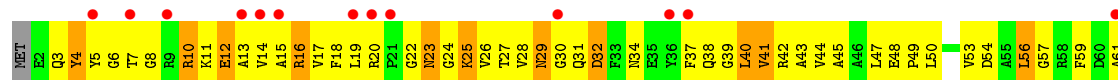
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



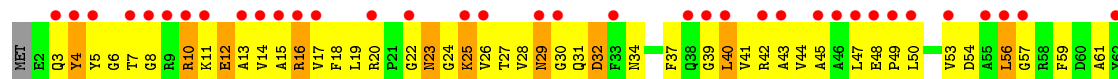
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

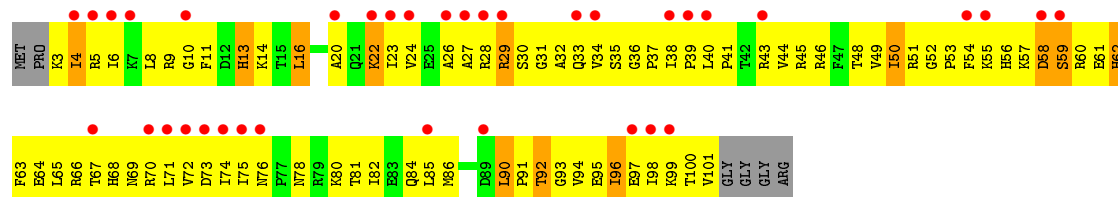


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

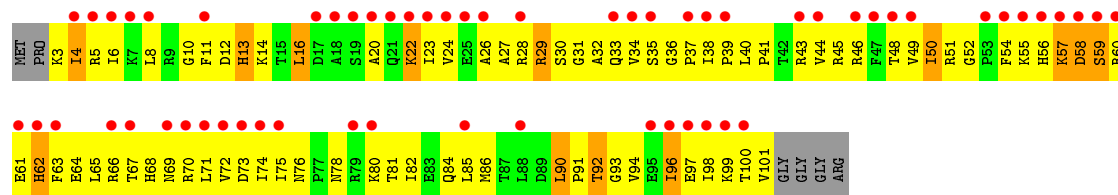




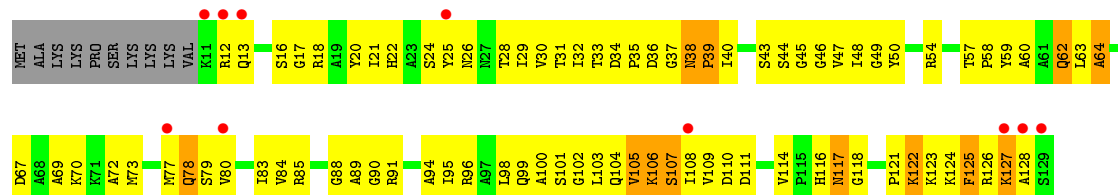
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



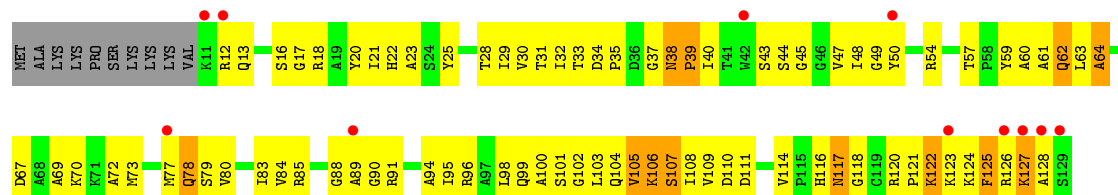
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

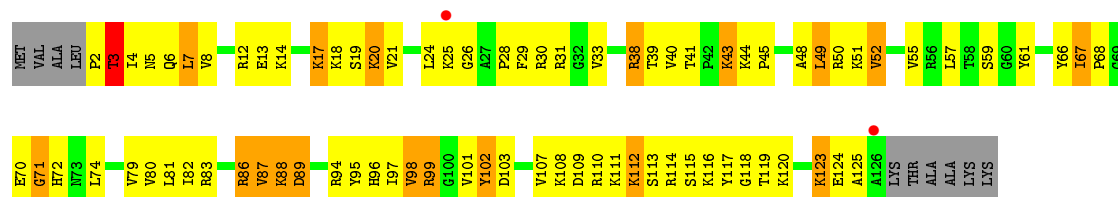


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

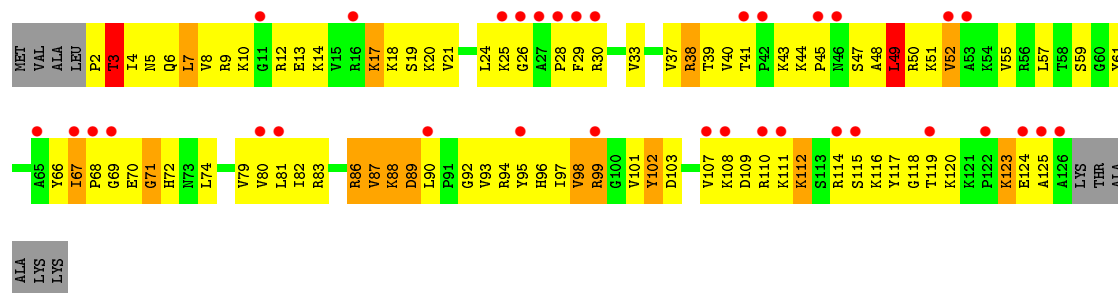


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

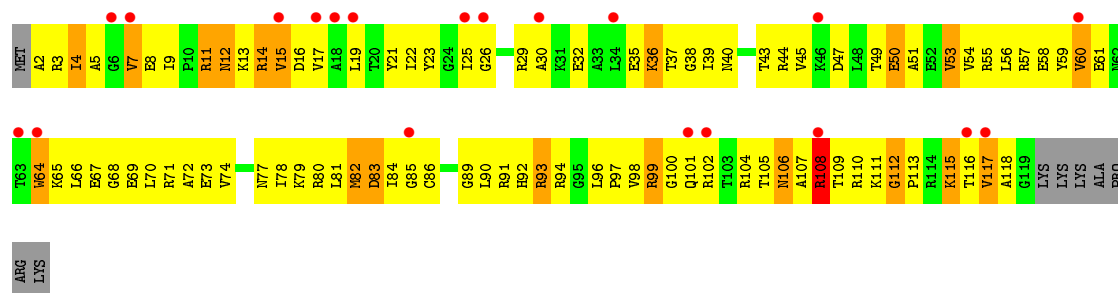




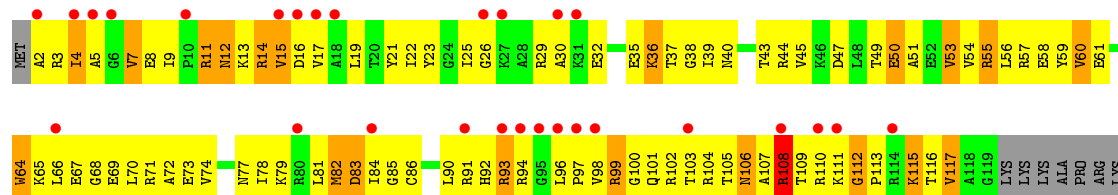
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



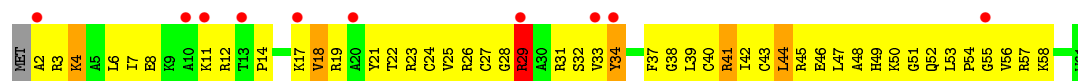
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



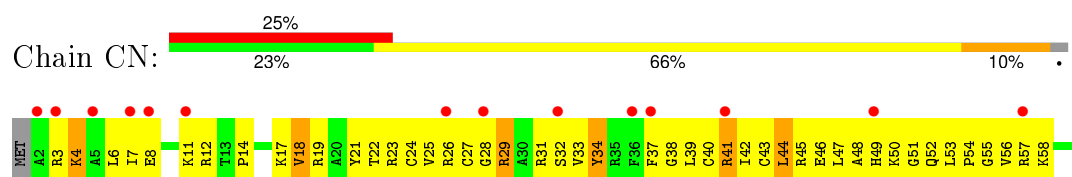
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



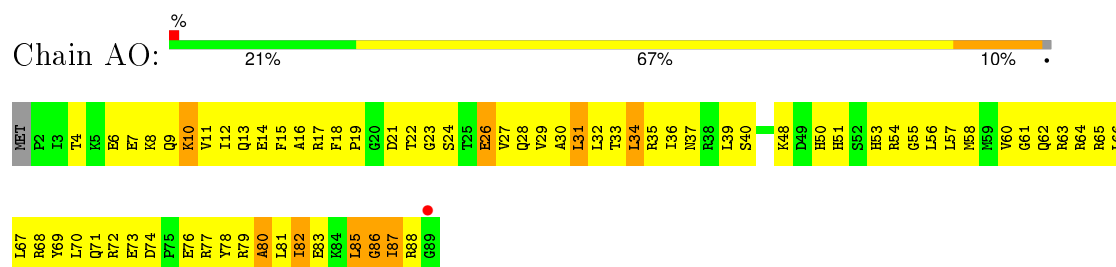
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



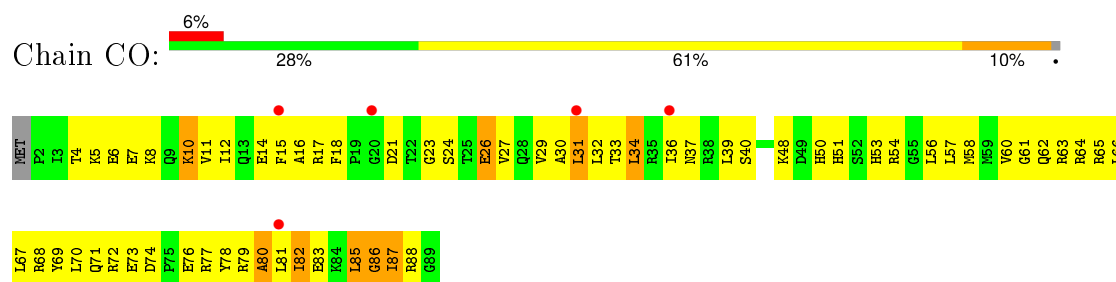
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



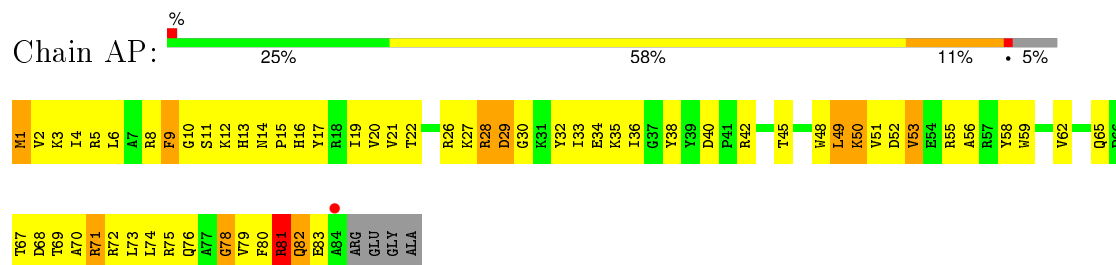
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



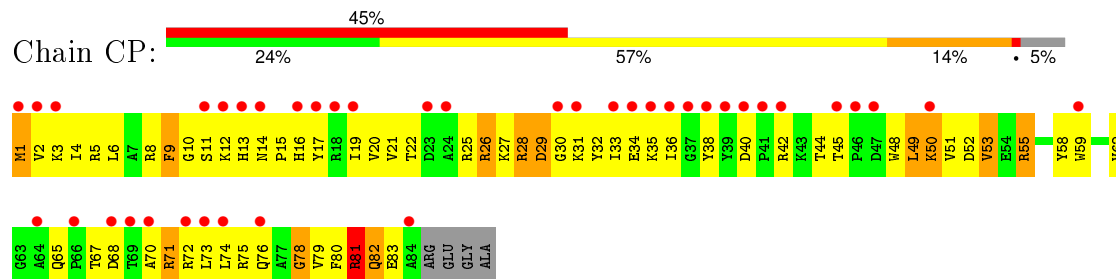
- Molecule 15: 30S RIBOSOMAL PROTEIN S15



- Molecule 16: 30S RIBOSOMAL PROTEIN S16

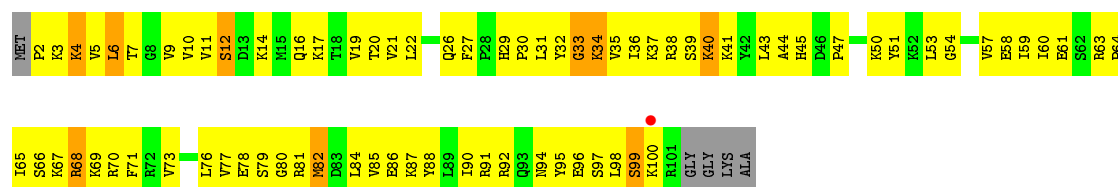


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

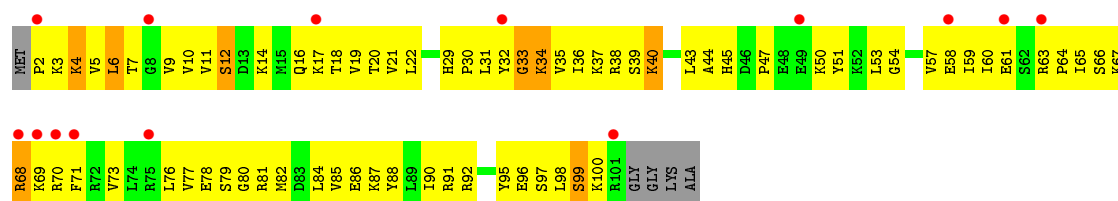


- Molecule 17: 30S RIBOSOMAL PROTEIN S17

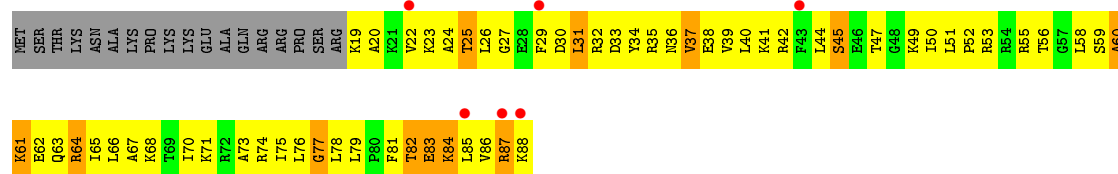
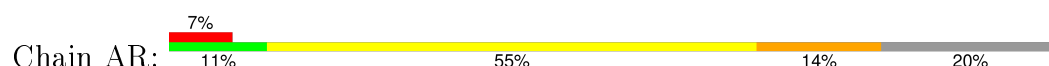




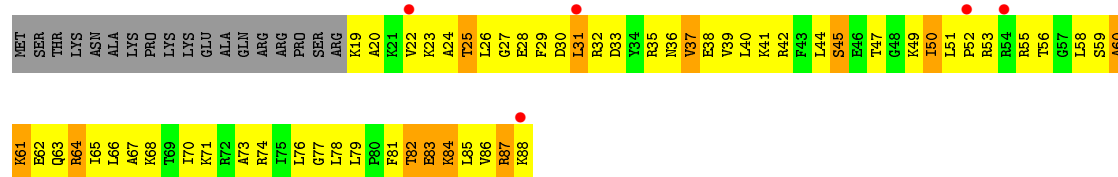
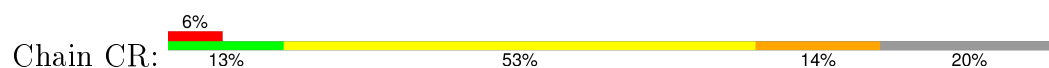
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



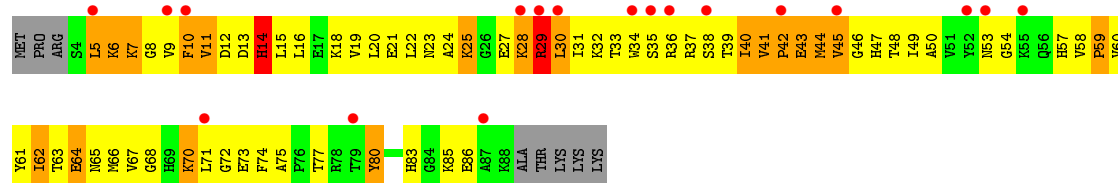
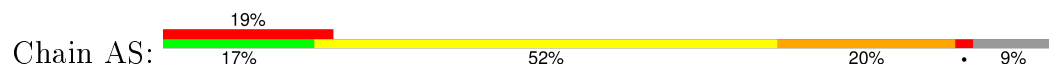
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

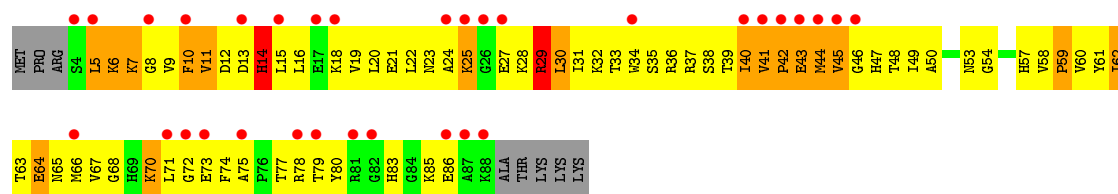


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

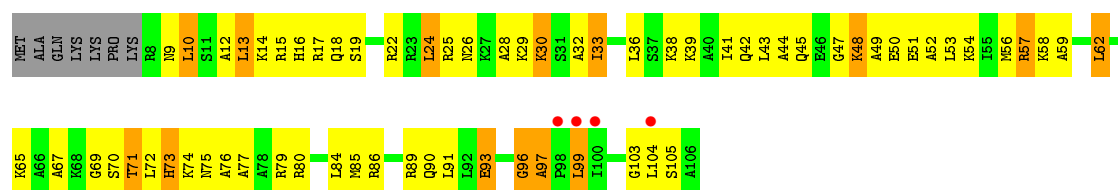


• Molecule 19: 30S RIBOSOMAL PROTEIN S19

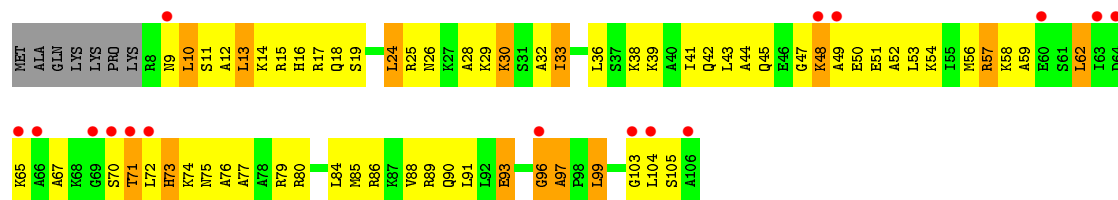




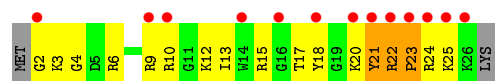
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



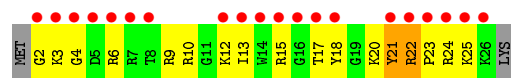
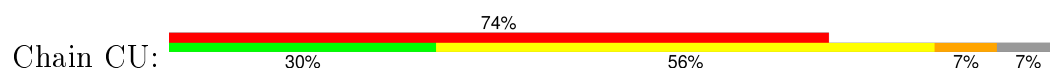
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



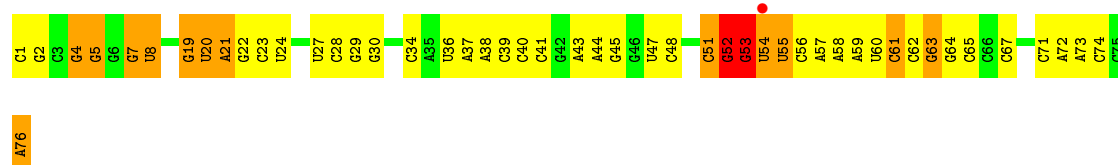
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

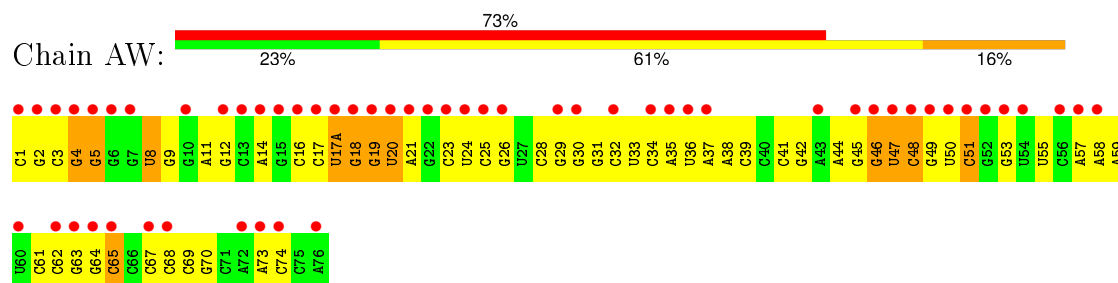


• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

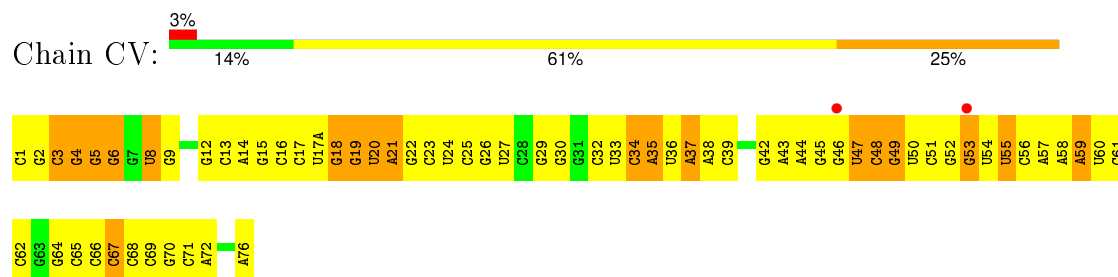




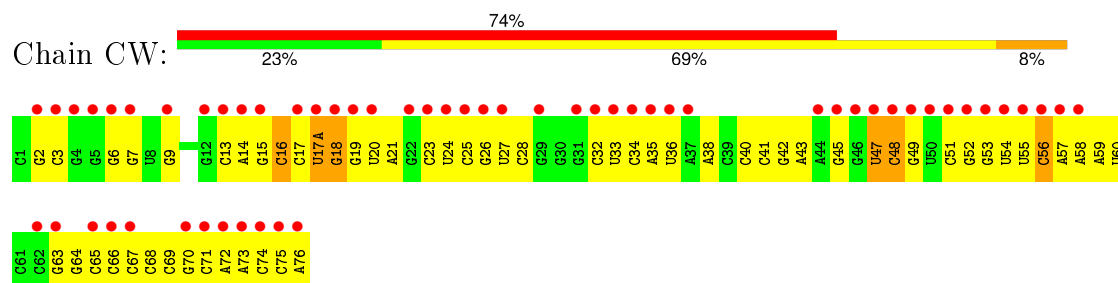
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



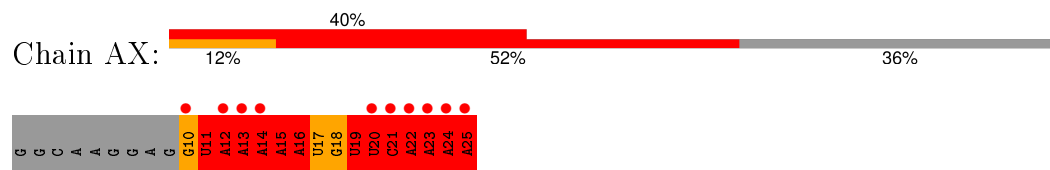
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



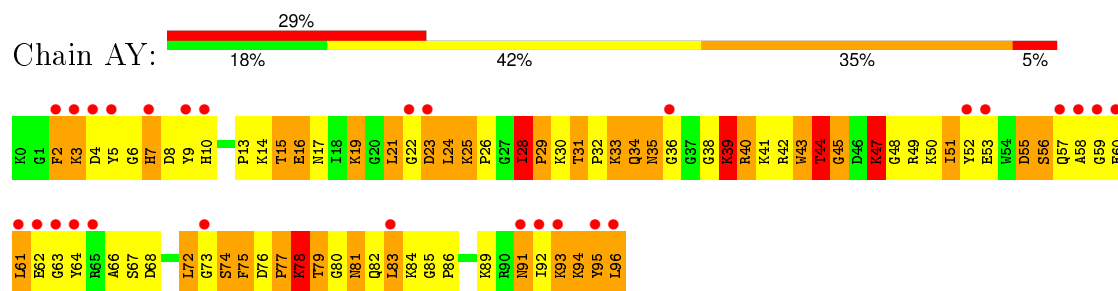
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



- Molecule 23: MRNA

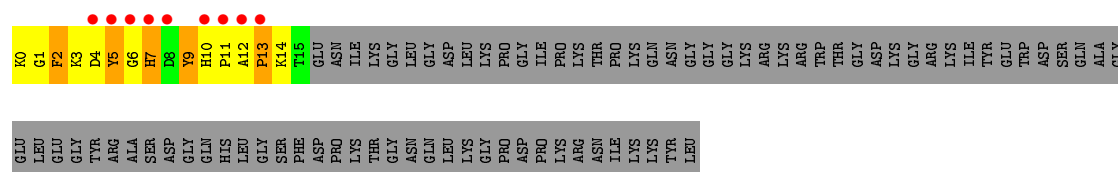


- Molecule 24: COLICIN-E3

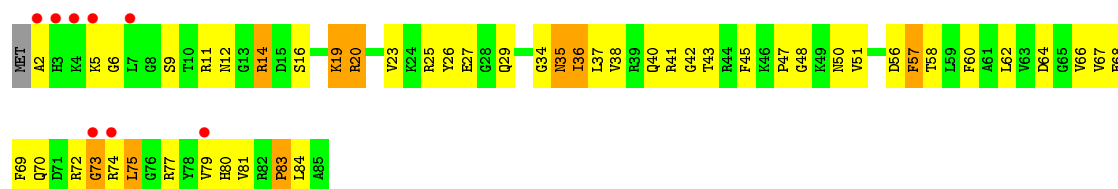


- Molecule 24: COLICIN-E3

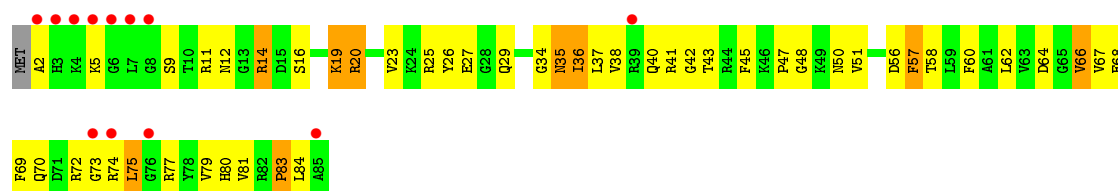




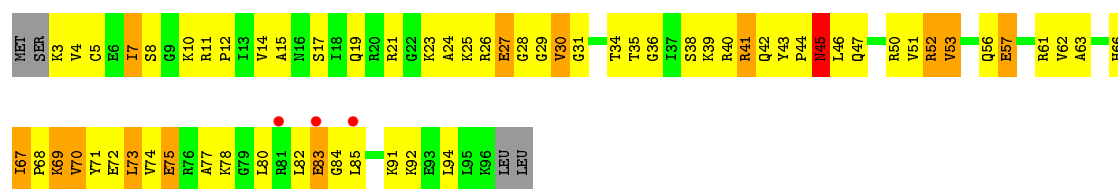
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



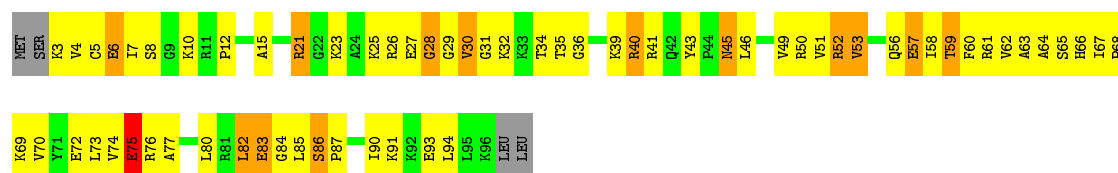
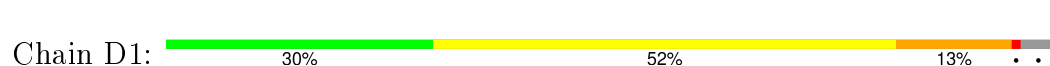
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



• Molecule 26: 50S RIBOSOMAL PROTEIN L28

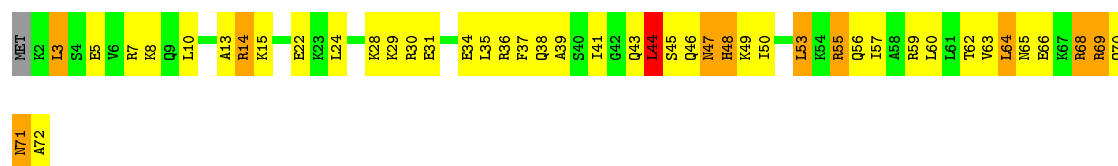


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

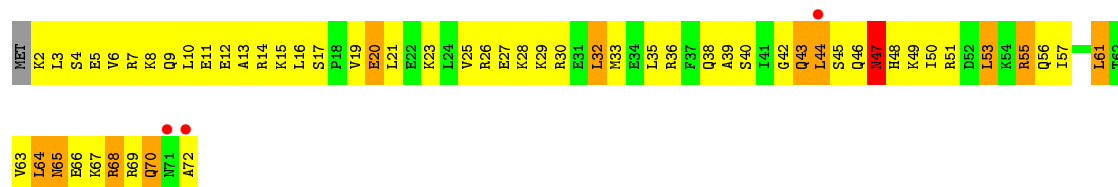


• Molecule 27: 50S RIBOSOMAL PROTEIN L29

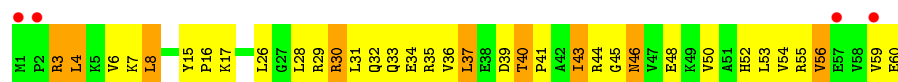
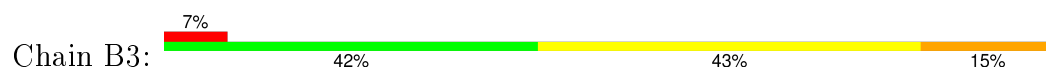




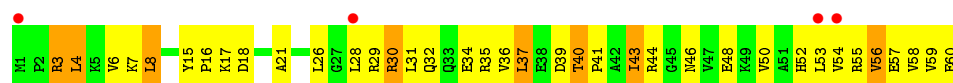
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30



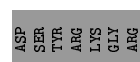
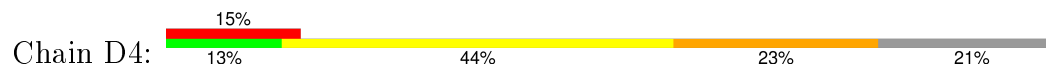
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



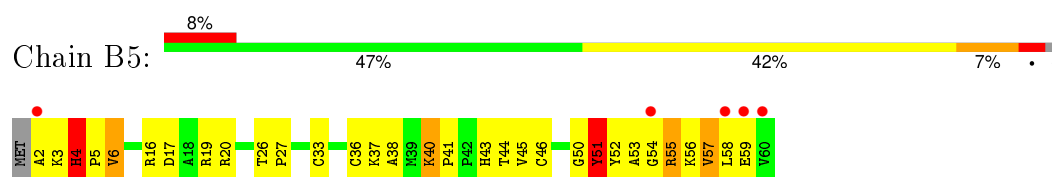
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



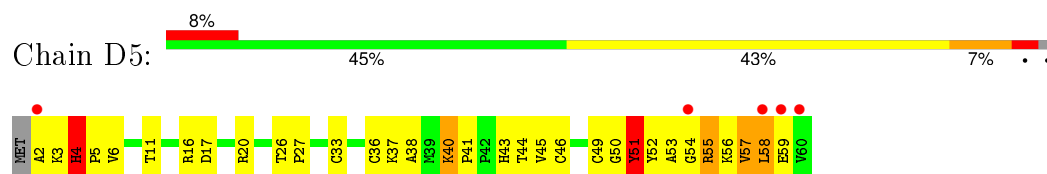
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



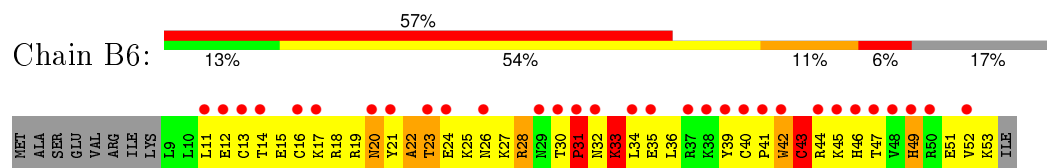
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



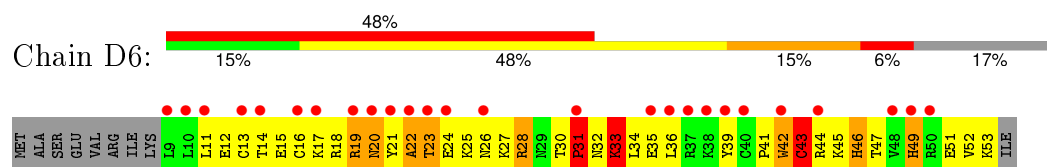
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



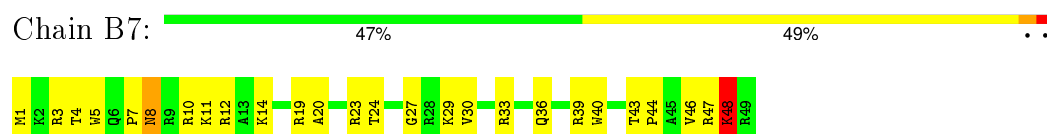
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



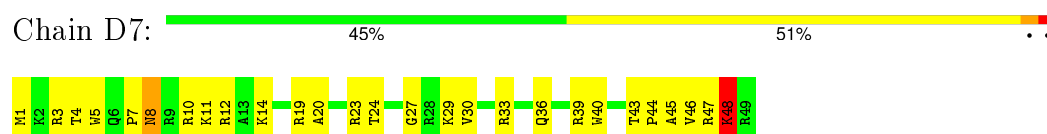
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



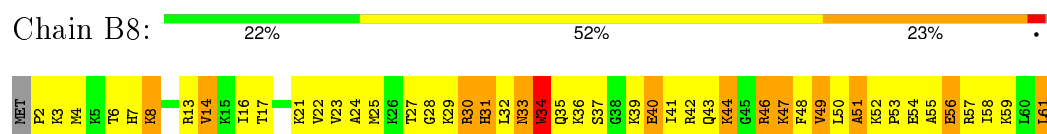
- Molecule 32: 50S RIBOSOMAL PROTEIN L34



- Molecule 32: 50S RIBOSOMAL PROTEIN L34



- Molecule 33: 50S RIBOSOMAL PROTEIN L35



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

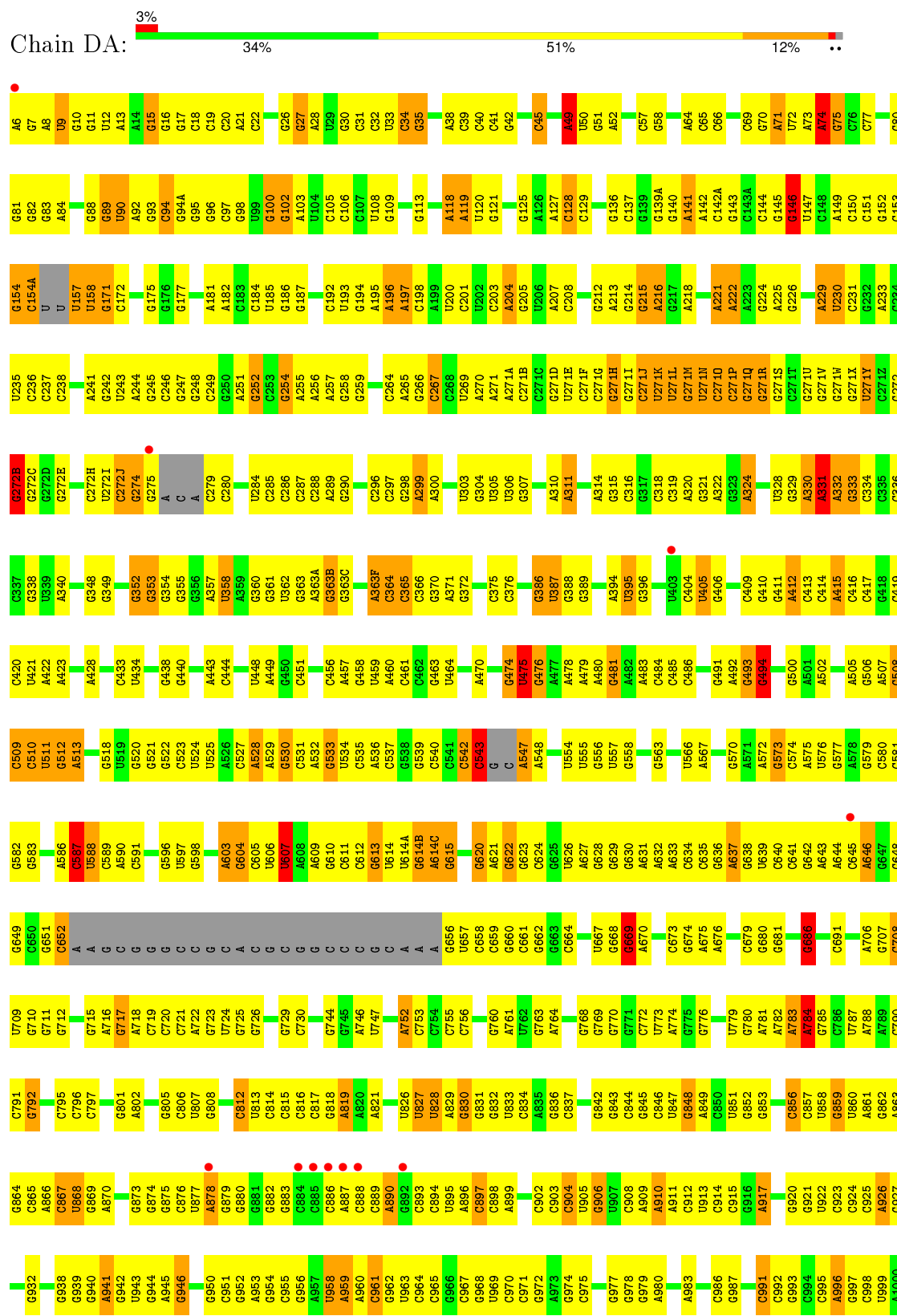




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C1743	C1561	G1561	G1500	G1435	G1358	A1276	G1196	A1126	C1004	G932	A863	A789	C708	G647
C1744	A1562	G1562	C1501	G1436	G1359	G1278	U1198		C1006	G938	G864	C791	U709	G648
C1745	C1563	G1563	C1502	G1437	G1360	G1279	U1203	A1129	G1011	A941	A866	A792	G711	G649
G1746	C1564	G1564	U1503	U1438	G1361	G1280	G1205	U1130	U1012			A793	G712	C652
A1682	C1565	C1565	C1504	A1439	G1362	G1281	U1206		U1013	G942	G869	C796		A
G1683	A1566	A1566	C1505	G1440	G1363	U1282	G1205	C1135	C1013	G943	A870	C797	G715	A
A1654	G1568	G1568	C1506	G1441	G1364	U1283	A1210	G1136	U1014	G944	G873	C797	A716	G
C1657	C1569	G1569	A1507	G1442	A1365	G1283	U1211	G1137	G1015	G945	G874		G717	C
C1658	A1570	A1570	A1508	G1443	G1368	A1284	G1212	G1138	G1016	G946	G875	A802	A718	G
A1571	C1509	A1571	C1509	A1445	G1369	G1285		G1139			G876		C719	G
G1685	A1572	A1572	A1509A	C1446A				G1140	U1019	G950	C876		G720	G
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U1687	C1587	C1587		G1461	G1389	G1309	G1231	G1154	G1034	C964	A892	A821	G745	G
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A1791	A1609	A1609	U	G1478	G1413	G1332		G1173	G1051	A980	C908	G842	G768	G
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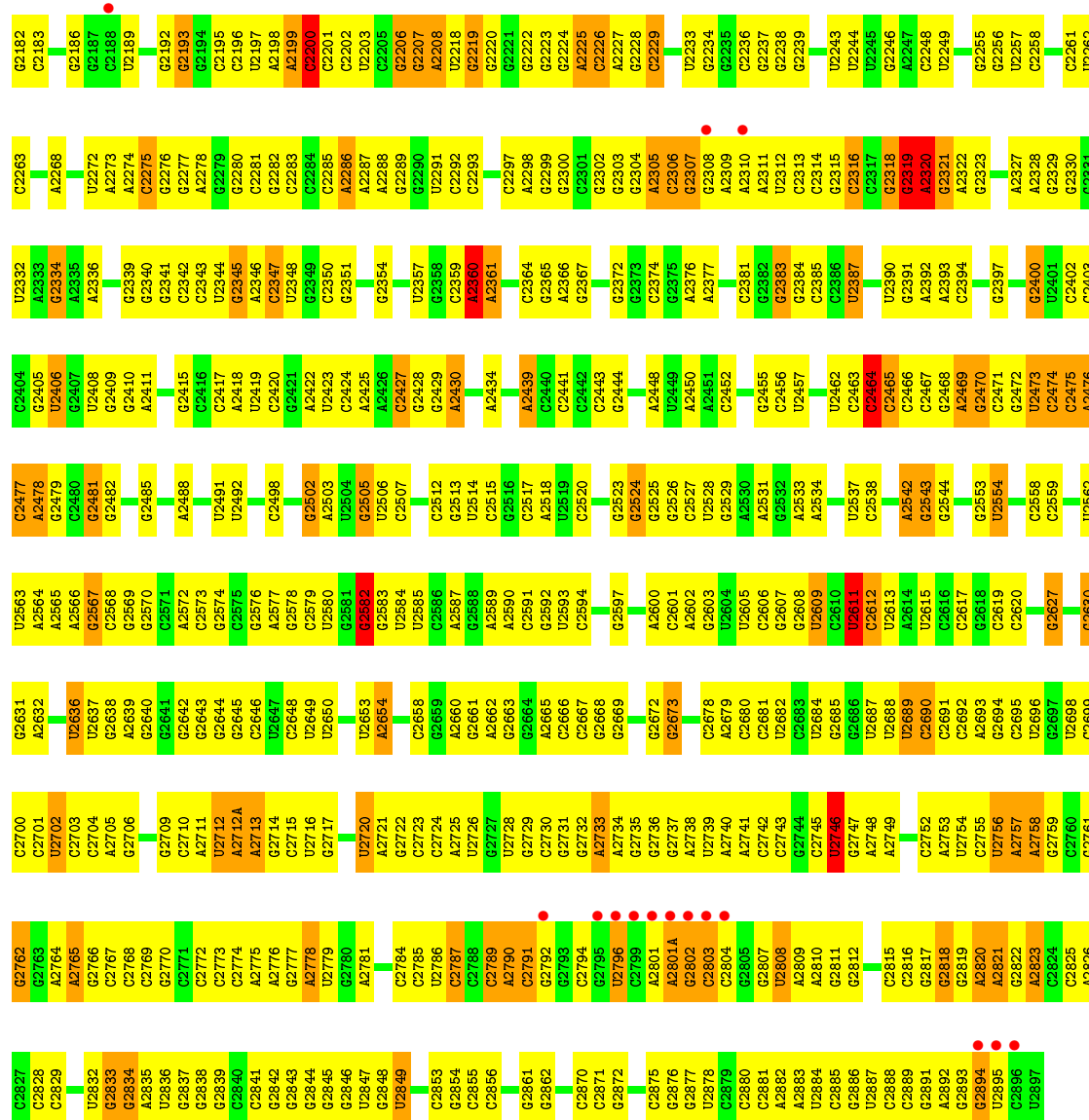


● Molecule 35: RNA (2848-MER)

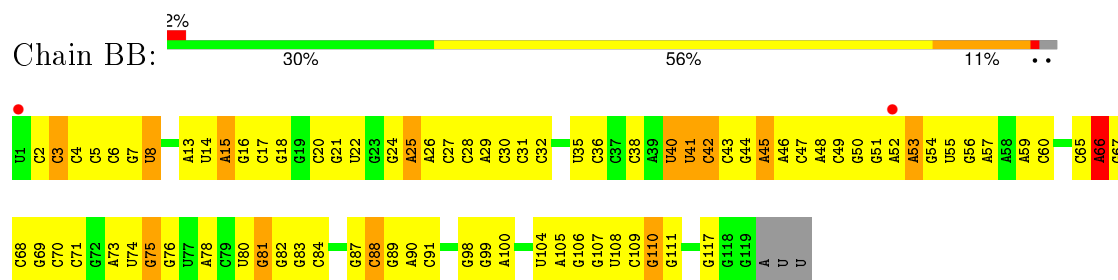




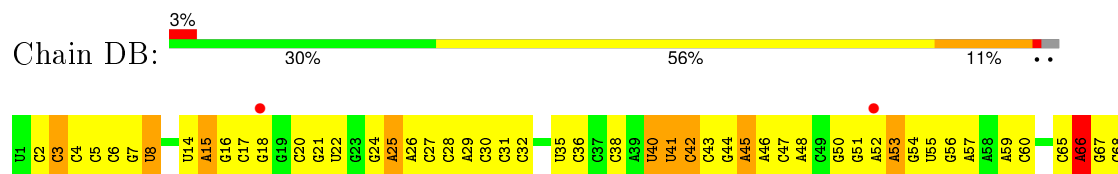
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C2076	A1918	A1918	A1918	C1839	G1773	A1889	G1594	C1531	C1468		G1228	G1151	
U2077	A1919	A1919	A1919	C1844	G1776	U1892	G1595	C1532	C1403	C1314			A1032
G2080	G1920	G1920	G1920	C1845	U1777	U1692	A1596	G1533	C1404	G1315	G1231	G1154	U1033
C2081	A1921	A1921	A1921	G1846	U1778	U1693	A1597	U1534	C1405	G1316	G1232	G1155	U1034
U2082	U1922	U1922	U1922	A1847	U1779	C1694	C1598	A1535	C1406	A1317	G1233	A1156	U1035
G2083	C1923	C1923	C1923	U1848	C1780	G1695	C1607	C1536	G1407	G1332	G1239	U1159	G1037
C2084	A1924	A1924	A1924	A1849	C1781	G1696	A1608	G1537	G1475	C1333	U1240	G1160	G1038
G2085	G1925	G1925	G1925	C1850	C1782	G1697	A1609	C1538	G1476	A1336	G1241	G1161	G1039
C2086	U1851	U1851	U1851	G1854	A1783	U1697	A1610	C1539	G1477	A1337	A1242	C1162	C1040
U2087	C1855	C1855	C1855	A1854	A1784	G1698	U1611	C1540	G1478	G1338	G1243	G1163	G1041
A2014	G1856	G1856	G1856	U1855	A1785	U1700	G1613	C1541	U1481	G1339	A1246	G1164	G1044
A2015	G1857	G1857	G1857	C1856	A1786	A1701	G1614	C1542	G1482		A1247	U1185	A1045
U2016	U1858	U1858	U1858	G1858	A1787	G1702	G1815	C1543	G1483	G1344	G1250	G1169	A1046
C2017	A1859	A1859	A1859	C1859	C1788	U1705	A1616	C1544	G1484	C1345	G1251	G1170	A1047
A2019	G1860	G1860	G1860	U1860	A1789	U1706	C1617	C1545	A1486	G1346	G1252	G1171	C1048
C2020	G1861	G1861	G1861	C1861	C1790	U1709	A1618	C1546	G1487	G1347	G1253	G1173	C1049
C2021	G1862	G1862	G1862	U1862	A1791	C1710	G1625	C1547	U1488	G1348	A1253	A1174	A1050
G2104	G1863	G1863	G1863	U1863	C1792	C1711	G1626	C1548	U1489	A1349	G1256	U1175	G1051
U2022	U1864	U1864	U1864	C1864	C1793	C1712	C1636	C1550	G1490	G1352	G1257	U1176	C1052
C2023	A1937	A1937	A1937	C1865	U1794	U1713	A1637	C1551	G1491	A1352	G1258	A1177	C1053
G2024	C1938	C1938	C1938	U1866	C1795	C1714	C1638	C1552	G1492	A1353	G1259	G1178	A1053
C2025	U1867	U1867	U1867	C1867	U1796	U1715	C1639	C1553	A1493	A1354	A1260	C1179	C1054
C2026	G1877	G1877	G1877	C1877	C1797	G1717	U1639	C1554	A1494	G1355	A1262	C1180	G1108
G2027	A1878	A1878	A1878	U1878	U1798	G1718	C1640	C1555	A1495	G1356	U1263	C1181	C1109
U2028	C1879	C1879	C1879	C1880	G1799	G1719	A1641	C1556	U1496	G1357	G1264	A1182	G1110
C2029	U1880	U1880	U1880	C1881	C1800	U1720	A1642	C1557	U1497	U1357	G1265	G1187	G1111
A2030	C1881	C1881	C1881	C1882	G1801	U1721	G1643	C1558	U1498	G1358	A1266	U1188	G1112
C2031	U1882	U1882	U1882	C1883	C1802	G1722	C1644	C1559	U1499	U1359	U1267	G1189	G1113
A2032	G1883	G1883	G1883	A1884	C1804	U1723	C1645	C1560	G1500	A1360	G1268	G1190	U1109
G2033	U1884	U1884	U1884	C1885	U1805	U1724	C1646	C1561	G1501	G1361	A1269	G1191	G1110
C2034	A1885	A1885	A1885	U1886	C1806	G1740	C1647	C1562	C1502	G1362	G1270	G1192	G1111
G2035	C1886	C1886	C1886	C1887	G1807	A1741	C1648	C1563	C1503	C1363	G1271	G1193	G1112
U2036	U1887	U1887	U1887	C1888	U1808	G1742	A1652	C1564	U1504	G1364	G1272	G1194	G1113
C2037	G1888	G1888	G1888	C1889	A1810	C1744	A1654	C1565	C1505	U1365	G1273	G1195	G1114
A1960	C1889	C1889	C1889	C1890				C1566	C1506	G1366			G1115
U1887	C1890	C1890	C1890	C1891				C1567	C1507	G1367			G1116
C2038	C1891	C1891	C1891	C1892				C1568	C1508	G1368			G1117
G2039	U1963	U1963	U1963	C1893				C1569	C1509	G1369			G1118

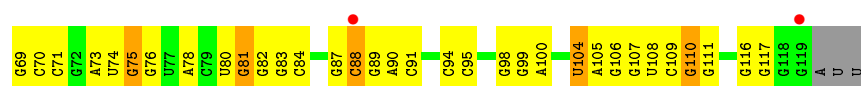


• Molecule 36: RNA (119-MER)

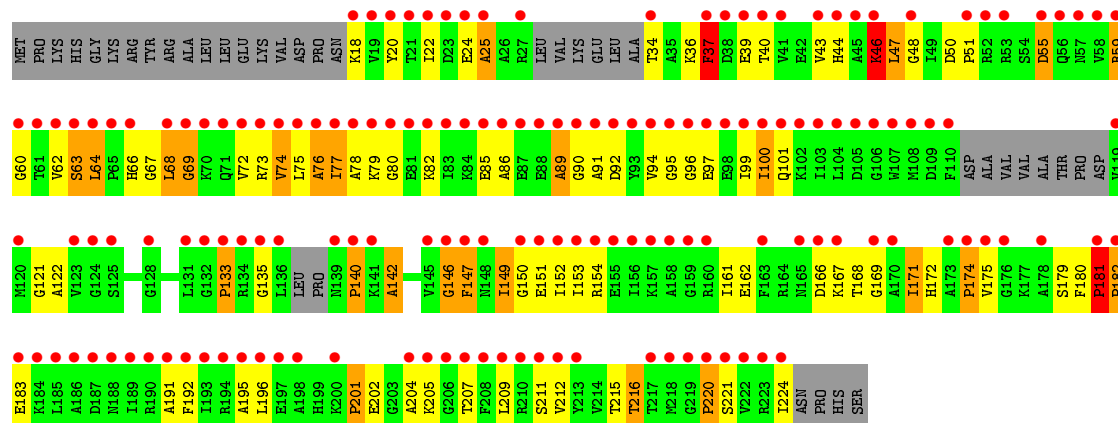
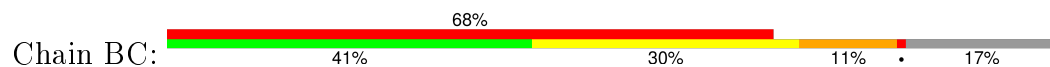


• Molecule 36: RNA (119-MER)

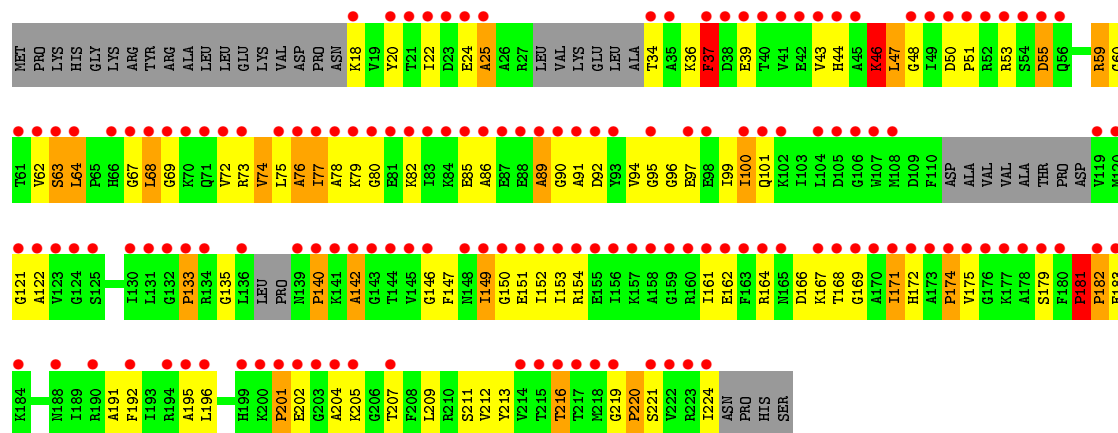
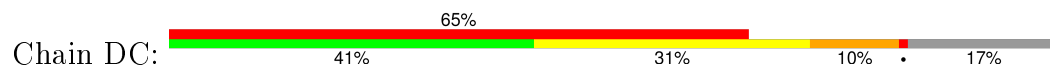




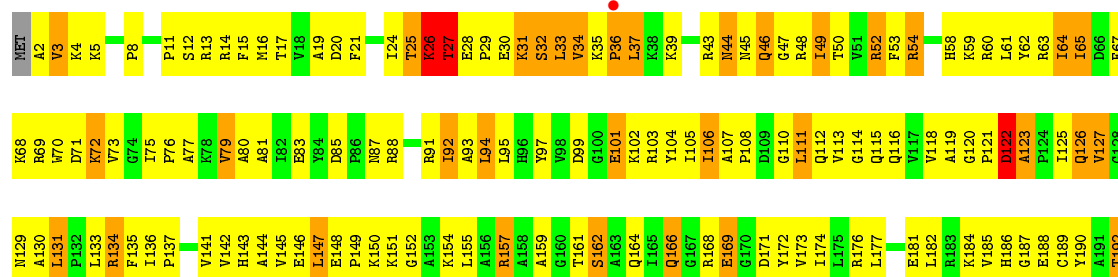
• Molecule 37: 50S RIBOSOMAL PROTEIN L1



• Molecule 37: 50S RIBOSOMAL PROTEIN L1

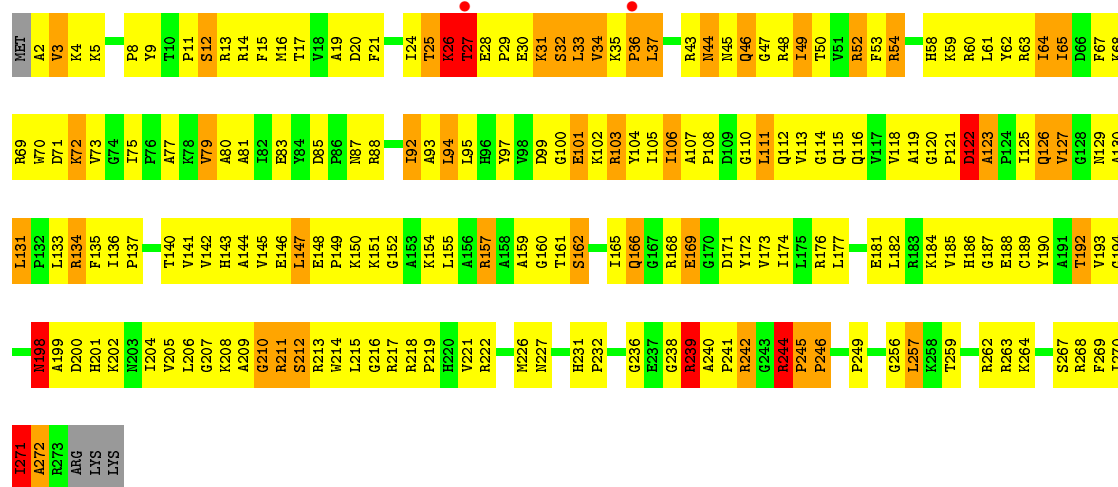


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

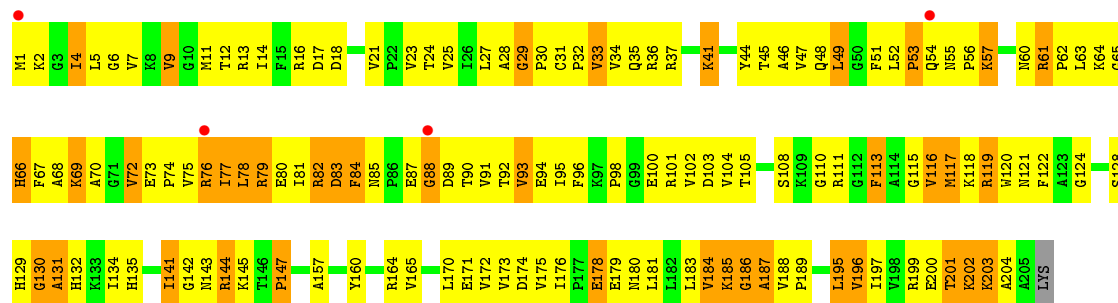




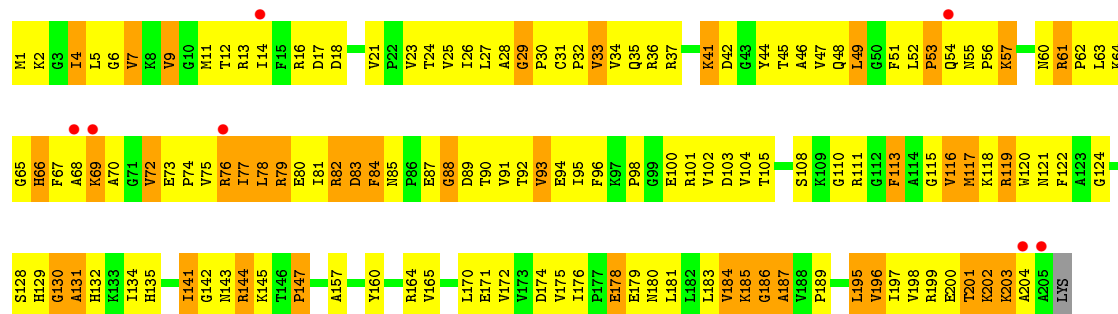
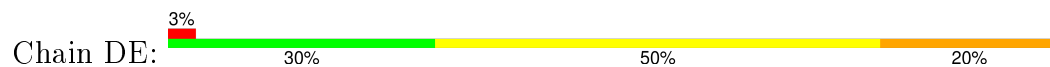
• Molecule 38: 50S RIBOSOMAL PROTEIN L2



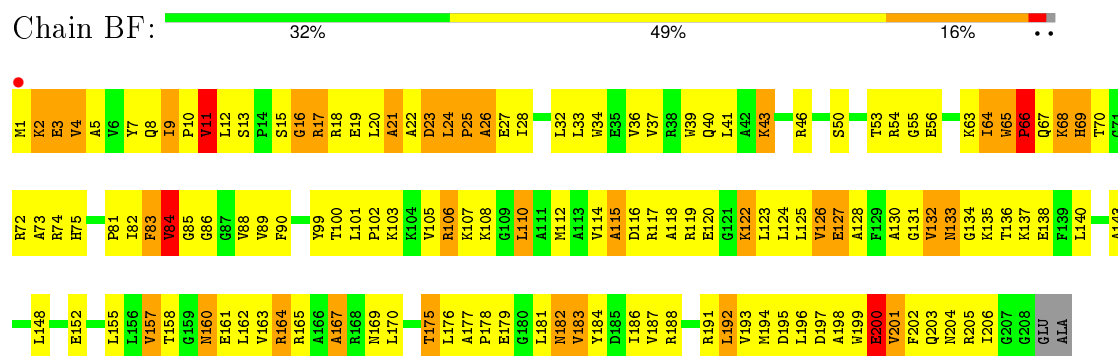
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



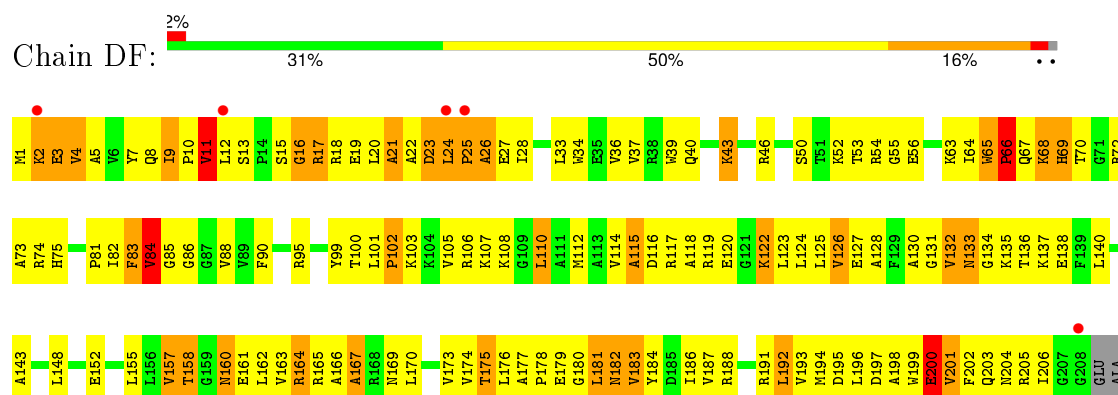
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



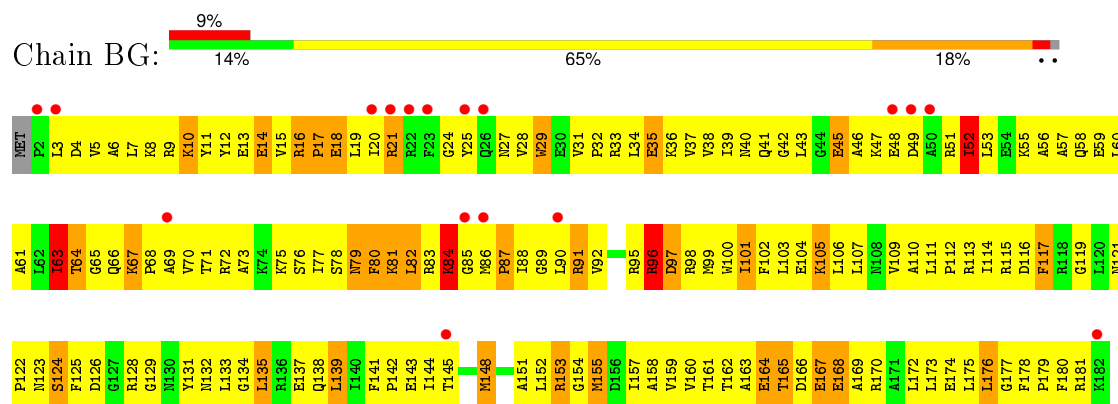
- Molecule 40: 50S RIBOSOMAL PROTEIN L4



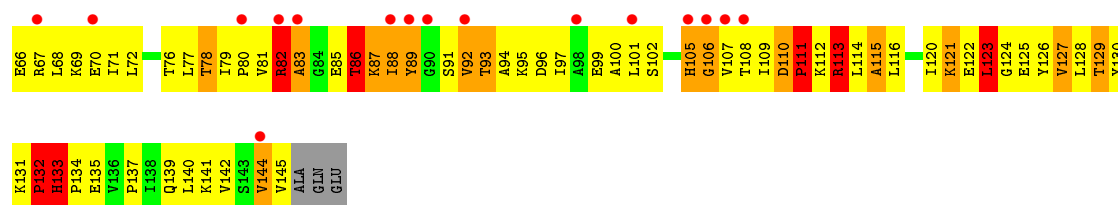
- Molecule 40: 50S RIBOSOMAL PROTEIN L4



- Molecule 41: 50S RIBOSOMAL PROTEIN L5

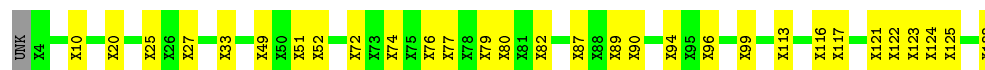






• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ: 76% 23%



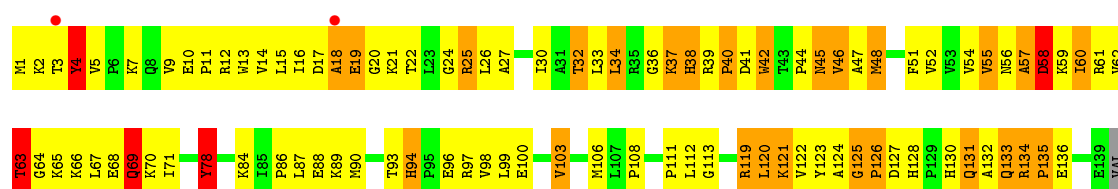
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ: 63% 37%



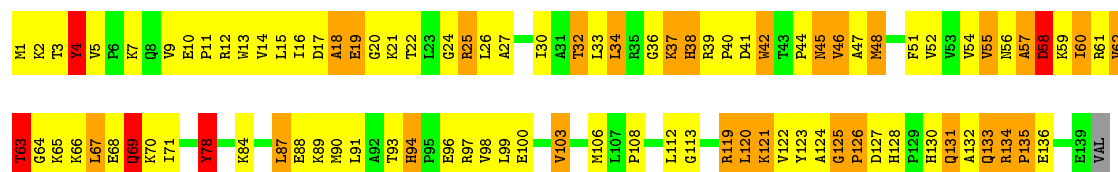
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN: 30% 47% 19%



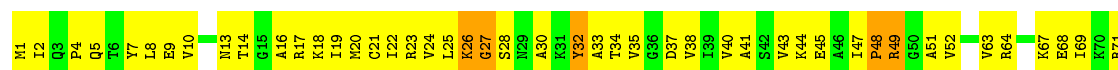
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

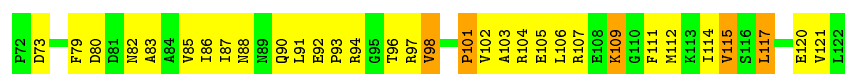
Chain DN: 31% 45% 20%



• Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO: 36% 56% 8%

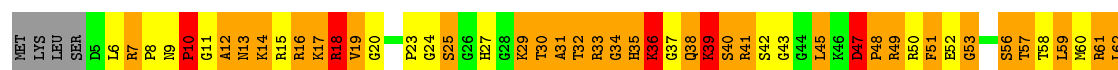
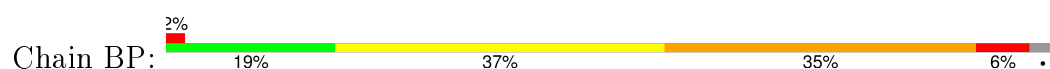




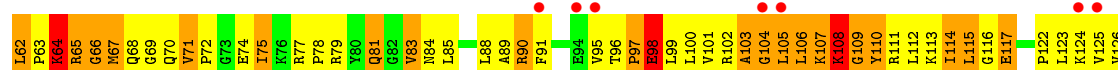
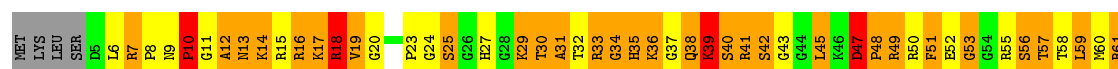
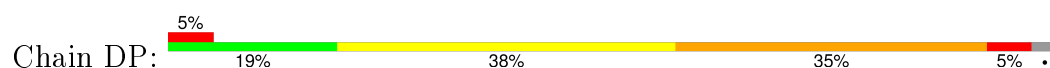
• Molecule 46: 50S RIBOSOMAL PROTEIN L14



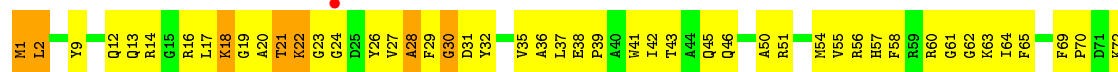
• Molecule 47: 50S RIBOSOMAL PROTEIN L15



• Molecule 47: 50S RIBOSOMAL PROTEIN L15

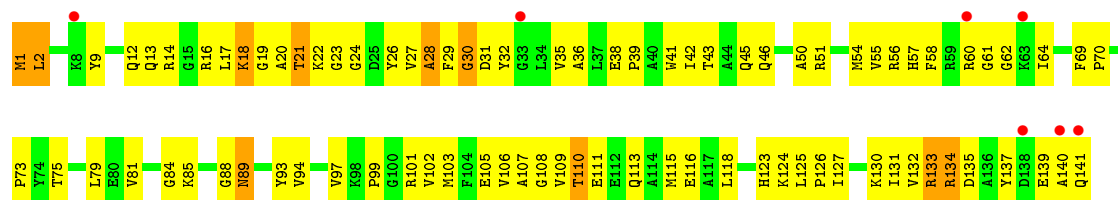


• Molecule 48: 50S RIBOSOMAL PROTEIN L16

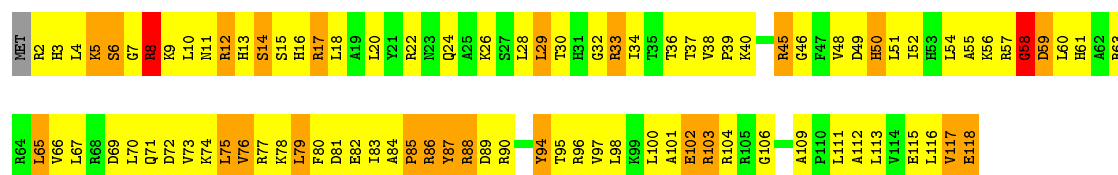


• Molecule 48: 50S RIBOSOMAL PROTEIN L16

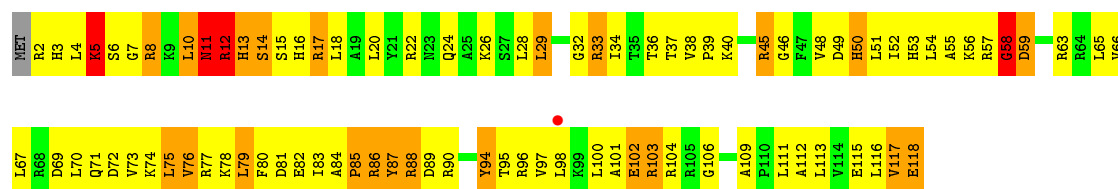




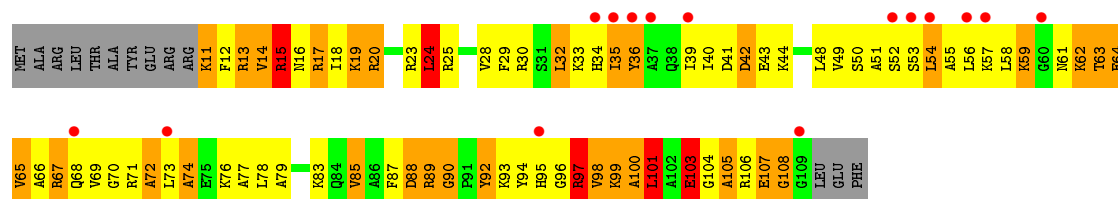
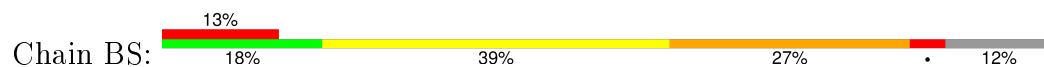
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



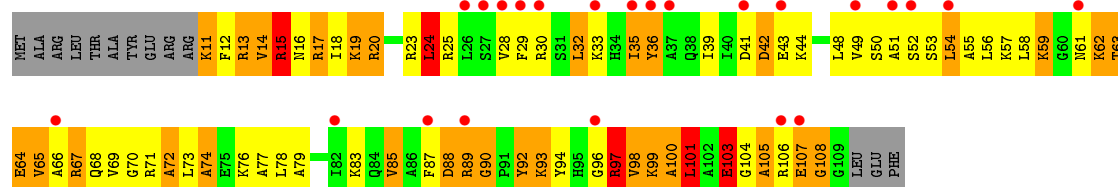
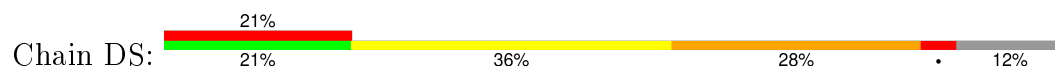
• Molecule 49: 50S RIBOSOMAL PROTEIN L17



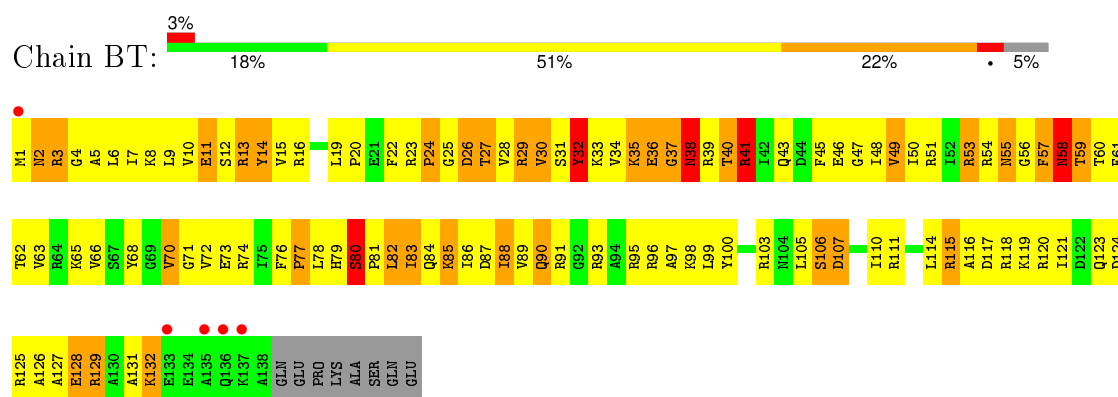
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



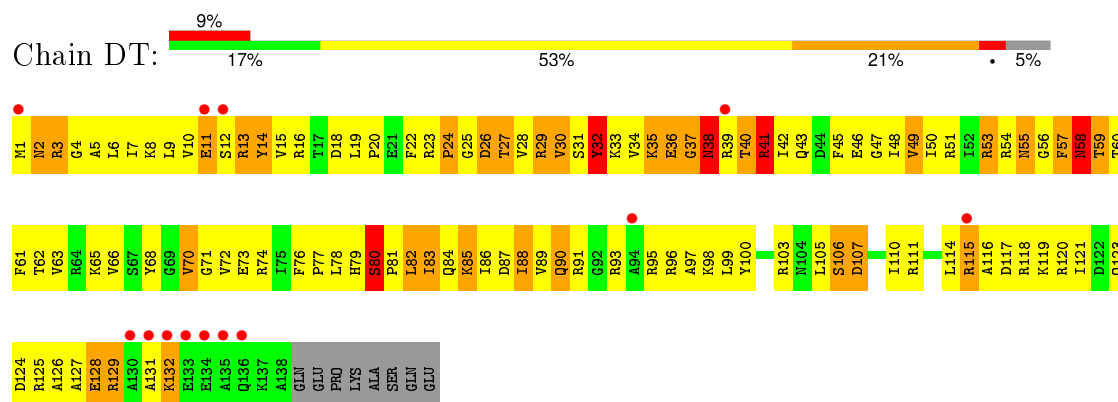
• Molecule 50: 50S RIBOSOMAL PROTEIN L18



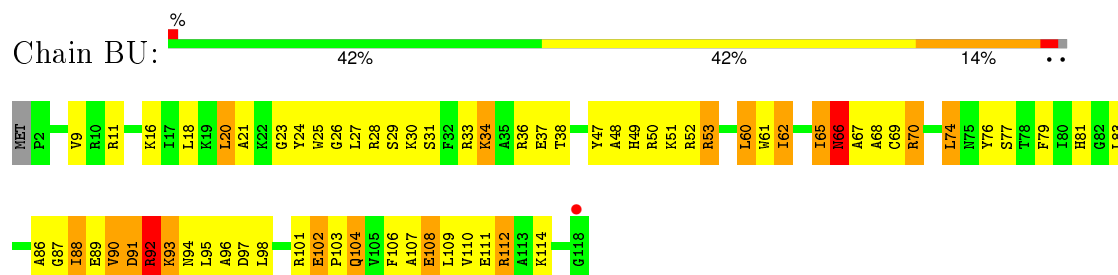
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



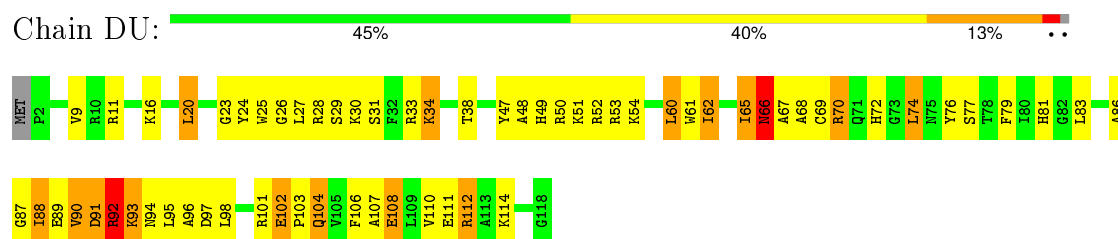
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



• Molecule 52: 50S RIBOSOMAL PROTEIN L20

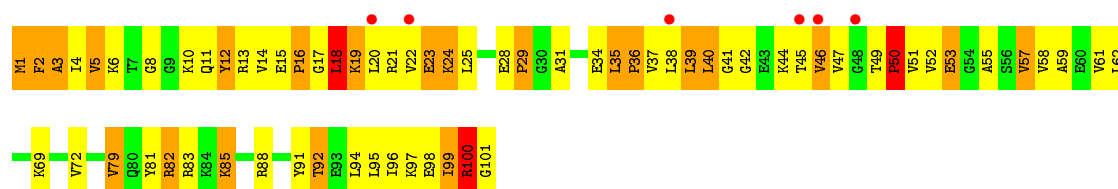


• Molecule 52: 50S RIBOSOMAL PROTEIN L20

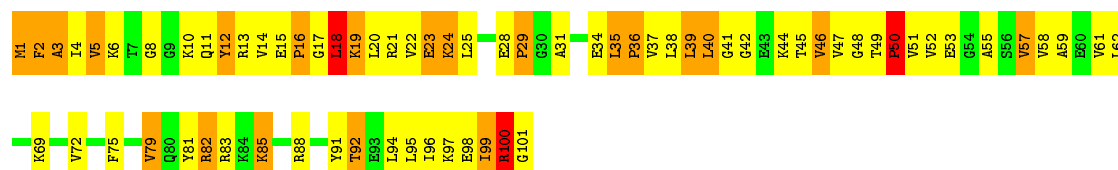
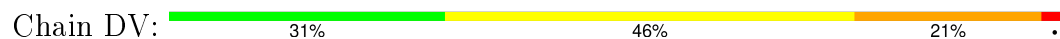


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

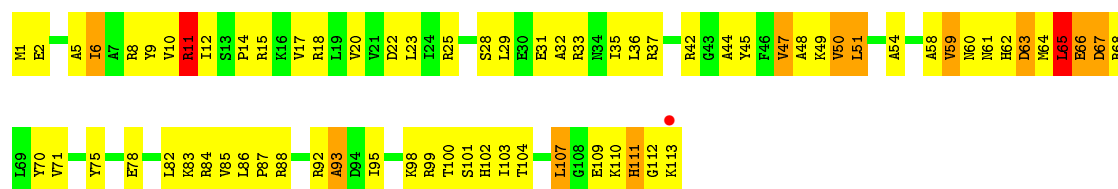




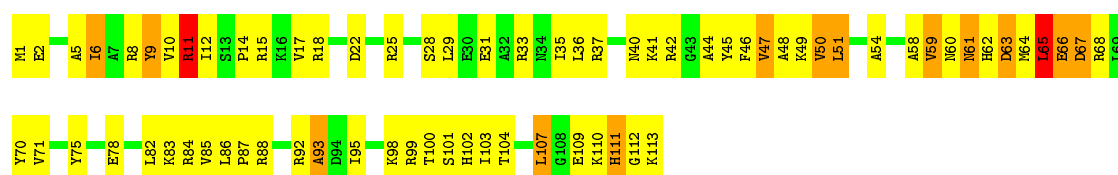
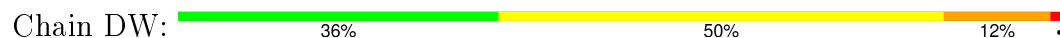
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



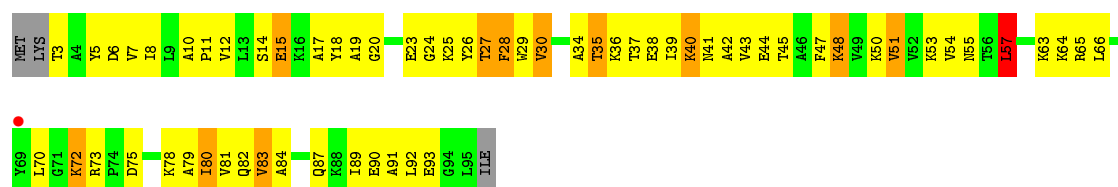
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



• Molecule 54: 50S RIBOSOMAL PROTEIN L22

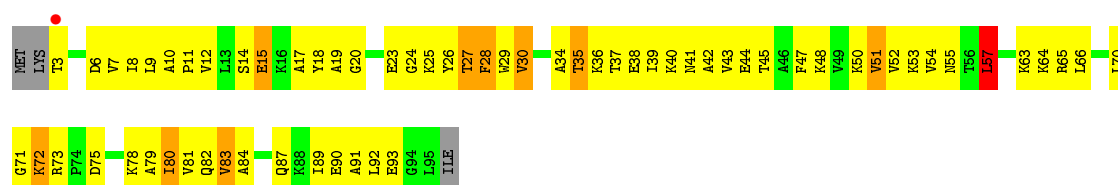


• Molecule 55: 50S RIBOSOMAL PROTEIN L23

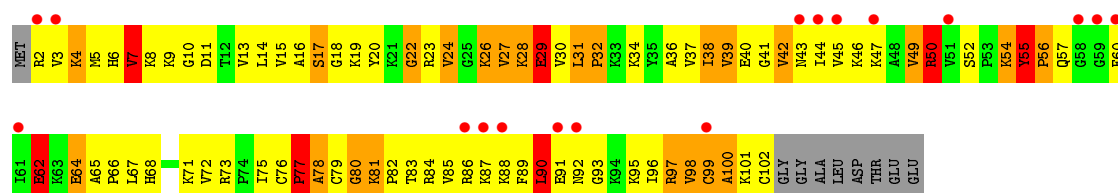
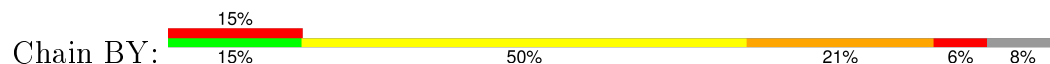


• Molecule 55: 50S RIBOSOMAL PROTEIN L23

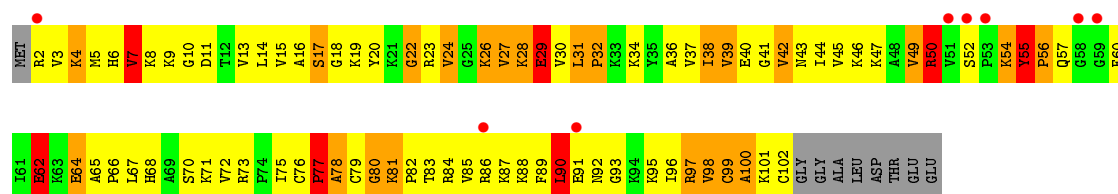
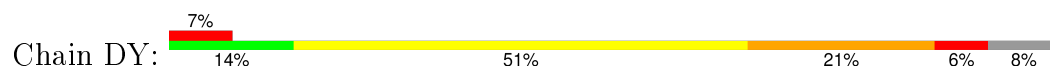




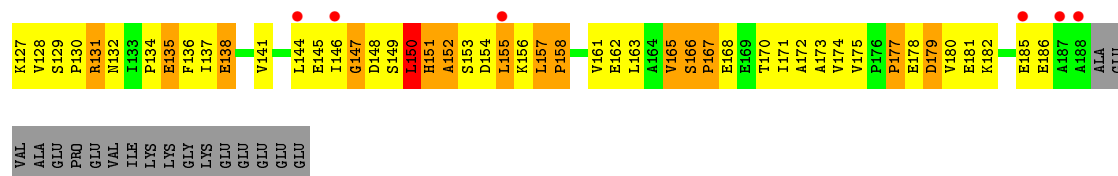
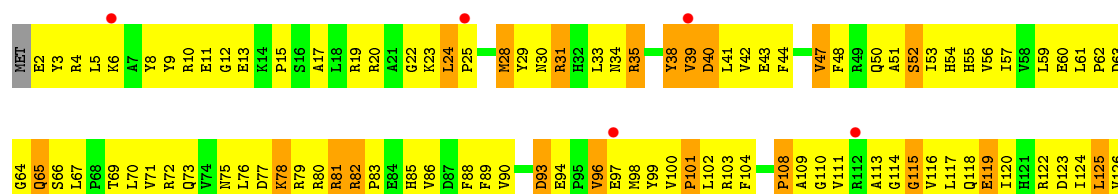
• Molecule 56: 50S RIBOSOMAL PROTEIN L24



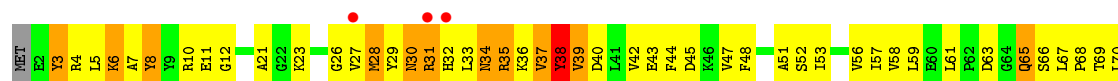
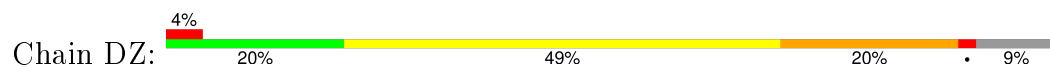
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

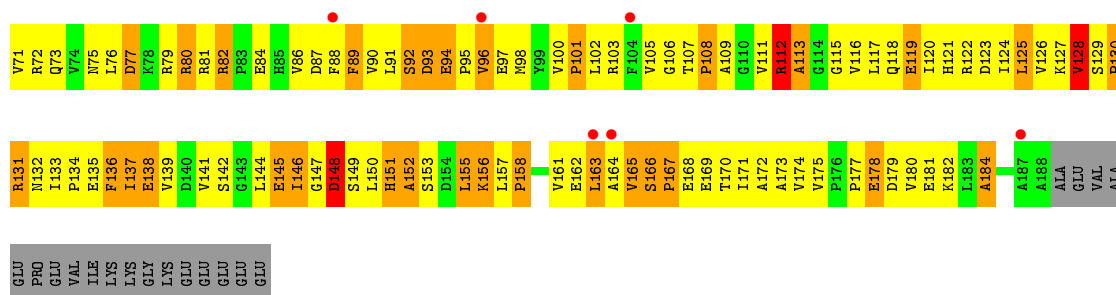


• Molecule 57: 50S RIBOSOMAL PROTEIN L25

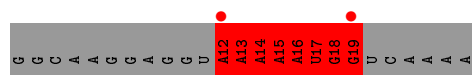


• Molecule 57: 50S RIBOSOMAL PROTEIN L25





- Molecule 58: mRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.04Å 453.51Å 616.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.53 – 3.20 44.53 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.53-3.20) 99.5 (44.53-3.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.228 , 0.270 0.230 , 0.272	Depositor DCC
$R_{free}$ test set	44837 reflections (4.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	87.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 108.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 960332 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	296762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A3P, 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	0.39	0/36252	0.68	9/56580 (0.0%)
1	CA	0.37	1/36253 (0.0%)	0.70	17/56582 (0.0%)
2	AB	0.32	0/1936	0.59	0/2611
2	CB	0.32	0/1936	0.59	0/2611
3	AC	0.30	0/1637	0.55	0/2207
3	CC	0.31	0/1637	0.55	0/2207
4	AD	0.37	0/1722	0.85	6/2306 (0.3%)
4	CD	0.35	0/1722	0.85	6/2306 (0.3%)
5	AE	0.34	0/1163	0.62	0/1566
5	CE	0.34	0/1163	0.61	0/1566
6	AF	0.32	0/856	0.62	0/1154
6	CF	0.34	0/856	0.63	0/1154
7	AG	0.29	0/1276	0.52	0/1709
7	CG	0.29	0/1276	0.51	0/1709
8	AH	0.33	0/1136	0.60	0/1527
8	CH	0.31	0/1136	0.60	0/1527
9	AI	0.32	0/1027	0.57	0/1372
9	CI	0.32	0/1027	0.57	0/1372
10	AJ	0.33	0/808	0.55	0/1087
10	CJ	0.33	0/808	0.55	0/1087
11	AK	0.31	0/900	0.58	0/1213
11	CK	0.33	0/900	0.58	0/1213
12	AL	0.38	0/987	0.87	3/1322 (0.2%)
12	CL	0.37	0/987	0.89	3/1322 (0.2%)
13	AM	0.31	0/941	0.62	0/1258
13	CM	0.32	0/941	0.61	0/1258
14	AN	0.33	0/501	0.54	0/664
14	CN	0.33	0/501	0.54	0/664
15	AO	0.35	0/745	0.60	0/992
15	CO	0.34	0/745	0.60	0/992
16	AP	0.37	0/717	0.61	0/965
16	CP	0.35	0/717	0.59	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.37	0/837	0.62	0/1119
17	CQ	0.34	0/837	0.62	0/1119
18	AR	0.33	0/579	0.60	0/768
18	CR	0.33	0/579	0.59	0/768
19	AS	0.33	0/685	0.54	0/922
19	CS	0.34	0/685	0.54	0/922
20	AT	0.31	0/765	0.57	0/1007
20	CT	0.29	0/765	0.57	0/1007
21	AU	0.45	0/213	0.53	0/279
21	CU	0.45	0/213	0.54	0/279
22	AV	2.00	34/1832 (1.9%)	2.16	50/2855 (1.8%)
22	AW	0.41	0/1832	0.71	0/2855
22	CV	0.44	1/1832 (0.1%)	0.72	0/2855
22	CW	0.40	0/1832	0.71	0/2855
23	AX	2.66	24/383 (6.3%)	4.32	117/595 (19.7%)
24	AY	1.30	4/790 (0.5%)	1.44	14/1055 (1.3%)
24	CY	1.10	0/132	1.27	0/177
25	B0	0.39	0/671	0.64	0/892
25	D0	0.39	0/671	0.63	0/892
26	B1	0.47	0/741	0.75	0/986
26	D1	0.47	0/741	0.78	0/986
27	B2	0.36	0/600	0.63	0/793
27	D2	0.45	0/600	0.71	0/793
28	B3	0.42	0/473	0.68	0/636
28	D3	0.41	0/473	0.67	0/636
29	B4	0.39	0/444	0.65	0/602
29	D4	0.40	0/444	0.65	0/602
30	B5	0.48	0/473	0.76	0/639
30	D5	0.48	0/473	0.76	0/639
31	B6	0.41	0/387	0.64	0/517
31	D6	0.41	0/387	0.64	0/517
32	B7	0.52	0/427	0.68	0/563
32	D7	0.56	0/427	0.71	0/563
33	B8	0.56	0/516	0.94	1/681 (0.1%)
33	D8	0.53	0/516	0.93	1/681 (0.1%)
34	B9	0.33	0/302	0.62	0/397
34	D9	0.34	0/302	0.62	0/397
35	BA	0.60	55/67715 (0.1%)	0.77	106/105714 (0.1%)
35	DA	0.60	28/67714 (0.0%)	0.78	109/105710 (0.1%)
36	BB	0.38	0/2853	0.69	0/4451
36	DB	0.38	0/2853	0.69	0/4451
37	BC	0.33	0/1145	0.60	7/1556 (0.4%)
37	DC	0.33	0/1145	0.60	7/1556 (0.4%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	BD	0.48	0/2155	0.78	1/2907 (0.0%)
38	DD	0.51	0/2155	0.80	1/2907 (0.0%)
39	BE	0.45	0/1597	0.74	0/2155
39	DE	0.44	0/1597	0.75	0/2155
40	BF	0.47	0/1659	0.75	1/2246 (0.0%)
40	DF	0.50	0/1659	0.75	0/2246
41	BG	0.33	0/1498	0.62	0/2013
41	DG	0.34	0/1498	0.64	0/2013
42	BH	0.61	1/1285 (0.1%)	0.85	3/1741 (0.2%)
42	DH	0.61	1/1285 (0.1%)	0.85	3/1741 (0.2%)
43	BI	0.38	0/1140	1.09	9/1543 (0.6%)
43	DI	0.37	0/1140	1.07	9/1543 (0.6%)
45	BN	0.41	0/1132	0.75	0/1527
45	DN	0.44	0/1132	0.76	0/1527
46	BO	0.44	0/943	0.71	0/1269
46	DO	0.41	0/943	0.69	0/1269
47	BP	0.57	0/1131	1.03	4/1504 (0.3%)
47	DP	0.56	0/1131	1.02	5/1504 (0.3%)
48	BQ	0.40	0/1143	0.63	0/1527
48	DQ	0.37	0/1143	0.63	0/1527
49	BR	0.40	0/974	0.70	1/1302 (0.1%)
49	DR	0.75	3/974 (0.3%)	0.95	6/1302 (0.5%)
50	BS	0.39	0/779	0.67	0/1038
50	DS	0.40	0/779	0.67	0/1038
51	BT	0.42	0/1156	0.74	1/1544 (0.1%)
51	DT	0.40	0/1156	0.72	1/1544 (0.1%)
52	BU	0.43	0/975	0.68	0/1297
52	DU	0.49	0/975	0.71	0/1297
53	BV	0.42	0/790	0.74	0/1057
53	DV	0.46	0/790	0.76	0/1057
54	BW	0.48	0/907	0.75	0/1216
54	DW	0.50	1/907 (0.1%)	0.76	0/1216
55	BX	0.48	0/740	0.71	1/995 (0.1%)
55	DX	0.54	0/740	0.73	1/995 (0.1%)
56	BY	0.48	0/789	0.79	1/1053 (0.1%)
56	DY	0.51	0/789	0.80	1/1053 (0.1%)
57	BZ	0.37	0/1514	0.67	0/2056
57	DZ	0.36	0/1514	0.64	0/2056
58	CX	3.13	24/195 (12.3%)	4.52	67/303 (22.1%)
All	All	0.53	177/318302 (0.1%)	0.78	572/475638 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	10
1	CA	1	9
22	AV	0	1
22	CV	0	1
24	AY	0	1
35	BA	20	57
35	DA	20	70
36	BB	0	1
36	DB	0	2
42	BH	0	1
42	DH	0	1
49	BR	0	1
49	DR	0	2
All	All	42	157

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	53	G	N3-C4	-27.79	1.16	1.35
22	AV	53	G	C2-N3	-27.03	1.11	1.32
22	AV	52	G	N7-C5	-25.47	1.24	1.39
22	AV	52	G	N9-C4	-25.25	1.17	1.38
22	AV	52	G	C5-C6	-22.33	1.20	1.42

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	52	G	C4-C5-N7	30.84	123.13	110.80
22	AV	53	G	N3-C2-N2	-29.82	99.03	119.90
22	AV	52	G	C5-N7-C8	-28.61	89.99	104.30
22	AV	53	G	C5'-C4'-O4'	-26.14	77.74	109.10
22	AV	53	G	N3-C4-N9	-25.89	110.46	126.00

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	575	G	C3'
35	BA	100	G	C1'
35	BA	474	G	C3'
35	BA	587	C	C3'

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Mol	Chain	Res	Type	Atom
35	BA	669	G	C4',C3',C1'

5 of 157 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	115	G	Sidechain
1	AA	120	A	Sidechain
1	AA	575	G	Sidechain
1	AA	587	G	Sidechain
1	AA	731	G	Sidechain

## 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	32412	0	16354	1303	0
1	CA	32413	0	16353	1699	0
2	AB	1901	0	1951	297	0
2	CB	1901	0	1951	304	0
3	AC	1613	0	1676	245	0
3	CC	1613	0	1677	238	0
4	AD	1692	0	1751	196	0
4	CD	1692	0	1753	218	0
5	AE	1147	0	1206	172	0
5	CE	1147	0	1207	191	0
6	AF	843	0	857	95	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	146	0
8	AH	1116	0	1177	159	0
8	CH	1116	0	1177	167	0
9	AI	1011	0	1041	160	0
9	CI	1011	0	1041	161	0
10	AJ	795	0	840	156	0
10	CJ	795	0	840	157	0
11	AK	885	0	904	99	0
11	CK	885	0	904	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1055	117	0
12	CL	971	0	1056	116	0
13	AM	934	0	989	124	0
13	CM	934	0	987	135	0
14	AN	492	0	530	74	0
14	CN	492	0	533	78	0
15	AO	734	0	771	82	0
15	CO	734	0	771	77	0
16	AP	701	0	719	93	0
16	CP	701	0	720	105	0
17	AQ	824	0	890	88	0
17	CQ	824	0	891	91	0
18	AR	574	0	644	90	0
18	CR	574	0	644	88	0
19	AS	671	0	689	118	0
19	CS	671	0	689	112	0
20	AT	763	0	861	74	0
20	CT	763	0	861	75	0
21	AU	209	0	221	42	0
21	CU	209	0	221	39	0
22	AV	1640	0	832	85	0
22	AW	1640	0	837	60	0
22	CV	1640	0	833	134	0
22	CW	1640	0	837	71	0
23	AX	341	0	174	126	0
24	AY	769	0	763	234	0
24	CY	126	0	115	33	0
25	B0	662	0	688	60	0
25	D0	662	0	688	56	0
26	B1	734	0	808	85	0
26	D1	734	0	808	83	0
27	B2	598	0	653	65	0
27	D2	598	0	653	79	0
28	B3	468	0	523	42	0
28	D3	468	0	523	45	0
29	B4	434	0	424	92	0
29	D4	434	0	424	69	0
30	B5	459	0	480	45	0
30	D5	459	0	479	45	0
31	B6	381	0	390	61	0
31	D6	381	0	390	63	0
32	B7	419	0	467	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	D7	419	0	467	34	0
33	B8	508	0	576	123	0
33	D8	508	0	576	122	0
34	B9	299	0	326	28	0
34	D9	299	0	326	30	0
35	BA	60459	0	30475	1946	0
35	DA	60459	0	30466	2110	1
36	BB	2551	0	1295	101	0
36	DB	2551	0	1294	90	1
37	BC	1142	0	865	72	0
37	DC	1142	0	865	71	0
38	BD	2105	0	2182	299	0
38	DD	2105	0	2182	311	0
39	BE	1564	0	1628	223	0
39	DE	1564	0	1628	233	0
40	BF	1624	0	1677	218	0
40	DF	1624	0	1676	225	0
41	BG	1474	0	1534	280	0
41	DG	1474	0	1534	306	0
42	BH	1260	0	1326	250	0
42	DH	1260	0	1326	242	0
43	BI	1125	0	1209	181	0
43	DI	1125	0	1209	169	0
44	BJ	651	0	165	21	0
44	DJ	651	0	166	35	0
45	BN	1105	0	1180	139	0
45	DN	1105	0	1180	133	0
46	BO	933	0	996	101	0
46	DO	933	0	996	114	0
47	BP	1114	0	1187	315	0
47	DP	1114	0	1187	310	0
48	BQ	1122	0	1179	113	0
48	DQ	1122	0	1179	112	0
49	BR	960	0	1021	132	0
49	DR	960	0	1019	127	0
50	BS	771	0	832	143	0
50	DS	771	0	832	132	0
51	BT	1142	0	1202	223	0
51	DT	1142	0	1201	226	0
52	BU	958	0	1015	121	0
52	DU	958	0	1015	116	0
53	BV	779	0	852	162	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	DV	779	0	852	158	0
54	BW	896	0	953	80	0
54	DW	896	0	952	77	0
55	BX	726	0	778	71	0
55	DX	726	0	778	73	0
56	BY	776	0	870	194	0
56	DY	776	0	870	192	0
57	BZ	1482	0	1503	210	0
57	DZ	1482	0	1503	244	0
58	CX	173	0	89	53	0
59	AA	373	0	0	0	0
59	AC	2	0	0	0	0
59	AD	3	0	0	0	0
59	AH	1	0	0	0	0
59	AI	3	0	0	0	0
59	AL	6	0	0	0	0
59	AN	2	0	0	0	0
59	AO	2	0	0	0	0
59	AP	1	0	0	0	0
59	AQ	3	0	0	0	0
59	AT	1	0	0	0	0
59	AV	7	0	0	0	0
59	AX	4	0	0	0	0
59	AY	3	0	0	0	0
59	B0	2	0	0	0	0
59	B1	1	0	0	0	0
59	B5	3	0	0	0	0
59	B6	1	0	0	0	0
59	B7	1	0	0	0	0
59	BA	709	0	0	0	0
59	BB	6	0	0	0	0
59	BD	5	0	0	0	0
59	BE	4	0	0	0	0
59	BF	1	0	0	0	0
59	BH	4	0	0	0	0
59	BN	1	0	0	0	0
59	BO	1	0	0	0	0
59	BP	4	0	0	5	0
59	BQ	1	0	0	0	0
59	BR	5	0	0	0	0
59	BT	1	0	0	0	0
59	BU	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BY	1	0	0	0	0
59	CA	184	0	0	0	0
59	CC	3	0	0	0	0
59	CD	1	0	0	0	0
59	CH	1	0	0	0	0
59	CJ	2	0	0	0	0
59	CM	3	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	1	0	0	0	0
59	CS	2	0	0	0	0
59	CV	12	0	0	0	0
59	CY	1	0	0	0	0
59	D0	4	0	0	0	0
59	D1	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D5	3	0	0	0	0
59	D6	2	0	0	0	0
59	D7	4	0	0	0	0
59	D8	1	0	0	0	0
59	D9	1	0	0	0	0
59	DA	897	0	0	0	0
59	DB	11	0	0	0	0
59	DD	6	0	0	0	0
59	DE	4	0	0	0	0
59	DF	3	0	0	0	0
59	DN	3	0	0	0	0
59	DO	1	0	0	0	0
59	DP	6	0	0	0	0
59	DR	2	0	0	0	0
59	DT	1	0	0	0	0
59	DU	4	0	0	0	0
59	DW	1	0	0	0	0
59	DY	1	0	0	0	0
60	AD	2	0	0	0	0
60	AN	1	0	0	0	0
60	CD	1	0	0	0	0
61	AA	2	0	0	0	0
All	All	296762	0	199834	19831	1

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 40.

The worst 5 of 19831 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)
3:AC:162:GLN:HB2	23:AX:23:A:C5	1.34	1.59
42:BH:11:VAL:HG22	42:BH:49:VAL:CG1	1.08	1.56
42:DH:11:VAL:HG22	42:DH:49:VAL:CG1	1.08	1.55
1:CA:644:G:C2'	1:CA:645:C:H5''	1.39	1.53
24:AY:57:GLN:HG3	35:BA:1913:A:C2	1.45	1.47

All (1) 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)
35:DA:1411:C:O3'	36:DB:53:A:O2'[1_655]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	133 (57%)	67 (29%)	33 (14%)	0	1
2	CB	233/256 (91%)	133 (57%)	68 (29%)	32 (14%)	0	1
3	AC	205/239 (86%)	130 (63%)	50 (24%)	25 (12%)	0	2
3	CC	205/239 (86%)	128 (62%)	52 (25%)	25 (12%)	0	2
4	AD	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	0	3
4	CD	206/209 (99%)	138 (67%)	46 (22%)	22 (11%)	0	3
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1	4
5	CE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1	4
6	AF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	0	2
6	CF	99/101 (98%)	74 (75%)	13 (13%)	12 (12%)	0	2
7	AG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	107 (70%)	35 (23%)	11 (7%)	1	10
8	AH	136/138 (99%)	99 (73%)	31 (23%)	6 (4%)	3	24
8	CH	136/138 (99%)	99 (73%)	30 (22%)	7 (5%)	2	20
9	AI	121/128 (94%)	75 (62%)	31 (26%)	15 (12%)	0	2
9	CI	121/128 (94%)	74 (61%)	33 (27%)	14 (12%)	0	3
10	AJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	2	19
10	CJ	97/105 (92%)	64 (66%)	28 (29%)	5 (5%)	2	19
11	AK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	0	3
11	CK	117/129 (91%)	76 (65%)	28 (24%)	13 (11%)	0	3
12	AL	123/135 (91%)	89 (72%)	21 (17%)	13 (11%)	0	3
12	CL	123/135 (91%)	87 (71%)	22 (18%)	14 (11%)	0	3
13	AM	110/126 (87%)	62 (56%)	27 (24%)	21 (19%)	0	0
13	CM	110/126 (87%)	63 (57%)	26 (24%)	21 (19%)	0	0
14	AN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	2
14	CN	58/61 (95%)	36 (62%)	16 (28%)	6 (10%)	1	4
15	AO	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	7
15	CO	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	7
16	AP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	0	3
16	CP	82/88 (93%)	55 (67%)	18 (22%)	9 (11%)	0	3
17	AQ	98/105 (93%)	65 (66%)	21 (21%)	12 (12%)	0	2
17	CQ	98/105 (93%)	66 (67%)	20 (20%)	12 (12%)	0	2
18	AR	68/88 (77%)	36 (53%)	22 (32%)	10 (15%)	0	1
18	CR	68/88 (77%)	35 (52%)	23 (34%)	10 (15%)	0	1
19	AS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
19	CS	83/93 (89%)	48 (58%)	18 (22%)	17 (20%)	0	0
20	AT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	1	4
20	CT	97/106 (92%)	62 (64%)	25 (26%)	10 (10%)	1	4
21	AU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	5
21	CU	23/27 (85%)	11 (48%)	10 (44%)	2 (9%)	1	5
24	AY	95/97 (98%)	81 (85%)	10 (10%)	4 (4%)	3	26
24	CY	14/97 (14%)	8 (57%)	4 (29%)	2 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	2	15
25	D0	82/85 (96%)	66 (80%)	10 (12%)	6 (7%)	1	9
26	B1	92/98 (94%)	70 (76%)	16 (17%)	6 (6%)	1	13
26	D1	92/98 (94%)	74 (80%)	9 (10%)	9 (10%)	1	4
27	B2	69/72 (96%)	51 (74%)	13 (19%)	5 (7%)	1	10
27	D2	69/72 (96%)	47 (68%)	18 (26%)	4 (6%)	2	17
28	B3	58/60 (97%)	49 (84%)	8 (14%)	1 (2%)	11	52
28	D3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	11	52
29	B4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
29	D4	54/71 (76%)	28 (52%)	12 (22%)	14 (26%)	0	0
30	B5	57/60 (95%)	42 (74%)	9 (16%)	6 (10%)	1	4
30	D5	57/60 (95%)	41 (72%)	10 (18%)	6 (10%)	1	4
31	B6	41/54 (76%)	17 (42%)	15 (37%)	9 (22%)	0	0
31	D6	41/54 (76%)	16 (39%)	16 (39%)	9 (22%)	0	0
32	B7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	9	46
32	D7	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	9	46
33	B8	62/65 (95%)	35 (56%)	15 (24%)	12 (19%)	0	0
33	D8	62/65 (95%)	34 (55%)	15 (24%)	13 (21%)	0	0
34	B9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	2	16
34	D9	34/37 (92%)	24 (71%)	8 (24%)	2 (6%)	2	16
37	BC	183/229 (80%)	75 (41%)	67 (37%)	41 (22%)	0	0
37	DC	183/229 (80%)	76 (42%)	65 (36%)	42 (23%)	0	0
38	BD	270/276 (98%)	199 (74%)	48 (18%)	23 (8%)	1	6
38	DD	270/276 (98%)	198 (73%)	47 (17%)	25 (9%)	1	5
39	BE	203/206 (98%)	142 (70%)	37 (18%)	24 (12%)	0	3
39	DE	203/206 (98%)	143 (70%)	36 (18%)	24 (12%)	0	3
40	BF	206/210 (98%)	137 (66%)	40 (19%)	29 (14%)	0	1
40	DF	206/210 (98%)	137 (66%)	41 (20%)	28 (14%)	0	1
41	BG	177/182 (97%)	109 (62%)	44 (25%)	24 (14%)	0	1
41	DG	177/182 (97%)	107 (60%)	43 (24%)	27 (15%)	0	1
42	BH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DH	163/180 (91%)	90 (55%)	42 (26%)	31 (19%)	0	0
43	BI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
43	DI	143/148 (97%)	80 (56%)	36 (25%)	27 (19%)	0	0
45	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	1
45	DN	137/140 (98%)	96 (70%)	21 (15%)	20 (15%)	0	1
46	BO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	3	21
46	DO	120/122 (98%)	99 (82%)	15 (12%)	6 (5%)	3	21
47	BP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
47	DP	144/150 (96%)	70 (49%)	34 (24%)	40 (28%)	0	0
48	BQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	5
48	DQ	139/141 (99%)	108 (78%)	18 (13%)	13 (9%)	1	5
49	BR	115/118 (98%)	80 (70%)	20 (17%)	15 (13%)	0	2
49	DR	115/118 (98%)	82 (71%)	20 (17%)	13 (11%)	0	3
50	BS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
50	DS	97/112 (87%)	46 (47%)	20 (21%)	31 (32%)	0	0
51	BT	136/146 (93%)	79 (58%)	33 (24%)	24 (18%)	0	0
51	DT	136/146 (93%)	80 (59%)	31 (23%)	25 (18%)	0	0
52	BU	115/118 (98%)	87 (76%)	18 (16%)	10 (9%)	1	5
52	DU	115/118 (98%)	88 (76%)	17 (15%)	10 (9%)	1	5
53	BV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
53	DV	99/101 (98%)	72 (73%)	12 (12%)	15 (15%)	0	1
54	BW	111/113 (98%)	84 (76%)	17 (15%)	10 (9%)	1	5
54	DW	111/113 (98%)	85 (77%)	16 (14%)	10 (9%)	1	5
55	BX	91/96 (95%)	73 (80%)	15 (16%)	3 (3%)	5	32
55	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	5	32
56	BY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
56	DY	99/110 (90%)	50 (50%)	23 (23%)	26 (26%)	0	0
57	BZ	185/206 (90%)	123 (66%)	38 (20%)	24 (13%)	0	2
57	DZ	185/206 (90%)	101 (55%)	49 (26%)	35 (19%)	0	0
All	All	11855/12786 (93%)	7751 (65%)	2556 (22%)	1548 (13%)	0	2

5 of 1548 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	75	LYS
2	AB	83	MET
2	AB	101	MET
2	AB	150	SER
2	AB	238	LEU

### 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	AB	202/220 (92%)	185 (92%)	17 (8%)	14	48
2	CB	202/220 (92%)	185 (92%)	17 (8%)	14	48
3	AC	160/188 (85%)	151 (94%)	9 (6%)	26	68
3	CC	160/188 (85%)	151 (94%)	9 (6%)	26	68
4	AD	179/181 (99%)	165 (92%)	14 (8%)	16	53
4	CD	179/181 (99%)	164 (92%)	15 (8%)	14	48
5	AE	115/123 (94%)	105 (91%)	10 (9%)	13	45
5	CE	115/123 (94%)	105 (91%)	10 (9%)	13	45
6	AF	90/90 (100%)	87 (97%)	3 (3%)	45	81
6	CF	90/90 (100%)	87 (97%)	3 (3%)	45	81
7	AG	126/127 (99%)	124 (98%)	2 (2%)	70	91
7	CG	126/127 (99%)	124 (98%)	2 (2%)	70	91
8	AH	119/119 (100%)	110 (92%)	9 (8%)	16	55
8	CH	119/119 (100%)	110 (92%)	9 (8%)	16	55
9	AI	98/99 (99%)	88 (90%)	10 (10%)	9	36
9	CI	98/99 (99%)	88 (90%)	10 (10%)	9	36
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	7	31
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	7	31
11	AK	90/99 (91%)	85 (94%)	5 (6%)	26	68
11	CK	90/99 (91%)	85 (94%)	5 (6%)	26	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	104/111 (94%)	95 (91%)	9 (9%)	13	45
12	CL	104/111 (94%)	95 (91%)	9 (9%)	13	45
13	AM	94/101 (93%)	86 (92%)	8 (8%)	13	47
13	CM	94/101 (93%)	86 (92%)	8 (8%)	13	47
14	AN	49/50 (98%)	45 (92%)	4 (8%)	14	50
14	CN	49/50 (98%)	45 (92%)	4 (8%)	14	50
15	AO	79/80 (99%)	74 (94%)	5 (6%)	22	63
15	CO	79/80 (99%)	74 (94%)	5 (6%)	22	63
16	AP	72/74 (97%)	67 (93%)	5 (7%)	19	59
16	CP	72/74 (97%)	66 (92%)	6 (8%)	14	49
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	81
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	61	88
18	AR	61/77 (79%)	59 (97%)	2 (3%)	45	81
18	CR	61/77 (79%)	59 (97%)	2 (3%)	45	81
19	AS	72/80 (90%)	62 (86%)	10 (14%)	4	20
19	CS	72/80 (90%)	62 (86%)	10 (14%)	4	20
20	AT	76/82 (93%)	67 (88%)	9 (12%)	6	29
20	CT	76/82 (93%)	67 (88%)	9 (12%)	6	29
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	35
21	CU	19/22 (86%)	18 (95%)	1 (5%)	28	69
24	AY	78/78 (100%)	42 (54%)	36 (46%)	0	0
24	CY	12/78 (15%)	8 (67%)	4 (33%)	0	0
25	B0	66/67 (98%)	58 (88%)	8 (12%)	6	28
25	D0	66/67 (98%)	58 (88%)	8 (12%)	6	28
26	B1	78/83 (94%)	67 (86%)	11 (14%)	4	20
26	D1	78/83 (94%)	67 (86%)	11 (14%)	4	20
27	B2	66/67 (98%)	59 (89%)	7 (11%)	8	34
27	D2	66/67 (98%)	56 (85%)	10 (15%)	3	17
28	B3	51/52 (98%)	41 (80%)	10 (20%)	1	9
28	D3	51/52 (98%)	41 (80%)	10 (20%)	1	9
29	B4	49/63 (78%)	40 (82%)	9 (18%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	D4	49/63 (78%)	42 (86%)	7 (14%)	4	19
30	B5	51/52 (98%)	47 (92%)	4 (8%)	16	53
30	D5	51/52 (98%)	47 (92%)	4 (8%)	16	53
31	B6	43/52 (83%)	39 (91%)	4 (9%)	11	41
31	D6	43/52 (83%)	38 (88%)	5 (12%)	7	30
32	B7	41/42 (98%)	36 (88%)	5 (12%)	6	27
32	D7	41/42 (98%)	36 (88%)	5 (12%)	6	27
33	B8	53/55 (96%)	45 (85%)	8 (15%)	3	17
33	D8	53/55 (96%)	45 (85%)	8 (15%)	3	17
34	B9	33/34 (97%)	32 (97%)	1 (3%)	48	82
34	D9	33/34 (97%)	32 (97%)	1 (3%)	48	82
37	BC	61/181 (34%)	57 (93%)	4 (7%)	21	61
37	DC	61/181 (34%)	57 (93%)	4 (7%)	21	61
38	BD	213/218 (98%)	176 (83%)	37 (17%)	2	12
38	DD	213/218 (98%)	176 (83%)	37 (17%)	2	12
39	BE	165/166 (99%)	142 (86%)	23 (14%)	4	20
39	DE	165/166 (99%)	142 (86%)	23 (14%)	4	20
40	BF	165/166 (99%)	143 (87%)	22 (13%)	5	23
40	DF	165/166 (99%)	143 (87%)	22 (13%)	5	23
41	BG	155/156 (99%)	133 (86%)	22 (14%)	4	19
41	DG	155/156 (99%)	135 (87%)	20 (13%)	5	24
42	BH	137/148 (93%)	122 (89%)	15 (11%)	8	33
42	DH	137/148 (93%)	122 (89%)	15 (11%)	8	33
43	BI	121/124 (98%)	104 (86%)	17 (14%)	4	20
43	DI	121/124 (98%)	103 (85%)	18 (15%)	4	17
45	BN	117/119 (98%)	97 (83%)	20 (17%)	2	12
45	DN	117/119 (98%)	96 (82%)	21 (18%)	2	11
46	BO	100/100 (100%)	95 (95%)	5 (5%)	30	71
46	DO	100/100 (100%)	94 (94%)	6 (6%)	24	65
47	BP	112/116 (97%)	80 (71%)	32 (29%)	0	1
47	DP	112/116 (97%)	81 (72%)	31 (28%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BQ	111/111 (100%)	104 (94%)	7 (6%)	22	63
48	DQ	111/111 (100%)	104 (94%)	7 (6%)	22	63
49	BR	100/101 (99%)	86 (86%)	14 (14%)	4	20
49	DR	100/101 (99%)	84 (84%)	16 (16%)	3	14
50	BS	77/88 (88%)	64 (83%)	13 (17%)	2	13
50	DS	77/88 (88%)	64 (83%)	13 (17%)	2	13
51	BT	120/127 (94%)	99 (82%)	21 (18%)	2	12
51	DT	120/127 (94%)	100 (83%)	20 (17%)	3	13
52	BU	92/94 (98%)	80 (87%)	12 (13%)	5	24
52	DU	92/94 (98%)	81 (88%)	11 (12%)	6	28
53	BV	82/82 (100%)	68 (83%)	14 (17%)	2	12
53	DV	82/82 (100%)	68 (83%)	14 (17%)	2	12
54	BW	91/92 (99%)	81 (89%)	10 (11%)	8	33
54	DW	91/92 (99%)	81 (89%)	10 (11%)	8	33
55	BX	74/78 (95%)	62 (84%)	12 (16%)	3	14
55	DX	74/78 (95%)	62 (84%)	12 (16%)	3	14
56	BY	84/91 (92%)	70 (83%)	14 (17%)	3	13
56	DY	84/91 (92%)	70 (83%)	14 (17%)	3	13
57	BZ	163/179 (91%)	147 (90%)	16 (10%)	10	38
57	DZ	163/179 (91%)	143 (88%)	20 (12%)	6	27
All	All	9806/10588 (93%)	8674 (88%)	1132 (12%)	7	30

5 of 1132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
52	BU	112	ARG
7	CG	57	GLU
51	DT	85	LYS
54	BW	11	ARG
57	BZ	150	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 302 such sidechains are listed below:

Mol	Chain	Res	Type
50	BS	95	HIS
3	CC	136	GLN
49	DR	71	GLN
52	BU	49	HIS
57	BZ	34	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1522 (98%)	206 (13%)	21 (1%)
1	CA	1505/1522 (98%)	235 (15%)	24 (1%)
22	AV	76/77 (98%)	18 (23%)	1 (1%)
22	AW	76/77 (98%)	14 (18%)	1 (1%)
22	CV	76/77 (98%)	20 (26%)	1 (1%)
22	CW	76/77 (98%)	8 (10%)	0
23	AX	15/25 (60%)	14 (93%)	10 (66%)
35	BA	2805/2848 (98%)	485 (17%)	58 (2%)
35	DA	2804/2848 (98%)	487 (17%)	58 (2%)
36	BB	118/122 (96%)	20 (16%)	1 (0%)
36	DB	118/122 (96%)	20 (16%)	1 (0%)
58	CX	8/25 (32%)	7 (87%)	5 (62%)
All	All	9182/9342 (98%)	1534 (16%)	181 (1%)

5 of 1534 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	31	G

5 of 181 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	2126	A
1	CA	428	G
35	DA	1992	G
35	BA	2422	A
36	BB	66	A



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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	A3P	AA	1493	1	19,28,29	0.83	0	22,42,45	2.02	3 (13%)
1	A3P	CA	1493	1	19,28,29	0.76	0	22,42,45	0.92	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A3P	AA	1493	1	-	0/8/30/31	0/3/3/3
1	A3P	CA	1493	1	-	0/8/30/31	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1493	A3P	P1-O3'-C3'	-4.71	110.27	121.56
1	CA	1493	A3P	C2'-C1'-N9	2.15	117.58	114.29
1	AA	1493	A3P	O2P-P1-O1P	2.64	119.09	110.58
1	CA	1493	A3P	O2P-P1-O1P	2.66	119.13	110.58
1	AA	1493	A3P	O3'-P1-O1P	7.27	125.27	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1493	A3P	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	CA	1493	A3P	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2338 ligands modelled in this entry, 2338 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	3
13	AM	3
9	AI	2
9	CI	2
41	DG	1
41	BG	1
31	D6	1
31	B6	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B6	46:HIS	C	47:THR	N	7.76
1	D6	46:HIS	C	47:THR	N	7.76
1	BG	112:PRO	C	113:ARG	N	4.73
1	DG	112:PRO	C	113:ARG	N	4.47
1	AM	69:GLU	C	70:LEU	N	4.25

## 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	1507/1522 (99%)	0.13	41 (2%) 58 44	54, 107, 196, 201	0
1	CA	1507/1522 (99%)	0.88	195 (12%) 5 3	60, 169, 201, 201	0
2	AB	235/256 (91%)	0.44	18 (7%) 16 9	77, 152, 197, 201	0
2	CB	235/256 (91%)	1.04	45 (19%) 2 1	90, 173, 201, 201	0
3	AC	207/239 (86%)	0.55	20 (9%) 10 6	83, 149, 188, 201	0
3	CC	207/239 (86%)	1.44	52 (25%) 1 1	106, 175, 201, 201	0
4	AD	208/209 (99%)	0.01	2 (0%) 84 75	65, 105, 149, 180	0
4	CD	208/209 (99%)	1.48	58 (27%) 1 0	85, 173, 201, 201	0
5	AE	151/162 (93%)	0.18	4 (2%) 59 45	70, 107, 155, 198	0
5	CE	151/162 (93%)	1.19	39 (25%) 1 0	89, 155, 197, 201	0
6	AF	101/101 (100%)	0.18	3 (2%) 54 39	70, 125, 163, 190	0
6	CF	101/101 (100%)	-0.00	1 (0%) 84 75	65, 110, 155, 184	0
7	AG	155/156 (99%)	0.46	14 (9%) 12 6	85, 141, 184, 201	0
7	CG	155/156 (99%)	1.04	38 (24%) 1 1	86, 164, 200, 201	0
8	AH	138/138 (100%)	0.13	2 (1%) 78 65	66, 108, 151, 171	0
8	CH	138/138 (100%)	0.95	25 (18%) 2 1	79, 157, 189, 201	0
9	AI	127/128 (99%)	1.17	30 (23%) 1 1	94, 164, 200, 201	0
9	CI	127/128 (99%)	2.34	63 (49%) 0 0	115, 177, 201, 201	0
10	AJ	99/105 (94%)	1.71	36 (36%) 0 0	105, 169, 201, 201	0
10	CJ	99/105 (94%)	3.20	59 (59%) 0 0	125, 181, 201, 201	0
11	AK	119/129 (92%)	0.42	10 (8%) 14 7	60, 113, 168, 197	0
11	CK	119/129 (92%)	0.65	11 (9%) 11 6	78, 139, 188, 200	0
12	AL	125/135 (92%)	0.22	2 (1%) 74 62	59, 90, 144, 201	0
12	CL	125/135 (92%)	1.26	34 (27%) 1 0	63, 139, 187, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	118/126 (93%)	0.83	20 (16%)	2	1	96, 152, 189, 201	0
13	CM	118/126 (93%)	1.28	28 (23%)	1	1	102, 165, 201, 201	0
14	AN	60/61 (98%)	0.99	10 (16%)	2	1	99, 153, 198, 201	0
14	CN	60/61 (98%)	1.49	15 (25%)	1	1	118, 171, 200, 201	0
15	AO	88/89 (98%)	0.13	1 (1%)	82	72	69, 102, 149, 171	0
15	CO	88/89 (98%)	0.44	5 (5%)	27	15	75, 123, 163, 176	0
16	AP	84/88 (95%)	0.07	1 (1%)	81	69	60, 92, 143, 195	0
16	CP	84/88 (95%)	2.04	40 (47%)	0	0	112, 172, 198, 201	0
17	AQ	100/105 (95%)	-0.05	1 (1%)	84	75	63, 97, 134, 156	0
17	CQ	100/105 (95%)	0.70	14 (14%)	4	2	102, 142, 181, 195	0
18	AR	70/88 (79%)	0.51	6 (8%)	13	7	78, 116, 165, 178	0
18	CR	70/88 (79%)	0.59	5 (7%)	19	10	79, 120, 180, 196	0
19	AS	85/93 (91%)	1.15	18 (21%)	1	1	101, 164, 198, 201	0
19	CS	85/93 (91%)	1.88	32 (37%)	0	0	118, 176, 199, 201	0
20	AT	99/106 (93%)	0.24	4 (4%)	42	27	60, 104, 163, 191	0
20	CT	99/106 (93%)	1.02	16 (16%)	3	2	113, 169, 198, 201	0
21	AU	25/27 (92%)	2.43	13 (52%)	0	0	91, 151, 184, 201	0
21	CU	25/27 (92%)	4.29	20 (80%)	0	0	84, 159, 199, 201	0
22	AV	77/77 (100%)	-0.08	1 (1%)	79	67	55, 106, 161, 194	0
22	AW	77/77 (100%)	2.95	56 (72%)	0	0	125, 201, 201, 201	0
22	CV	77/77 (100%)	0.14	2 (2%)	59	45	50, 131, 175, 182	0
22	CW	77/77 (100%)	3.14	57 (74%)	0	0	146, 201, 201, 201	0
23	AX	16/25 (64%)	2.50	10 (62%)	0	0	84, 199, 201, 201	0
24	AY	97/97 (100%)	1.33	28 (28%)	1	0	99, 149, 192, 201	1 (1%)
24	CY	16/97 (16%)	2.40	9 (56%)	0	0	130, 157, 201, 201	0
25	B0	84/85 (98%)	0.67	8 (9%)	10	6	51, 90, 164, 196	0
25	D0	84/85 (98%)	0.92	12 (14%)	4	2	70, 105, 166, 191	0
26	B1	94/98 (95%)	0.08	3 (3%)	51	36	44, 76, 145, 161	0
26	D1	94/98 (95%)	-0.02	0	100	100	41, 74, 139, 159	0
27	B2	71/72 (98%)	0.16	0	100	100	65, 103, 150, 169	0
27	D2	71/72 (98%)	-0.20	3 (4%)	40	26	42, 71, 129, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
28	B3	60/60 (100%)	0.42	4 (6%)	21 12	42, 88, 148, 201	0
28	D3	60/60 (100%)	0.38	4 (6%)	21 12	50, 87, 142, 200	0
29	B4	56/71 (78%)	0.23	5 (8%)	12 6	96, 160, 187, 197	0
29	D4	56/71 (78%)	0.93	11 (19%)	1 1	122, 176, 201, 201	0
30	B5	59/60 (98%)	0.29	5 (8%)	13 7	37, 70, 174, 181	0
30	D5	59/60 (98%)	0.50	5 (8%)	13 7	27, 75, 177, 201	0
31	B6	45/54 (83%)	2.92	31 (68%)	0 0	97, 141, 184, 187	0
31	D6	45/54 (83%)	2.27	26 (57%)	0 0	103, 161, 195, 199	0
32	B7	49/49 (100%)	-0.15	0	100 100	38, 55, 112, 194	0
32	D7	49/49 (100%)	-0.13	0	100 100	21, 40, 108, 159	0
33	B8	64/65 (98%)	0.01	0	100 100	32, 72, 132, 200	0
33	D8	64/65 (98%)	0.27	2 (3%)	52 38	41, 83, 148, 201	0
34	B9	36/37 (97%)	2.01	18 (50%)	0 0	83, 123, 168, 201	0
34	D9	36/37 (97%)	1.98	15 (41%)	0 0	91, 128, 167, 197	0
35	BA	2807/2848 (98%)	0.09	108 (3%)	44 29	32, 74, 188, 201	0
35	DA	2807/2848 (98%)	0.14	92 (3%)	50 35	29, 77, 189, 201	0
36	BB	119/122 (97%)	0.06	2 (1%)	73 60	76, 130, 181, 201	0
36	DB	119/122 (97%)	0.30	4 (3%)	49 34	87, 151, 189, 200	0
37	BC	191/229 (83%)	4.26	156 (81%)	0 0	160, 198, 201, 201	0
37	DC	191/229 (83%)	4.12	149 (78%)	0 0	154, 197, 201, 201	0
38	BD	272/276 (98%)	-0.15	1 (0%)	93 90	38, 71, 107, 184	0
38	DD	272/276 (98%)	-0.04	2 (0%)	89 83	32, 68, 111, 185	0
39	BE	205/206 (99%)	0.01	4 (1%)	68 54	36, 83, 157, 201	0
39	DE	205/206 (99%)	0.18	7 (3%)	49 34	25, 91, 157, 201	0
40	BF	208/210 (99%)	-0.20	1 (0%)	91 87	30, 73, 156, 186	0
40	DF	208/210 (99%)	-0.10	5 (2%)	62 47	24, 78, 165, 196	0
41	BG	181/182 (99%)	0.57	17 (9%)	11 6	79, 142, 188, 201	0
41	DG	181/182 (99%)	0.69	20 (11%)	7 4	92, 155, 193, 201	0
42	BH	165/180 (91%)	1.49	54 (32%)	1 0	90, 157, 193, 201	0
42	DH	165/180 (91%)	0.30	11 (6%)	21 12	55, 112, 158, 182	0
43	BI	145/148 (97%)	2.54	55 (37%)	0 0	60, 161, 201, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	DI	145/148 (97%)	0.93	23 (15%) 3 2	70, 130, 200, 201	0
44	BJ	0/131	-	-	-	-
44	DJ	0/131	-	-	-	-
45	BN	139/140 (99%)	-0.03	2 (1%) 78 65	52, 88, 145, 201	0
45	DN	139/140 (99%)	-0.14	0 100 100	44, 79, 140, 189	0
46	BO	122/122 (100%)	-0.34	0 100 100	42, 72, 101, 178	0
46	DO	122/122 (100%)	0.31	1 (0%) 87 80	59, 104, 154, 201	0
47	BP	146/150 (97%)	0.22	3 (2%) 67 52	26, 92, 150, 197	0
47	DP	146/150 (97%)	0.44	8 (5%) 29 16	35, 96, 170, 198	0
48	BQ	141/141 (100%)	0.04	2 (1%) 78 65	48, 89, 132, 201	0
48	DQ	141/141 (100%)	0.37	7 (4%) 32 19	53, 106, 159, 191	0
49	BR	117/118 (99%)	-0.15	0 100 100	39, 76, 125, 150	0
49	DR	117/118 (99%)	0.28	1 (0%) 85 78	53, 90, 147, 162	0
50	BS	99/112 (88%)	0.70	15 (15%) 3 2	75, 133, 182, 189	0
50	DS	99/112 (88%)	1.09	23 (23%) 1 1	95, 145, 196, 201	0
51	BT	138/146 (94%)	0.02	5 (3%) 46 31	51, 87, 182, 201	0
51	DT	138/146 (94%)	0.63	13 (9%) 11 6	68, 131, 194, 201	0
52	BU	117/118 (99%)	-0.09	1 (0%) 85 78	37, 73, 137, 201	0
52	DU	117/118 (99%)	-0.27	0 100 100	25, 62, 114, 174	0
53	BV	101/101 (100%)	0.16	6 (5%) 26 14	35, 103, 143, 201	0
53	DV	101/101 (100%)	-0.14	0 100 100	33, 80, 126, 180	0
54	BW	113/113 (100%)	-0.18	1 (0%) 85 78	43, 70, 133, 201	0
54	DW	113/113 (100%)	-0.25	0 100 100	37, 60, 118, 187	0
55	BX	93/96 (96%)	-0.07	1 (1%) 82 72	43, 89, 125, 140	0
55	DX	93/96 (96%)	-0.20	1 (1%) 82 72	43, 65, 114, 153	0
56	BY	101/110 (91%)	0.98	17 (16%) 2 1	63, 109, 182, 201	0
56	DY	101/110 (91%)	0.49	8 (7%) 15 9	54, 99, 176, 201	0
57	BZ	187/206 (90%)	0.33	11 (5%) 26 14	74, 121, 171, 201	0
57	DZ	187/206 (90%)	0.26	9 (4%) 34 21	76, 133, 187, 201	0
58	CX	8/25 (32%)	1.24	2 (25%) 1 1	106, 165, 200, 201	0
All	All	21297/22390 (95%)	0.51	2214 (10%) 8 5	21, 111, 198, 201	1 (0%)

The worst 5 of 2214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
43	BI	111	PRO	29.5
3	CC	169	ALA	20.0
10	CJ	72	VAL	18.0
37	DC	176	GLY	17.6
10	CJ	35	SER	16.9

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

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
1	A3P	CA	1493	26/27	0.63	0.44	-	191,200,203,203	0
1	A3P	AA	1493	26/27	0.90	0.20	-	151,182,188,189	0

## 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
59	MG	BA	3204	1/1	0.92	0.89	127.77	71,71,71,71	0
59	MG	DA	3140	1/1	0.92	0.66	114.26	77,77,77,77	0
59	MG	DA	3349	1/1	0.44	1.17	83.04	141,141,141,141	0
59	MG	DA	3406	1/1	0.84	1.62	78.72	38,38,38,38	1
59	MG	BA	3055	1/1	0.97	0.74	78.42	92,92,92,92	0
59	MG	DA	3522	1/1	0.83	0.53	73.02	56,56,56,56	0
59	MG	DA	3169	1/1	0.85	1.38	71.66	67,67,67,67	0
59	MG	BA	3040	1/1	0.87	0.65	68.76	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
59	MG	BA	3428	1/1	0.89	1.06	67.66	72,72,72,72	0
59	MG	DA	2935	1/1	0.90	1.25	67.21	12,12,12,12	1
59	MG	BA	3053	1/1	0.94	1.01	66.93	62,62,62,62	0
59	MG	BA	3463	1/1	0.93	0.68	58.17	66,66,66,66	0
59	MG	DA	3019	1/1	0.96	0.67	54.28	92,92,92,92	0
59	MG	BA	3527	1/1	0.96	0.63	53.06	86,86,86,86	0
59	MG	BA	3039	1/1	0.64	0.76	49.92	81,81,81,81	0
59	MG	DA	3217	1/1	0.97	0.63	48.03	69,69,69,69	0
59	MG	DA	3271	1/1	0.22	0.69	45.48	96,96,96,96	0
59	MG	DA	3339	1/1	0.99	0.47	44.39	37,37,37,37	0
59	MG	BA	3221	1/1	0.95	0.59	43.54	42,42,42,42	0
59	MG	BA	3037	1/1	0.62	0.68	43.00	64,64,64,64	0
59	MG	DA	3589	1/1	0.96	0.71	42.54	47,47,47,47	0
59	MG	CA	1680	1/1	0.79	0.99	41.13	102,102,102,102	0
59	MG	DA	3401	1/1	0.86	0.80	40.89	65,65,65,65	0
59	MG	DA	2930	1/1	0.87	1.30	40.50	1,1,1,1	1
59	MG	BA	3010	1/1	0.91	0.65	40.46	95,95,95,95	0
59	MG	BA	2993	1/1	0.77	0.87	40.01	86,86,86,86	0
59	MG	AV	102	1/1	0.91	0.79	38.97	106,106,106,106	0
59	MG	DA	3257	1/1	0.95	0.70	38.89	29,29,29,29	0
59	MG	BA	3162	1/1	0.91	0.68	38.55	41,41,41,41	0
59	MG	BA	3337	1/1	0.95	0.75	37.84	37,37,37,37	0
59	MG	DA	3335	1/1	0.85	0.50	37.56	48,48,48,48	0
59	MG	BA	3257	1/1	0.97	0.74	37.24	42,42,42,42	0
59	MG	DA	3381	1/1	0.95	0.67	36.27	43,43,43,43	0
59	MG	DA	3366	1/1	0.72	0.75	35.95	9,9,9,9	1
59	MG	DA	3345	1/1	0.04	1.22	34.29	25,25,25,25	1
59	MG	BA	3066	1/1	0.94	0.66	34.04	57,57,57,57	0
59	MG	D7	103	1/1	0.83	1.99	33.97	69,69,69,69	0
59	MG	BA	3273	1/1	0.97	0.56	33.51	31,31,31,31	0
59	MG	DA	3462	1/1	0.82	0.87	33.19	78,78,78,78	0
59	MG	BA	3019	1/1	0.68	0.95	32.70	66,66,66,66	0
59	MG	DA	3696	1/1	0.90	0.53	32.51	80,80,80,80	0
59	MG	BA	2985	1/1	0.92	0.74	32.02	84,84,84,84	0
59	MG	BA	2953	1/1	0.65	0.58	31.97	84,84,84,84	0
59	MG	AA	1938	1/1	0.66	1.01	31.92	124,124,124,124	0
59	MG	DA	3625	1/1	0.98	0.43	31.64	29,29,29,29	0
59	MG	DA	3635	1/1	0.98	0.44	31.12	31,31,31,31	0
59	MG	DA	3553	1/1	0.75	0.70	31.06	68,68,68,68	0
59	MG	BA	3488	1/1	0.81	0.53	30.60	66,66,66,66	1
59	MG	BA	3012	1/1	0.95	0.46	29.27	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3271	1/1	0.99	0.47	28.82	29,29,29,29	0
59	MG	DA	3468	1/1	0.77	0.47	28.70	76,76,76,76	0
59	MG	DA	3364	1/1	0.93	0.34	28.50	59,59,59,59	0
59	MG	BA	3081	1/1	0.96	0.58	28.45	64,64,64,64	0
59	MG	DA	3122	1/1	0.99	0.69	28.25	38,38,38,38	0
59	MG	DA	3459	1/1	0.60	0.55	27.82	92,92,92,92	0
59	MG	BA	3249	1/1	0.82	0.92	27.76	79,79,79,79	0
59	MG	AA	1790	1/1	0.84	0.41	27.67	96,96,96,96	0
59	MG	DA	3060	1/1	0.80	0.59	26.48	77,77,77,77	0
59	MG	BA	3510	1/1	0.93	0.71	26.45	41,41,41,41	0
59	MG	BA	3413	1/1	0.92	0.70	26.38	73,73,73,73	0
59	MG	BA	3583	1/1	0.62	0.56	26.04	81,81,81,81	1
59	MG	DA	3305	1/1	0.93	0.56	26.04	52,52,52,52	0
59	MG	DA	3022	1/1	0.70	0.47	25.97	71,71,71,71	0
59	MG	BA	2975	1/1	0.92	0.58	25.78	57,57,57,57	0
59	MG	AA	1697	1/1	0.95	0.83	25.75	76,76,76,76	0
59	MG	DA	3397	1/1	0.90	0.56	25.27	72,72,72,72	0
59	MG	DA	2964	1/1	0.95	0.44	24.86	54,54,54,54	0
59	MG	DA	3771	1/1	0.96	0.68	24.81	71,71,71,71	0
59	MG	DA	3763	1/1	0.79	0.51	24.66	62,62,62,62	1
59	MG	BA	2974	1/1	0.97	0.54	24.42	38,38,38,38	0
59	MG	DA	3390	1/1	0.79	0.55	23.62	60,60,60,60	1
59	MG	AA	1905	1/1	0.67	0.68	23.35	71,71,71,71	1
59	MG	BA	3052	1/1	0.71	0.44	23.10	64,64,64,64	0
59	MG	BA	3456	1/1	0.93	0.58	22.97	33,33,33,33	0
59	MG	AA	1862	1/1	0.90	0.37	22.92	65,65,65,65	0
59	MG	DA	3641	1/1	0.97	0.70	22.66	68,68,68,68	0
59	MG	DA	3247	1/1	0.96	0.58	22.43	41,41,41,41	0
59	MG	BA	3214	1/1	0.93	0.56	22.27	85,85,85,85	0
59	MG	BA	3068	1/1	0.92	0.63	22.09	59,59,59,59	0
59	MG	BA	3031	1/1	0.95	0.44	22.08	58,58,58,58	0
59	MG	DA	2904	1/1	0.88	1.08	21.58	66,66,66,66	0
59	MG	BA	3460	1/1	0.77	0.55	21.51	40,40,40,40	0
59	MG	BA	3410	1/1	0.91	0.47	21.32	42,42,42,42	0
59	MG	DA	3277	1/1	0.94	0.40	21.15	42,42,42,42	0
59	MG	DA	3219	1/1	0.85	0.47	21.02	62,62,62,62	0
59	MG	DA	3489	1/1	0.52	0.55	20.97	59,59,59,59	1
59	MG	DA	3398	1/1	0.97	0.47	20.93	31,31,31,31	1
59	MG	BA	3490	1/1	0.98	0.60	20.63	19,19,19,19	0
59	MG	DA	3012	1/1	0.99	0.60	20.40	30,30,30,30	0
59	MG	DA	2942	1/1	0.79	0.79	20.30	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3412	1/1	0.83	0.48	20.22	42,42,42,42	0
59	MG	BA	3035	1/1	0.95	0.68	20.05	42,42,42,42	0
59	MG	BA	3191	1/1	0.92	0.75	19.96	78,78,78,78	0
59	MG	DA	2908	1/1	0.71	1.43	19.92	97,97,97,97	0
59	MG	BA	3323	1/1	0.97	0.53	19.73	36,36,36,36	0
59	MG	DA	3341	1/1	0.76	0.57	19.61	62,62,62,62	0
59	MG	AA	1915	1/1	0.76	0.48	19.50	75,75,75,75	0
59	MG	BA	2925	1/1	0.96	0.45	19.45	33,33,33,33	0
59	MG	BA	3032	1/1	0.79	0.36	19.39	88,88,88,88	0
59	MG	DA	3343	1/1	0.82	0.43	19.31	69,69,69,69	0
59	MG	BA	3445	1/1	0.77	0.51	19.11	111,111,111,111	0
59	MG	DA	3187	1/1	0.99	0.56	19.01	44,44,44,44	0
59	MG	DA	2953	1/1	0.68	0.65	18.79	99,99,99,99	0
59	MG	DA	3356	1/1	0.98	0.55	18.78	32,32,32,32	0
59	MG	DA	3416	1/1	0.98	0.35	18.51	35,35,35,35	0
59	MG	BU	201	1/1	0.90	0.51	18.46	46,46,46,46	0
59	MG	BA	3465	1/1	0.88	0.55	17.86	37,37,37,37	0
59	MG	DA	3176	1/1	0.99	0.47	17.74	37,37,37,37	0
59	MG	BA	3582	1/1	0.81	0.46	17.73	63,63,63,63	0
59	MG	DA	3042	1/1	0.35	0.42	17.50	60,60,60,60	0
59	MG	BA	3450	1/1	0.94	0.61	17.48	60,60,60,60	0
59	MG	DA	3292	1/1	0.94	0.47	17.38	106,106,106,106	0
59	MG	AA	1872	1/1	0.72	0.67	17.37	77,77,77,77	0
59	MG	BA	2940	1/1	0.86	0.42	17.23	63,63,63,63	0
59	MG	BA	3509	1/1	0.83	0.52	17.06	58,58,58,58	0
59	MG	DA	3426	1/1	0.96	0.38	17.02	28,28,28,28	0
59	MG	DA	3759	1/1	0.91	0.58	16.65	49,49,49,49	0
59	MG	BA	3414	1/1	0.78	0.36	16.33	67,67,67,67	0
59	MG	BA	2979	1/1	0.80	0.41	16.15	66,66,66,66	0
59	MG	BA	3210	1/1	0.60	0.51	15.88	106,106,106,106	0
59	MG	BA	3330	1/1	0.90	0.39	15.83	88,88,88,88	0
59	MG	DA	3350	1/1	0.98	0.49	15.82	34,34,34,34	0
59	MG	BA	3521	1/1	0.88	0.33	15.67	119,119,119,119	0
59	MG	DA	3458	1/1	0.92	0.51	15.64	59,59,59,59	0
59	MG	BA	3329	1/1	0.88	0.46	15.32	1,1,1,1	1
59	MG	DA	3333	1/1	0.98	0.35	15.26	55,55,55,55	0
59	MG	DA	3281	1/1	0.94	0.45	15.12	31,31,31,31	0
59	MG	BA	3155	1/1	0.97	0.48	14.92	29,29,29,29	0
59	MG	BA	3395	1/1	0.63	0.64	14.83	84,84,84,84	0
59	MG	BA	2980	1/1	0.92	0.32	14.78	47,47,47,47	0
59	MG	BA	3265	1/1	0.70	0.32	14.59	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3649	1/1	0.69	0.47	14.49	66,66,66,66	0
59	MG	DA	3017	1/1	0.47	0.42	14.39	70,70,70,70	0
59	MG	BA	3405	1/1	0.96	0.46	14.36	44,44,44,44	0
59	MG	AA	1691	1/1	0.89	0.59	14.16	90,90,90,90	0
59	MG	DA	3031	1/1	0.99	0.38	14.05	51,51,51,51	0
59	MG	DA	2959	1/1	0.80	0.38	13.92	61,61,61,61	0
59	MG	DA	3500	1/1	0.83	0.47	13.80	84,84,84,84	0
59	MG	DA	3454	1/1	0.96	0.48	13.76	35,35,35,35	0
59	MG	BA	3256	1/1	0.88	0.32	13.64	122,122,122,122	0
59	MG	BA	3327	1/1	0.68	0.55	13.57	59,59,59,59	0
59	MG	DA	3244	1/1	0.85	0.30	13.25	29,29,29,29	0
59	MG	AA	1737	1/1	0.93	0.54	13.12	69,69,69,69	0
59	MG	BA	3305	1/1	0.98	0.41	13.09	28,28,28,28	0
59	MG	DU	202	1/1	0.94	0.31	13.06	8,8,8,8	1
59	MG	BA	3168	1/1	0.96	0.32	12.93	24,24,24,24	0
59	MG	BA	3187	1/1	0.89	0.57	12.76	37,37,37,37	0
59	MG	BA	3402	1/1	0.96	0.46	12.66	37,37,37,37	0
59	MG	DA	2927	1/1	0.84	0.35	12.54	1,1,1,1	1
59	MG	BA	3094	1/1	0.95	0.41	12.38	32,32,32,32	0
59	MG	DA	3477	1/1	0.90	0.62	12.32	76,76,76,76	0
59	MG	CA	1700	1/1	0.36	0.43	11.75	104,104,104,104	0
59	MG	DA	3037	1/1	0.88	0.54	11.71	58,58,58,58	0
59	MG	BA	3448	1/1	0.97	0.40	11.67	40,40,40,40	0
59	MG	BA	3452	1/1	0.96	0.45	11.59	45,45,45,45	0
59	MG	BA	3003	1/1	0.82	0.33	11.53	75,75,75,75	0
59	MG	AA	1829	1/1	0.69	0.55	11.39	91,91,91,91	0
59	MG	DA	3068	1/1	0.74	0.34	11.29	51,51,51,51	0
59	MG	BA	3184	1/1	0.93	0.34	11.01	38,38,38,38	0
59	MG	DA	3028	1/1	0.83	0.40	10.93	79,79,79,79	0
59	MG	DA	3032	1/1	0.97	0.37	10.88	34,34,34,34	0
59	MG	BA	3064	1/1	0.86	0.41	10.80	45,45,45,45	0
59	MG	DA	3604	1/1	0.96	0.49	10.78	39,39,39,39	0
59	MG	BA	3167	1/1	0.97	0.28	10.58	36,36,36,36	0
59	MG	DA	3488	1/1	0.91	0.28	10.43	28,28,28,28	0
59	MG	DA	3705	1/1	0.97	0.55	10.40	58,58,58,58	0
59	MG	DA	3444	1/1	0.94	0.42	10.33	31,31,31,31	0
59	MG	DA	2946	1/1	0.94	0.35	10.30	96,96,96,96	0
59	MG	AA	1616	1/1	0.94	0.53	10.25	61,61,61,61	0
59	MG	BA	3462	1/1	0.95	0.46	10.22	28,28,28,28	0
59	MG	DA	2939	1/1	0.93	0.81	10.14	1,1,1,1	1
59	MG	DA	3224	1/1	0.84	0.39	10.14	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3669	1/1	0.92	0.40	10.07	39,39,39,39	0
59	MG	BR	203	1/1	0.94	0.45	10.07	83,83,83,83	0
59	MG	DA	3677	1/1	0.94	0.31	9.99	45,45,45,45	0
59	MG	DA	3087	1/1	0.94	0.33	9.96	33,33,33,33	0
59	MG	DA	3282	1/1	0.96	0.38	9.93	31,31,31,31	0
59	MG	BA	3171	1/1	0.87	0.30	9.89	29,29,29,29	0
59	MG	DA	3452	1/1	0.98	0.45	9.89	30,30,30,30	0
59	MG	DA	2997	1/1	0.94	0.53	9.86	43,43,43,43	0
59	MG	DA	3611	1/1	0.95	0.46	9.84	31,31,31,31	0
59	MG	DA	3502	1/1	0.88	0.28	9.75	74,74,74,74	0
59	MG	BA	3074	1/1	0.84	0.48	9.74	36,36,36,36	0
59	MG	DA	3215	1/1	0.93	0.48	9.69	69,69,69,69	0
59	MG	BA	3496	1/1	0.94	0.32	9.58	44,44,44,44	0
59	MG	BE	304	1/1	0.73	0.44	9.49	46,46,46,46	1
59	MG	DA	3268	1/1	0.86	0.30	9.47	35,35,35,35	0
59	MG	DA	3535	1/1	0.95	0.52	9.47	52,52,52,52	0
59	MG	BA	3213	1/1	0.67	0.63	9.46	135,135,135,135	0
59	MG	DA	3473	1/1	0.98	0.53	9.36	38,38,38,38	0
59	MG	AA	1899	1/1	0.94	0.37	9.33	63,63,63,63	0
59	MG	DA	3050	1/1	0.93	0.54	9.26	40,40,40,40	0
59	MG	DA	3284	1/1	0.97	0.39	9.25	25,25,25,25	0
59	MG	DA	2990	1/1	0.71	0.45	9.17	43,43,43,43	1
59	MG	DA	3236	1/1	0.81	0.37	9.05	63,63,63,63	0
59	MG	DA	3600	1/1	0.97	0.30	8.96	30,30,30,30	0
59	MG	AA	1948	1/1	0.76	0.60	8.88	114,114,114,114	0
59	MG	BA	3043	1/1	0.77	0.38	8.83	80,80,80,80	0
59	MG	DA	3232	1/1	0.97	0.32	8.81	59,59,59,59	0
59	MG	AA	1968	1/1	0.76	0.51	8.63	95,95,95,95	0
59	MG	DA	3494	1/1	0.94	0.38	8.48	41,41,41,41	0
59	MG	BA	3248	1/1	0.63	0.35	8.35	101,101,101,101	0
59	MG	BA	3594	1/1	0.78	0.23	8.25	83,83,83,83	0
59	MG	BA	3169	1/1	0.99	0.36	8.24	24,24,24,24	0
59	MG	BA	3028	1/1	0.95	0.33	8.20	58,58,58,58	0
59	MG	DA	3344	1/1	0.84	0.27	8.13	75,75,75,75	0
59	MG	BA	3468	1/1	0.98	0.44	7.98	36,36,36,36	0
59	MG	BA	3558	1/1	0.89	0.40	7.92	78,78,78,78	0
59	MG	BA	3368	1/1	0.95	0.37	7.89	62,62,62,62	0
59	MG	DA	3084	1/1	0.97	0.39	7.88	57,57,57,57	0
59	MG	DA	3126	1/1	0.86	0.28	7.81	60,60,60,60	0
59	MG	BA	3517	1/1	0.94	0.25	7.78	98,98,98,98	0
59	MG	DA	2913	1/1	0.91	0.37	7.75	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3351	1/1	0.97	0.29	7.75	26,26,26,26	0
59	MG	BA	3512	1/1	0.75	0.28	7.75	51,51,51,51	0
59	MG	DA	3795	1/1	0.95	0.44	7.72	25,25,25,25	0
59	MG	DA	3255	1/1	0.93	0.41	7.69	51,51,51,51	0
59	MG	AA	1812	1/1	0.97	1.00	7.62	70,70,70,70	0
59	MG	DA	3788	1/1	0.88	0.25	7.61	124,124,124,124	0
59	MG	DA	3365	1/1	0.89	0.48	7.56	92,92,92,92	0
59	MG	DA	3608	1/1	0.96	0.35	7.55	61,61,61,61	0
59	MG	DA	3638	1/1	0.96	0.33	7.50	21,21,21,21	0
59	MG	DA	3141	1/1	0.98	0.36	7.49	99,99,99,99	0
59	MG	BA	2927	1/1	0.78	0.33	7.38	83,83,83,83	1
59	MG	BA	3397	1/1	0.98	0.34	7.33	75,75,75,75	0
59	MG	BA	3177	1/1	0.97	0.36	7.23	45,45,45,45	0
59	MG	BA	3063	1/1	0.91	0.34	7.17	59,59,59,59	0
59	MG	DA	3402	1/1	0.95	0.29	7.14	16,16,16,16	0
59	MG	DA	3026	1/1	0.96	0.34	7.06	60,60,60,60	0
59	MG	BA	2989	1/1	0.85	0.26	7.03	82,82,82,82	0
59	MG	BA	3119	1/1	0.97	0.34	6.92	30,30,30,30	0
59	MG	DP	202	1/1	0.60	0.59	6.82	49,49,49,49	1
59	MG	BA	3243	1/1	0.97	0.46	6.72	25,25,25,25	0
59	MG	DA	3290	1/1	0.97	0.36	6.66	32,32,32,32	0
59	MG	BA	3099	1/1	0.97	0.37	6.66	30,30,30,30	0
59	MG	BA	3246	1/1	0.87	0.24	6.65	68,68,68,68	0
59	MG	BA	3206	1/1	0.97	0.51	6.63	59,59,59,59	0
59	MG	BA	2920	1/1	0.92	0.28	6.58	42,42,42,42	0
59	MG	DA	3624	1/1	0.91	0.43	6.57	71,71,71,71	0
59	MG	DA	3178	1/1	0.97	0.35	6.42	29,29,29,29	0
59	MG	BA	3484	1/1	0.96	0.31	6.42	94,94,94,94	0
59	MG	DA	3579	1/1	0.91	0.34	6.31	110,110,110,110	0
59	MG	DA	3180	1/1	0.91	0.34	6.31	115,115,115,115	0
59	MG	D6	102	1/1	0.53	0.92	6.23	97,97,97,97	0
59	MG	DA	3276	1/1	0.93	0.30	6.21	58,58,58,58	0
59	MG	DA	3363	1/1	0.79	0.39	6.20	69,69,69,69	0
59	MG	BA	3312	1/1	0.82	0.28	6.19	53,53,53,53	0
59	MG	DA	2901	1/1	0.85	0.33	6.12	51,51,51,51	0
59	MG	DA	2967	1/1	0.84	0.33	6.09	35,35,35,35	1
59	MG	DA	3199	1/1	0.97	0.41	6.06	30,30,30,30	0
59	MG	DA	2919	1/1	0.75	0.23	6.04	57,57,57,57	0
59	MG	DA	2918	1/1	0.80	0.49	6.01	91,91,91,91	0
59	MG	BA	3197	1/1	0.96	0.31	5.99	54,54,54,54	0
59	MG	AA	1845	1/1	0.97	0.28	5.98	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
59	MG	BA	2947	1/1	0.96	0.31	5.93	45,45,45,45	0
59	MG	BA	3286	1/1	0.69	0.27	5.84	57,57,57,57	0
59	MG	DA	3003	1/1	0.95	0.30	5.82	36,36,36,36	0
59	MG	AA	1692	1/1	0.85	0.32	5.76	89,89,89,89	0
59	MG	BA	3514	1/1	0.68	0.39	5.74	76,76,76,76	0
59	MG	CA	1626	1/1	0.69	0.53	5.60	112,112,112,112	0
59	MG	DA	3717	1/1	0.13	0.31	5.59	155,155,155,155	0
59	MG	BA	3419	1/1	0.97	0.23	5.49	49,49,49,49	0
59	MG	BN	201	1/1	0.60	0.43	5.46	64,64,64,64	0
59	MG	DA	3631	1/1	0.88	0.41	5.44	41,41,41,41	0
59	MG	DA	3266	1/1	0.84	0.37	5.44	57,57,57,57	0
59	MG	BU	202	1/1	0.95	0.37	5.43	39,39,39,39	0
59	MG	DA	3298	1/1	0.58	0.34	5.40	65,65,65,65	0
59	MG	BA	3381	1/1	0.97	0.29	5.40	42,42,42,42	0
59	MG	DP	203	1/1	0.95	0.37	5.39	53,53,53,53	0
59	MG	BA	3446	1/1	0.90	0.30	5.39	99,99,99,99	0
59	MG	BA	3172	1/1	0.90	0.43	5.34	80,80,80,80	0
59	MG	BA	3161	1/1	0.97	0.27	5.31	39,39,39,39	0
59	MG	CA	1752	1/1	0.74	0.58	5.31	113,113,113,113	0
59	MG	BA	3574	1/1	0.89	0.30	5.28	53,53,53,53	0
59	MG	DA	3015	1/1	0.79	0.37	5.28	81,81,81,81	0
59	MG	DA	3264	1/1	0.99	0.30	5.20	47,47,47,47	1
59	MG	DA	3503	1/1	0.82	0.30	5.17	59,59,59,59	0
59	MG	BF	301	1/1	0.93	0.37	5.07	60,60,60,60	0
59	MG	BA	2954	1/1	0.87	0.28	5.03	59,59,59,59	0
59	MG	CA	1765	1/1	0.79	1.08	4.99	94,94,94,94	0
59	MG	BA	2997	1/1	0.94	0.37	4.97	82,82,82,82	0
59	MG	DA	3543	1/1	0.95	0.32	4.93	71,71,71,71	0
59	MG	AA	1726	1/1	0.82	0.32	4.93	70,70,70,70	1
59	MG	DA	3396	1/1	0.87	0.30	4.85	62,62,62,62	0
59	MG	AA	1858	1/1	0.96	0.28	4.79	60,60,60,60	0
59	MG	AA	1729	1/1	0.88	0.23	4.78	50,50,50,50	0
59	MG	DA	3301	1/1	0.86	0.20	4.77	32,32,32,32	0
59	MG	BA	3439	1/1	0.98	0.25	4.74	37,37,37,37	0
59	MG	DA	3662	1/1	0.94	0.28	4.70	59,59,59,59	0
59	MG	BA	2969	1/1	0.97	0.26	4.69	41,41,41,41	0
59	MG	AA	1893	1/1	0.97	0.27	4.69	56,56,56,56	0
59	MG	BA	3292	1/1	0.95	0.26	4.63	29,29,29,29	0
59	MG	DA	3262	1/1	0.96	0.29	4.63	59,59,59,59	1
59	MG	D7	102	1/1	0.90	0.30	4.62	75,75,75,75	0
59	MG	BA	3584	1/1	0.88	0.26	4.61	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	DD	303	1/1	0.71	0.38	4.58	64,64,64,64	0
59	MG	DA	3300	1/1	0.92	0.32	4.51	67,67,67,67	0
59	MG	DP	205	1/1	0.84	0.42	4.49	63,63,63,63	0
59	MG	DA	3303	1/1	0.97	0.28	4.49	54,54,54,54	0
59	MG	BA	3211	1/1	0.55	0.20	4.48	67,67,67,67	0
59	MG	DU	203	1/1	0.98	0.47	4.47	36,36,36,36	0
59	MG	DA	3251	1/1	0.96	0.23	4.40	53,53,53,53	0
59	MG	CA	1611	1/1	0.74	0.42	4.40	86,86,86,86	0
59	MG	DA	3394	1/1	0.92	0.30	4.40	63,63,63,63	0
59	MG	CH	201	1/1	0.83	0.63	4.36	37,37,37,37	1
59	MG	BD	301	1/1	0.98	0.37	4.31	25,25,25,25	0
59	MG	BA	3352	1/1	0.83	0.24	4.23	72,72,72,72	0
59	MG	DA	3013	1/1	0.91	0.45	4.09	68,68,68,68	0
59	MG	AA	1760	1/1	0.92	0.37	4.08	45,45,45,45	0
59	MG	AA	1650	1/1	0.96	0.33	4.05	73,73,73,73	0
59	MG	DA	3346	1/1	0.69	0.35	3.88	59,59,59,59	0
59	MG	BA	2937	1/1	0.96	0.34	3.88	40,40,40,40	0
59	MG	BA	3261	1/1	0.98	0.28	3.75	41,41,41,41	0
59	MG	AA	1630	1/1	0.77	0.31	3.71	57,57,57,57	0
59	MG	DA	2924	1/1	0.93	0.30	3.62	65,65,65,65	0
59	MG	CA	1631	1/1	0.81	0.35	3.58	59,59,59,59	0
59	MG	DA	3782	1/1	0.89	0.27	3.58	51,51,51,51	0
59	MG	AA	1932	1/1	0.69	0.30	3.58	82,82,82,82	0
59	MG	DA	3722	1/1	0.94	0.56	3.57	86,86,86,86	0
59	MG	BA	3309	1/1	0.82	0.25	3.53	58,58,58,58	0
59	MG	AA	1669	1/1	0.94	0.28	3.50	50,50,50,50	0
59	MG	DA	3072	1/1	0.65	0.44	3.44	81,81,81,81	0
59	MG	DA	3536	1/1	0.92	0.26	3.44	37,37,37,37	1
59	MG	AA	1820	1/1	0.71	0.31	3.40	97,97,97,97	0
59	MG	AA	1848	1/1	0.89	0.29	3.35	117,117,117,117	0
59	MG	BA	3137	1/1	0.98	0.22	3.27	43,43,43,43	0
59	MG	DA	3342	1/1	0.97	0.29	3.26	58,58,58,58	0
59	MG	DA	3071	1/1	0.95	0.25	3.25	71,71,71,71	0
59	MG	BA	2992	1/1	0.75	0.29	3.24	50,50,50,50	1
59	MG	BA	3176	1/1	0.80	0.25	3.18	50,50,50,50	0
59	MG	BA	3603	1/1	0.87	0.25	3.10	74,74,74,74	0
59	MG	DA	3408	1/1	0.90	0.30	3.07	41,41,41,41	0
59	MG	DA	3157	1/1	0.93	0.23	3.06	52,52,52,52	0
59	MG	BA	3255	1/1	0.96	0.24	3.06	55,55,55,55	0
59	MG	BA	3438	1/1	0.99	0.23	3.01	29,29,29,29	0
59	MG	DA	3025	1/1	0.93	0.24	2.97	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DE	301	1/1	0.58	0.36	2.91	67,67,67,67	0
59	MG	BA	3412	1/1	0.84	0.36	2.84	95,95,95,95	0
59	MG	DA	3741	1/1	0.96	0.26	2.84	43,43,43,43	0
59	MG	DA	3679	1/1	0.82	0.29	2.77	51,51,51,51	0
59	MG	BA	3247	1/1	0.97	0.21	2.62	62,62,62,62	1
59	MG	DA	3278	1/1	0.95	0.25	2.61	57,57,57,57	0
59	MG	BD	302	1/1	0.86	0.32	2.58	52,52,52,52	0
59	MG	BA	3373	1/1	0.92	0.21	2.57	56,56,56,56	0
59	MG	CA	1668	1/1	0.87	0.31	2.53	94,94,94,94	0
59	MG	DA	3372	1/1	0.84	0.24	2.47	82,82,82,82	0
59	MG	DA	3211	1/1	0.86	0.23	2.43	65,65,65,65	0
59	MG	DA	3729	1/1	0.95	0.23	2.42	96,96,96,96	0
59	MG	DA	3086	1/1	0.81	0.26	2.40	60,60,60,60	0
59	MG	AA	1662	1/1	0.92	0.43	2.28	68,68,68,68	0
59	MG	BA	3525	1/1	0.97	0.26	2.27	44,44,44,44	0
59	MG	DA	3090	1/1	0.97	0.24	2.25	35,35,35,35	0
59	MG	AA	1888	1/1	0.98	0.22	2.24	58,58,58,58	0
59	MG	DA	3080	1/1	0.88	0.19	2.17	56,56,56,56	0
59	MG	BA	3559	1/1	0.96	0.22	2.14	45,45,45,45	0
59	MG	BA	3058	1/1	0.91	0.26	2.09	74,74,74,74	0
59	MG	AA	1694	1/1	0.88	0.24	2.05	56,56,56,56	1
59	MG	DA	3197	1/1	0.81	0.21	2.03	67,67,67,67	0
59	MG	DA	3137	1/1	0.68	0.27	2.02	70,70,70,70	0
59	MG	AA	1857	1/1	0.68	0.18	2.01	57,57,57,57	0
59	MG	AA	1887	1/1	0.93	0.24	1.96	72,72,72,72	0
59	MG	BA	3298	1/1	0.96	0.25	1.92	67,67,67,67	0
59	MG	AL	205	1/1	0.91	0.28	1.87	47,47,47,47	1
59	MG	DA	3010	1/1	0.99	0.23	1.84	49,49,49,49	0
59	MG	DA	3063	1/1	0.86	0.23	1.75	50,50,50,50	0
59	MG	DU	204	1/1	0.98	0.29	1.70	19,19,19,19	0
59	MG	BP	203	1/1	0.98	0.23	1.68	88,88,88,88	0
59	MG	DA	3280	1/1	0.90	0.21	1.65	58,58,58,58	0
59	MG	BA	3250	1/1	0.91	0.25	1.65	51,51,51,51	0
59	MG	CA	1720	1/1	0.42	0.31	1.64	106,106,106,106	0
59	MG	AA	1908	1/1	0.62	0.30	1.57	65,65,65,65	0
59	MG	BA	3151	1/1	0.90	0.20	1.42	65,65,65,65	0
59	MG	AA	1622	1/1	0.93	0.30	1.40	70,70,70,70	0
59	MG	BA	3259	1/1	0.82	0.23	1.39	59,59,59,59	0
59	MG	DA	3580	1/1	0.90	0.26	1.37	34,34,34,34	0
59	MG	AA	1864	1/1	0.89	0.20	1.30	67,67,67,67	0
59	MG	BA	3404	1/1	0.96	0.31	1.30	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BD	303	1/1	0.96	0.23	1.19	35,35,35,35	0
59	MG	BA	3225	1/1	0.73	0.20	1.18	62,62,62,62	0
59	MG	DA	3308	1/1	0.92	0.23	1.18	103,103,103,103	0
59	MG	CA	1601	1/1	0.70	0.27	1.14	96,96,96,96	0
59	MG	BA	3142	1/1	0.79	0.17	1.11	67,67,67,67	0
59	MG	BP	204	1/1	0.96	0.27	1.09	24,24,24,24	1
59	MG	B5	102	1/1	0.91	0.21	0.98	32,32,32,32	1
59	MG	DA	3425	1/1	0.97	0.21	0.98	56,56,56,56	0
59	MG	BA	3049	1/1	0.86	0.19	0.98	66,66,66,66	0
59	MG	DA	3735	1/1	0.85	0.16	0.91	90,90,90,90	0
59	MG	DA	3749	1/1	0.97	0.22	0.87	80,80,80,80	1
59	MG	BQ	201	1/1	0.89	0.27	0.86	72,72,72,72	0
59	MG	DA	3029	1/1	0.98	0.19	0.85	30,30,30,30	0
59	MG	AA	1762	1/1	0.68	0.19	0.81	74,74,74,74	0
59	MG	DA	3272	1/1	0.90	0.22	0.78	79,79,79,79	1
59	MG	DA	3191	1/1	0.80	0.21	0.74	83,83,83,83	0
59	MG	DA	3064	1/1	0.94	0.22	0.69	51,51,51,51	0
59	MG	BA	2926	1/1	0.97	0.22	0.68	20,20,20,20	0
59	MG	BA	3590	1/1	0.79	0.17	0.64	90,90,90,90	0
59	MG	BA	3436	1/1	0.89	0.16	0.59	62,62,62,62	0
59	MG	DA	3599	1/1	1.00	0.22	0.59	39,39,39,39	0
59	MG	BA	3067	1/1	0.90	0.21	0.51	34,34,34,34	0
59	MG	DA	3175	1/1	0.92	0.20	0.47	28,28,28,28	0
59	MG	BA	3201	1/1	0.86	0.23	0.45	50,50,50,50	0
59	MG	DA	3057	1/1	0.94	0.22	0.41	32,32,32,32	0
59	MG	DA	3207	1/1	0.93	0.19	0.39	84,84,84,84	0
59	MG	BA	3469	1/1	0.99	0.17	0.36	102,102,102,102	0
59	MG	DA	3385	1/1	0.88	0.23	0.35	43,43,43,43	0
59	MG	D0	102	1/1	0.74	0.40	0.31	75,75,75,75	0
59	MG	DA	3794	1/1	0.89	0.17	0.30	79,79,79,79	0
59	MG	AA	1960	1/1	0.90	0.18	0.30	72,72,72,72	0
59	MG	DE	303	1/1	0.91	0.23	0.30	42,42,42,42	0
59	MG	AA	1721	1/1	0.95	0.14	0.29	111,111,111,111	0
59	MG	AA	1859	1/1	0.93	0.20	0.26	44,44,44,44	0
59	MG	BA	3491	1/1	0.70	0.17	0.26	70,70,70,70	0
59	MG	BA	2908	1/1	0.74	0.16	0.26	84,84,84,84	0
59	MG	AA	1643	1/1	0.84	0.17	0.25	92,92,92,92	0
59	MG	DA	3577	1/1	0.78	0.16	0.25	92,92,92,92	0
59	MG	DA	3713	1/1	0.92	0.18	0.24	67,67,67,67	0
59	MG	BA	3235	1/1	0.98	0.20	0.19	40,40,40,40	0
59	MG	DA	3698	1/1	0.86	0.18	0.19	25,25,25,25	0
59	MG	BA	3183	1/1	0.89	0.17	0.18	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3130	1/1	0.84	0.17	0.15	62,62,62,62	0
59	MG	DA	3715	1/1	0.97	0.20	0.13	64,64,64,64	0
59	MG	AA	1937	1/1	0.86	0.18	0.12	58,58,58,58	0
59	MG	DA	3314	1/1	0.85	0.15	0.10	71,71,71,71	0
59	MG	AA	1660	1/1	0.70	0.21	0.10	82,82,82,82	0
59	MG	AA	1910	1/1	0.79	0.17	0.03	120,120,120,120	0
59	MG	BA	3451	1/1	0.94	0.17	0.02	55,55,55,55	0
59	MG	CA	1686	1/1	0.74	0.28	0.01	74,74,74,74	0
59	MG	BA	3076	1/1	0.96	0.23	-0.02	30,30,30,30	0
59	MG	DA	3288	1/1	0.76	0.13	-0.03	60,60,60,60	0
59	MG	DA	3116	1/1	0.81	0.16	-0.05	78,78,78,78	0
59	MG	BA	3303	1/1	0.78	0.14	-0.11	88,88,88,88	0
59	MG	BY	201	1/1	0.88	0.23	-0.11	50,50,50,50	0
59	MG	BA	2984	1/1	0.68	0.33	-0.12	92,92,92,92	0
59	MG	AA	1695	1/1	0.88	0.19	-0.13	65,65,65,65	0
59	MG	DA	3523	1/1	0.98	0.18	-0.14	34,34,34,34	0
59	MG	DA	2934	1/1	0.93	0.19	-0.18	48,48,48,48	1
59	MG	BA	3266	1/1	0.85	0.17	-0.19	65,65,65,65	0
59	MG	BA	2931	1/1	0.95	0.19	-0.19	44,44,44,44	0
59	MG	DA	3703	1/1	0.88	0.19	-0.21	41,41,41,41	0
59	MG	DA	3082	1/1	0.97	0.17	-0.24	82,82,82,82	0
59	MG	BA	3535	1/1	0.95	0.18	-0.25	81,81,81,81	0
59	MG	DD	302	1/1	0.95	0.20	-0.29	53,53,53,53	0
59	MG	BA	3170	1/1	0.81	0.15	-0.33	56,56,56,56	0
59	MG	CA	1713	1/1	0.91	0.26	-0.34	65,65,65,65	1
59	MG	BH	204	1/1	0.41	0.21	-0.35	57,57,57,57	1
59	MG	CD	302	1/1	0.88	0.25	-0.38	68,68,68,68	0
59	MG	AA	1641	1/1	0.86	0.15	-0.38	68,68,68,68	1
59	MG	DA	2980	1/1	0.97	0.20	-0.41	69,69,69,69	0
59	MG	BA	3051	1/1	0.91	0.17	-0.45	68,68,68,68	0
59	MG	AA	1703	1/1	0.79	0.15	-0.46	44,44,44,44	1
59	MG	DA	3202	1/1	0.86	0.17	-0.46	70,70,70,70	0
59	MG	B6	101	1/1	0.56	0.42	-0.48	111,111,111,111	0
59	MG	CA	1728	1/1	0.96	0.18	-0.50	88,88,88,88	0
59	MG	AA	1926	1/1	0.92	0.16	-0.50	59,59,59,59	0
59	MG	AA	1911	1/1	0.95	0.14	-0.50	55,55,55,55	0
59	MG	AA	1652	1/1	0.75	0.18	-0.50	95,95,95,95	0
59	MG	DA	2958	1/1	0.68	0.20	-0.53	59,59,59,59	1
59	MG	BA	2988	1/1	0.93	0.14	-0.63	35,35,35,35	0
59	MG	AI	201	1/1	0.90	0.29	-0.65	163,163,163,163	0
59	MG	BA	3233	1/1	0.87	0.15	-0.69	73,73,73,73	0
59	MG	AA	1795	1/1	0.67	0.12	-0.70	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	ZN	AD	305	1/1	1.00	0.22	-0.74	88,88,88,88	0
59	MG	CA	1732	1/1	0.73	0.19	-0.79	70,70,70,70	0
60	ZN	AD	301	1/1	1.00	0.23	-0.84	106,106,106,106	0
59	MG	DA	3186	1/1	0.90	0.18	-0.87	42,42,42,42	0
59	MG	DA	3560	1/1	0.97	0.19	-0.90	58,58,58,58	0
59	MG	DA	3687	1/1	0.97	0.16	-0.90	43,43,43,43	0
59	MG	DA	3701	1/1	0.98	0.11	-0.91	55,55,55,55	0
59	MG	BA	3492	1/1	0.79	0.15	-0.91	31,31,31,31	1
59	MG	CM	202	1/1	0.96	0.20	-0.92	151,151,151,151	0
59	MG	AA	1882	1/1	0.95	0.20	-0.94	57,57,57,57	0
59	MG	DB	208	1/1	0.95	0.17	-0.97	86,86,86,86	0
59	MG	D5	103	1/1	0.96	0.11	-0.98	88,88,88,88	0
59	MG	AA	1878	1/1	0.91	0.16	-0.99	76,76,76,76	0
59	MG	BA	3018	1/1	0.91	0.15	-1.04	38,38,38,38	0
59	MG	DA	3533	1/1	0.96	0.19	-1.08	100,100,100,100	0
60	ZN	CD	301	1/1	0.86	0.24	-1.14	151,151,151,151	0
59	MG	BA	3287	1/1	0.85	0.14	-1.16	104,104,104,104	0
59	MG	CS	101	1/1	0.81	0.15	-1.18	97,97,97,97	1
60	ZN	AN	101	1/1	0.96	0.14	-1.22	153,153,153,153	0
59	MG	BP	202	1/1	0.99	0.14	-1.22	69,69,69,69	1
59	MG	AN	103	1/1	0.98	0.25	-1.23	147,147,147,147	0
59	MG	DA	3603	1/1	0.96	0.18	-1.23	60,60,60,60	0
59	MG	BA	3269	1/1	0.94	0.15	-1.25	63,63,63,63	0
59	MG	DA	2971	1/1	0.98	0.19	-1.25	20,20,20,20	0
59	MG	AD	304	1/1	0.94	0.19	-1.26	135,135,135,135	0
59	MG	AA	1913	1/1	0.97	0.10	-1.27	72,72,72,72	0
59	MG	AC	302	1/1	0.89	0.12	-1.28	163,163,163,163	0
59	MG	CQ	201	1/1	0.90	0.08	-1.33	98,98,98,98	1
59	MG	CA	1706	1/1	0.91	0.09	-1.35	47,47,47,47	0
59	MG	DP	201	1/1	0.93	0.11	-1.41	36,36,36,36	1
59	MG	AA	1647	1/1	0.94	0.15	-1.42	35,35,35,35	0
59	MG	DA	3318	1/1	0.94	0.12	-1.43	59,59,59,59	0
59	MG	AI	203	1/1	0.83	0.27	-1.46	138,138,138,138	0
59	MG	AD	302	1/1	0.87	0.07	-1.47	96,96,96,96	0
59	MG	DA	3085	1/1	0.81	0.14	-1.51	68,68,68,68	0
59	MG	BE	302	1/1	0.96	0.14	-1.59	30,30,30,30	0
59	MG	AA	1778	1/1	0.97	0.12	-1.60	84,84,84,84	0
59	MG	CA	1745	1/1	0.69	0.28	-1.66	112,112,112,112	0
59	MG	CA	1768	1/1	0.85	0.15	-1.78	71,71,71,71	0
59	MG	BA	3334	1/1	0.96	0.17	-1.79	60,60,60,60	0
59	MG	BA	2961	1/1	0.86	0.13	-1.82	79,79,79,79	0
59	MG	BA	3252	1/1	0.99	0.15	-1.82	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
59	MG	BA	3134	1/1	0.74	0.10	-1.84	65,65,65,65	0
59	MG	AA	1612	1/1	0.96	0.09	-1.87	55,55,55,55	0
59	MG	DA	3755	1/1	0.88	0.15	-1.92	128,128,128,128	0
59	MG	DA	3306	1/1	0.76	0.11	-1.93	56,56,56,56	0
59	MG	BA	3038	1/1	0.96	0.18	-1.94	17,17,17,17	0
59	MG	DA	3319	1/1	0.93	0.13	-1.96	47,47,47,47	0
59	MG	CM	201	1/1	0.72	0.12	-1.99	131,131,131,131	0
59	MG	CM	203	1/1	0.97	0.12	-1.99	123,123,123,123	0
59	MG	DA	3733	1/1	0.81	0.13	-2.11	43,43,43,43	0
59	MG	DA	3069	1/1	0.97	0.18	-2.12	50,50,50,50	0
59	MG	D5	102	1/1	0.99	0.07	-2.17	63,63,63,63	0
59	MG	AP	101	1/1	0.99	0.16	-2.17	93,93,93,93	0
59	MG	CA	1731	1/1	0.67	0.21	-2.19	76,76,76,76	0
59	MG	BA	3114	1/1	0.95	0.10	-2.28	80,80,80,80	0
59	MG	BA	3441	1/1	0.99	0.15	-2.34	40,40,40,40	0
59	MG	DA	3274	1/1	0.83	0.08	-2.40	73,73,73,73	0
59	MG	CA	1734	1/1	0.98	0.14	-2.40	56,56,56,56	0
59	MG	AA	1930	1/1	0.90	0.17	-2.48	64,64,64,64	0
59	MG	BA	3449	1/1	0.95	0.14	-2.50	69,69,69,69	0
59	MG	DA	3652	1/1	0.90	0.13	-2.55	74,74,74,74	0
59	MG	DD	306	1/1	0.96	0.09	-2.59	60,60,60,60	0
59	MG	CA	1678	1/1	0.93	0.14	-2.59	45,45,45,45	1
59	MG	DA	3691	1/1	0.88	0.10	-2.66	59,59,59,59	0
59	MG	BA	3188	1/1	0.90	0.09	-2.71	58,58,58,58	0
59	MG	CA	1704	1/1	0.92	0.11	-2.79	71,71,71,71	0
59	MG	CA	1742	1/1	0.98	0.09	-2.92	81,81,81,81	0
59	MG	DA	3382	1/1	0.87	0.11	-2.93	101,101,101,101	0
59	MG	CA	1666	1/1	0.97	0.08	-2.99	63,63,63,63	0
59	MG	BD	305	1/1	0.93	0.14	-3.15	168,168,168,168	0
59	MG	BB	204	1/1	0.55	0.15	-3.16	109,109,109,109	0
59	MG	BA	3453	1/1	0.94	0.07	-3.18	120,120,120,120	0
59	MG	BA	3090	1/1	0.98	0.14	-3.19	27,27,27,27	0
59	MG	AN	102	1/1	0.66	0.12	-3.20	141,141,141,141	0
59	MG	AA	1925	1/1	0.94	0.13	-3.27	72,72,72,72	0
59	MG	BA	3538	1/1	0.96	0.09	-3.30	37,37,37,37	0
59	MG	DA	3557	1/1	0.95	0.14	-3.40	64,64,64,64	0
59	MG	DA	3283	1/1	0.95	0.12	-3.41	65,65,65,65	0
59	MG	DA	3490	1/1	0.95	0.13	-3.43	29,29,29,29	1
59	MG	AA	1920	1/1	0.88	0.14	-3.47	73,73,73,73	0
59	MG	CA	1645	1/1	0.97	0.12	-3.62	50,50,50,50	0
59	MG	BA	3200	1/1	0.84	0.12	-4.39	31,31,31,31	0
59	MG	DA	3258	1/1	0.95	0.18	-4.44	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3045	1/1	0.98	0.16	-4.76	47,47,47,47	0
59	MG	DA	3033	1/1	0.97	0.14	-4.79	50,50,50,50	0
59	MG	DA	3405	1/1	0.96	0.11	-5.32	63,63,63,63	0
59	MG	CA	1781	1/1	0.94	0.16	-5.58	74,74,74,74	0
59	MG	BA	3022	1/1	0.95	0.08	-5.65	43,43,43,43	0
59	MG	AA	1693	1/1	0.91	0.10	-6.04	56,56,56,56	1
59	MG	BA	3593	1/1	0.96	0.09	-6.92	41,41,41,41	0
59	MG	DA	3681	1/1	0.95	0.10	-7.32	28,28,28,28	0
59	MG	BA	3106	1/1	0.96	0.11	-8.51	35,35,35,35	0
59	MG	BA	3489	1/1	0.94	0.10	-8.56	22,22,22,22	0
59	MG	AA	1973	1/1	0.94	0.22	-	69,69,69,69	0
59	MG	BA	3093	1/1	0.92	0.21	-	52,52,52,52	0
59	MG	AA	1842	1/1	0.83	0.12	-	58,58,58,58	0
59	MG	BA	2977	1/1	0.83	1.03	-	93,93,93,93	0
59	MG	CA	1604	1/1	0.94	0.20	-	63,63,63,63	0
59	MG	AA	1603	1/1	0.90	0.20	-	74,74,74,74	0
59	MG	DA	3131	1/1	0.14	0.50	-	154,154,154,154	0
59	MG	DA	3518	1/1	0.81	0.36	-	62,62,62,62	1
59	MG	BA	3196	1/1	0.76	0.48	-	64,64,64,64	0
59	MG	BE	301	1/1	0.81	0.46	-	88,88,88,88	0
59	MG	BA	3262	1/1	0.92	0.27	-	50,50,50,50	0
59	MG	DA	3136	1/1	0.80	0.47	-	97,97,97,97	0
59	MG	DA	2985	1/1	0.96	0.46	-	39,39,39,39	0
59	MG	DA	3230	1/1	0.82	0.31	-	94,94,94,94	0
59	MG	DD	304	1/1	0.60	0.40	-	97,97,97,97	0
59	MG	BA	3354	1/1	0.47	0.59	-	76,76,76,76	0
59	MG	CA	1675	1/1	0.92	0.59	-	93,93,93,93	0
59	MG	DA	3228	1/1	0.81	0.31	-	79,79,79,79	0
59	MG	DA	3295	1/1	0.87	0.78	-	99,99,99,99	0
59	MG	CV	110	1/1	0.24	0.46	-	105,105,105,105	0
59	MG	DA	2903	1/1	0.93	0.48	-	43,43,43,43	0
59	MG	DA	3449	1/1	0.52	0.46	-	71,71,71,71	0
59	MG	BA	3338	1/1	0.69	0.43	-	97,97,97,97	0
59	MG	AA	1752	1/1	0.81	0.38	-	51,51,51,51	1
59	MG	DA	3464	1/1	0.77	0.67	-	62,62,62,62	1
59	MG	DA	3471	1/1	0.92	0.56	-	63,63,63,63	0
59	MG	CA	1684	1/1	0.74	0.47	-	64,64,64,64	0
59	MG	BA	3218	1/1	0.73	0.34	-	111,111,111,111	0
59	MG	DA	3410	1/1	0.99	0.41	-	25,25,25,25	0
59	MG	DA	3226	1/1	0.95	0.70	-	54,54,54,54	0
59	MG	BA	3295	1/1	0.95	0.59	-	51,51,51,51	0
59	MG	BA	3586	1/1	0.95	0.91	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3693	1/1	0.74	0.42	-	33,33,33,33	1
59	MG	DA	3443	1/1	0.69	0.41	-	133,133,133,133	0
59	MG	BB	203	1/1	0.72	0.36	-	59,59,59,59	0
59	MG	BA	3289	1/1	0.97	0.33	-	39,39,39,39	0
59	MG	BA	3411	1/1	0.94	0.50	-	76,76,76,76	0
59	MG	BA	3091	1/1	0.97	0.30	-	62,62,62,62	0
59	MG	BA	3555	1/1	0.85	0.69	-	60,60,60,60	0
59	MG	AQ	203	1/1	0.89	1.00	-	130,130,130,130	0
59	MG	DA	3145	1/1	0.58	1.01	-	120,120,120,120	0
59	MG	BA	3545	1/1	0.94	0.42	-	79,79,79,79	0
59	MG	DA	3144	1/1	0.82	0.50	-	131,131,131,131	0
59	MG	BA	2965	1/1	0.73	0.77	-	84,84,84,84	0
59	MG	DA	3702	1/1	0.80	0.43	-	80,80,80,80	0
59	MG	DA	3103	1/1	0.98	0.35	-	60,60,60,60	0
59	MG	BA	3430	1/1	0.78	0.36	-	68,68,68,68	0
59	MG	DA	3460	1/1	0.94	0.17	-	73,73,73,73	0
59	MG	CA	1775	1/1	0.82	0.12	-	70,70,70,70	1
59	MG	AA	1743	1/1	0.81	0.21	-	87,87,87,87	0
59	MG	BE	303	1/1	0.97	0.34	-	22,22,22,22	0
59	MG	DA	3467	1/1	0.80	0.36	-	109,109,109,109	0
59	MG	BA	3382	1/1	0.82	0.12	-	77,77,77,77	0
59	MG	DA	3354	1/1	0.78	0.27	-	52,52,52,52	0
59	MG	DA	3450	1/1	0.96	0.17	-	100,100,100,100	0
59	MG	BA	3435	1/1	0.89	0.61	-	70,70,70,70	0
59	MG	DA	2943	1/1	0.96	0.07	-	71,71,71,71	1
59	MG	DF	303	1/1	0.90	0.21	-	22,22,22,22	1
59	MG	BA	3131	1/1	0.99	0.35	-	43,43,43,43	0
59	MG	BA	2949	1/1	0.56	0.52	-	102,102,102,102	0
59	MG	AL	204	1/1	0.96	0.05	-	90,90,90,90	0
59	MG	BA	3075	1/1	0.85	0.44	-	87,87,87,87	0
59	MG	AA	1671	1/1	0.80	1.37	-	107,107,107,107	0
59	MG	AA	1757	1/1	0.49	1.54	-	111,111,111,111	0
59	MG	DA	3248	1/1	0.85	0.26	-	62,62,62,62	0
59	MG	DA	2933	1/1	0.93	0.25	-	51,51,51,51	0
59	MG	DA	3172	1/1	0.73	1.02	-	102,102,102,102	0
59	MG	DA	3243	1/1	0.97	0.81	-	64,64,64,64	0
59	MG	AA	1825	1/1	0.83	0.72	-	71,71,71,71	0
59	MG	AA	1814	1/1	0.74	1.04	-	77,77,77,77	0
59	MG	AA	1771	1/1	0.88	0.59	-	95,95,95,95	0
59	MG	DA	3155	1/1	0.70	0.88	-	78,78,78,78	0
59	MG	AO	102	1/1	0.76	1.05	-	77,77,77,77	0
59	MG	AA	1822	1/1	0.95	0.33	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3478	1/1	0.93	1.02	-	112,112,112,112	0
59	MG	DA	3112	1/1	0.79	0.10	-	87,87,87,87	0
59	MG	AA	1847	1/1	0.90	0.37	-	76,76,76,76	0
59	MG	BA	3472	1/1	0.88	0.97	-	100,100,100,100	0
59	MG	AA	1811	1/1	0.92	0.25	-	49,49,49,49	0
59	MG	DA	3665	1/1	0.67	0.57	-	96,96,96,96	0
59	MG	AA	1724	1/1	0.95	0.16	-	86,86,86,86	1
59	MG	BA	3136	1/1	0.98	0.19	-	34,34,34,34	0
59	MG	BA	3503	1/1	0.85	0.37	-	65,65,65,65	1
59	MG	DA	3697	1/1	0.99	0.30	-	32,32,32,32	0
59	MG	BA	2982	1/1	0.92	0.13	-	58,58,58,58	1
59	MG	DN	203	1/1	0.73	0.83	-	64,64,64,64	1
59	MG	DA	3158	1/1	0.77	0.55	-	130,130,130,130	0
59	MG	DA	3761	1/1	0.46	0.59	-	96,96,96,96	0
59	MG	DA	3322	1/1	0.93	0.56	-	89,89,89,89	0
59	MG	CA	1726	1/1	0.57	1.02	-	107,107,107,107	0
59	MG	BA	3245	1/1	0.51	0.21	-	116,116,116,116	0
59	MG	DA	3789	1/1	0.77	0.40	-	68,68,68,68	0
59	MG	AA	1611	1/1	0.86	0.39	-	66,66,66,66	0
59	MG	BA	3166	1/1	0.98	0.47	-	89,89,89,89	0
59	MG	DA	3059	1/1	0.90	0.59	-	77,77,77,77	0
59	MG	BA	3340	1/1	0.63	0.94	-	99,99,99,99	0
59	MG	BA	2957	1/1	0.91	0.46	-	81,81,81,81	0
59	MG	DA	3507	1/1	0.90	0.32	-	5,5,5,5	1
59	MG	DA	3463	1/1	0.89	0.56	-	83,83,83,83	0
59	MG	AA	1681	1/1	0.88	0.24	-	106,106,106,106	0
59	MG	DA	3592	1/1	0.94	0.49	-	58,58,58,58	0
59	MG	AA	1604	1/1	0.50	0.30	-	118,118,118,118	0
59	MG	DA	2960	1/1	0.88	0.91	-	57,57,57,57	1
59	MG	DA	3753	1/1	0.88	0.80	-	83,83,83,83	0
59	MG	DA	3245	1/1	0.89	0.31	-	78,78,78,78	0
59	MG	DA	3590	1/1	0.36	0.46	-	67,67,67,67	0
59	MG	AA	1917	1/1	0.87	0.31	-	78,78,78,78	0
59	MG	CA	1603	1/1	0.91	0.32	-	112,112,112,112	0
59	MG	CA	1763	1/1	-0.10	0.59	-	105,105,105,105	0
59	MG	DA	3475	1/1	0.66	0.39	-	115,115,115,115	0
59	MG	DA	3653	1/1	0.95	0.55	-	82,82,82,82	0
59	MG	AA	1824	1/1	0.95	0.15	-	83,83,83,83	0
59	MG	AA	1741	1/1	0.96	0.17	-	54,54,54,54	0
59	MG	DA	3511	1/1	0.67	1.33	-	83,83,83,83	0
59	MG	DA	3630	1/1	0.85	0.40	-	99,99,99,99	0
59	MG	AA	1950	1/1	0.62	0.36	-	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
59	MG	BA	3504	1/1	0.92	0.23	-	59,59,59,59	0
59	MG	AY	101	1/1	0.94	1.20	-	6,6,6,6	1
59	MG	CA	1693	1/1	0.82	0.70	-	73,73,73,73	0
59	MG	AA	1747	1/1	0.81	0.77	-	119,119,119,119	0
59	MG	CA	1703	1/1	0.81	1.03	-	82,82,82,82	0
59	MG	BA	3347	1/1	0.98	0.50	-	30,30,30,30	0
59	MG	DA	3152	1/1	0.95	0.42	-	108,108,108,108	0
59	MG	BA	3422	1/1	0.90	0.16	-	68,68,68,68	0
59	MG	AA	1955	1/1	0.84	0.30	-	64,64,64,64	1
59	MG	DA	3361	1/1	0.97	0.37	-	42,42,42,42	0
59	MG	B0	102	1/1	0.71	0.27	-	91,91,91,91	0
59	MG	CA	1683	1/1	0.71	0.36	-	60,60,60,60	0
59	MG	DA	3746	1/1	0.94	0.69	-	71,71,71,71	0
59	MG	DA	3567	1/1	0.84	1.22	-	98,98,98,98	0
59	MG	BA	3542	1/1	0.87	0.35	-	102,102,102,102	0
59	MG	CA	1746	1/1	0.77	0.53	-	85,85,85,85	0
59	MG	DA	3778	1/1	0.86	0.22	-	115,115,115,115	0
59	MG	BA	3158	1/1	0.90	0.22	-	33,33,33,33	0
59	MG	DA	3214	1/1	0.56	0.53	-	102,102,102,102	0
59	MG	DA	3171	1/1	0.95	0.27	-	71,71,71,71	0
59	MG	CA	1662	1/1	0.76	0.12	-	79,79,79,79	0
59	MG	DA	3009	1/1	0.68	1.71	-	83,83,83,83	0
59	MG	DA	3070	1/1	0.84	0.12	-	59,59,59,59	0
59	MG	DA	3660	1/1	0.94	0.66	-	78,78,78,78	0
59	MG	BA	3346	1/1	0.79	0.52	-	71,71,71,71	0
59	MG	DA	3683	1/1	0.94	0.69	-	46,46,46,46	0
59	MG	AA	1863	1/1	0.91	0.30	-	80,80,80,80	0
59	MG	BA	2946	1/1	0.94	0.42	-	49,49,49,49	0
59	MG	AA	1754	1/1	0.78	0.13	-	124,124,124,124	0
59	MG	DA	3263	1/1	0.84	0.33	-	125,125,125,125	0
59	MG	DA	3008	1/1	0.95	0.28	-	70,70,70,70	0
59	MG	BA	3386	1/1	0.92	0.34	-	72,72,72,72	0
59	MG	CA	1762	1/1	0.69	0.20	-	95,95,95,95	0
59	MG	DA	3770	1/1	0.69	0.31	-	85,85,85,85	1
59	MG	DA	3546	1/1	0.73	0.85	-	11,11,11,11	1
59	MG	AT	201	1/1	0.92	0.23	-	76,76,76,76	1
59	MG	BA	3495	1/1	0.90	0.20	-	69,69,69,69	0
59	MG	AA	1625	1/1	0.77	0.48	-	73,73,73,73	1
59	MG	AA	1655	1/1	0.98	0.05	-	101,101,101,101	0
59	MG	BA	2960	1/1	0.98	0.58	-	84,84,84,84	0
59	MG	DA	3650	1/1	0.84	0.36	-	106,106,106,106	0
59	MG	BA	3180	1/1	0.89	0.29	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3651	1/1	0.87	0.34	-	93,93,93,93	0
59	MG	DA	3707	1/1	0.95	0.38	-	55,55,55,55	1
59	MG	BA	2907	1/1	0.63	0.32	-	108,108,108,108	0
59	MG	DA	3188	1/1	0.96	0.31	-	31,31,31,31	0
59	MG	DA	3747	1/1	0.68	0.54	-	38,38,38,38	1
59	MG	DA	3694	1/1	0.96	0.25	-	107,107,107,107	0
59	MG	DA	3479	1/1	0.88	0.59	-	127,127,127,127	0
59	MG	BA	3157	1/1	0.80	0.56	-	60,60,60,60	0
59	MG	CV	111	1/1	0.95	0.13	-	71,71,71,71	0
59	MG	AA	1952	1/1	0.92	0.88	-	97,97,97,97	0
59	MG	DA	3710	1/1	0.76	0.61	-	92,92,92,92	0
59	MG	DA	3328	1/1	0.95	0.28	-	34,34,34,34	0
59	MG	AA	1678	1/1	0.81	0.37	-	76,76,76,76	0
59	MG	DA	3777	1/1	0.76	0.27	-	70,70,70,70	0
59	MG	CA	1606	1/1	0.94	0.10	-	60,60,60,60	0
59	MG	CA	1782	1/1	0.97	0.24	-	52,52,52,52	0
59	MG	BA	3378	1/1	0.80	0.40	-	79,79,79,79	0
59	MG	AA	1723	1/1	0.83	0.16	-	91,91,91,91	0
59	MG	BA	3364	1/1	0.89	0.91	-	66,66,66,66	1
59	MG	DA	3016	1/1	0.92	0.28	-	51,51,51,51	0
59	MG	AA	1766	1/1	0.67	0.71	-	74,74,74,74	0
59	MG	CA	1730	1/1	0.66	0.18	-	106,106,106,106	0
59	MG	BA	3258	1/1	0.87	0.52	-	69,69,69,69	0
59	MG	AA	1606	1/1	0.94	0.24	-	77,77,77,77	0
59	MG	BA	3129	1/1	0.94	0.41	-	42,42,42,42	0
59	MG	CA	1738	1/1	0.81	0.18	-	80,80,80,80	0
59	MG	DA	3636	1/1	0.91	0.15	-	50,50,50,50	0
59	MG	BA	3375	1/1	0.76	1.10	-	74,74,74,74	0
59	MG	DA	3108	1/1	0.91	0.24	-	81,81,81,81	0
59	MG	DA	2972	1/1	0.42	1.11	-	97,97,97,97	0
59	MG	BA	2981	1/1	0.92	0.20	-	80,80,80,80	0
59	MG	BA	3104	1/1	0.79	0.51	-	78,78,78,78	0
59	MG	BA	3548	1/1	0.70	0.36	-	92,92,92,92	0
59	MG	AA	1831	1/1	0.89	0.84	-	89,89,89,89	0
59	MG	DA	3034	1/1	0.88	0.45	-	98,98,98,98	0
59	MG	DA	3368	1/1	0.80	0.52	-	104,104,104,104	0
59	MG	DA	3721	1/1	0.92	0.19	-	171,171,171,171	0
59	MG	CA	1677	1/1	0.80	0.97	-	88,88,88,88	1
59	MG	CA	1708	1/1	0.90	0.20	-	64,64,64,64	1
59	MG	BA	3357	1/1	0.56	0.28	-	78,78,78,78	1
59	MG	BA	3501	1/1	0.76	0.25	-	112,112,112,112	0
59	MG	CA	1610	1/1	0.74	2.00	-	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1642	1/1	0.53	0.16	-	108,108,108,108	0
59	MG	BA	3467	1/1	0.98	0.15	-	93,93,93,93	0
59	MG	CA	1691	1/1	0.42	0.08	-	103,103,103,103	0
59	MG	DA	3565	1/1	0.95	0.16	-	54,54,54,54	0
59	MG	DA	3357	1/1	0.76	0.33	-	64,64,64,64	0
59	MG	DA	2965	1/1	0.94	0.65	-	52,52,52,52	0
59	MG	BA	3279	1/1	0.93	0.35	-	59,59,59,59	0
59	MG	DA	3537	1/1	0.79	0.49	-	56,56,56,56	0
59	MG	BA	3571	1/1	0.74	0.45	-	77,77,77,77	0
59	MG	BA	3341	1/1	0.94	0.41	-	33,33,33,33	0
59	MG	CA	1705	1/1	0.85	0.45	-	62,62,62,62	0
59	MG	BA	3149	1/1	0.86	0.32	-	86,86,86,86	0
59	MG	AA	1710	1/1	0.54	0.23	-	77,77,77,77	0
59	MG	BA	3526	1/1	0.83	1.19	-	76,76,76,76	0
59	MG	AA	1865	1/1	0.80	0.37	-	96,96,96,96	0
59	MG	AA	1839	1/1	0.83	0.36	-	74,74,74,74	0
59	MG	BA	2936	1/1	0.96	0.30	-	43,43,43,43	0
59	MG	AD	303	1/1	0.68	0.47	-	134,134,134,134	0
59	MG	DA	3675	1/1	0.96	0.42	-	39,39,39,39	0
59	MG	BA	3348	1/1	0.88	0.26	-	61,61,61,61	0
59	MG	DA	3330	1/1	0.81	0.34	-	1,1,1,1	1
59	MG	DA	3238	1/1	0.66	0.28	-	134,134,134,134	0
59	MG	AA	1819	1/1	0.88	0.08	-	75,75,75,75	0
59	MG	AA	1717	1/1	0.86	0.32	-	120,120,120,120	0
59	MG	BA	3291	1/1	0.96	0.54	-	41,41,41,41	0
59	MG	BA	3483	1/1	0.88	0.53	-	60,60,60,60	0
59	MG	DA	3061	1/1	0.97	0.30	-	67,67,67,67	0
59	MG	AA	1807	1/1	0.88	0.42	-	61,61,61,61	0
59	MG	DA	2998	1/1	0.97	0.28	-	49,49,49,49	0
59	MG	BA	3054	1/1	0.93	0.27	-	100,100,100,100	0
59	MG	DA	2989	1/1	0.59	0.26	-	83,83,83,83	0
59	MG	BA	3361	1/1	0.76	1.62	-	105,105,105,105	0
59	MG	DA	3617	1/1	0.67	0.42	-	111,111,111,111	0
59	MG	DA	3040	1/1	0.82	0.58	-	81,81,81,81	0
59	MG	AA	1866	1/1	0.74	0.34	-	74,74,74,74	0
59	MG	AA	1733	1/1	0.90	0.14	-	71,71,71,71	0
59	MG	BA	3585	1/1	0.52	1.84	-	143,143,143,143	0
59	MG	BA	3046	1/1	0.88	0.12	-	90,90,90,90	0
59	MG	DA	3640	1/1	0.59	0.46	-	81,81,81,81	1
59	MG	BA	2924	1/1	0.94	0.52	-	73,73,73,73	0
59	MG	AA	1644	1/1	0.79	0.32	-	84,84,84,84	0
59	MG	DA	3734	1/1	0.95	0.17	-	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
59	MG	DA	3758	1/1	0.80	0.89	-	95,95,95,95	0
59	MG	AA	1923	1/1	0.89	0.43	-	55,55,55,55	0
59	MG	BA	3089	1/1	0.93	0.33	-	33,33,33,33	0
59	MG	DA	3682	1/1	0.87	0.18	-	103,103,103,103	0
59	MG	DA	3221	1/1	0.90	0.73	-	77,77,77,77	0
59	MG	DA	3089	1/1	0.94	0.19	-	81,81,81,81	0
59	MG	BA	3124	1/1	0.86	0.45	-	62,62,62,62	0
59	MG	CA	1737	1/1	0.78	0.12	-	120,120,120,120	0
59	MG	BA	3029	1/1	0.83	0.31	-	92,92,92,92	0
59	MG	BA	3112	1/1	0.67	0.41	-	101,101,101,101	0
59	MG	BA	3285	1/1	0.88	0.18	-	96,96,96,96	0
59	MG	BA	3519	1/1	0.93	0.82	-	88,88,88,88	0
59	MG	DA	3109	1/1	0.71	0.44	-	90,90,90,90	0
59	MG	BA	3367	1/1	0.69	1.57	-	96,96,96,96	0
59	MG	BA	3036	1/1	0.87	0.34	-	98,98,98,98	0
59	MG	AY	103	1/1	0.68	0.63	-	108,108,108,108	0
59	MG	DA	3483	1/1	0.96	0.57	-	55,55,55,55	0
59	MG	AA	1667	1/1	0.70	0.25	-	49,49,49,49	0
59	MG	DA	3628	1/1	0.77	1.26	-	93,93,93,93	0
59	MG	AA	1947	1/1	0.84	0.66	-	79,79,79,79	0
59	MG	BA	3534	1/1	0.88	0.56	-	56,56,56,56	0
59	MG	BA	3193	1/1	0.62	0.71	-	109,109,109,109	0
59	MG	BA	3599	1/1	0.97	0.07	-	83,83,83,83	0
59	MG	BA	3111	1/1	0.45	0.53	-	79,79,79,79	0
59	MG	BA	3296	1/1	0.99	0.55	-	27,27,27,27	0
59	MG	DA	3732	1/1	0.74	0.30	-	67,67,67,67	0
59	MG	AA	1796	1/1	0.94	0.14	-	61,61,61,61	0
59	MG	DA	2936	1/1	0.69	0.67	-	81,81,81,81	0
59	MG	BA	2958	1/1	0.87	0.28	-	46,46,46,46	0
59	MG	CA	1751	1/1	0.78	0.26	-	69,69,69,69	1
59	MG	BA	3322	1/1	0.99	0.68	-	24,24,24,24	0
59	MG	DA	3404	1/1	0.68	0.43	-	87,87,87,87	0
59	MG	AA	1828	1/1	0.56	0.25	-	86,86,86,86	0
59	MG	DA	3077	1/1	0.96	0.77	-	68,68,68,68	0
59	MG	AA	1813	1/1	0.88	0.40	-	134,134,134,134	0
59	MG	BA	2943	1/1	0.84	0.17	-	92,92,92,92	1
59	MG	AA	1834	1/1	0.89	0.35	-	94,94,94,94	0
59	MG	AA	1794	1/1	0.78	0.48	-	106,106,106,106	0
59	MG	DA	3304	1/1	0.87	0.48	-	84,84,84,84	0
59	MG	DN	201	1/1	0.78	0.23	-	19,19,19,19	1
59	MG	BA	2990	1/1	0.87	0.21	-	77,77,77,77	0
59	MG	DA	3551	1/1	0.95	0.55	-	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
59	MG	BA	3272	1/1	0.67	1.25	-	126,126,126,126	0
59	MG	AA	1750	1/1	0.94	0.20	-	54,54,54,54	1
59	MG	BA	3437	1/1	0.89	0.31	-	60,60,60,60	0
59	MG	CA	1764	1/1	0.82	0.19	-	82,82,82,82	0
59	MG	DA	3239	1/1	0.84	0.14	-	96,96,96,96	0
59	MG	BR	201	1/1	0.71	0.46	-	47,47,47,47	1
59	MG	CA	1711	1/1	0.82	0.11	-	65,65,65,65	1
59	MG	BA	3551	1/1	0.84	0.95	-	82,82,82,82	0
59	MG	DA	3780	1/1	0.68	0.46	-	77,77,77,77	0
59	MG	DA	3620	1/1	0.91	0.13	-	70,70,70,70	0
59	MG	DA	3594	1/1	0.85	0.23	-	63,63,63,63	1
59	MG	AA	1683	1/1	0.83	0.57	-	47,47,47,47	1
59	MG	DA	3760	1/1	0.97	0.32	-	52,52,52,52	0
59	MG	DA	3525	1/1	0.71	0.99	-	63,63,63,63	0
59	MG	DA	3286	1/1	0.82	0.42	-	112,112,112,112	0
59	MG	AA	1716	1/1	0.90	0.23	-	82,82,82,82	0
59	MG	DA	3521	1/1	0.87	0.22	-	99,99,99,99	0
59	MG	DA	3558	1/1	0.95	0.42	-	88,88,88,88	0
59	MG	AA	1631	1/1	0.82	1.13	-	85,85,85,85	0
59	MG	AA	1624	1/1	0.76	0.73	-	98,98,98,98	0
59	MG	DA	2977	1/1	0.97	0.41	-	60,60,60,60	0
59	MG	BO	201	1/1	0.83	0.25	-	88,88,88,88	0
59	MG	DA	3499	1/1	0.90	0.35	-	90,90,90,90	0
59	MG	BA	3236	1/1	0.94	0.88	-	86,86,86,86	0
59	MG	AA	1746	1/1	0.93	0.31	-	66,66,66,66	0
59	MG	DA	3586	1/1	0.94	0.54	-	34,34,34,34	0
59	MG	BA	2901	1/1	0.68	1.43	-	113,113,113,113	0
59	MG	DA	3194	1/1	0.94	0.23	-	92,92,92,92	0
59	MG	BA	2968	1/1	0.93	0.59	-	72,72,72,72	0
59	MG	DF	301	1/1	0.89	0.35	-	17,17,17,17	1
59	MG	BA	3418	1/1	0.96	1.27	-	69,69,69,69	0
59	MG	BA	3121	1/1	0.66	1.00	-	125,125,125,125	0
59	MG	BA	3350	1/1	0.69	0.98	-	118,118,118,118	0
59	MG	DA	3399	1/1	0.96	0.22	-	62,62,62,62	0
59	MG	DA	3596	1/1	0.95	0.42	-	54,54,54,54	1
59	MG	BA	2996	1/1	0.89	0.28	-	68,68,68,68	0
59	MG	DA	3520	1/1	0.92	0.41	-	103,103,103,103	0
59	MG	BA	2928	1/1	0.85	0.80	-	116,116,116,116	0
59	MG	DA	3371	1/1	0.89	0.14	-	59,59,59,59	1
59	MG	BA	3485	1/1	0.88	0.64	-	103,103,103,103	0
59	MG	DA	3205	1/1	0.84	0.47	-	130,130,130,130	0
59	MG	AV	106	1/1	0.69	0.24	-	87,87,87,87	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3439	1/1	0.56	0.28	-	54,54,54,54	1
59	MG	DA	3293	1/1	0.82	0.70	-	70,70,70,70	0
59	MG	BA	3128	1/1	0.90	0.53	-	92,92,92,92	0
59	MG	AA	1884	1/1	0.95	0.08	-	89,89,89,89	0
59	MG	DA	3783	1/1	0.88	1.06	-	90,90,90,90	0
59	MG	DA	3325	1/1	0.94	0.33	-	109,109,109,109	0
59	MG	BA	3315	1/1	0.93	0.67	-	74,74,74,74	0
59	MG	AA	1763	1/1	0.96	0.24	-	88,88,88,88	0
59	MG	BA	3116	1/1	0.73	0.53	-	81,81,81,81	0
59	MG	CA	1697	1/1	0.48	0.58	-	83,83,83,83	0
59	MG	CA	1602	1/1	0.93	0.15	-	76,76,76,76	0
59	MG	CA	1722	1/1	0.68	0.32	-	73,73,73,73	0
59	MG	AA	1734	1/1	0.81	0.21	-	9,9,9,9	1
59	MG	CA	1627	1/1	0.76	0.17	-	71,71,71,71	0
59	MG	AA	1800	1/1	0.80	0.95	-	114,114,114,114	0
59	MG	DA	3542	1/1	0.94	0.18	-	74,74,74,74	0
59	MG	DA	3391	1/1	0.62	0.44	-	73,73,73,73	0
59	MG	DA	3744	1/1	0.92	0.27	-	93,93,93,93	1
59	MG	BA	3228	1/1	0.89	0.62	-	99,99,99,99	0
59	MG	DA	3052	1/1	0.95	0.30	-	68,68,68,68	0
59	MG	AA	1684	1/1	0.95	0.19	-	87,87,87,87	0
59	MG	CA	1614	1/1	0.85	0.42	-	72,72,72,72	0
59	MG	BA	3071	1/1	0.71	0.72	-	110,110,110,110	0
59	MG	BA	3332	1/1	0.99	0.46	-	19,19,19,19	0
59	MG	DA	3078	1/1	0.82	0.65	-	73,73,73,73	0
59	MG	DA	3648	1/1	0.87	0.63	-	100,100,100,100	0
59	MG	AA	1713	1/1	0.85	0.12	-	70,70,70,70	0
59	MG	DA	2975	1/1	0.98	0.32	-	56,56,56,56	0
59	MG	AA	1702	1/1	0.71	0.28	-	64,64,64,64	0
59	MG	AI	202	1/1	0.92	0.17	-	117,117,117,117	0
59	MG	DA	3058	1/1	0.96	0.28	-	32,32,32,32	0
59	MG	BA	3523	1/1	0.84	1.10	-	122,122,122,122	0
59	MG	DA	3776	1/1	0.88	0.45	-	58,58,58,58	0
59	MG	DA	3731	1/1	0.93	0.26	-	45,45,45,45	1
59	MG	DA	3054	1/1	0.93	0.08	-	69,69,69,69	0
59	MG	BA	2902	1/1	0.88	0.32	-	79,79,79,79	0
59	MG	BA	3109	1/1	0.92	0.31	-	35,35,35,35	0
59	MG	BA	3431	1/1	0.92	0.58	-	79,79,79,79	0
59	MG	BA	3267	1/1	0.87	1.17	-	94,94,94,94	0
59	MG	DA	3465	1/1	0.96	0.43	-	26,26,26,26	0
59	MG	BA	3417	1/1	0.63	0.48	-	68,68,68,68	0
59	MG	BA	3458	1/1	0.54	1.16	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
59	MG	AA	1687	1/1	0.93	0.11	-	101,101,101,101	0
59	MG	CA	1661	1/1	0.90	0.19	-	65,65,65,65	0
59	MG	CA	1712	1/1	0.49	0.52	-	88,88,88,88	1
59	MG	CA	1648	1/1	0.93	0.80	-	90,90,90,90	0
59	MG	DA	3485	1/1	0.48	1.83	-	8,8,8,8	1
59	MG	BA	3240	1/1	0.91	0.60	-	55,55,55,55	0
59	MG	BA	3487	1/1	0.72	0.29	-	64,64,64,64	0
59	MG	CA	1621	1/1	0.84	0.38	-	89,89,89,89	0
59	MG	BA	3083	1/1	0.82	0.27	-	80,80,80,80	0
59	MG	DA	3714	1/1	0.81	1.07	-	109,109,109,109	0
59	MG	AA	1605	1/1	0.48	0.33	-	152,152,152,152	0
59	MG	DA	3627	1/1	0.86	0.31	-	70,70,70,70	0
59	MG	DA	3568	1/1	0.90	0.64	-	73,73,73,73	0
59	MG	AA	1698	1/1	0.20	0.64	-	103,103,103,103	0
59	MG	BA	3160	1/1	0.98	0.33	-	49,49,49,49	0
59	MG	DA	2928	1/1	0.63	0.33	-	61,61,61,61	1
59	MG	AA	1775	1/1	0.76	0.26	-	92,92,92,92	0
59	MG	CA	1632	1/1	0.86	0.47	-	94,94,94,94	0
59	MG	DA	2970	1/1	0.93	0.36	-	41,41,41,41	1
59	MG	DA	3227	1/1	0.80	0.44	-	73,73,73,73	0
59	MG	AA	1770	1/1	0.78	0.38	-	76,76,76,76	0
59	MG	BA	3536	1/1	0.75	0.84	-	73,73,73,73	0
59	MG	AA	1767	1/1	0.93	0.35	-	77,77,77,77	0
59	MG	DA	3389	1/1	0.67	1.20	-	145,145,145,145	0
59	MG	DA	3311	1/1	0.92	0.92	-	96,96,96,96	0
59	MG	BA	3016	1/1	0.70	0.36	-	66,66,66,66	0
59	MG	BA	2915	1/1	0.88	0.37	-	70,70,70,70	0
59	MG	DA	3098	1/1	0.84	0.87	-	86,86,86,86	0
59	MG	DA	3575	1/1	0.81	0.72	-	89,89,89,89	0
59	MG	CA	1769	1/1	0.93	0.23	-	68,68,68,68	0
59	MG	D9	101	1/1	0.77	0.34	-	92,92,92,92	1
59	MG	BA	3073	1/1	0.94	0.49	-	52,52,52,52	0
59	MG	AA	1700	1/1	0.82	0.62	-	90,90,90,90	0
59	MG	DA	3544	1/1	0.77	0.14	-	62,62,62,62	0
59	MG	DA	2931	1/1	0.24	0.73	-	151,151,151,151	1
59	MG	DA	3774	1/1	0.93	0.64	-	84,84,84,84	0
59	MG	CA	1640	1/1	0.63	0.41	-	76,76,76,76	0
59	MG	AA	1614	1/1	0.49	0.33	-	113,113,113,113	0
59	MG	BA	3475	1/1	0.94	0.19	-	59,59,59,59	0
59	MG	DA	3762	1/1	0.93	0.13	-	99,99,99,99	0
59	MG	DA	3181	1/1	0.85	0.36	-	49,49,49,49	0
59	MG	DA	3204	1/1	0.92	0.22	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1904	1/1	0.77	0.44	-	81,81,81,81	0
59	MG	AA	1918	1/1	0.89	0.29	-	64,64,64,64	0
59	MG	DA	2902	1/1	0.90	0.41	-	42,42,42,42	0
59	MG	DA	3772	1/1	0.94	0.17	-	69,69,69,69	0
59	MG	BA	3006	1/1	0.52	0.95	-	68,68,68,68	0
59	MG	DA	3142	1/1	0.62	0.29	-	90,90,90,90	0
59	MG	AA	1958	1/1	0.88	0.12	-	106,106,106,106	0
59	MG	AA	1783	1/1	0.95	0.55	-	73,73,73,73	0
59	MG	DA	3750	1/1	0.82	0.85	-	84,84,84,84	0
59	MG	BA	3369	1/1	0.96	0.25	-	65,65,65,65	0
59	MG	CV	101	1/1	0.75	0.31	-	93,93,93,93	1
59	MG	DA	3556	1/1	0.74	0.56	-	97,97,97,97	0
59	MG	DA	3726	1/1	0.95	0.22	-	65,65,65,65	0
59	MG	CA	1748	1/1	0.97	0.08	-	102,102,102,102	0
59	MG	B5	103	1/1	0.97	0.33	-	36,36,36,36	0
59	MG	BA	3563	1/1	0.80	0.49	-	80,80,80,80	0
59	MG	DA	3480	1/1	0.86	0.27	-	87,87,87,87	0
59	MG	DA	2981	1/1	0.88	0.37	-	127,127,127,127	0
59	MG	AA	1696	1/1	0.96	0.21	-	90,90,90,90	0
59	MG	DA	3049	1/1	0.89	1.46	-	96,96,96,96	0
59	MG	B1	101	1/1	0.95	0.14	-	50,50,50,50	1
59	MG	BA	3401	1/1	0.90	0.09	-	75,75,75,75	0
59	MG	AA	1601	1/1	0.89	0.17	-	74,74,74,74	0
59	MG	BA	3567	1/1	0.74	0.29	-	76,76,76,76	0
59	MG	DA	3362	1/1	0.97	0.42	-	39,39,39,39	0
59	MG	AA	1666	1/1	0.52	2.56	-	127,127,127,127	0
59	MG	DA	3530	1/1	0.93	0.29	-	122,122,122,122	0
59	MG	CA	1641	1/1	0.51	0.34	-	84,84,84,84	0
59	MG	BA	3304	1/1	0.73	1.24	-	90,90,90,90	0
59	MG	DA	3481	1/1	0.84	0.52	-	73,73,73,73	0
59	MG	AA	1943	1/1	0.52	1.38	-	60,60,60,60	1
59	MG	BA	3084	1/1	0.45	0.29	-	88,88,88,88	0
59	MG	AV	105	1/1	0.89	0.15	-	80,80,80,80	0
59	MG	DA	3213	1/1	0.89	0.65	-	67,67,67,67	0
59	MG	AA	1772	1/1	0.72	0.50	-	85,85,85,85	0
59	MG	BA	3360	1/1	0.93	0.39	-	80,80,80,80	0
59	MG	DA	3796	1/1	0.89	0.28	-	95,95,95,95	1
59	MG	DY	201	1/1	-0.34	3.38	-	168,168,168,168	0
59	MG	CA	1637	1/1	0.78	0.14	-	114,114,114,114	0
59	MG	B5	101	1/1	0.70	0.57	-	83,83,83,83	0
59	MG	DA	3403	1/1	0.76	0.23	-	109,109,109,109	0
59	MG	CA	1747	1/1	0.62	0.17	-	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
59	MG	DA	3209	1/1	0.93	0.49	-	50,50,50,50	0
59	MG	B0	101	1/1	0.96	0.89	-	73,73,73,73	0
59	MG	DA	3195	1/1	0.63	0.55	-	96,96,96,96	0
59	MG	AA	1727	1/1	0.93	0.13	-	84,84,84,84	1
59	MG	DA	3021	1/1	0.49	1.34	-	87,87,87,87	0
59	MG	DA	3622	1/1	0.94	0.06	-	58,58,58,58	0
59	MG	AA	1801	1/1	0.89	0.22	-	130,130,130,130	0
59	MG	BA	3195	1/1	0.89	0.35	-	85,85,85,85	0
59	MG	BA	3470	1/1	0.98	0.42	-	35,35,35,35	0
59	MG	BA	2966	1/1	0.93	0.55	-	64,64,64,64	0
59	MG	BA	2933	1/1	0.96	0.25	-	36,36,36,36	0
59	MG	BA	3113	1/1	0.66	0.13	-	95,95,95,95	0
59	MG	DA	3581	1/1	0.84	0.26	-	88,88,88,88	1
59	MG	DA	3585	1/1	0.88	0.35	-	78,78,78,78	0
59	MG	DA	3414	1/1	0.67	0.88	-	121,121,121,121	0
59	MG	BA	3409	1/1	0.89	0.55	-	104,104,104,104	0
59	MG	BA	3013	1/1	0.84	0.44	-	60,60,60,60	0
59	MG	DA	3020	1/1	0.96	0.28	-	52,52,52,52	0
59	MG	DA	3127	1/1	0.38	0.32	-	93,93,93,93	0
59	MG	CA	1654	1/1	0.77	0.57	-	77,77,77,77	0
59	MG	DA	3629	1/1	0.81	0.32	-	45,45,45,45	0
59	MG	AA	1636	1/1	0.97	0.22	-	53,53,53,53	0
59	MG	D8	101	1/1	0.86	0.19	-	74,74,74,74	0
59	MG	DA	3684	1/1	0.90	0.29	-	82,82,82,82	0
59	MG	CA	1667	1/1	0.98	0.07	-	66,66,66,66	0
59	MG	DA	3668	1/1	0.92	0.29	-	93,93,93,93	0
59	MG	BA	2912	1/1	0.93	0.48	-	57,57,57,57	0
59	MG	DA	2941	1/1	0.95	0.08	-	27,27,27,27	1
59	MG	DA	3340	1/1	0.79	0.28	-	96,96,96,96	0
59	MG	DA	2994	1/1	0.97	0.63	-	60,60,60,60	0
59	MG	AA	1789	1/1	0.51	0.33	-	108,108,108,108	0
59	MG	BA	2944	1/1	0.94	0.29	-	43,43,43,43	0
59	MG	CV	112	1/1	0.79	0.20	-	69,69,69,69	0
59	MG	DA	3506	1/1	0.81	1.06	-	73,73,73,73	1
59	MG	AA	1679	1/1	0.89	0.32	-	53,53,53,53	1
59	MG	BA	2995	1/1	0.94	0.35	-	84,84,84,84	0
59	MG	DA	3757	1/1	0.89	0.65	-	86,86,86,86	0
59	MG	CA	1729	1/1	0.95	0.24	-	88,88,88,88	0
59	MG	DA	2982	1/1	0.85	0.33	-	97,97,97,97	0
59	MG	AA	1916	1/1	0.93	0.09	-	70,70,70,70	0
59	MG	DA	3027	1/1	0.76	0.44	-	69,69,69,69	0
59	MG	DA	3514	1/1	0.80	0.40	-	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
59	MG	BA	3280	1/1	0.98	0.43	-	38,38,38,38	0
59	MG	CA	1671	1/1	0.60	0.43	-	99,99,99,99	0
59	MG	DA	3633	1/1	0.93	0.65	-	75,75,75,75	0
59	MG	CA	1628	1/1	0.76	0.19	-	88,88,88,88	0
59	MG	DA	2923	1/1	0.88	0.16	-	94,94,94,94	0
59	MG	DA	3690	1/1	0.88	0.30	-	62,62,62,62	0
59	MG	DA	3067	1/1	0.88	0.29	-	106,106,106,106	0
59	MG	BA	3163	1/1	0.98	0.42	-	35,35,35,35	0
59	MG	DA	3562	1/1	0.98	0.13	-	25,25,25,25	1
59	MG	AA	1782	1/1	0.86	0.36	-	103,103,103,103	0
59	MG	CA	1754	1/1	0.37	0.31	-	78,78,78,78	1
59	MG	DA	3374	1/1	0.70	0.36	-	91,91,91,91	0
59	MG	CA	1740	1/1	0.95	0.88	-	85,85,85,85	0
59	MG	BA	3524	1/1	0.83	0.42	-	103,103,103,103	0
59	MG	BA	3270	1/1	0.84	0.27	-	60,60,60,60	0
59	MG	BA	3281	1/1	0.78	0.47	-	94,94,94,94	0
59	MG	DA	3001	1/1	0.87	0.07	-	79,79,79,79	0
59	MG	BA	3045	1/1	0.85	0.16	-	75,75,75,75	0
59	MG	DA	3752	1/1	0.90	0.38	-	96,96,96,96	0
59	MG	BA	3374	1/1	0.73	0.73	-	74,74,74,74	0
59	MG	BB	206	1/1	0.74	0.63	-	90,90,90,90	1
59	MG	CA	1759	1/1	0.91	0.78	-	98,98,98,98	0
59	MG	BA	3459	1/1	0.96	0.33	-	44,44,44,44	0
59	MG	BA	3299	1/1	0.95	0.40	-	66,66,66,66	0
59	MG	BA	3442	1/1	0.98	0.25	-	65,65,65,65	0
59	MG	DA	3113	1/1	0.67	1.30	-	109,109,109,109	0
59	MG	AA	1810	1/1	0.89	0.24	-	71,71,71,71	0
59	MG	DA	3048	1/1	0.84	0.71	-	63,63,63,63	0
59	MG	BH	202	1/1	0.83	0.13	-	95,95,95,95	0
59	MG	AA	1876	1/1	0.91	0.27	-	92,92,92,92	1
59	MG	BA	3173	1/1	0.78	0.30	-	102,102,102,102	1
59	MG	DA	3440	1/1	0.96	0.16	-	50,50,50,50	1
59	MG	AA	1761	1/1	0.90	1.23	-	83,83,83,83	0
59	MG	DA	3419	1/1	0.73	0.89	-	122,122,122,122	0
59	MG	DB	204	1/1	0.33	0.20	-	110,110,110,110	0
59	MG	DA	3719	1/1	0.95	0.45	-	73,73,73,73	0
59	MG	CA	1685	1/1	0.78	0.37	-	92,92,92,92	0
59	MG	DA	3745	1/1	0.90	0.51	-	56,56,56,56	0
59	MG	CV	108	1/1	0.89	0.25	-	101,101,101,101	0
59	MG	DA	3754	1/1	0.89	0.79	-	34,34,34,34	1
59	MG	BA	3420	1/1	0.99	0.35	-	71,71,71,71	0
59	MG	DA	3143	1/1	0.42	0.71	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3057	1/1	0.97	0.44	-	68,68,68,68	0
59	MG	DA	3100	1/1	0.90	0.55	-	67,67,67,67	0
59	MG	DA	3011	1/1	0.92	0.27	-	40,40,40,40	0
59	MG	AA	1875	1/1	0.89	0.23	-	62,62,62,62	0
59	MG	CA	1647	1/1	0.74	0.42	-	77,77,77,77	0
59	MG	BA	3263	1/1	0.88	0.99	-	76,76,76,76	0
59	MG	DA	3413	1/1	0.89	1.26	-	84,84,84,84	0
59	MG	DA	3515	1/1	0.64	1.29	-	108,108,108,108	0
59	MG	BA	3216	1/1	0.84	0.38	-	73,73,73,73	0
59	MG	BA	3400	1/1	0.72	0.10	-	87,87,87,87	0
59	MG	AA	1798	1/1	0.67	0.40	-	114,114,114,114	0
59	MG	BA	3608	1/1	0.98	0.42	-	31,31,31,31	0
59	MG	DA	2993	1/1	0.81	0.79	-	96,96,96,96	0
59	MG	DW	201	1/1	0.94	0.30	-	36,36,36,36	1
59	MG	BA	3203	1/1	0.92	0.40	-	75,75,75,75	0
59	MG	AA	1672	1/1	0.97	0.16	-	77,77,77,77	0
59	MG	DA	3723	1/1	0.93	0.48	-	101,101,101,101	0
59	MG	BA	3100	1/1	0.95	0.23	-	47,47,47,47	0
59	MG	AA	1953	1/1	0.62	0.49	-	120,120,120,120	0
59	MG	BA	3336	1/1	0.66	0.24	-	99,99,99,99	0
59	MG	CA	1659	1/1	0.69	1.53	-	100,100,100,100	0
59	MG	DA	3107	1/1	0.78	0.61	-	103,103,103,103	0
59	MG	BA	3102	1/1	0.76	0.67	-	64,64,64,64	0
59	MG	BA	3198	1/1	0.88	0.35	-	102,102,102,102	0
59	MG	BA	3041	1/1	0.96	0.42	-	37,37,37,37	0
59	MG	BA	3217	1/1	0.71	0.17	-	72,72,72,72	0
59	MG	AA	1788	1/1	0.74	0.33	-	80,80,80,80	0
59	MG	DA	2956	1/1	0.95	0.26	-	38,38,38,38	0
59	MG	BA	3324	1/1	0.80	0.41	-	63,63,63,63	0
59	MG	DA	3073	1/1	0.93	0.42	-	64,64,64,64	0
59	MG	DA	2955	1/1	0.86	0.33	-	34,34,34,34	1
59	MG	DA	3447	1/1	0.94	0.77	-	70,70,70,70	0
59	MG	BA	2903	1/1	0.96	0.42	-	37,37,37,37	0
59	MG	DA	3125	1/1	0.86	0.46	-	118,118,118,118	0
59	MG	DA	3716	1/1	0.91	0.50	-	103,103,103,103	0
59	MG	AA	1966	1/1	0.83	0.27	-	99,99,99,99	0
59	MG	DA	3574	1/1	0.82	0.68	-	70,70,70,70	1
59	MG	CJ	202	1/1	0.74	0.09	-	130,130,130,130	0
59	MG	AA	1921	1/1	0.94	0.47	-	86,86,86,86	0
59	MG	DA	3606	1/1	0.97	0.11	-	88,88,88,88	1
59	MG	DA	3689	1/1	0.66	0.15	-	123,123,123,123	0
59	MG	DA	2969	1/1	0.85	1.03	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3678	1/1	0.86	0.47	-	100,100,100,100	0
59	MG	BA	3190	1/1	0.28	1.46	-	117,117,117,117	0
59	MG	DA	3569	1/1	0.92	0.61	-	102,102,102,102	0
59	MG	DA	3400	1/1	0.54	0.64	-	63,63,63,63	1
59	MG	CA	1624	1/1	0.88	0.35	-	86,86,86,86	0
59	MG	DA	3791	1/1	0.83	0.62	-	76,76,76,76	0
59	MG	D6	101	1/1	0.72	0.60	-	95,95,95,95	0
59	MG	BA	2935	1/1	0.77	0.43	-	102,102,102,102	0
59	MG	DA	3006	1/1	0.90	0.38	-	107,107,107,107	0
59	MG	AX	101	1/1	0.82	0.44	-	113,113,113,113	0
59	MG	DA	2973	1/1	0.99	0.41	-	21,21,21,21	0
59	MG	DA	2976	1/1	0.56	0.65	-	1,1,1,1	1
59	MG	BA	2913	1/1	0.96	0.72	-	51,51,51,51	0
59	MG	DA	3654	1/1	0.86	0.36	-	78,78,78,78	0
59	MG	CV	103	1/1	0.90	0.16	-	67,67,67,67	0
59	MG	AA	1935	1/1	0.65	0.25	-	96,96,96,96	0
59	MG	DA	3047	1/1	0.86	0.75	-	88,88,88,88	0
59	MG	AA	1677	1/1	0.89	0.28	-	76,76,76,76	1
59	MG	AA	1823	1/1	0.97	0.29	-	68,68,68,68	0
59	MG	DA	3309	1/1	0.92	0.59	-	76,76,76,76	0
59	MG	DA	3004	1/1	0.68	0.91	-	122,122,122,122	0
59	MG	AA	1797	1/1	0.86	0.27	-	76,76,76,76	0
59	MG	DA	3587	1/1	0.82	0.75	-	74,74,74,74	0
59	MG	DA	3246	1/1	0.99	0.30	-	32,32,32,32	0
59	MG	DA	3161	1/1	0.80	0.64	-	61,61,61,61	0
59	MG	DA	3738	1/1	0.94	0.21	-	89,89,89,89	0
59	MG	DA	3094	1/1	0.63	0.53	-	87,87,87,87	0
59	MG	BA	2991	1/1	0.71	0.98	-	60,60,60,60	1
59	MG	DA	3493	1/1	0.79	0.39	-	90,90,90,90	0
59	MG	BA	3011	1/1	0.85	0.92	-	107,107,107,107	0
59	MG	BA	3145	1/1	0.86	0.35	-	89,89,89,89	0
59	MG	BA	3508	1/1	0.94	0.51	-	39,39,39,39	0
59	MG	DA	3769	1/1	0.45	0.17	-	142,142,142,142	0
59	MG	AA	1919	1/1	0.83	0.16	-	78,78,78,78	0
59	MG	BA	2932	1/1	0.96	0.49	-	63,63,63,63	0
59	MG	AA	1818	1/1	0.71	0.13	-	60,60,60,60	0
59	MG	BA	3429	1/1	0.89	1.00	-	67,67,67,67	0
59	MG	DA	3742	1/1	0.98	0.58	-	51,51,51,51	0
59	MG	DA	3673	1/1	0.78	0.81	-	116,116,116,116	0
59	MG	BA	3606	1/1	0.94	0.55	-	65,65,65,65	0
59	MG	AA	1646	1/1	0.81	0.61	-	106,106,106,106	0
59	MG	BA	3034	1/1	0.85	0.23	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3107	1/1	0.86	0.63	-	87,87,87,87	0
59	MG	DA	3433	1/1	0.89	0.66	-	1,1,1,1	1
59	MG	BA	3572	1/1	0.88	0.90	-	68,68,68,68	0
59	MG	CA	1660	1/1	0.88	0.35	-	99,99,99,99	0
59	MG	BA	3282	1/1	0.89	0.38	-	47,47,47,47	0
59	MG	DD	305	1/1	0.71	0.28	-	1,1,1,1	1
59	MG	CC	301	1/1	0.75	0.86	-	117,117,117,117	0
59	MG	AA	1663	1/1	0.82	0.50	-	95,95,95,95	0
59	MG	D0	103	1/1	0.93	0.35	-	74,74,74,74	0
59	MG	AA	1869	1/1	0.78	0.59	-	75,75,75,75	0
59	MG	AA	1675	1/1	0.79	0.35	-	52,52,52,52	1
59	MG	BA	3343	1/1	0.99	0.50	-	32,32,32,32	0
59	MG	BA	3007	1/1	0.89	0.34	-	93,93,93,93	0
59	MG	DA	3018	1/1	0.99	0.13	-	76,76,76,76	0
59	MG	DA	3380	1/1	0.89	0.31	-	43,43,43,43	0
59	MG	BA	3321	1/1	0.90	0.34	-	58,58,58,58	0
59	MG	BA	2948	1/1	0.86	0.21	-	64,64,64,64	0
59	MG	DA	3552	1/1	0.64	0.42	-	120,120,120,120	0
59	MG	BA	3001	1/1	0.89	0.28	-	117,117,117,117	0
59	MG	BA	3607	1/1	0.96	0.71	-	95,95,95,95	0
59	MG	CA	1625	1/1	0.86	0.16	-	62,62,62,62	0
59	MG	BA	3042	1/1	0.75	0.35	-	103,103,103,103	0
59	MG	BA	3502	1/1	0.83	1.81	-	132,132,132,132	0
59	MG	DA	2954	1/1	0.91	0.51	-	47,47,47,47	1
59	MG	CA	1776	1/1	0.68	0.83	-	83,83,83,83	0
59	MG	BA	3497	1/1	0.81	1.27	-	85,85,85,85	0
59	MG	DA	3162	1/1	0.94	0.36	-	122,122,122,122	0
59	MG	CA	1736	1/1	0.98	0.14	-	60,60,60,60	0
59	MG	DA	2995	1/1	0.95	0.13	-	44,44,44,44	0
59	MG	DA	3496	1/1	0.75	0.26	-	83,83,83,83	0
59	MG	CA	1755	1/1	0.73	0.29	-	100,100,100,100	0
59	MG	DA	3254	1/1	0.96	0.08	-	59,59,59,59	0
59	MG	DA	3347	1/1	0.94	0.21	-	71,71,71,71	0
59	MG	BA	3152	1/1	0.99	0.33	-	34,34,34,34	0
59	MG	AA	1827	1/1	0.84	0.20	-	85,85,85,85	0
59	MG	DA	3655	1/1	0.93	0.78	-	91,91,91,91	0
59	MG	AA	1883	1/1	0.58	0.85	-	58,58,58,58	0
59	MG	DA	2992	1/1	0.96	0.77	-	103,103,103,103	0
59	MG	AA	1804	1/1	0.93	0.47	-	90,90,90,90	0
59	MG	BA	3156	1/1	0.98	0.34	-	27,27,27,27	0
59	MG	AA	1833	1/1	0.86	0.28	-	87,87,87,87	0
59	MG	AA	1832	1/1	0.89	0.51	-	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3024	1/1	0.98	0.35	-	79,79,79,79	0
59	MG	AA	1777	1/1	0.77	0.38	-	115,115,115,115	0
59	MG	BA	2918	1/1	0.97	0.56	-	76,76,76,76	1
59	MG	BA	3530	1/1	0.99	0.22	-	33,33,33,33	0
59	MG	DA	3377	1/1	0.97	0.26	-	16,16,16,16	0
59	MG	AA	1837	1/1	0.82	0.26	-	75,75,75,75	0
59	MG	DA	3430	1/1	0.95	0.23	-	25,25,25,25	0
59	MG	AA	1787	1/1	0.79	0.20	-	109,109,109,109	0
59	MG	DA	3097	1/1	0.95	0.32	-	69,69,69,69	0
59	MG	CV	104	1/1	0.76	0.18	-	86,86,86,86	0
59	MG	AA	1856	1/1	0.83	0.47	-	80,80,80,80	0
59	MG	DA	2951	1/1	0.78	0.46	-	102,102,102,102	0
59	MG	AA	1885	1/1	0.93	0.37	-	57,57,57,57	0
59	MG	DA	3338	1/1	0.79	0.21	-	68,68,68,68	0
59	MG	DA	2983	1/1	0.69	0.57	-	79,79,79,79	1
59	MG	BA	3110	1/1	0.88	0.23	-	55,55,55,55	0
59	MG	AX	104	1/1	0.94	0.45	-	43,43,43,43	0
59	MG	DA	3659	1/1	0.88	0.45	-	88,88,88,88	0
59	MG	BA	3597	1/1	0.85	0.72	-	53,53,53,53	1
59	MG	AA	1892	1/1	0.94	0.19	-	75,75,75,75	0
59	MG	BA	3479	1/1	0.79	0.52	-	133,133,133,133	0
59	MG	DA	3206	1/1	0.89	0.32	-	66,66,66,66	0
59	MG	BA	3391	1/1	0.76	1.34	-	91,91,91,91	1
59	MG	DA	3256	1/1	0.95	0.58	-	42,42,42,42	0
59	MG	BA	3148	1/1	0.90	0.76	-	106,106,106,106	0
59	MG	DA	3081	1/1	0.84	0.26	-	75,75,75,75	0
59	MG	BA	3561	1/1	0.92	1.31	-	122,122,122,122	0
59	MG	DA	3639	1/1	0.95	0.32	-	37,37,37,37	0
59	MG	CA	1715	1/1	0.81	0.16	-	80,80,80,80	0
59	MG	AA	1971	1/1	0.80	0.66	-	125,125,125,125	0
59	MG	CA	1644	1/1	0.81	0.36	-	92,92,92,92	0
59	MG	CA	1620	1/1	0.96	0.70	-	87,87,87,87	0
59	MG	BA	3140	1/1	0.48	0.76	-	113,113,113,113	0
59	MG	CV	106	1/1	0.74	0.38	-	101,101,101,101	0
59	MG	BA	3605	1/1	0.95	0.83	-	79,79,79,79	0
59	MG	AA	1809	1/1	0.88	1.31	-	92,92,92,92	0
59	MG	DA	3711	1/1	0.78	0.36	-	55,55,55,55	1
59	MG	BA	2909	1/1	0.94	0.20	-	50,50,50,50	0
59	MG	AA	1740	1/1	0.86	0.39	-	94,94,94,94	0
59	MG	CA	1753	1/1	0.91	0.09	-	103,103,103,103	0
59	MG	DA	3779	1/1	0.73	0.75	-	122,122,122,122	0
59	MG	BA	3533	1/1	0.95	0.44	-	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
59	MG	BA	3026	1/1	0.93	0.43	-	105,105,105,105	0
59	MG	BA	3539	1/1	0.82	0.30	-	97,97,97,97	1
59	MG	DA	3563	1/1	0.57	0.52	-	68,68,68,68	1
59	MG	BA	3587	1/1	0.74	0.54	-	47,47,47,47	0
59	MG	CA	1784	1/1	0.95	0.65	-	76,76,76,76	0
59	MG	DA	3539	1/1	0.64	0.58	-	70,70,70,70	0
59	MG	BA	2999	1/1	0.69	0.12	-	86,86,86,86	0
59	MG	DO	201	1/1	0.72	0.18	-	117,117,117,117	0
59	MG	CA	1778	1/1	0.93	0.35	-	88,88,88,88	0
59	MG	AA	1711	1/1	0.69	0.25	-	90,90,90,90	0
59	MG	AA	1936	1/1	0.85	0.20	-	135,135,135,135	0
59	MG	BA	3208	1/1	0.89	0.37	-	27,27,27,27	0
59	MG	BA	3595	1/1	0.86	0.63	-	65,65,65,65	0
59	MG	AA	1758	1/1	0.71	0.43	-	98,98,98,98	0
59	MG	DA	3270	1/1	0.83	0.17	-	55,55,55,55	0
59	MG	AA	1656	1/1	0.87	0.30	-	98,98,98,98	1
59	MG	DA	3720	1/1	0.97	0.14	-	66,66,66,66	0
59	MG	AA	1774	1/1	0.88	0.52	-	120,120,120,120	0
59	MG	DA	3066	1/1	0.82	0.18	-	113,113,113,113	0
59	MG	BA	3537	1/1	0.91	0.30	-	28,28,28,28	0
59	MG	BA	3389	1/1	0.96	0.45	-	56,56,56,56	0
59	MG	AA	1707	1/1	0.91	0.26	-	97,97,97,97	0
59	MG	DA	3466	1/1	0.90	0.56	-	40,40,40,40	0
59	MG	BH	203	1/1	0.86	0.46	-	75,75,75,75	0
59	MG	BA	3560	1/1	0.63	0.99	-	83,83,83,83	0
59	MG	DA	3088	1/1	0.97	0.10	-	65,65,65,65	0
59	MG	BA	3174	1/1	0.90	0.25	-	83,83,83,83	0
59	MG	DA	3706	1/1	0.84	0.74	-	66,66,66,66	0
59	MG	AA	1731	1/1	0.86	0.34	-	81,81,81,81	0
59	MG	DA	3044	1/1	0.92	0.23	-	78,78,78,78	0
59	MG	DA	3307	1/1	0.77	0.32	-	77,77,77,77	0
59	MG	BA	3358	1/1	0.83	0.11	-	100,100,100,100	0
59	MG	BA	3494	1/1	0.96	0.57	-	77,77,77,77	0
59	MG	DA	3267	1/1	0.88	0.36	-	62,62,62,62	0
59	MG	DA	3614	1/1	0.89	0.26	-	100,100,100,100	0
59	MG	CC	302	1/1	0.95	0.68	-	114,114,114,114	0
59	MG	DB	211	1/1	0.74	0.34	-	80,80,80,80	0
59	MG	BA	3477	1/1	0.84	1.31	-	128,128,128,128	0
59	MG	AA	1941	1/1	0.90	0.56	-	63,63,63,63	0
59	MG	DA	3549	1/1	0.54	0.55	-	97,97,97,97	0
59	MG	BA	3277	1/1	0.95	0.48	-	44,44,44,44	0
59	MG	DA	3578	1/1	0.81	0.65	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AV	101	1/1	0.92	0.74	-	52,52,52,52	1
59	MG	AA	1649	1/1	0.97	0.17	-	63,63,63,63	0
59	MG	DA	2948	1/1	0.98	0.34	-	75,75,75,75	0
59	MG	BA	3147	1/1	0.94	0.50	-	72,72,72,72	0
59	MG	CA	1780	1/1	0.83	0.68	-	47,47,47,47	1
59	MG	CA	1710	1/1	0.95	0.21	-	51,51,51,51	0
59	MG	DA	2968	1/1	0.97	0.13	-	1,1,1,1	1
59	MG	AA	1877	1/1	0.96	0.40	-	61,61,61,61	0
59	MG	DA	2957	1/1	0.92	0.41	-	47,47,47,47	0
59	MG	BA	3317	1/1	0.68	0.88	-	64,64,64,64	1
59	MG	CA	1643	1/1	0.83	0.12	-	80,80,80,80	0
59	MG	DA	3091	1/1	0.85	0.39	-	119,119,119,119	0
59	MG	DA	3571	1/1	0.61	0.58	-	96,96,96,96	0
59	MG	DA	3456	1/1	0.97	0.73	-	56,56,56,56	0
59	MG	DA	3183	1/1	0.93	0.28	-	94,94,94,94	0
59	MG	DA	3646	1/1	0.97	0.81	-	57,57,57,57	0
59	MG	DA	3420	1/1	0.78	0.63	-	100,100,100,100	0
59	MG	BA	3078	1/1	0.99	0.20	-	18,18,18,18	0
59	MG	BA	3575	1/1	0.87	0.36	-	92,92,92,92	0
59	MG	DA	3461	1/1	0.94	0.54	-	77,77,77,77	0
59	MG	DA	3316	1/1	0.69	0.45	-	59,59,59,59	1
59	MG	AA	1851	1/1	0.66	0.48	-	62,62,62,62	0
59	MG	AA	1712	1/1	0.85	0.77	-	188,188,188,188	0
59	MG	DA	3105	1/1	0.80	0.89	-	92,92,92,92	0
59	MG	BA	3406	1/1	0.96	0.47	-	52,52,52,52	0
59	MG	DA	3208	1/1	0.76	0.43	-	91,91,91,91	0
59	MG	BA	3566	1/1	0.67	0.39	-	66,66,66,66	1
59	MG	AA	1633	1/1	0.88	1.30	-	72,72,72,72	1
59	MG	AA	1954	1/1	0.97	1.03	-	67,67,67,67	0
59	MG	AA	1961	1/1	0.94	0.24	-	87,87,87,87	0
59	MG	DB	209	1/1	0.73	0.24	-	95,95,95,95	0
59	MG	DA	3708	1/1	0.88	1.27	-	100,100,100,100	0
59	MG	DA	3438	1/1	0.85	0.23	-	76,76,76,76	0
59	MG	DA	3014	1/1	0.78	0.47	-	108,108,108,108	0
59	MG	BP	201	1/1	0.87	0.31	-	24,24,24,24	0
59	MG	CA	1771	1/1	0.81	0.82	-	96,96,96,96	0
59	MG	DA	3513	1/1	0.94	0.13	-	95,95,95,95	0
59	MG	DA	3337	1/1	0.74	0.25	-	90,90,90,90	0
59	MG	CA	1658	1/1	0.62	0.52	-	97,97,97,97	0
59	MG	DA	2921	1/1	0.81	1.66	-	114,114,114,114	0
59	MG	BA	3050	1/1	0.89	0.12	-	73,73,73,73	0
59	MG	AA	1706	1/1	0.97	0.06	-	44,44,44,44	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1689	1/1	0.72	0.16	-	82,82,82,82	1
59	MG	AV	103	1/1	0.87	0.12	-	72,72,72,72	0
59	MG	DA	3431	1/1	0.95	0.33	-	38,38,38,38	0
59	MG	DA	3312	1/1	0.90	0.29	-	48,48,48,48	0
59	MG	AA	1843	1/1	0.89	0.71	-	99,99,99,99	0
59	MG	CA	1699	1/1	0.92	0.21	-	64,64,64,64	0
59	MG	AC	301	1/1	0.91	0.14	-	173,173,173,173	0
59	MG	AA	1894	1/1	0.86	0.21	-	90,90,90,90	0
59	MG	BA	3072	1/1	0.92	0.33	-	101,101,101,101	0
59	MG	DA	3273	1/1	0.90	0.58	-	54,54,54,54	0
59	MG	DA	3764	1/1	0.94	0.24	-	75,75,75,75	0
59	MG	BA	3146	1/1	0.79	1.09	-	113,113,113,113	0
59	MG	BA	3547	1/1	0.79	0.26	-	78,78,78,78	0
59	MG	BA	3318	1/1	0.96	0.48	-	63,63,63,63	0
59	MG	AA	1610	1/1	0.83	0.49	-	77,77,77,77	0
59	MG	DA	3415	1/1	0.90	0.53	-	41,41,41,41	0
59	MG	BA	3238	1/1	0.98	0.52	-	110,110,110,110	0
59	MG	BA	2910	1/1	0.92	0.23	-	83,83,83,83	1
59	MG	AA	1674	1/1	0.85	0.26	-	48,48,48,48	0
59	MG	AA	1849	1/1	0.84	0.20	-	80,80,80,80	0
59	MG	DA	3527	1/1	0.95	0.06	-	46,46,46,46	0
59	MG	DA	3484	1/1	0.92	0.86	-	58,58,58,58	0
59	MG	BA	3254	1/1	0.98	0.28	-	93,93,93,93	0
59	MG	CA	1735	1/1	0.45	0.63	-	127,127,127,127	0
59	MG	BA	3005	1/1	0.84	1.23	-	105,105,105,105	0
59	MG	DA	3423	1/1	0.73	0.45	-	51,51,51,51	1
59	MG	AA	1931	1/1	0.88	0.25	-	87,87,87,87	0
59	MG	CA	1707	1/1	0.97	0.10	-	79,79,79,79	0
59	MG	DA	3036	1/1	0.87	0.47	-	76,76,76,76	0
59	MG	DA	3531	1/1	0.94	0.32	-	82,82,82,82	0
59	MG	DA	3613	1/1	0.97	0.13	-	56,56,56,56	1
59	MG	BA	3407	1/1	0.92	0.30	-	64,64,64,64	0
59	MG	AA	1755	1/1	0.88	0.25	-	34,34,34,34	1
59	MG	DA	3351	1/1	0.97	0.17	-	77,77,77,77	0
59	MG	BA	3308	1/1	0.88	0.27	-	53,53,53,53	1
59	MG	DA	3046	1/1	0.83	0.36	-	95,95,95,95	0
59	MG	DA	3023	1/1	0.82	0.38	-	41,41,41,41	0
59	MG	AA	1738	1/1	0.75	0.83	-	59,59,59,59	0
59	MG	BA	3466	1/1	0.95	0.26	-	38,38,38,38	0
59	MG	AA	1764	1/1	0.80	1.02	-	65,65,65,65	0
59	MG	BA	3455	1/1	0.93	0.79	-	65,65,65,65	0
59	MG	CA	1669	1/1	0.97	0.15	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1725	1/1	0.65	0.50	-	70,70,70,70	1
59	MG	CA	1701	1/1	0.85	0.27	-	83,83,83,83	0
59	MG	BA	3363	1/1	0.81	0.50	-	92,92,92,92	0
59	MG	AA	1962	1/1	0.74	0.79	-	65,65,65,65	0
59	MG	BA	3394	1/1	0.88	0.32	-	85,85,85,85	0
59	MG	AA	1688	1/1	0.98	0.07	-	22,22,22,22	1
59	MG	DB	203	1/1	0.84	0.17	-	30,30,30,30	1
59	MG	AA	1658	1/1	0.99	0.17	-	106,106,106,106	0
59	MG	CA	1608	1/1	0.67	0.72	-	124,124,124,124	0
59	MG	DA	3538	1/1	0.67	0.59	-	118,118,118,118	0
59	MG	BA	3306	1/1	0.92	0.25	-	57,57,57,57	0
59	MG	BA	3511	1/1	0.90	0.33	-	73,73,73,73	0
59	MG	BA	3288	1/1	0.97	0.45	-	38,38,38,38	0
59	MG	BA	3294	1/1	0.97	0.30	-	73,73,73,73	0
59	MG	DA	3643	1/1	0.68	0.35	-	113,113,113,113	0
59	MG	BA	3059	1/1	0.91	0.23	-	98,98,98,98	0
59	MG	AQ	201	1/1	0.90	0.09	-	97,97,97,97	1
59	MG	DA	3051	1/1	0.96	0.34	-	36,36,36,36	0
59	MG	AA	1860	1/1	0.96	0.38	-	61,61,61,61	0
59	MG	BA	3601	1/1	0.69	0.41	-	79,79,79,79	0
59	MG	D3	101	1/1	0.80	1.94	-	1,1,1,1	1
59	MG	DA	3474	1/1	0.82	2.41	-	99,99,99,99	0
59	MG	D7	101	1/1	0.92	0.55	-	89,89,89,89	0
59	MG	DA	3111	1/1	0.62	0.34	-	83,83,83,83	0
59	MG	BA	3353	1/1	0.84	0.65	-	107,107,107,107	0
59	MG	DA	3092	1/1	0.83	0.68	-	106,106,106,106	0
59	MG	DA	3730	1/1	0.78	0.50	-	91,91,91,91	0
59	MG	DA	3632	1/1	0.86	0.49	-	56,56,56,56	0
59	MG	BA	3284	1/1	0.64	0.55	-	97,97,97,97	0
59	MG	DA	3285	1/1	0.96	0.31	-	37,37,37,37	0
59	MG	DA	3766	1/1	0.93	0.79	-	100,100,100,100	0
59	MG	BA	3528	1/1	0.79	0.46	-	73,73,73,73	0
59	MG	BA	2967	1/1	0.65	0.28	-	95,95,95,95	0
59	MG	DA	3360	1/1	0.89	0.22	-	99,99,99,99	0
59	MG	DA	3332	1/1	0.97	0.31	-	26,26,26,26	0
59	MG	CA	1757	1/1	0.93	0.14	-	83,83,83,83	0
59	MG	DA	3573	1/1	0.84	0.35	-	86,86,86,86	0
59	MG	DA	2937	1/1	0.85	0.33	-	63,63,63,63	1
59	MG	BA	3127	1/1	0.81	0.41	-	71,71,71,71	0
59	MG	AA	1665	1/1	0.83	0.67	-	60,60,60,60	0
59	MG	DA	3656	1/1	0.98	0.17	-	75,75,75,75	0
59	MG	BA	3328	1/1	0.85	0.66	-	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
59	MG	AA	1806	1/1	0.82	0.17	-	81,81,81,81	0
59	MG	CA	1773	1/1	0.68	0.42	-	106,106,106,106	0
59	MG	DA	3359	1/1	0.87	0.33	-	64,64,64,64	0
59	MG	BA	3117	1/1	0.92	0.77	-	98,98,98,98	0
59	MG	DA	3595	1/1	0.83	0.79	-	75,75,75,75	0
59	MG	BB	201	1/1	0.94	0.38	-	46,46,46,46	0
59	MG	CA	1709	1/1	0.69	0.15	-	85,85,85,85	1
59	MG	BA	3600	1/1	0.74	0.54	-	63,63,63,63	0
59	MG	DA	3455	1/1	0.90	0.47	-	71,71,71,71	0
59	MG	AA	1963	1/1	0.89	0.76	-	74,74,74,74	0
59	MG	BA	3212	1/1	0.89	0.57	-	52,52,52,52	0
59	MG	AA	1889	1/1	0.68	0.42	-	115,115,115,115	0
59	MG	DA	3797	1/1	0.88	0.36	-	56,56,56,56	0
59	MG	CA	1716	1/1	0.78	0.53	-	110,110,110,110	0
59	MG	DA	3123	1/1	0.67	1.02	-	91,91,91,91	0
59	MG	DA	3160	1/1	0.95	0.32	-	68,68,68,68	0
59	MG	BA	3550	1/1	0.94	0.42	-	103,103,103,103	0
59	MG	AA	1949	1/1	0.85	0.48	-	42,42,42,42	1
59	MG	DA	3369	1/1	0.72	0.26	-	95,95,95,95	0
59	MG	DA	3326	1/1	0.73	0.54	-	63,63,63,63	0
59	MG	DA	3114	1/1	0.96	0.52	-	55,55,55,55	0
59	MG	DA	3584	1/1	0.63	0.64	-	80,80,80,80	0
59	MG	DA	3299	1/1	0.87	0.47	-	75,75,75,75	0
59	MG	DA	3559	1/1	0.74	0.32	-	74,74,74,74	0
59	MG	AA	1602	1/1	0.85	0.18	-	71,71,71,71	0
59	MG	DA	3661	1/1	0.56	0.35	-	100,100,100,100	0
59	MG	DA	3790	1/1	0.95	1.41	-	29,29,29,29	1
59	MG	BR	204	1/1	0.97	0.21	-	26,26,26,26	0
59	MG	DA	2999	1/1	0.98	0.05	-	91,91,91,91	0
59	MG	BA	3461	1/1	0.95	0.51	-	41,41,41,41	0
59	MG	DA	3132	1/1	0.88	0.59	-	49,49,49,49	0
59	MG	BA	3579	1/1	0.91	0.71	-	71,71,71,71	0
59	MG	CA	1618	1/1	0.87	0.31	-	79,79,79,79	0
59	MG	DA	3442	1/1	0.88	0.45	-	71,71,71,71	0
59	MG	BA	3480	1/1	0.80	0.35	-	55,55,55,55	0
59	MG	DA	3422	1/1	0.96	0.74	-	63,63,63,63	0
59	MG	CA	1664	1/1	0.81	0.24	-	91,91,91,91	0
59	MG	AA	1867	1/1	0.81	0.36	-	65,65,65,65	0
59	MG	DA	2961	1/1	0.76	0.52	-	126,126,126,126	0
59	MG	CA	1670	1/1	0.82	0.28	-	66,66,66,66	0
59	MG	BA	3415	1/1	0.85	0.43	-	69,69,69,69	1
59	MG	BA	2951	1/1	0.48	1.42	-	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3056	1/1	0.83	0.71	-	65,65,65,65	0
59	MG	CA	1656	1/1	0.89	0.50	-	73,73,73,73	0
59	MG	DA	3634	1/1	0.70	0.34	-	83,83,83,83	0
59	MG	AV	107	1/1	0.91	0.25	-	58,58,58,58	0
59	MG	D5	101	1/1	0.98	0.30	-	48,48,48,48	0
59	MG	DA	3220	1/1	0.79	0.91	-	117,117,117,117	0
59	MG	AA	1722	1/1	0.67	0.76	-	116,116,116,116	0
59	MG	CV	107	1/1	0.76	0.29	-	115,115,115,115	0
59	MG	DA	3130	1/1	0.82	1.23	-	108,108,108,108	0
59	MG	BA	3080	1/1	0.87	0.60	-	83,83,83,83	0
59	MG	CA	1613	1/1	0.86	0.37	-	73,73,73,73	0
59	MG	DA	3554	1/1	0.92	0.08	-	95,95,95,95	0
59	MG	BA	3087	1/1	0.68	0.44	-	87,87,87,87	0
59	MG	D1	102	1/1	0.91	0.27	-	80,80,80,80	0
59	MG	AO	101	1/1	0.64	0.39	-	111,111,111,111	0
59	MG	DA	2949	1/1	0.85	0.33	-	98,98,98,98	1
59	MG	BA	3562	1/1	0.89	0.52	-	71,71,71,71	0
59	MG	AA	1799	1/1	0.93	0.13	-	80,80,80,80	0
59	MG	BA	3349	1/1	0.93	0.33	-	68,68,68,68	0
59	MG	BA	3219	1/1	0.93	0.43	-	57,57,57,57	0
59	MG	DA	3564	1/1	0.97	0.32	-	42,42,42,42	0
59	MG	AA	1946	1/1	0.92	0.40	-	77,77,77,77	0
59	MG	BA	3564	1/1	0.86	0.67	-	113,113,113,113	0
59	MG	DA	3074	1/1	0.49	0.55	-	129,129,129,129	0
59	MG	BA	3432	1/1	0.86	0.45	-	59,59,59,59	0
59	MG	BA	3062	1/1	0.97	0.21	-	61,61,61,61	0
59	MG	BA	3570	1/1	0.67	0.54	-	115,115,115,115	0
59	MG	DA	3566	1/1	0.62	0.15	-	106,106,106,106	0
59	MG	D7	104	1/1	0.82	0.22	-	82,82,82,82	1
59	MG	DA	3547	1/1	0.80	0.72	-	89,89,89,89	0
59	MG	DA	2944	1/1	0.33	2.47	-	109,109,109,109	1
59	MG	AA	1942	1/1	0.84	0.22	-	98,98,98,98	0
59	MG	DA	3582	1/1	0.72	0.58	-	47,47,47,47	1
59	MG	BA	3532	1/1	0.70	1.45	-	88,88,88,88	0
59	MG	BA	2964	1/1	0.97	0.17	-	96,96,96,96	0
59	MG	DA	3756	1/1	0.80	0.44	-	106,106,106,106	0
59	MG	BA	3133	1/1	0.85	0.21	-	57,57,57,57	0
59	MG	AA	1619	1/1	0.62	0.50	-	111,111,111,111	0
59	MG	AA	1709	1/1	0.92	0.27	-	85,85,85,85	1
59	MG	BA	2976	1/1	0.82	0.13	-	97,97,97,97	0
59	MG	AA	1728	1/1	0.70	0.30	-	78,78,78,78	0
59	MG	AA	1830	1/1	0.96	0.36	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1972	1/1	0.47	1.62	-	98,98,98,98	1
59	MG	DA	3663	1/1	0.98	0.60	-	55,55,55,55	0
59	MG	AA	1874	1/1	0.42	0.26	-	111,111,111,111	0
59	MG	AA	1634	1/1	0.92	0.47	-	70,70,70,70	1
59	MG	BA	3085	1/1	0.79	0.45	-	68,68,68,68	0
59	MG	DA	3642	1/1	0.81	0.56	-	88,88,88,88	0
59	MG	BA	3194	1/1	0.86	0.12	-	67,67,67,67	0
59	MG	DA	2910	1/1	0.84	0.80	-	68,68,68,68	0
59	MG	AA	1840	1/1	0.92	0.34	-	76,76,76,76	0
59	MG	DA	3189	1/1	0.90	0.26	-	80,80,80,80	0
59	MG	BA	2986	1/1	0.74	0.36	-	52,52,52,52	0
59	MG	DA	3516	1/1	0.91	0.85	-	97,97,97,97	0
59	MG	BA	3359	1/1	0.59	0.82	-	101,101,101,101	0
59	MG	DA	3736	1/1	0.71	0.18	-	77,77,77,77	1
59	MG	DA	3792	1/1	0.84	0.44	-	77,77,77,77	0
59	MG	BA	3393	1/1	0.88	0.20	-	104,104,104,104	0
59	MG	CA	1609	1/1	0.71	1.04	-	93,93,93,93	0
59	MG	BA	2983	1/1	0.84	0.19	-	63,63,63,63	0
59	MG	BA	3103	1/1	0.95	0.30	-	69,69,69,69	0
59	MG	AA	1792	1/1	0.71	0.17	-	102,102,102,102	0
59	MG	DA	3441	1/1	0.97	0.64	-	55,55,55,55	0
59	MG	BA	3474	1/1	0.92	0.56	-	53,53,53,53	0
59	MG	BA	3061	1/1	0.92	0.32	-	63,63,63,63	0
59	MG	AA	1951	1/1	0.92	0.33	-	82,82,82,82	0
59	MG	CA	1657	1/1	0.58	0.52	-	85,85,85,85	0
59	MG	BA	3440	1/1	0.89	0.42	-	72,72,72,72	0
59	MG	BA	3159	1/1	0.94	0.45	-	72,72,72,72	0
59	MG	DA	3055	1/1	0.96	0.49	-	51,51,51,51	0
59	MG	BA	3234	1/1	0.59	0.59	-	90,90,90,90	0
59	MG	AL	201	1/1	0.98	0.11	-	87,87,87,87	0
59	MG	AA	1871	1/1	0.94	0.22	-	144,144,144,144	0
59	MG	BA	3175	1/1	0.97	0.35	-	25,25,25,25	0
59	MG	DA	3748	1/1	0.85	0.67	-	125,125,125,125	0
59	MG	AA	1886	1/1	0.96	0.64	-	84,84,84,84	0
59	MG	DA	3528	1/1	0.90	0.28	-	80,80,80,80	0
59	MG	CA	1651	1/1	0.90	0.17	-	84,84,84,84	0
59	MG	CA	1663	1/1	0.72	0.20	-	97,97,97,97	0
59	MG	AA	1928	1/1	0.93	0.34	-	42,42,42,42	0
59	MG	BA	3376	1/1	0.89	0.24	-	68,68,68,68	1
59	MG	DA	3348	1/1	0.96	0.58	-	43,43,43,43	0
59	MG	AA	1735	1/1	0.68	0.77	-	85,85,85,85	0
59	MG	BA	3226	1/1	0.95	0.48	-	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
59	MG	DA	3216	1/1	0.98	0.36	-	36,36,36,36	0
59	MG	DA	3043	1/1	0.81	0.37	-	80,80,80,80	0
59	MG	DA	3434	1/1	0.95	0.55	-	44,44,44,44	0
59	MG	DA	3168	1/1	0.71	1.16	-	100,100,100,100	0
59	MG	DA	3154	1/1	0.84	0.34	-	58,58,58,58	0
59	MG	AA	1940	1/1	0.87	0.25	-	86,86,86,86	0
59	MG	AA	1608	1/1	0.87	0.41	-	58,58,58,58	0
59	MG	AL	202	1/1	0.59	0.12	-	73,73,73,73	0
59	MG	DA	3110	1/1	0.98	0.72	-	200,200,200,200	0
59	MG	AA	1670	1/1	0.93	0.21	-	28,28,28,28	1
59	MG	DA	3260	1/1	0.89	0.69	-	33,33,33,33	0
59	MG	DA	3784	1/1	0.91	0.34	-	123,123,123,123	0
59	MG	DA	3615	1/1	0.86	0.79	-	86,86,86,86	0
59	MG	DA	3504	1/1	0.97	0.27	-	60,60,60,60	0
59	MG	BA	3143	1/1	0.98	0.37	-	149,149,149,149	0
59	MG	DA	3190	1/1	0.85	0.35	-	97,97,97,97	0
59	MG	BA	3486	1/1	0.67	0.26	-	54,54,54,54	0
59	MG	D1	101	1/1	0.72	0.23	-	75,75,75,75	0
59	MG	BA	3515	1/1	0.94	0.15	-	47,47,47,47	1
59	MG	BA	3385	1/1	0.80	0.35	-	63,63,63,63	1
59	MG	BA	3505	1/1	0.71	0.47	-	95,95,95,95	0
59	MG	BA	2987	1/1	0.74	0.24	-	104,104,104,104	0
59	MG	BA	3141	1/1	0.79	0.60	-	104,104,104,104	0
59	MG	CA	1665	1/1	0.92	0.13	-	79,79,79,79	0
59	MG	BA	3454	1/1	0.98	0.56	-	64,64,64,64	0
59	MG	BA	3447	1/1	0.97	0.10	-	90,90,90,90	0
59	MG	BA	3297	1/1	0.94	0.22	-	34,34,34,34	0
59	MG	DA	3147	1/1	0.85	0.17	-	90,90,90,90	0
59	MG	DA	3096	1/1	0.68	0.44	-	80,80,80,80	0
59	MG	CA	1717	1/1	0.95	0.14	-	78,78,78,78	0
59	MG	DA	3317	1/1	0.94	0.50	-	62,62,62,62	0
59	MG	AA	1836	1/1	0.94	0.34	-	114,114,114,114	0
59	MG	DA	2987	1/1	0.90	0.28	-	68,68,68,68	0
59	MG	CA	1766	1/1	0.65	0.30	-	118,118,118,118	0
59	MG	BA	3082	1/1	0.68	0.29	-	90,90,90,90	0
59	MG	DA	3666	1/1	0.58	1.13	-	66,66,66,66	0
59	MG	DA	3593	1/1	0.81	0.32	-	61,61,61,61	0
59	MG	BA	2921	1/1	0.88	0.12	-	51,51,51,51	0
59	MG	DB	210	1/1	0.90	0.36	-	56,56,56,56	0
59	MG	DA	3718	1/1	0.71	0.77	-	92,92,92,92	0
59	MG	DA	3395	1/1	0.89	0.41	-	83,83,83,83	0
59	MG	AA	1959	1/1	0.69	0.83	-	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	2919	1/1	0.92	0.44	-	44,44,44,44	1
59	MG	DA	3421	1/1	0.78	0.18	-	71,71,71,71	0
59	MG	DA	3601	1/1	0.90	0.25	-	39,39,39,39	0
59	MG	BA	3396	1/1	0.94	0.66	-	86,86,86,86	0
59	MG	DA	3775	1/1	0.94	0.66	-	86,86,86,86	0
59	MG	BA	3433	1/1	0.95	0.22	-	61,61,61,61	0
59	MG	BA	3573	1/1	0.90	0.70	-	75,75,75,75	0
59	MG	DA	3148	1/1	0.84	1.15	-	120,120,120,120	0
59	MG	DB	202	1/1	0.80	0.46	-	55,55,55,55	0
59	MG	BA	3105	1/1	0.83	1.08	-	79,79,79,79	0
59	MG	BA	3387	1/1	0.69	0.42	-	87,87,87,87	0
59	MG	AA	1637	1/1	0.95	0.15	-	78,78,78,78	1
59	MG	DA	3083	1/1	0.81	0.45	-	104,104,104,104	0
59	MG	DA	3501	1/1	0.90	0.49	-	59,59,59,59	0
59	MG	DA	3002	1/1	0.91	0.07	-	78,78,78,78	0
59	MG	DA	2912	1/1	0.95	0.30	-	68,68,68,68	0
59	MG	BA	3345	1/1	0.94	0.59	-	37,37,37,37	0
59	MG	AA	1780	1/1	0.82	0.44	-	154,154,154,154	0
59	MG	AA	1784	1/1	0.89	0.30	-	92,92,92,92	0
59	MG	BA	3179	1/1	0.85	0.26	-	66,66,66,66	0
59	MG	BA	2963	1/1	0.85	1.12	-	113,113,113,113	0
59	MG	BR	202	1/1	0.96	0.18	-	24,24,24,24	0
59	MG	DA	3378	1/1	0.90	0.45	-	96,96,96,96	0
59	MG	AA	1924	1/1	0.96	1.03	-	84,84,84,84	0
59	MG	DA	3476	1/1	0.77	0.41	-	120,120,120,120	0
59	MG	BA	3516	1/1	0.97	0.80	-	64,64,64,64	0
59	MG	BA	3023	1/1	0.92	0.28	-	64,64,64,64	0
59	MG	AA	1779	1/1	0.84	0.22	-	114,114,114,114	0
59	MG	DA	3296	1/1	0.82	0.28	-	46,46,46,46	1
59	MG	AA	1639	1/1	0.88	1.32	-	79,79,79,79	0
59	MG	DA	3323	1/1	0.94	0.75	-	58,58,58,58	0
59	MG	CA	1760	1/1	0.83	0.24	-	52,52,52,52	1
59	MG	BA	3434	1/1	0.96	0.38	-	68,68,68,68	0
59	MG	AA	1659	1/1	0.86	0.20	-	107,107,107,107	0
59	MG	AA	1618	1/1	0.81	0.54	-	78,78,78,78	0
59	MG	AA	1657	1/1	0.98	0.14	-	77,77,77,77	0
59	MG	DA	3165	1/1	0.76	0.51	-	121,121,121,121	0
59	MG	BA	3540	1/1	0.87	0.86	-	66,66,66,66	1
59	MG	DA	3781	1/1	0.37	0.77	-	143,143,143,143	0
59	MG	DA	3315	1/1	0.94	0.46	-	77,77,77,77	0
59	MG	CA	1721	1/1	0.81	0.71	-	111,111,111,111	0
59	MG	BA	3565	1/1	0.85	0.38	-	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
59	MG	AX	103	1/1	0.61	0.62	-	112,112,112,112	0
59	MG	BA	2923	1/1	0.64	1.07	-	96,96,96,96	0
59	MG	CA	1696	1/1	0.80	1.10	-	79,79,79,79	0
59	MG	DA	3407	1/1	0.83	0.52	-	77,77,77,77	1
59	MG	DA	3253	1/1	0.67	0.45	-	52,52,52,52	0
59	MG	DA	3786	1/1	0.60	0.38	-	144,144,144,144	0
59	MG	AA	1668	1/1	0.89	0.66	-	78,78,78,78	0
59	MG	DA	3336	1/1	0.96	0.56	-	31,31,31,31	0
59	MG	BA	2914	1/1	0.67	1.75	-	106,106,106,106	0
59	MG	BA	3481	1/1	0.95	0.44	-	59,59,59,59	0
59	MG	BA	3220	1/1	0.96	0.64	-	54,54,54,54	0
59	MG	CA	1783	1/1	0.96	0.10	-	83,83,83,83	0
59	MG	DA	3618	1/1	0.96	0.66	-	72,72,72,72	0
59	MG	CA	1774	1/1	0.86	1.64	-	111,111,111,111	1
59	MG	DA	3291	1/1	0.87	0.37	-	88,88,88,88	0
59	MG	BA	3568	1/1	0.70	0.46	-	58,58,58,58	0
59	MG	AA	1682	1/1	0.74	1.09	-	104,104,104,104	0
59	MG	BA	3108	1/1	0.96	0.67	-	56,56,56,56	0
59	MG	AA	1748	1/1	0.88	0.47	-	23,23,23,23	1
59	MG	CA	1739	1/1	0.68	0.53	-	104,104,104,104	0
59	MG	DA	2938	1/1	0.80	0.17	-	17,17,17,17	1
59	MG	DA	3193	1/1	0.83	0.17	-	68,68,68,68	0
59	MG	DA	3727	1/1	0.58	0.44	-	70,70,70,70	1
59	MG	BA	3153	1/1	0.96	0.12	-	93,93,93,93	0
59	MG	CA	1634	1/1	0.77	0.12	-	97,97,97,97	0
59	MG	BA	3223	1/1	0.92	0.22	-	80,80,80,80	0
59	MG	CA	1629	1/1	0.89	0.29	-	98,98,98,98	0
59	MG	AA	1903	1/1	0.86	0.39	-	79,79,79,79	0
59	MG	BA	2939	1/1	0.86	0.32	-	80,80,80,80	0
59	MG	D0	101	1/1	0.89	0.16	-	16,16,16,16	1
59	MG	BA	3030	1/1	0.72	0.54	-	79,79,79,79	0
59	MG	DA	2940	1/1	0.82	0.45	-	106,106,106,106	0
59	MG	AA	1690	1/1	0.76	0.22	-	81,81,81,81	1
59	MG	CV	102	1/1	0.91	0.08	-	92,92,92,92	0
59	MG	BA	3192	1/1	0.87	0.70	-	90,90,90,90	0
59	MG	BA	2930	1/1	0.90	0.20	-	85,85,85,85	0
59	MG	BA	3522	1/1	0.82	0.20	-	74,74,74,74	0
59	MG	AA	1705	1/1	0.89	1.06	-	105,105,105,105	0
59	MG	B7	101	1/1	0.94	0.89	-	93,93,93,93	0
59	MG	BA	3580	1/1	0.51	0.23	-	135,135,135,135	0
59	MG	DA	3540	1/1	0.77	0.32	-	152,152,152,152	0
59	MG	DA	3093	1/1	0.85	0.36	-	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
59	MG	DA	3115	1/1	0.94	0.47	-	39,39,39,39	0
59	MG	DA	3725	1/1	0.97	0.36	-	71,71,71,71	0
59	MG	BA	2950	1/1	0.89	0.29	-	55,55,55,55	1
59	MG	DA	3030	1/1	0.94	0.74	-	59,59,59,59	0
59	MG	AA	1965	1/1	0.95	1.21	-	97,97,97,97	0
59	MG	BA	3578	1/1	0.82	0.18	-	76,76,76,76	0
59	MG	AA	1835	1/1	0.69	1.83	-	102,102,102,102	0
59	MG	BA	3015	1/1	0.88	0.07	-	105,105,105,105	0
59	MG	CA	1694	1/1	0.90	0.20	-	93,93,93,93	0
59	MG	BA	3476	1/1	0.94	0.27	-	58,58,58,58	0
59	MG	DA	3457	1/1	0.83	0.74	-	68,68,68,68	0
59	MG	DA	3075	1/1	0.73	0.15	-	98,98,98,98	0
59	MG	BA	3421	1/1	0.78	0.33	-	68,68,68,68	0
59	MG	BB	202	1/1	0.89	0.50	-	62,62,62,62	0
59	MG	DA	3185	1/1	0.88	0.23	-	79,79,79,79	0
59	MG	DA	3409	1/1	0.70	0.18	-	53,53,53,53	1
59	MG	DA	3451	1/1	0.85	0.15	-	80,80,80,80	1
59	MG	DA	3250	1/1	0.87	0.28	-	69,69,69,69	0
59	MG	DA	3200	1/1	0.78	0.57	-	62,62,62,62	0
59	MG	DA	3297	1/1	0.93	0.65	-	53,53,53,53	0
59	MG	BA	2952	1/1	0.92	0.46	-	96,96,96,96	0
59	MG	BA	3135	1/1	0.91	0.24	-	86,86,86,86	0
59	MG	BA	3000	1/1	0.90	0.10	-	80,80,80,80	0
59	MG	BA	3370	1/1	0.86	0.52	-	105,105,105,105	0
59	MG	DA	3218	1/1	0.90	0.38	-	130,130,130,130	0
59	MG	CA	1655	1/1	0.43	0.26	-	84,84,84,84	0
59	MG	DA	3607	1/1	0.79	0.29	-	104,104,104,104	0
59	MG	DA	3388	1/1	0.83	0.66	-	78,78,78,78	0
59	MG	AA	1898	1/1	0.93	0.27	-	65,65,65,65	0
59	MG	BA	3207	1/1	0.94	0.43	-	43,43,43,43	0
59	MG	AA	1933	1/1	0.97	0.21	-	67,67,67,67	0
59	MG	BR	205	1/1	0.95	0.16	-	76,76,76,76	0
59	MG	DR	202	1/1	0.67	0.38	-	65,65,65,65	1
59	MG	DA	3541	1/1	0.90	0.21	-	96,96,96,96	0
59	MG	AA	1640	1/1	0.70	1.74	-	127,127,127,127	0
59	MG	DA	3375	1/1	0.92	0.43	-	57,57,57,57	0
59	MG	CA	1679	1/1	0.82	0.15	-	65,65,65,65	1
59	MG	AA	1805	1/1	0.90	0.19	-	102,102,102,102	0
59	MG	BA	3065	1/1	0.95	0.38	-	50,50,50,50	0
59	MG	AA	1654	1/1	0.94	0.13	-	58,58,58,58	1
59	MG	AA	1873	1/1	0.92	0.43	-	117,117,117,117	0
59	MG	BA	3253	1/1	0.88	0.37	-	52,52,52,52	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1749	1/1	0.60	0.28	-	74,74,74,74	1
59	MG	AY	102	1/1	0.91	0.74	-	104,104,104,104	1
59	MG	BA	3592	1/1	0.84	0.25	-	100,100,100,100	0
59	MG	AA	1808	1/1	0.97	0.48	-	57,57,57,57	0
59	MG	BA	3520	1/1	0.91	0.23	-	80,80,80,80	0
59	MG	DA	2925	1/1	0.68	1.06	-	108,108,108,108	0
59	MG	CA	1615	1/1	0.64	1.21	-	104,104,104,104	0
59	MG	AA	1821	1/1	0.90	0.40	-	65,65,65,65	0
59	MG	DA	3310	1/1	0.96	0.39	-	90,90,90,90	1
59	MG	DA	3437	1/1	0.98	0.18	-	12,12,12,12	1
59	MG	AA	1632	1/1	0.95	0.24	-	97,97,97,97	0
59	MG	DA	2988	1/1	0.66	0.54	-	40,40,40,40	1
59	MG	DA	2962	1/1	0.85	0.69	-	84,84,84,84	0
59	MG	DA	3664	1/1	0.95	0.14	-	85,85,85,85	0
59	MG	DB	205	1/1	0.88	0.49	-	82,82,82,82	0
59	MG	CA	1642	1/1	0.80	0.25	-	85,85,85,85	0
59	MG	BA	2905	1/1	0.94	0.34	-	52,52,52,52	0
59	MG	DA	3201	1/1	0.87	0.35	-	62,62,62,62	0
59	MG	DA	3508	1/1	0.84	0.29	-	88,88,88,88	0
59	MG	AA	1736	1/1	0.79	1.18	-	101,101,101,101	0
59	MG	DA	3000	1/1	0.92	0.06	-	105,105,105,105	0
59	MG	DA	3124	1/1	0.63	0.53	-	81,81,81,81	0
59	MG	DA	3519	1/1	0.81	0.33	-	77,77,77,77	0
59	MG	D2	101	1/1	0.85	0.36	-	62,62,62,62	0
59	MG	BA	2962	1/1	0.91	0.63	-	70,70,70,70	0
59	MG	DA	2945	1/1	0.87	0.73	-	102,102,102,102	0
59	MG	AA	1901	1/1	0.94	0.69	-	65,65,65,65	0
59	MG	DA	3149	1/1	0.94	0.31	-	26,26,26,26	0
59	MG	BA	3268	1/1	0.83	0.18	-	88,88,88,88	1
59	MG	BA	3120	1/1	0.69	0.13	-	101,101,101,101	0
59	MG	BA	2971	1/1	0.72	1.10	-	92,92,92,92	0
59	MG	DA	3370	1/1	0.95	0.54	-	68,68,68,68	0
59	MG	DA	2947	1/1	0.97	0.15	-	86,86,86,86	0
59	MG	BA	3301	1/1	0.60	0.63	-	67,67,67,67	0
59	MG	DA	3561	1/1	0.76	0.46	-	81,81,81,81	1
59	MG	BA	3025	1/1	0.78	0.22	-	83,83,83,83	0
59	MG	DA	2905	1/1	0.80	0.08	-	80,80,80,80	0
59	MG	BA	2941	1/1	0.90	0.27	-	62,62,62,62	0
59	MG	AA	1957	1/1	0.81	0.80	-	75,75,75,75	0
59	MG	DA	3203	1/1	0.71	0.75	-	112,112,112,112	0
59	MG	BA	2916	1/1	0.58	0.35	-	78,78,78,78	0
59	MG	BA	3138	1/1	0.85	0.13	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3344	1/1	0.98	0.51	-	45,45,45,45	0
59	MG	DA	3053	1/1	0.94	0.38	-	33,33,33,33	0
59	MG	BA	3237	1/1	0.95	0.20	-	58,58,58,58	0
59	MG	DA	3242	1/1	0.94	0.34	-	31,31,31,31	0
59	MG	DA	2917	1/1	0.83	0.99	-	89,89,89,89	0
59	MG	DA	3453	1/1	0.85	0.22	-	84,84,84,84	0
59	MG	DA	3550	1/1	0.92	0.46	-	86,86,86,86	0
59	MG	AA	1793	1/1	0.73	0.17	-	75,75,75,75	0
59	MG	BA	3596	1/1	0.77	1.24	-	107,107,107,107	0
59	MG	CA	1623	1/1	0.88	0.08	-	81,81,81,81	0
59	MG	DA	3129	1/1	0.98	0.41	-	72,72,72,72	0
59	MG	DA	3612	1/1	0.82	0.50	-	77,77,77,77	0
59	MG	DA	3616	1/1	0.93	0.36	-	51,51,51,51	0
59	MG	AA	1765	1/1	0.92	0.09	-	107,107,107,107	1
59	MG	AA	1922	1/1	0.67	0.27	-	82,82,82,82	0
59	MG	DA	3671	1/1	0.79	0.90	-	103,103,103,103	0
59	MG	BA	3320	1/1	0.70	0.32	-	92,92,92,92	0
59	MG	BA	3531	1/1	0.93	0.54	-	53,53,53,53	0
59	MG	BA	2998	1/1	0.95	0.23	-	54,54,54,54	0
59	MG	DA	3102	1/1	0.82	0.40	-	86,86,86,86	0
59	MG	DA	3510	1/1	0.89	0.10	-	59,59,59,59	0
59	MG	BA	3086	1/1	0.86	0.18	-	123,123,123,123	0
59	MG	DA	3352	1/1	0.93	0.31	-	58,58,58,58	0
59	MG	BA	3215	1/1	0.71	0.57	-	4,4,4,4	1
59	MG	DA	3038	1/1	0.96	0.35	-	32,32,32,32	0
59	MG	BA	2959	1/1	0.94	0.26	-	65,65,65,65	0
59	MG	DA	3491	1/1	0.72	1.06	-	107,107,107,107	0
59	MG	BA	3518	1/1	0.92	0.30	-	64,64,64,64	0
59	MG	AA	1907	1/1	0.82	0.52	-	96,96,96,96	0
59	MG	DA	3174	1/1	0.95	0.38	-	93,93,93,93	0
59	MG	CA	1724	1/1	0.94	0.52	-	102,102,102,102	0
59	MG	DA	3355	1/1	0.93	0.15	-	80,80,80,80	0
59	MG	DA	2963	1/1	0.86	0.33	-	39,39,39,39	1
59	MG	BA	3185	1/1	0.76	0.34	-	75,75,75,75	0
59	MG	AA	1680	1/1	0.91	0.27	-	75,75,75,75	0
59	MG	DA	3234	1/1	0.96	0.42	-	118,118,118,118	0
59	MG	DA	3225	1/1	0.96	0.44	-	32,32,32,32	0
59	MG	BA	3060	1/1	0.87	1.10	-	98,98,98,98	0
59	MG	CA	1743	1/1	0.69	1.95	-	81,81,81,81	0
59	MG	BA	3314	1/1	0.96	0.52	-	29,29,29,29	0
59	MG	BA	3088	1/1	0.97	0.86	-	62,62,62,62	0
59	MG	DA	3133	1/1	0.69	0.90	-	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3457	1/1	0.92	0.53	-	72,72,72,72	0
59	MG	BA	3426	1/1	0.91	0.76	-	77,77,77,77	0
59	MG	DA	3686	1/1	0.79	0.34	-	107,107,107,107	0
59	MG	DA	3383	1/1	0.82	0.63	-	135,135,135,135	0
59	MG	CA	1688	1/1	0.95	0.11	-	79,79,79,79	0
59	MG	AA	1880	1/1	0.77	0.51	-	102,102,102,102	0
59	MG	BA	3311	1/1	0.77	0.36	-	80,80,80,80	0
59	MG	BA	3004	1/1	0.78	1.52	-	84,84,84,84	0
59	MG	BA	3189	1/1	0.86	0.36	-	62,62,62,62	0
59	MG	DA	3572	1/1	0.88	0.52	-	56,56,56,56	1
59	MG	DA	3231	1/1	0.69	0.42	-	98,98,98,98	0
59	MG	DA	3192	1/1	0.72	1.03	-	70,70,70,70	0
59	MG	BA	3182	1/1	0.98	0.25	-	60,60,60,60	0
59	MG	CA	1725	1/1	0.82	0.47	-	76,76,76,76	1
59	MG	CA	1695	1/1	0.72	0.51	-	110,110,110,110	0
59	MG	BA	3319	1/1	0.91	0.52	-	33,33,33,33	0
59	MG	AA	1776	1/1	0.71	0.69	-	119,119,119,119	0
59	MG	BA	3355	1/1	0.86	0.24	-	26,26,26,26	0
59	MG	BA	3425	1/1	0.84	0.44	-	48,48,48,48	0
59	MG	CA	1674	1/1	0.95	0.18	-	90,90,90,90	0
59	MG	CA	1607	1/1	0.77	0.11	-	94,94,94,94	0
59	MG	DA	3104	1/1	0.99	0.11	-	63,63,63,63	0
59	MG	DA	3210	1/1	0.71	0.29	-	71,71,71,71	0
59	MG	DA	3555	1/1	0.90	1.20	-	105,105,105,105	0
59	MG	BA	2934	1/1	0.97	0.36	-	57,57,57,57	0
59	MG	CA	1653	1/1	0.99	0.35	-	39,39,39,39	0
59	MG	DA	3327	1/1	0.92	0.12	-	39,39,39,39	1
59	MG	AA	1906	1/1	0.87	0.36	-	65,65,65,65	1
59	MG	AA	1617	1/1	0.80	0.16	-	109,109,109,109	0
59	MG	CA	1692	1/1	0.77	0.23	-	140,140,140,140	0
59	MG	BA	3115	1/1	0.78	0.41	-	93,93,93,93	0
59	MG	DA	2929	1/1	0.96	0.20	-	10,10,10,10	1
59	MG	DA	3688	1/1	0.80	0.34	-	107,107,107,107	1
59	MG	BA	3499	1/1	0.93	0.36	-	43,43,43,43	0
59	MG	DA	3379	1/1	0.85	0.46	-	72,72,72,72	0
59	MG	DA	3179	1/1	0.96	0.53	-	66,66,66,66	0
59	MG	BA	3278	1/1	0.86	0.43	-	71,71,71,71	0
59	MG	DA	3373	1/1	0.88	0.69	-	75,75,75,75	0
59	MG	DA	3163	1/1	0.88	0.33	-	49,49,49,49	0
59	MG	CA	1617	1/1	0.96	0.06	-	66,66,66,66	0
59	MG	CA	1714	1/1	0.93	0.61	-	83,83,83,83	0
59	MG	CA	1689	1/1	0.86	0.13	-	96,96,96,96	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3002	1/1	0.83	1.67	-	83,83,83,83	0
59	MG	AA	1732	1/1	0.73	0.11	-	52,52,52,52	0
59	MG	BA	3372	1/1	0.90	0.37	-	70,70,70,70	0
59	MG	DA	2926	1/1	0.85	0.44	-	45,45,45,45	1
59	MG	AA	1676	1/1	0.88	0.29	-	68,68,68,68	0
59	MG	DA	3728	1/1	0.88	0.42	-	46,46,46,46	1
59	MG	BA	3181	1/1	0.87	0.51	-	42,42,42,42	0
59	MG	AA	1815	1/1	0.96	0.21	-	76,76,76,76	0
59	MG	DA	3482	1/1	0.86	0.34	-	37,37,37,37	1
59	MG	DA	3647	1/1	0.95	0.50	-	36,36,36,36	0
59	MG	AA	1661	1/1	0.84	0.44	-	34,34,34,34	1
59	MG	BA	3097	1/1	0.65	0.45	-	89,89,89,89	0
59	MG	AA	1879	1/1	0.81	0.48	-	74,74,74,74	0
59	MG	CA	1687	1/1	0.92	0.08	-	63,63,63,63	0
59	MG	AA	1855	1/1	0.86	0.31	-	69,69,69,69	0
59	MG	DA	2952	1/1	0.86	0.49	-	44,44,44,44	0
59	MG	BA	3044	1/1	0.81	0.65	-	64,64,64,64	0
59	MG	BA	3609	1/1	0.97	0.20	-	56,56,56,56	0
59	MG	DA	3177	1/1	0.83	0.22	-	71,71,71,71	0
59	MG	BA	3209	1/1	0.80	0.31	-	61,61,61,61	0
59	MG	DA	3134	1/1	0.69	0.33	-	74,74,74,74	0
59	MG	DA	3486	1/1	0.94	0.62	-	38,38,38,38	0
59	MG	BA	3283	1/1	0.92	0.29	-	58,58,58,58	0
59	MG	DF	302	1/1	0.53	1.29	-	98,98,98,98	0
59	MG	DA	3570	1/1	0.93	0.38	-	62,62,62,62	0
59	MG	DA	3324	1/1	0.64	0.33	-	66,66,66,66	1
59	MG	DA	3787	1/1	0.95	0.53	-	95,95,95,95	0
59	MG	DA	3041	1/1	0.94	0.22	-	78,78,78,78	0
59	MG	DA	3740	1/1	0.93	0.21	-	50,50,50,50	0
59	MG	DA	2991	1/1	0.88	0.35	-	44,44,44,44	1
59	MG	BA	3423	1/1	0.86	0.40	-	67,67,67,67	1
59	MG	DA	3261	1/1	0.91	0.76	-	34,34,34,34	1
59	MG	AA	1704	1/1	0.83	0.29	-	84,84,84,84	0
59	MG	AA	1648	1/1	0.64	0.78	-	108,108,108,108	0
59	MG	AA	1673	1/1	0.42	0.94	-	90,90,90,90	0
59	MG	DA	3367	1/1	0.86	0.57	-	28,28,28,28	1
59	MG	BA	3362	1/1	0.93	0.51	-	43,43,43,43	0
59	MG	BA	3557	1/1	0.90	1.00	-	37,37,37,37	1
59	MG	BA	3552	1/1	0.92	0.17	-	54,54,54,54	1
59	MG	BA	3333	1/1	0.81	0.36	-	72,72,72,72	0
59	MG	CA	1744	1/1	0.89	0.22	-	57,57,57,57	0
59	MG	DA	3685	1/1	0.92	0.15	-	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
59	MG	DA	2966	1/1	0.92	0.96	-	51,51,51,51	1
59	MG	AA	1615	1/1	0.88	1.12	-	67,67,67,67	0
59	MG	BA	3017	1/1	0.78	0.95	-	93,93,93,93	0
59	MG	BA	3339	1/1	0.82	0.80	-	63,63,63,63	1
59	MG	DA	3233	1/1	0.94	0.20	-	152,152,152,152	0
59	MG	DA	3159	1/1	0.83	0.41	-	85,85,85,85	0
59	MG	DA	3150	1/1	0.69	0.16	-	98,98,98,98	0
59	MG	AA	1626	1/1	0.97	0.64	-	89,89,89,89	0
59	MG	BA	2972	1/1	0.89	0.49	-	63,63,63,63	1
59	MG	DB	207	1/1	0.77	0.41	-	53,53,53,53	1
59	MG	AA	1902	1/1	0.87	0.10	-	90,90,90,90	0
59	MG	BA	3165	1/1	0.84	0.71	-	77,77,77,77	0
59	MG	DA	3252	1/1	0.86	0.19	-	87,87,87,87	0
59	MG	DA	3334	1/1	0.93	0.19	-	56,56,56,56	0
59	MG	AA	1781	1/1	0.80	0.32	-	111,111,111,111	0
59	MG	AV	104	1/1	0.36	0.29	-	133,133,133,133	0
59	MG	BA	3506	1/1	0.97	0.16	-	42,42,42,42	0
59	MG	DA	3626	1/1	0.96	0.33	-	34,34,34,34	0
59	MG	BA	2978	1/1	0.98	0.48	-	75,75,75,75	0
59	MG	BA	3302	1/1	0.97	1.20	-	69,69,69,69	0
59	MG	BA	3101	1/1	0.81	0.42	-	79,79,79,79	0
59	MG	CP	101	1/1	0.93	0.06	-	81,81,81,81	0
59	MG	DA	2950	1/1	0.61	0.21	-	80,80,80,80	1
59	MG	DA	3302	1/1	0.81	0.64	-	57,57,57,57	0
59	MG	CA	1756	1/1	0.56	0.66	-	87,87,87,87	0
59	MG	CA	1758	1/1	0.78	0.56	-	126,126,126,126	0
59	MG	DA	3235	1/1	0.78	0.47	-	110,110,110,110	0
59	MG	DA	3275	1/1	0.96	0.28	-	63,63,63,63	0
59	MG	DA	2932	1/1	0.93	0.21	-	1,1,1,1	1
59	MG	AA	1719	1/1	0.85	0.84	-	76,76,76,76	1
59	MG	AA	1701	1/1	0.92	0.34	-	77,77,77,77	0
59	MG	AA	1929	1/1	0.88	0.26	-	69,69,69,69	0
59	MG	DA	3135	1/1	0.88	0.29	-	51,51,51,51	0
59	MG	BA	3478	1/1	0.95	0.44	-	28,28,28,28	0
59	MG	AA	1964	1/1	0.74	1.22	-	106,106,106,106	0
59	MG	DA	3576	1/1	0.74	0.35	-	87,87,87,87	0
59	MG	BA	3388	1/1	0.93	0.59	-	100,100,100,100	0
59	MG	BA	3274	1/1	0.82	0.46	-	83,83,83,83	0
59	MG	DA	3497	1/1	0.72	0.28	-	103,103,103,103	0
59	MG	CV	109	1/1	0.81	0.13	-	95,95,95,95	0
59	MG	BA	3598	1/1	0.83	0.49	-	110,110,110,110	0
59	MG	AA	1969	1/1	0.83	0.71	-	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
59	MG	BA	3588	1/1	0.77	1.38	-	90,90,90,90	0
59	MG	DA	3605	1/1	0.95	0.32	-	63,63,63,63	0
59	MG	DA	2911	1/1	0.75	0.65	-	91,91,91,91	0
59	MG	DA	3767	1/1	0.90	0.64	-	67,67,67,67	0
59	MG	BA	3325	1/1	0.75	0.38	-	84,84,84,84	0
59	MG	BA	2945	1/1	0.93	0.34	-	113,113,113,113	0
59	MG	BA	3408	1/1	0.87	0.39	-	73,73,73,73	0
59	MG	BA	3356	1/1	0.97	0.25	-	45,45,45,45	0
59	MG	DA	3739	1/1	0.84	0.27	-	95,95,95,95	0
59	MG	DA	3446	1/1	0.88	0.37	-	52,52,52,52	0
59	MG	BA	3202	1/1	0.97	0.28	-	24,24,24,24	0
59	MG	BA	2973	1/1	0.61	0.91	-	85,85,85,85	0
59	MG	AA	1745	1/1	0.65	0.54	-	50,50,50,50	1
59	MG	DB	206	1/1	0.94	0.09	-	65,65,65,65	1
59	MG	AA	1914	1/1	0.97	0.24	-	56,56,56,56	0
59	MG	DA	3384	1/1	0.60	0.85	-	120,120,120,120	0
59	MG	CA	1733	1/1	0.77	0.17	-	76,76,76,76	0
59	MG	BA	3069	1/1	0.93	0.57	-	100,100,100,100	0
59	MG	DA	3164	1/1	0.82	0.26	-	55,55,55,55	0
59	MG	DA	3393	1/1	0.94	0.28	-	6,6,6,6	1
59	MG	DA	3329	1/1	0.74	0.41	-	110,110,110,110	0
59	MG	DA	3166	1/1	0.96	0.29	-	30,30,30,30	0
59	MG	CA	1681	1/1	0.64	0.42	-	95,95,95,95	0
59	MG	BA	3399	1/1	0.97	0.58	-	146,146,146,146	0
59	MG	DD	301	1/1	0.89	0.38	-	57,57,57,57	0
59	MG	DA	3035	1/1	0.81	0.27	-	84,84,84,84	0
59	MG	CA	1749	1/1	0.76	0.52	-	16,16,16,16	1
59	MG	AA	1816	1/1	0.96	0.28	-	64,64,64,64	0
59	MG	AA	1742	1/1	0.86	0.27	-	63,63,63,63	1
59	MG	DA	3548	1/1	0.81	0.38	-	50,50,50,50	1
59	MG	DA	3591	1/1	0.84	0.65	-	19,19,19,19	1
59	MG	DA	3121	1/1	0.84	0.35	-	69,69,69,69	0
59	MG	DA	3417	1/1	0.64	0.57	-	48,48,48,48	1
59	MG	BT	201	1/1	0.08	0.38	-	117,117,117,117	0
59	MG	AA	1844	1/1	0.92	0.21	-	107,107,107,107	0
59	MG	AA	1653	1/1	0.98	0.07	-	68,68,68,68	1
59	MG	BA	3365	1/1	0.85	1.28	-	112,112,112,112	0
59	MG	AA	1718	1/1	0.99	0.17	-	98,98,98,98	0
59	MG	DA	3249	1/1	0.94	0.26	-	68,68,68,68	0
59	MG	BA	3604	1/1	0.68	0.66	-	82,82,82,82	0
59	MG	BA	3331	1/1	0.71	1.51	-	92,92,92,92	0
59	MG	DA	3700	1/1	0.95	0.32	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3070	1/1	0.83	0.47	-	108,108,108,108	0
59	MG	DE	302	1/1	0.92	0.24	-	39,39,39,39	1
59	MG	DA	3709	1/1	0.90	0.22	-	61,61,61,61	0
59	MG	DA	3692	1/1	0.95	0.87	-	61,61,61,61	0
59	MG	AA	1868	1/1	0.89	0.25	-	100,100,100,100	0
59	MG	DT	201	1/1	0.84	0.78	-	5,5,5,5	1
59	MG	DA	3785	1/1	0.75	1.05	-	35,35,35,35	1
59	MG	BA	3602	1/1	0.62	1.44	-	122,122,122,122	1
59	MG	DE	304	1/1	0.98	0.35	-	22,22,22,22	0
59	MG	CA	1652	1/1	0.95	0.48	-	78,78,78,78	0
59	MG	DA	3623	1/1	0.94	0.16	-	28,28,28,28	0
59	MG	DA	3436	1/1	0.86	0.33	-	104,104,104,104	0
59	MG	AA	1854	1/1	0.84	0.20	-	71,71,71,71	0
59	MG	CA	1698	1/1	0.44	0.61	-	73,73,73,73	1
59	MG	DA	3139	1/1	0.86	0.27	-	89,89,89,89	0
59	MG	BA	3543	1/1	0.90	0.69	-	71,71,71,71	0
59	MG	DA	3099	1/1	0.96	0.31	-	67,67,67,67	0
59	MG	BA	3205	1/1	0.48	0.57	-	78,78,78,78	0
59	MG	BA	3444	1/1	0.84	0.76	-	69,69,69,69	0
59	MG	AA	1699	1/1	0.87	0.19	-	71,71,71,71	0
59	MG	AA	1730	1/1	0.81	0.27	-	77,77,77,77	1
59	MG	AA	1607	1/1	0.80	0.26	-	73,73,73,73	0
59	MG	CA	1639	1/1	0.96	0.18	-	95,95,95,95	0
59	MG	CA	1636	1/1	0.86	0.53	-	77,77,77,77	0
59	MG	DA	2909	1/1	0.74	0.49	-	83,83,83,83	0
59	MG	BA	3383	1/1	0.67	0.11	-	126,126,126,126	0
59	MG	DA	3429	1/1	0.83	0.66	-	23,23,23,23	1
59	MG	AA	1970	1/1	0.80	0.33	-	107,107,107,107	0
59	MG	BA	3384	1/1	0.76	0.82	-	95,95,95,95	0
59	MG	AA	1768	1/1	0.67	0.89	-	107,107,107,107	0
59	MG	DA	3294	1/1	0.97	0.09	-	80,80,80,80	1
59	MG	DR	201	1/1	0.81	0.22	-	108,108,108,108	0
59	MG	AQ	202	1/1	0.60	0.47	-	97,97,97,97	0
59	MG	BA	3229	1/1	0.84	1.19	-	88,88,88,88	0
59	MG	AL	206	1/1	0.92	0.19	-	53,53,53,53	1
59	MG	CA	1633	1/1	0.93	0.09	-	70,70,70,70	0
59	MG	AA	1685	1/1	0.77	0.39	-	30,30,30,30	1
59	MG	AA	1967	1/1	0.98	0.28	-	67,67,67,67	0
59	MG	DA	3376	1/1	0.81	0.80	-	93,93,93,93	0
59	MG	BA	2994	1/1	0.83	0.48	-	80,80,80,80	0
59	MG	BD	304	1/1	0.89	0.32	-	49,49,49,49	0
59	MG	AA	1817	1/1	0.90	0.14	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3602	1/1	0.90	0.29	-	76,76,76,76	0
59	MG	BA	3033	1/1	0.91	0.33	-	69,69,69,69	0
59	MG	BA	3150	1/1	0.84	0.40	-	145,145,145,145	0
59	MG	DA	3428	1/1	0.92	0.33	-	65,65,65,65	0
59	MG	DA	3358	1/1	0.81	0.26	-	93,93,93,93	0
59	MG	BA	3443	1/1	0.80	0.14	-	76,76,76,76	0
59	MG	DA	3609	1/1	0.91	0.53	-	63,63,63,63	0
59	MG	AA	1628	1/1	0.96	0.10	-	84,84,84,84	0
59	MG	DA	3712	1/1	0.81	0.95	-	108,108,108,108	0
59	MG	CA	1750	1/1	0.73	1.38	-	102,102,102,102	0
59	MG	CA	1622	1/1	0.78	0.75	-	99,99,99,99	0
59	MG	DA	3167	1/1	0.87	0.32	-	40,40,40,40	0
59	MG	AA	1838	1/1	0.73	0.74	-	80,80,80,80	0
59	MG	BA	3290	1/1	0.78	0.38	-	86,86,86,86	0
59	MG	DA	3495	1/1	0.68	0.62	-	75,75,75,75	0
59	MG	AA	1715	1/1	0.82	0.99	-	126,126,126,126	0
59	MG	DA	3424	1/1	0.91	1.01	-	84,84,84,84	0
59	MG	DA	3392	1/1	0.77	0.36	-	81,81,81,81	0
59	MG	BA	3500	1/1	0.92	0.35	-	79,79,79,79	0
59	MG	BA	3098	1/1	0.86	0.41	-	62,62,62,62	0
59	MG	AA	1896	1/1	0.94	0.20	-	78,78,78,78	0
59	MG	DA	3065	1/1	0.39	0.71	-	128,128,128,128	0
59	MG	CA	1779	1/1	0.66	0.51	-	102,102,102,102	0
59	MG	BA	3392	1/1	0.94	0.85	-	87,87,87,87	0
59	MG	DA	3418	1/1	0.73	0.14	-	88,88,88,88	0
59	MG	BA	3126	1/1	0.98	0.12	-	36,36,36,36	0
59	MG	BA	2938	1/1	0.91	0.19	-	64,64,64,64	1
59	MG	DA	3793	1/1	0.59	0.33	-	130,130,130,130	0
59	MG	CV	105	1/1	0.84	0.17	-	82,82,82,82	0
59	MG	DA	3289	1/1	0.62	0.56	-	78,78,78,78	0
59	MG	AA	1756	1/1	0.87	0.19	-	91,91,91,91	0
59	MG	BA	3251	1/1	0.76	0.67	-	100,100,100,100	0
59	MG	BB	205	1/1	0.91	0.12	-	69,69,69,69	1
59	MG	CC	303	1/1	0.88	0.12	-	113,113,113,113	0
59	MG	DA	3313	1/1	0.98	0.29	-	101,101,101,101	0
59	MG	CA	1770	1/1	0.72	0.67	-	54,54,54,54	1
59	MG	BA	3056	1/1	0.94	0.24	-	156,156,156,156	0
59	MG	AA	1786	1/1	0.93	0.14	-	123,123,123,123	0
59	MG	AA	1744	1/1	0.96	0.08	-	80,80,80,80	0
59	MG	BA	3342	1/1	0.72	0.58	-	127,127,127,127	0
59	MG	DA	3524	1/1	0.72	0.58	-	61,61,61,61	0
59	MG	AA	1939	1/1	0.86	0.29	-	74,74,74,74	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3427	1/1	0.91	0.61	-	63,63,63,63	0
59	MG	CA	1649	1/1	0.68	1.08	-	92,92,92,92	0
59	MG	BA	3507	1/1	0.86	0.42	-	55,55,55,55	0
59	MG	AA	1664	1/1	0.94	0.15	-	17,17,17,17	1
59	MG	AA	1623	1/1	0.96	1.02	-	66,66,66,66	0
59	MG	BA	3541	1/1	0.83	0.93	-	82,82,82,82	0
59	MG	DA	3583	1/1	0.83	0.48	-	64,64,64,64	0
59	MG	BA	3178	1/1	0.94	0.96	-	79,79,79,79	0
59	MG	BA	3482	1/1	0.98	0.49	-	144,144,144,144	0
59	MG	D0	104	1/1	0.29	0.68	-	98,98,98,98	0
59	MG	DA	3621	1/1	0.90	0.35	-	76,76,76,76	1
59	MG	DA	3448	1/1	0.97	0.20	-	55,55,55,55	0
59	MG	DA	3509	1/1	0.89	0.47	-	39,39,39,39	0
59	MG	AA	1934	1/1	0.93	0.23	-	68,68,68,68	0
59	MG	BA	3132	1/1	0.35	0.42	-	81,81,81,81	0
59	MG	DA	3196	1/1	0.97	0.19	-	100,100,100,100	0
59	MG	BA	3186	1/1	0.67	0.11	-	81,81,81,81	0
59	MG	DA	3529	1/1	0.86	0.10	-	42,42,42,42	0
59	MG	BA	3239	1/1	0.84	0.29	-	77,77,77,77	0
59	MG	BA	2970	1/1	0.49	1.54	-	101,101,101,101	0
59	MG	BA	3307	1/1	0.97	0.44	-	75,75,75,75	0
59	MG	AA	1651	1/1	0.69	0.20	-	76,76,76,76	0
59	MG	AA	1720	1/1	0.93	0.55	-	37,37,37,37	1
59	MG	DA	2978	1/1	0.93	0.34	-	33,33,33,33	0
59	MG	DA	2907	1/1	0.87	0.41	-	83,83,83,83	0
59	MG	CA	1619	1/1	0.76	0.21	-	116,116,116,116	0
59	MG	DA	3156	1/1	0.89	0.56	-	73,73,73,73	0
59	MG	DA	3472	1/1	0.90	0.35	-	79,79,79,79	1
59	MG	BH	201	1/1	0.76	0.29	-	71,71,71,71	1
59	MG	DA	3645	1/1	0.95	0.24	-	78,78,78,78	0
59	MG	BA	3230	1/1	0.87	0.52	-	85,85,85,85	0
59	MG	AA	1897	1/1	0.95	0.23	-	68,68,68,68	0
59	MG	BA	3335	1/1	0.35	1.65	-	113,113,113,113	0
59	MG	BA	3380	1/1	0.79	1.22	-	133,133,133,133	0
59	MG	CA	1723	1/1	0.72	0.49	-	82,82,82,82	0
59	MG	AA	1841	1/1	0.94	0.39	-	42,42,42,42	0
59	MG	BA	3231	1/1	0.95	0.39	-	28,28,28,28	0
59	MG	DA	3432	1/1	0.50	0.58	-	86,86,86,86	1
59	MG	DA	3287	1/1	0.93	0.14	-	66,66,66,66	0
59	MG	BA	3553	1/1	0.83	0.32	-	106,106,106,106	0
59	MG	BA	3513	1/1	0.90	0.38	-	77,77,77,77	0
59	MG	DA	2920	1/1	0.47	0.23	-	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	3569	1/1	0.72	1.14	-	113,113,113,113	0
59	MG	DA	3598	1/1	0.88	0.62	-	83,83,83,83	0
59	MG	DA	3765	1/1	0.93	0.56	-	69,69,69,69	0
59	MG	BA	3498	1/1	0.86	1.06	-	85,85,85,85	1
59	MG	AA	1609	1/1	0.82	0.56	-	59,59,59,59	0
59	MG	BA	3096	1/1	0.81	0.91	-	102,102,102,102	0
59	MG	DA	3680	1/1	0.70	0.76	-	98,98,98,98	0
59	MG	BA	3549	1/1	0.94	0.63	-	84,84,84,84	0
59	MG	AA	1826	1/1	0.94	0.15	-	83,83,83,83	0
59	MG	AA	1900	1/1	0.54	0.22	-	128,128,128,128	0
59	MG	DA	3435	1/1	0.81	0.29	-	47,47,47,47	0
59	MG	BA	3260	1/1	0.83	0.40	-	77,77,77,77	0
59	MG	BA	3199	1/1	0.66	1.87	-	110,110,110,110	0
59	MG	CA	1672	1/1	0.95	0.16	-	92,92,92,92	0
59	MG	AA	1802	1/1	0.80	0.28	-	119,119,119,119	0
59	MG	CA	1673	1/1	0.95	0.28	-	62,62,62,62	0
59	MG	DA	3241	1/1	0.65	0.49	-	34,34,34,34	1
59	MG	DA	3751	1/1	0.80	0.59	-	82,82,82,82	0
59	MG	DA	3173	1/1	0.94	0.46	-	48,48,48,48	0
59	MG	AA	1751	1/1	0.96	0.07	-	104,104,104,104	0
59	MG	BA	3264	1/1	0.95	0.37	-	42,42,42,42	0
59	MG	DA	3117	1/1	0.91	0.43	-	88,88,88,88	0
59	MG	DA	3427	1/1	0.87	0.39	-	78,78,78,78	0
59	MG	CA	1727	1/1	0.95	0.14	-	74,74,74,74	0
59	MG	DA	3095	1/1	0.93	0.56	-	42,42,42,42	0
59	MG	AA	1686	1/1	0.87	0.17	-	81,81,81,81	0
59	MG	DA	3237	1/1	0.90	0.33	-	37,37,37,37	0
59	MG	BA	3144	1/1	0.87	0.32	-	73,73,73,73	0
59	MG	DA	2996	1/1	0.89	0.51	-	71,71,71,71	1
59	MG	DA	3637	1/1	0.46	1.11	-	88,88,88,88	0
59	MG	DA	3079	1/1	0.87	0.68	-	127,127,127,127	0
59	MG	DA	3387	1/1	0.87	0.42	-	77,77,77,77	0
59	MG	CA	1650	1/1	0.67	0.89	-	79,79,79,79	0
59	MG	DA	2979	1/1	0.84	0.37	-	42,42,42,42	0
59	MG	BA	3241	1/1	0.72	0.26	-	44,44,44,44	0
59	MG	AA	1629	1/1	0.92	0.31	-	80,80,80,80	0
59	MG	DA	2984	1/1	0.58	0.42	-	66,66,66,66	1
59	MG	BA	3316	1/1	0.45	0.62	-	98,98,98,98	0
59	MG	BA	3390	1/1	0.83	0.14	-	65,65,65,65	0
59	MG	AA	1769	1/1	0.82	0.48	-	101,101,101,101	0
59	MG	DA	3118	1/1	0.96	0.15	-	63,63,63,63	0
59	MG	AA	1870	1/1	0.70	0.38	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	BA	2906	1/1	0.92	0.36	-	92,92,92,92	0
59	MG	BA	3222	1/1	0.68	0.91	-	108,108,108,108	0
59	MG	CA	1682	1/1	0.92	0.33	-	53,53,53,53	0
59	MG	DA	3138	1/1	0.62	0.83	-	139,139,139,139	0
59	MG	BA	3581	1/1	0.73	1.48	-	95,95,95,95	0
59	MG	BA	3544	1/1	0.84	0.33	-	62,62,62,62	0
59	MG	BA	3326	1/1	0.78	0.61	-	77,77,77,77	0
59	MG	DA	3128	1/1	0.88	0.30	-	86,86,86,86	0
59	MG	DA	3670	1/1	0.76	0.47	-	88,88,88,88	0
59	MG	DA	3269	1/1	0.83	0.47	-	44,44,44,44	0
59	MG	DA	3039	1/1	0.96	0.36	-	88,88,88,88	0
59	MG	DA	3532	1/1	0.87	0.27	-	79,79,79,79	0
59	MG	BA	3577	1/1	0.99	0.44	-	38,38,38,38	0
59	MG	DA	3672	1/1	0.94	0.23	-	74,74,74,74	0
59	MG	BA	2955	1/1	0.95	0.69	-	84,84,84,84	0
59	MG	AH	201	1/1	0.81	0.89	-	102,102,102,102	0
59	MG	BA	3276	1/1	0.61	1.19	-	125,125,125,125	0
59	MG	BA	3154	1/1	0.83	0.34	-	54,54,54,54	0
59	MG	DA	3151	1/1	0.85	0.92	-	73,73,73,73	0
59	MG	CA	1761	1/1	0.81	0.26	-	87,87,87,87	0
59	MG	DA	3619	1/1	0.85	0.27	-	69,69,69,69	0
59	MG	DA	3259	1/1	0.97	0.52	-	32,32,32,32	0
59	MG	DA	3411	1/1	0.87	0.18	-	67,67,67,67	1
59	MG	BA	3227	1/1	0.94	0.23	-	78,78,78,78	0
59	MG	DA	3676	1/1	0.67	0.61	-	96,96,96,96	0
59	MG	DA	3470	1/1	0.69	0.59	-	75,75,75,75	0
59	MG	BA	3048	1/1	0.90	0.19	-	90,90,90,90	0
59	MG	BA	3122	1/1	0.73	0.91	-	106,106,106,106	0
59	MG	DA	3320	1/1	0.90	0.13	-	78,78,78,78	0
59	MG	DA	2916	1/1	0.90	0.15	-	57,57,57,57	0
59	MG	CA	1630	1/1	0.74	0.18	-	68,68,68,68	0
59	MG	BA	3139	1/1	0.99	0.33	-	27,27,27,27	0
59	MG	AA	1645	1/1	0.84	1.01	-	56,56,56,56	1
59	MG	BA	2911	1/1	0.93	0.30	-	94,94,94,94	0
59	MG	AA	1891	1/1	0.66	0.37	-	54,54,54,54	1
59	MG	CA	1702	1/1	0.93	0.17	-	104,104,104,104	0
59	MG	BA	3403	1/1	0.93	0.16	-	69,69,69,69	0
59	MG	DA	3534	1/1	0.92	0.47	-	73,73,73,73	1
59	MG	BA	3464	1/1	0.99	0.54	-	43,43,43,43	0
59	MG	DA	2986	1/1	0.98	0.21	-	142,142,142,142	0
59	MG	DA	3768	1/1	0.89	0.06	-	58,58,58,58	1
59	MG	DA	3773	1/1	0.83	0.28	-	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
59	MG	DA	2974	1/1	0.88	0.69	-	47,47,47,47	1
59	MG	DA	2922	1/1	0.86	0.33	-	65,65,65,65	0
59	MG	CA	1646	1/1	0.71	0.78	-	102,102,102,102	0
59	MG	DA	3153	1/1	0.89	0.56	-	68,68,68,68	0
59	MG	DA	3007	1/1	0.80	0.28	-	57,57,57,57	0
59	MG	AA	1846	1/1	0.95	0.46	-	45,45,45,45	0
59	MG	CA	1638	1/1	0.89	0.29	-	61,61,61,61	0
59	MG	DA	3667	1/1	0.86	0.43	-	46,46,46,46	1
59	MG	CA	1772	1/1	0.96	0.21	-	79,79,79,79	0
59	MG	CA	1777	1/1	-0.11	0.16	-	125,125,125,125	0
59	MG	AA	1714	1/1	0.93	0.21	-	66,66,66,66	0
59	MG	BA	2917	1/1	0.85	0.25	-	84,84,84,84	0
59	MG	DA	3222	1/1	0.78	0.30	-	79,79,79,79	0
59	MG	DB	201	1/1	0.91	0.15	-	59,59,59,59	0
59	MG	AA	1945	1/1	0.73	1.00	-	94,94,94,94	1
59	MG	CA	1612	1/1	0.94	0.24	-	58,58,58,58	0
59	MG	DA	3120	1/1	0.97	0.24	-	106,106,106,106	0
59	MG	CJ	201	1/1	0.67	0.41	-	115,115,115,115	0
59	MG	BA	3589	1/1	0.97	0.10	-	41,41,41,41	0
59	MG	DA	3695	1/1	0.79	0.42	-	81,81,81,81	0
59	MG	DA	3119	1/1	0.94	0.14	-	66,66,66,66	0
59	MG	BA	3244	1/1	0.88	0.48	-	88,88,88,88	0
59	MG	AA	1708	1/1	0.69	0.37	-	65,65,65,65	1
59	MG	BA	3310	1/1	0.93	0.64	-	68,68,68,68	0
59	MG	BA	2942	1/1	0.94	0.62	-	110,110,110,110	0
59	MG	BA	3014	1/1	0.89	0.35	-	79,79,79,79	0
59	MG	CY	101	1/1	0.81	0.41	-	143,143,143,143	0
59	MG	BA	3398	1/1	0.92	0.69	-	53,53,53,53	0
59	MG	AA	1861	1/1	0.74	0.62	-	77,77,77,77	0
59	MG	BA	3546	1/1	0.82	0.75	-	83,83,83,83	0
59	MG	AA	1852	1/1	0.92	0.37	-	56,56,56,56	0
59	MG	AA	1759	1/1	0.80	0.38	-	51,51,51,51	0
59	MG	DA	3588	1/1	0.93	0.40	-	83,83,83,83	0
59	MG	BA	3493	1/1	0.74	0.47	-	101,101,101,101	0
59	MG	DA	3737	1/1	0.73	0.80	-	74,74,74,74	0
59	MG	DA	3487	1/1	0.95	0.67	-	42,42,42,42	1
59	MG	DA	3146	1/1	0.70	0.59	-	85,85,85,85	0
59	MG	BA	3377	1/1	0.91	0.28	-	59,59,59,59	0
59	MG	DA	3743	1/1	0.93	0.26	-	50,50,50,50	1
59	MG	CA	1718	1/1	0.85	0.25	-	87,87,87,87	0
59	MG	DA	3657	1/1	0.92	0.32	-	59,59,59,59	0
59	MG	AA	1620	1/1	0.76	0.63	-	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	DA	3024	1/1	0.97	0.23	-	92,92,92,92	0
59	MG	DA	2906	1/1	0.86	0.34	-	93,93,93,93	1
59	MG	BA	3027	1/1	0.80	0.32	-	74,74,74,74	0
59	MG	BA	3021	1/1	0.93	0.57	-	78,78,78,78	0
59	MG	AA	1956	1/1	0.70	0.56	-	58,58,58,58	0
59	MG	BA	3232	1/1	0.84	0.31	-	64,64,64,64	0
59	MG	DA	3469	1/1	0.95	0.47	-	65,65,65,65	0
59	MG	BA	3554	1/1	0.39	0.26	-	109,109,109,109	0
59	MG	BA	2922	1/1	0.88	1.25	-	95,95,95,95	0
59	MG	DA	3279	1/1	0.95	0.59	-	70,70,70,70	0
59	MG	AA	1890	1/1	0.80	0.49	-	78,78,78,78	0
59	MG	BA	3366	1/1	0.93	0.54	-	71,71,71,71	0
59	MG	BA	3077	1/1	0.89	0.46	-	71,71,71,71	0
59	MG	DA	3106	1/1	0.88	0.24	-	77,77,77,77	0
59	MG	DA	3724	1/1	0.93	0.28	-	73,73,73,73	0
59	MG	BA	3529	1/1	0.36	0.70	-	70,70,70,70	0
59	MG	DA	3005	1/1	0.78	0.11	-	69,69,69,69	0
59	MG	DA	3229	1/1	0.98	0.08	-	51,51,51,51	0
59	MG	BA	3591	1/1	0.91	0.83	-	93,93,93,93	0
59	MG	DA	2915	1/1	0.91	0.35	-	48,48,48,48	0
59	MG	DP	206	1/1	0.72	1.12	-	82,82,82,82	0
59	MG	BA	3008	1/1	0.89	0.34	-	123,123,123,123	0
59	MG	DA	3704	1/1	0.81	0.22	-	74,74,74,74	0
59	MG	AA	1753	1/1	0.97	0.06	-	110,110,110,110	0
59	MG	DA	2914	1/1	0.68	0.59	-	83,83,83,83	0
59	MG	BA	3242	1/1	0.91	0.38	-	60,60,60,60	0
59	MG	DA	3184	1/1	0.91	0.27	-	63,63,63,63	0
59	MG	DA	3101	1/1	0.84	1.26	-	97,97,97,97	0
59	MG	DA	3545	1/1	0.91	0.11	-	58,58,58,58	0
59	MG	AA	1773	1/1	0.95	0.14	-	50,50,50,50	0
59	MG	DA	3699	1/1	0.98	0.19	-	62,62,62,62	0
59	MG	CA	1767	1/1	0.80	0.44	-	73,73,73,73	0
59	MG	DA	3498	1/1	0.85	0.42	-	82,82,82,82	0
59	MG	CA	1690	1/1	0.92	0.42	-	60,60,60,60	0
59	MG	DU	201	1/1	0.92	0.21	-	68,68,68,68	0
59	MG	BA	3416	1/1	0.94	0.72	-	58,58,58,58	0
59	MG	DN	202	1/1	0.47	0.61	-	78,78,78,78	0
59	MG	BA	3125	1/1	0.90	0.23	-	70,70,70,70	0
59	MG	AA	1613	1/1	0.86	0.93	-	74,74,74,74	0
59	MG	DA	3321	1/1	0.70	0.32	-	88,88,88,88	0
59	MG	AA	1638	1/1	0.95	0.36	-	119,119,119,119	0
59	MG	AA	1895	1/1	0.94	0.22	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
59	MG	AA	1853	1/1	0.95	0.29	-	74,74,74,74	0
59	MG	BA	2956	1/1	0.94	0.27	-	37,37,37,37	1
59	MG	CA	1635	1/1	0.90	0.22	-	93,93,93,93	0
59	MG	DA	3492	1/1	0.85	0.88	-	62,62,62,62	0
59	MG	AA	1927	1/1	0.92	0.13	-	113,113,113,113	0
59	MG	BA	2929	1/1	0.63	0.26	-	90,90,90,90	0
59	MG	BA	3275	1/1	0.88	0.19	-	38,38,38,38	0
59	MG	DA	3512	1/1	0.84	0.37	-	104,104,104,104	0
59	MG	DA	3331	1/1	0.97	0.16	-	45,45,45,45	1
59	MG	DA	3644	1/1	0.96	0.66	-	54,54,54,54	0
59	MG	CA	1605	1/1	0.85	0.85	-	49,49,49,49	1
59	MG	CA	1741	1/1	0.72	1.70	-	106,106,106,106	0
59	MG	BA	3424	1/1	0.95	0.36	-	64,64,64,64	0
59	MG	BA	3300	1/1	0.84	0.48	-	71,71,71,71	0
59	MG	CA	1719	1/1	0.84	0.28	-	95,95,95,95	0
59	MG	BA	3576	1/1	0.69	0.18	-	97,97,97,97	0
59	MG	BA	3224	1/1	0.97	0.36	-	79,79,79,79	0
59	MG	BA	3164	1/1	0.93	0.83	-	44,44,44,44	0
59	MG	BA	3020	1/1	0.85	0.50	-	103,103,103,103	0
59	MG	AA	1850	1/1	0.84	0.82	-	89,89,89,89	0
59	MG	DA	3610	1/1	0.96	0.20	-	112,112,112,112	0
59	MG	DA	3182	1/1	0.93	0.21	-	73,73,73,73	0
59	MG	AA	1621	1/1	0.80	1.25	-	98,98,98,98	0
59	MG	DP	204	1/1	0.96	0.28	-	15,15,15,15	0
59	MG	BA	3118	1/1	0.87	0.07	-	59,59,59,59	0
59	MG	CA	1616	1/1	0.93	0.15	-	62,62,62,62	0
59	MG	AA	1627	1/1	0.53	1.17	-	142,142,142,142	0
59	MG	DA	3223	1/1	0.86	0.38	-	37,37,37,37	0
59	MG	BA	3313	1/1	0.69	0.15	-	70,70,70,70	0
59	MG	DA	3505	1/1	0.26	1.03	-	125,125,125,125	0
59	MG	BA	3095	1/1	0.73	0.39	-	95,95,95,95	0
59	MG	AA	1912	1/1	0.78	0.32	-	57,57,57,57	1
59	MG	DA	3170	1/1	0.85	0.47	-	98,98,98,98	0
59	MG	CA	1676	1/1	0.57	0.30	-	88,88,88,88	0
59	MG	AA	1909	1/1	0.93	0.11	-	87,87,87,87	1
59	MG	BA	3473	1/1	0.87	0.91	-	87,87,87,87	0
59	MG	DA	3445	1/1	0.94	0.25	-	55,55,55,55	0
59	MG	DA	3674	1/1	0.94	0.70	-	55,55,55,55	0
59	MG	BA	3079	1/1	0.94	0.16	-	37,37,37,37	0
59	MG	DA	3517	1/1	0.29	0.39	-	107,107,107,107	0
59	MG	AA	1944	1/1	0.68	0.33	-	76,76,76,76	0
59	MG	CS	102	1/1	0.66	0.11	-	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
59	MG	DA	3240	1/1	0.60	0.08	-	128,128,128,128	0
59	MG	BA	3371	1/1	0.89	0.15	-	63,63,63,63	0
59	MG	DA	3386	1/1	0.86	0.40	-	99,99,99,99	0
59	MG	DA	3353	1/1	0.89	0.12	-	84,84,84,84	0
59	MG	BA	2904	1/1	0.73	1.74	-	104,104,104,104	0
59	MG	DA	3212	1/1	0.85	0.43	-	105,105,105,105	0
59	MG	DA	3658	1/1	0.96	0.27	-	53,53,53,53	0
59	MG	DA	3062	1/1	0.91	0.41	-	88,88,88,88	0
59	MG	AX	102	1/1	0.91	0.12	-	87,87,87,87	0
59	MG	BA	3379	1/1	0.69	1.75	-	114,114,114,114	0
59	MG	BA	3009	1/1	0.94	0.42	-	80,80,80,80	0
59	MG	BA	3556	1/1	0.81	1.12	-	116,116,116,116	0
59	MG	BA	3293	1/1	0.92	0.17	-	82,82,82,82	0
59	MG	AA	1785	1/1	0.98	0.03	-	108,108,108,108	0
59	MG	BA	3471	1/1	0.81	0.61	-	96,96,96,96	0
59	MG	BA	3047	1/1	0.88	0.69	-	89,89,89,89	0
59	MG	DA	3198	1/1	0.91	0.54	-	31,31,31,31	0
59	MG	AA	1803	1/1	0.74	0.53	-	98,98,98,98	0
59	MG	AA	1739	1/1	0.82	0.91	-	73,73,73,73	1
59	MG	AA	1791	1/1	0.88	0.30	-	93,93,93,93	0
59	MG	DA	3076	1/1	0.85	0.27	-	75,75,75,75	0
59	MG	DA	3597	1/1	0.74	0.28	-	66,66,66,66	0
59	MG	DA	3526	1/1	0.85	0.10	-	11,11,11,11	1
59	MG	BA	3123	1/1	0.90	0.41	-	105,105,105,105	0
59	MG	AL	203	1/1	0.95	0.25	-	81,81,81,81	0
59	MG	AA	1881	1/1	0.84	0.52	-	98,98,98,98	0
59	MG	DA	3265	1/1	0.85	0.79	-	82,82,82,82	0
59	MG	BA	3092	1/1	0.82	0.22	-	101,101,101,101	0
59	MG	AA	1635	1/1	0.57	0.70	-	108,108,108,108	0

## 6.5 Other polymers

There are no such residues in this entry.