



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:52 PM GMT

PDB ID : 4WPO  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G in the pre-translocational state  
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.  
Deposited on : 2014-10-20  
Resolution : 2.80 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

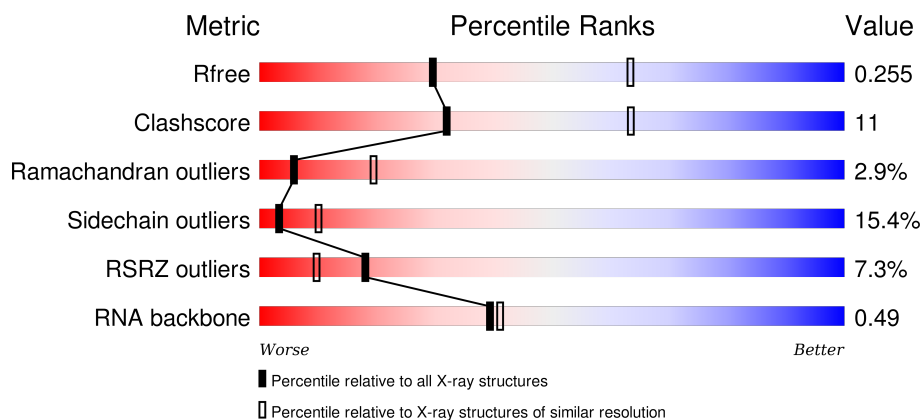
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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	2915	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>41%</div> <div>16%</div> <div>..</div> </div> </div>
1	CA	2915	<div> <div>4%</div> <div> <div></div> <div>48%</div> <div>37%</div> <div>12%</div> <div>..</div> </div> </div>
2	AB	121	<div> <div></div> <div> <div></div> <div>56%</div> <div>35%</div> <div>8%</div> <div>.</div> </div> </div>
2	CB	121	<div> <div></div> <div> <div></div> <div>58%</div> <div>31%</div> <div>10%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
13	CP	150	
14	AQ	141	
14	CQ	141	
15	AR	118	

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Mol	Chain	Length	Quality of chain
15	CR	118	
16	AS	112	
16	CS	112	
17	AT	146	
17	CT	146	
18	AU	118	
18	CU	118	
19	AV	101	
19	CV	101	
20	AW	113	
20	CW	113	
21	AX	96	
21	CX	96	
22	AY	110	
22	CY	110	
23	AZ	206	
23	CZ	206	
24	A0	85	
24	C0	85	
25	A1	98	
25	C1	98	
26	A2	72	
26	C2	72	
27	A3	60	
27	C3	60	

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Mol	Chain	Length	Quality of chain
28	A4	71	
28	C4	71	
29	A5	60	
29	C5	60	
30	A6	54	
30	C6	54	
31	A7	49	
31	C7	49	
32	A8	65	
32	C8	65	
33	A9	37	
33	C9	37	
34	BA	1521	
34	DA	1521	
35	BB	256	
35	DB	256	
36	BC	239	
36	DC	239	
37	BD	209	
37	DD	209	
38	BE	162	
38	DE	162	
39	BF	101	
39	DF	101	
40	BG	156	

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Mol	Chain	Length	Quality of chain
40	DG	156	
41	BH	138	
41	DH	138	
42	BI	128	
42	DI	128	
43	BJ	105	
43	DJ	105	
44	BK	129	
44	DK	129	
45	BL	132	
45	DL	132	
46	BM	126	
46	DM	126	
47	BN	61	
47	DN	61	
48	BO	89	
48	DO	89	
49	BP	88	
49	DP	88	
50	BQ	105	
50	DQ	105	
51	BR	88	
51	DR	88	
52	BS	93	
52	DS	93	

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Mol	Chain	Length	Quality of chain
53	BT	106	
53	DT	106	
54	BU	27	
54	DU	27	
55	BV	24	
55	DV	24	
56	BW	76	
56	DW	76	
57	BX	77	
57	DX	77	
58	BY	76	
58	DY	76	
59	BZ	758	
59	DZ	758	

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
60	MG	A0	101	-	-	-	X
60	MG	AA	3001	-	-	-	X
60	MG	AA	3008	-	-	-	X
60	MG	AA	3018	-	-	-	X
60	MG	AA	3019	-	-	-	X
60	MG	AA	3020	-	-	-	X
60	MG	AA	3021	-	-	-	X
60	MG	AA	3023	-	-	-	X
60	MG	AA	3033	-	-	-	X
60	MG	AA	3034	-	-	-	X
60	MG	AA	3035	-	-	-	X
60	MG	AA	3036	-	-	-	X
60	MG	AA	3038	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3039	-	-	-	X
60	MG	AA	3042	-	-	-	X
60	MG	AA	3043	-	-	-	X
60	MG	AA	3044	-	-	-	X
60	MG	AA	3045	-	-	-	X
60	MG	AA	3047	-	-	-	X
60	MG	AA	3050	-	-	-	X
60	MG	AA	3052	-	-	-	X
60	MG	AA	3060	-	-	-	X
60	MG	AA	3082	-	-	-	X
60	MG	AA	3101	-	-	-	X
60	MG	AA	3102	-	-	-	X
60	MG	AA	3109	-	-	-	X
60	MG	AA	3110	-	-	-	X
60	MG	AA	3112	-	-	-	X
60	MG	AA	3115	-	-	-	X
60	MG	AA	3116	-	-	-	X
60	MG	AA	3119	-	-	-	X
60	MG	AA	3120	-	-	-	X
60	MG	AA	3121	-	-	-	X
60	MG	AA	3127	-	-	-	X
60	MG	AA	3129	-	-	-	X
60	MG	AA	3131	-	-	-	X
60	MG	AA	3133	-	-	-	X
60	MG	AA	3134	-	-	-	X
60	MG	AA	3137	-	-	-	X
60	MG	AA	3141	-	-	-	X
60	MG	AA	3144	-	-	-	X
60	MG	AA	3149	-	-	-	X
60	MG	AA	3160	-	-	-	X
60	MG	AA	3167	-	-	-	X
60	MG	AA	3168	-	-	-	X
60	MG	AA	3170	-	-	-	X
60	MG	AA	3172	-	-	-	X
60	MG	AA	3173	-	-	-	X
60	MG	AA	3178	-	-	-	X
60	MG	AA	3180	-	-	-	X
60	MG	AA	3181	-	-	-	X
60	MG	AA	3183	-	-	-	X
60	MG	AA	3184	-	-	-	X
60	MG	AA	3185	-	-	-	X
60	MG	AA	3187	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3190	-	-	-	X
60	MG	AA	3196	-	-	-	X
60	MG	AA	3200	-	-	-	X
60	MG	AA	3206	-	-	-	X
60	MG	AA	3210	-	-	-	X
60	MG	AA	3211	-	-	-	X
60	MG	AA	3212	-	-	-	X
60	MG	AA	3213	-	-	-	X
60	MG	AA	3217	-	-	-	X
60	MG	AA	3218	-	-	-	X
60	MG	AA	3220	-	-	-	X
60	MG	AA	3222	-	-	-	X
60	MG	AA	3228	-	-	-	X
60	MG	AA	3231	-	-	-	X
60	MG	AA	3240	-	-	-	X
60	MG	AA	3241	-	-	-	X
60	MG	AA	3248	-	-	-	X
60	MG	AA	3250	-	-	-	X
60	MG	AA	3251	-	-	-	X
60	MG	AA	3253	-	-	-	X
60	MG	AA	3257	-	-	-	X
60	MG	AA	3258	-	-	-	X
60	MG	AA	3272	-	-	-	X
60	MG	AA	3274	-	-	-	X
60	MG	AA	3277	-	-	-	X
60	MG	AA	3281	-	-	-	X
60	MG	AA	3289	-	-	-	X
60	MG	AA	3294	-	-	-	X
60	MG	AA	3296	-	-	-	X
60	MG	AA	3300	-	-	-	X
60	MG	AA	3302	-	-	-	X
60	MG	AA	3309	-	-	-	X
60	MG	AA	3310	-	-	-	X
60	MG	AA	3313	-	-	-	X
60	MG	AA	3315	-	-	-	X
60	MG	AA	3323	-	-	-	X
60	MG	AA	3330	-	-	-	X
60	MG	AA	3339	-	-	-	X
60	MG	AA	3347	-	-	-	X
60	MG	AA	3352	-	-	-	X
60	MG	AA	3354	-	-	-	X
60	MG	AA	3357	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3369	-	-	-	X
60	MG	AA	3376	-	-	-	X
60	MG	AA	3378	-	-	-	X
60	MG	AA	3384	-	-	-	X
60	MG	AA	3385	-	-	-	X
60	MG	AA	3386	-	-	-	X
60	MG	AA	3387	-	-	-	X
60	MG	AA	3398	-	-	-	X
60	MG	AA	3401	-	-	-	X
60	MG	AA	3408	-	-	-	X
60	MG	AA	3415	-	-	-	X
60	MG	AA	3417	-	-	-	X
60	MG	AA	3430	-	-	-	X
60	MG	AA	3437	-	-	-	X
60	MG	AA	3438	-	-	-	X
60	MG	AA	3451	-	-	-	X
60	MG	AA	3454	-	-	-	X
60	MG	AA	3460	-	-	-	X
60	MG	AA	3461	-	-	-	X
60	MG	AA	3471	-	-	-	X
60	MG	AA	3486	-	-	-	X
60	MG	AA	3505	-	-	-	X
60	MG	AA	3506	-	-	-	X
60	MG	AA	3507	-	-	-	X
60	MG	AA	3510	-	-	-	X
60	MG	AA	3513	-	-	-	X
60	MG	AA	3514	-	-	-	X
60	MG	AA	3516	-	-	-	X
60	MG	AA	3517	-	-	-	X
60	MG	AA	3518	-	-	-	X
60	MG	AA	3523	-	-	-	X
60	MG	AA	3524	-	-	-	X
60	MG	AA	3525	-	-	-	X
60	MG	AA	3528	-	-	-	X
60	MG	AA	3529	-	-	-	X
60	MG	AA	3532	-	-	-	X
60	MG	AA	3535	-	-	-	X
60	MG	AA	3539	-	-	-	X
60	MG	AA	3540	-	-	-	X
60	MG	AA	3541	-	-	-	X
60	MG	AA	3551	-	-	-	X
60	MG	AA	3556	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3559	-	-	-	X
60	MG	AA	3564	-	-	-	X
60	MG	AA	3565	-	-	-	X
60	MG	AA	3572	-	-	-	X
60	MG	AA	3581	-	-	-	X
60	MG	AA	3582	-	-	-	X
60	MG	AA	3589	-	-	-	X
60	MG	AA	3596	-	-	-	X
60	MG	AA	3602	-	-	-	X
60	MG	AA	3604	-	-	-	X
60	MG	AA	3654	-	-	-	X
60	MG	AA	3662	-	-	-	X
60	MG	AA	3669	-	-	-	X
60	MG	AA	3671	-	-	-	X
60	MG	AA	3686	-	-	-	X
60	MG	AA	3692	-	-	-	X
60	MG	AA	3698	-	-	-	X
60	MG	AA	3702	-	-	-	X
60	MG	AA	3705	-	-	-	X
60	MG	AA	3706	-	-	-	X
60	MG	AA	3708	-	-	-	X
60	MG	AA	3711	-	-	-	X
60	MG	AA	3712	-	-	-	X
60	MG	AA	3714	-	-	-	X
60	MG	AA	3717	-	-	-	X
60	MG	AA	3721	-	-	-	X
60	MG	AA	3735	-	-	-	X
60	MG	AA	3739	-	-	-	X
60	MG	AA	3740	-	-	-	X
60	MG	AA	3741	-	-	-	X
60	MG	AA	3767	-	-	-	X
60	MG	AA	3769	-	-	-	X
60	MG	AA	3770	-	-	-	X
60	MG	AA	3772	-	-	-	X
60	MG	AA	3790	-	-	-	X
60	MG	AA	3792	-	-	-	X
60	MG	AA	3796	-	-	-	X
60	MG	AA	3797	-	-	-	X
60	MG	AA	3803	-	-	-	X
60	MG	AA	3806	-	-	-	X
60	MG	AA	3810	-	-	-	X
60	MG	AA	3816	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	3817	-	-	-	X
60	MG	AA	3818	-	-	-	X
60	MG	AA	3819	-	-	-	X
60	MG	AA	3822	-	-	-	X
60	MG	AA	3823	-	-	-	X
60	MG	AA	3824	-	-	-	X
60	MG	AA	3825	-	-	-	X
60	MG	AA	3826	-	-	-	X
60	MG	AA	3827	-	-	-	X
60	MG	AA	3828	-	-	-	X
60	MG	AA	3829	-	-	-	X
60	MG	AA	3830	-	-	-	X
60	MG	AA	3832	-	-	-	X
60	MG	AA	3833	-	-	-	X
60	MG	AA	3834	-	-	-	X
60	MG	AB	3008	-	-	-	X
60	MG	AB	3014	-	-	-	X
60	MG	AB	3016	-	-	-	X
60	MG	AD	301	-	-	-	X
60	MG	AD	302	-	-	-	X
60	MG	AD	304	-	-	-	X
60	MG	AD	305	-	-	-	X
60	MG	AD	308	-	-	-	X
60	MG	AD	309	-	-	-	X
60	MG	AD	310	-	-	-	X
60	MG	AE	305	-	-	-	X
60	MG	AF	301	-	-	-	X
60	MG	AF	303	-	-	-	X
60	MG	AH	201	-	-	-	X
60	MG	AN	3001	-	-	-	X
60	MG	AN	3002	-	-	-	X
60	MG	AP	201	-	-	-	X
60	MG	AQ	3001	-	-	-	X
60	MG	AU	201	-	-	-	X
60	MG	AU	202	-	-	-	X
60	MG	AU	203	-	-	-	X
60	MG	AU	204	-	-	-	X
60	MG	AW	3003	-	-	-	X
60	MG	AX	102	-	-	-	X
60	MG	BA	1601	-	-	-	X
60	MG	BA	1615	-	-	-	X
60	MG	BA	1626	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	1629	-	-	-	X
60	MG	BA	1630	-	-	-	X
60	MG	BA	1648	-	-	-	X
60	MG	BA	1655	-	-	-	X
60	MG	BA	1658	-	-	-	X
60	MG	BA	1662	-	-	-	X
60	MG	BA	1671	-	-	-	X
60	MG	BA	1675	-	-	-	X
60	MG	BA	1679	-	-	-	X
60	MG	BA	1683	-	-	-	X
60	MG	BA	1686	-	-	-	X
60	MG	BA	1687	-	-	-	X
60	MG	BA	1701	-	-	-	X
60	MG	BA	1705	-	-	-	X
60	MG	BA	1724	-	-	-	X
60	MG	BA	1749	-	-	-	X
60	MG	BA	1757	-	-	-	X
60	MG	BA	1765	-	-	-	X
60	MG	BA	1778	-	-	-	X
60	MG	BA	1785	-	-	-	X
60	MG	BA	1804	-	-	-	X
60	MG	BB	3001	-	-	-	X
60	MG	C3	101	-	-	-	X
60	MG	C5	101	-	-	-	X
60	MG	C7	101	-	-	-	X
60	MG	CA	3002	-	-	-	X
60	MG	CA	3004	-	-	-	X
60	MG	CA	3013	-	-	-	X
60	MG	CA	3018	-	-	-	X
60	MG	CA	3022	-	-	-	X
60	MG	CA	3026	-	-	-	X
60	MG	CA	3028	-	-	-	X
60	MG	CA	3032	-	-	-	X
60	MG	CA	3035	-	-	-	X
60	MG	CA	3038	-	-	-	X
60	MG	CA	3068	-	-	-	X
60	MG	CA	3082	-	-	-	X
60	MG	CA	3083	-	-	-	X
60	MG	CA	3084	-	-	-	X
60	MG	CA	3087	-	-	-	X
60	MG	CA	3099	-	-	-	X
60	MG	CA	3100	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	3102	-	-	-	X
60	MG	CA	3103	-	-	-	X
60	MG	CA	3106	-	-	-	X
60	MG	CA	3110	-	-	-	X
60	MG	CA	3114	-	-	-	X
60	MG	CA	3115	-	-	-	X
60	MG	CA	3121	-	-	-	X
60	MG	CA	3122	-	-	-	X
60	MG	CA	3129	-	-	-	X
60	MG	CA	3143	-	-	-	X
60	MG	CA	3154	-	-	-	X
60	MG	CA	3156	-	-	-	X
60	MG	CA	3157	-	-	-	X
60	MG	CA	3160	-	-	-	X
60	MG	CA	3163	-	-	-	X
60	MG	CA	3165	-	-	-	X
60	MG	CA	3166	-	-	-	X
60	MG	CA	3179	-	-	-	X
60	MG	CA	3181	-	-	-	X
60	MG	CA	3182	-	-	-	X
60	MG	CA	3184	-	-	-	X
60	MG	CA	3187	-	-	-	X
60	MG	CA	3198	-	-	-	X
60	MG	CA	3209	-	-	-	X
60	MG	CA	3210	-	-	-	X
60	MG	CA	3214	-	-	-	X
60	MG	CA	3215	-	-	-	X
60	MG	CA	3218	-	-	-	X
60	MG	CA	3220	-	-	-	X
60	MG	CA	3226	-	-	-	X
60	MG	CA	3227	-	-	-	X
60	MG	CA	3233	-	-	-	X
60	MG	CA	3236	-	-	-	X
60	MG	CA	3249	-	-	-	X
60	MG	CA	3264	-	-	-	X
60	MG	CA	3265	-	-	-	X
60	MG	CA	3274	-	-	-	X
60	MG	CA	3279	-	-	-	X
60	MG	CA	3282	-	-	-	X
60	MG	CA	3288	-	-	-	X
60	MG	CA	3293	-	-	-	X
60	MG	CA	3307	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	3311	-	-	-	X
60	MG	CA	3312	-	-	-	X
60	MG	CA	3315	-	-	-	X
60	MG	CA	3320	-	-	-	X
60	MG	CA	3324	-	-	-	X
60	MG	CA	3330	-	-	-	X
60	MG	CA	3346	-	-	-	X
60	MG	CA	3356	-	-	-	X
60	MG	CA	3359	-	-	-	X
60	MG	CA	3366	-	-	-	X
60	MG	CA	3381	-	-	-	X
60	MG	CA	3407	-	-	-	X
60	MG	CA	3408	-	-	-	X
60	MG	CA	3411	-	-	-	X
60	MG	CA	3413	-	-	-	X
60	MG	CA	3418	-	-	-	X
60	MG	CA	3423	-	-	-	X
60	MG	CA	3430	-	-	-	X
60	MG	CA	3431	-	-	-	X
60	MG	CA	3438	-	-	-	X
60	MG	CA	3439	-	-	-	X
60	MG	CA	3446	-	-	-	X
60	MG	CA	3449	-	-	-	X
60	MG	CA	3450	-	-	-	X
60	MG	CA	3454	-	-	-	X
60	MG	CA	3455	-	-	-	X
60	MG	CA	3460	-	-	-	X
60	MG	CA	3463	-	-	-	X
60	MG	CA	3464	-	-	-	X
60	MG	CA	3473	-	-	-	X
60	MG	CA	3488	-	-	-	X
60	MG	CA	3496	-	-	-	X
60	MG	CA	3500	-	-	-	X
60	MG	CA	3529	-	-	-	X
60	MG	CA	3541	-	-	-	X
60	MG	CA	3549	-	-	-	X
60	MG	CA	3558	-	-	-	X
60	MG	CA	3576	-	-	-	X
60	MG	CA	3595	-	-	-	X
60	MG	CA	3598	-	-	-	X
60	MG	CA	3601	-	-	-	X
60	MG	CA	3617	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	CA	3619	-	-	-	X
60	MG	CA	3625	-	-	-	X
60	MG	CA	3641	-	-	-	X
60	MG	CA	3652	-	-	-	X
60	MG	CA	3653	-	-	-	X
60	MG	CA	3655	-	-	-	X
60	MG	CA	3656	-	-	-	X
60	MG	CA	3659	-	-	-	X
60	MG	CA	3662	-	-	-	X
60	MG	CD	301	-	-	-	X
60	MG	CE	301	-	-	-	X
60	MG	CE	303	-	-	-	X
60	MG	CE	304	-	-	-	X
60	MG	CF	301	-	-	-	X
60	MG	CF	302	-	-	-	X
60	MG	CF	306	-	-	-	X
60	MG	CQ	201	-	-	-	X
60	MG	CQ	202	-	-	-	X
60	MG	CU	201	-	-	-	X
60	MG	CV	201	-	-	-	X
60	MG	CV	202	-	-	-	X
60	MG	DA	1602	-	-	-	X
60	MG	DA	1611	-	-	-	X
60	MG	DA	1619	-	-	-	X
60	MG	DA	1631	-	-	-	X
60	MG	DA	1637	-	-	-	X
60	MG	DA	1638	-	-	-	X
60	MG	DA	1646	-	-	-	X
60	MG	DA	1650	-	-	-	X
60	MG	DA	1651	-	-	-	X
60	MG	DA	1667	-	-	-	X
60	MG	DA	1674	-	-	-	X
60	MG	DA	1679	-	-	-	X
60	MG	DA	1686	-	-	-	X
60	MG	DA	1688	-	-	-	X
60	MG	DA	1694	-	-	-	X
60	MG	DA	1696	-	-	-	X
60	MG	DA	1706	-	-	-	X
60	MG	DA	1714	-	-	-	X
60	MG	DA	1719	-	-	-	X
60	MG	DA	1742	-	-	-	X
60	MG	DA	1767	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DE	201	-	-	-	X

## 2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 313372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2872	Total	C	N	O	P	0	0	0
			61861	27532	11574	19884	2871			
1	CA	2868	Total	C	N	O	P	0	0	0
			61771	27492	11554	19858	2867			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
2	CB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			
3	CC	137	Total	C	N	O	S	0	0	0
			1063	669	201	192	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
4	CD	275	Total	C	N	O	S	0	0	0
			2142	1352	426	361	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
5	CE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
6	CF	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
7	CG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
8	CH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AK	130	Total	C	N	O		0	0	0
			641	381	130	130				
9	CK	130	Total	C	N	O		0	0	0
			641	381	130	130				

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	66	Total	C	N	O	S	0	0	0
			498	310	93	92	3			

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
11	CN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
12	CO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	149	Total	C	N	O	S	0	0	0
			1139	709	231	196	3			
13	CP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
14	CQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
15	CR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			



- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	AS	110	Total	C	N	O	0	0	0
			877	553	175	149			
16	CS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
17	CT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
18	CU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
19	CV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
20	CW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
21	CX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
22	CY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
23	CZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
25	C1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	59	Total	C	N	O		0	0	0
			469	298	90	81				
27	C3	59	Total	C	N	O		0	0	0
			464	296	90	78				

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
28	C4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
29	C5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
30	C6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
31	C7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
32	C8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
33	C9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 34 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1497	Total	C	N	O	P	0	0	0
			32185	14324	5968	10396	1497			
34	DA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
35	DB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
36	DC	206	Total	C	N	O	S	0	0	0
			1544	970	300	273	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
37	DD	208	Total	C	N	O	S	0	0	0
			1678	1052	333	286	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
38	DE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	100	Total	C	N	O	S	0	0	0
			812	514	146	149	3			
39	DF	100	Total	C	N	O	S	0	0	0
			820	518	147	152	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
40	DG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
41	DH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	127	Total	C	N	O		0	0	0
			986	626	193	167				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	97	Total	C	N	O	0	0	0
			709	440	138	131			
43	DJ	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			
44	DK	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			
45	DL	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	123	Total	C	N	O	S	0	0	0
			966	598	200	166	2			
46	DM	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
48	DO	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
49	DP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
50	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BR	68	Total	C	N	O	0	0	0
			555	355	108	92			
51	DR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BS	84	Total	C	N	O	S	0	0	0
			661	423	122	114	2			
52	DS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
53	DT	96	Total	C	N	O	S	0	0	0
			731	449	156	124	2			

- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BU	23	Total	C	N	O		0	0	0
			199	122	48	29				
54	DU	23	Total	C	N	O		0	0	0
			199	122	48	29				

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
55	DV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 56 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	74	Total	C	N	O	P	0	0	0
			1599	722	287	515	73			
56	DW	72	Total	C	N	O	P	0	0	0
			1552	697	280	502	72			

- Molecule 57 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BX	76	Total	C	N	O	P	0	0	0
			1635	731	296	530	76			
57	DX	76	Total	C	N	O	P	0	0	0
			1635	731	296	530	76			

- Molecule 58 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BY	74	Total	C	N	O	P	0	0	0
			1581	707	285	515	73			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
58	DY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 59 is a protein called 50S ribosomal protein L9,Elongation factor G.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
59	BZ	728	Total	C	N	O	S		0	0	0
			5663	3599	973	1072	19				
59	DZ	730	Total	C	N	O	S		0	0	0
			5682	3611	978	1074	19				

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AP	2	Total	Mg	0	0
			2	2		
60	CR	2	Total	Mg	0	0
			2	2		
60	BA	213	Total	Mg	0	0
			213	213		
60	CA	664	Total	Mg	0	0
			664	664		
60	C8	1	Total	Mg	0	0
			1	1		
60	C5	1	Total	Mg	0	0
			1	1		
60	AB	23	Total	Mg	0	0
			23	23		
60	BL	2	Total	Mg	0	0
			2	2		
60	CV	2	Total	Mg	0	0
			2	2		
60	A6	1	Total	Mg	0	0
			1	1		
60	BE	1	Total	Mg	0	0
			1	1		
60	AW	4	Total	Mg	0	0
			4	4		
60	AN	3	Total	Mg	0	0
			3	3		
60	DZ	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	2	Total 2	Mg 2	0	0
60	CN	1	Total 1	Mg 1	0	0
60	A2	1	Total 1	Mg 1	0	0
60	DX	1	Total 1	Mg 1	0	0
60	CY	1	Total 1	Mg 1	0	0
60	DD	1	Total 1	Mg 1	0	0
60	BB	1	Total 1	Mg 1	0	0
60	BT	1	Total 1	Mg 1	0	0
60	AE	5	Total 5	Mg 5	0	0
60	BM	1	Total 1	Mg 1	0	0
60	CU	1	Total 1	Mg 1	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	1	Total 1	Mg 1	0	0
60	BX	15	Total 15	Mg 15	0	0
60	DA	168	Total 168	Mg 168	0	0
60	CB	13	Total 13	Mg 13	0	0
60	C0	2	Total 2	Mg 2	0	0
60	AA	834	Total 834	Mg 834	0	0
60	DF	1	Total 1	Mg 1	0	0
60	CQ	4	Total 4	Mg 4	0	0
60	A5	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AR	1	Total 1	Mg 1	0	0
60	CG	1	Total 1	Mg 1	0	0
60	DK	2	Total 2	Mg 2	0	0
60	A1	2	Total 2	Mg 2	0	0
60	AD	10	Total 10	Mg 10	0	0
60	BN	2	Total 2	Mg 2	0	0
60	DJ	1	Total 1	Mg 1	0	0
60	BY	2	Total 2	Mg 2	0	0
60	C7	1	Total 1	Mg 1	0	0
60	C3	1	Total 1	Mg 1	0	0
60	AZ	1	Total 1	Mg 1	0	0
60	A4	1	Total 1	Mg 1	0	0
60	BK	1	Total 1	Mg 1	0	0
60	AU	4	Total 4	Mg 4	0	0
60	DW	1	Total 1	Mg 1	0	0
60	A9	1	Total 1	Mg 1	0	0
60	CF	6	Total 6	Mg 6	0	0
60	BV	1	Total 1	Mg 1	0	0
60	A0	5	Total 5	Mg 5	0	0
60	AG	2	Total 2	Mg 2	0	0
60	DE	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AQ	3	Total 3	Mg 3	0	0
60	CE	6	Total 6	Mg 6	0	0
60	AH	1	Total 1	Mg 1	0	0
60	BZ	1	Total 1	Mg 1	0	0
60	CO	2	Total 2	Mg 2	0	0
60	CP	1	Total 1	Mg 1	0	0
60	A7	1	Total 1	Mg 1	0	0
60	CD	4	Total 4	Mg 4	0	0
60	BD	1	Total 1	Mg 1	0	0
60	DT	1	Total 1	Mg 1	0	0
60	A8	2	Total 2	Mg 2	0	0
60	AO	1	Total 1	Mg 1	0	0
60	BW	2	Total 2	Mg 2	0	0
60	AY	1	Total 1	Mg 1	0	0
60	AF	5	Total 5	Mg 5	0	0

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	1	Total 1	K 1	0	0

- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

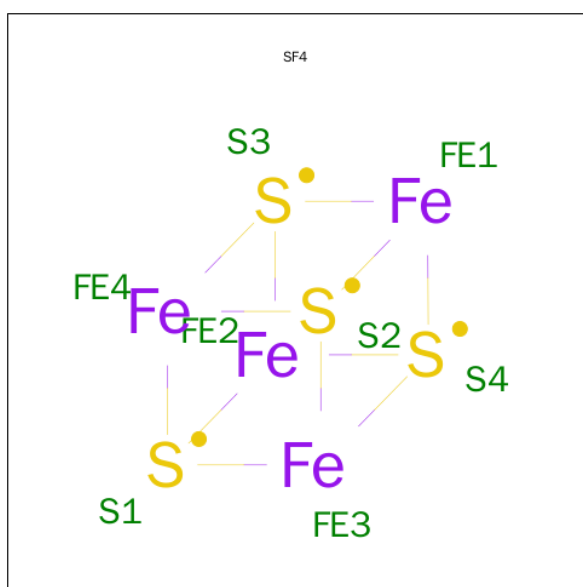
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	1	Total 1	Zn 1	0	0

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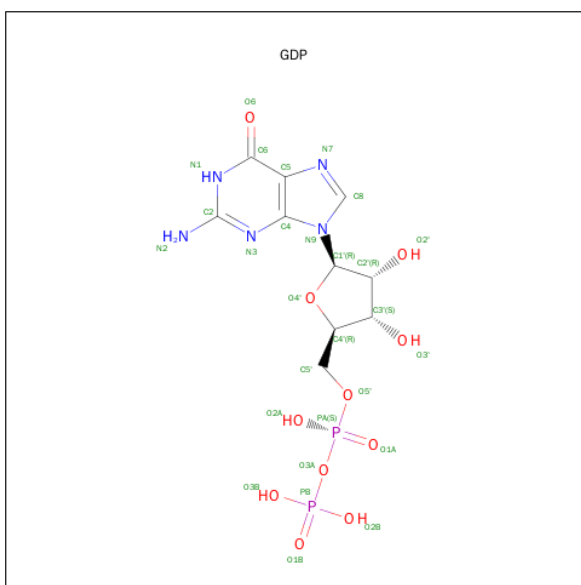
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	BN	1	Total	Zn	0	0
			1	1		
62	C4	1	Total	Zn	0	0
			1	1		
62	C5	1	Total	Zn	0	0
			1	1		
62	C6	1	Total	Zn	0	0
			1	1		
62	A6	1	Total	Zn	0	0
			1	1		
62	C9	1	Total	Zn	0	0
			1	1		
62	DN	1	Total	Zn	0	0
			1	1		
62	A4	1	Total	Zn	0	0
			1	1		
62	A5	1	Total	Zn	0	0
			1	1		
62	A9	1	Total	Zn	0	0
			1	1		
62	CY	1	Total	Zn	0	0
			1	1		

- Molecule 63 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	BD	1	Total	Fe	S	0	0
			8	4	4		
63	DD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
64	BZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
64	DZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AA	1408	Total	O	0	0
			1408	1408		
65	AB	36	Total	O	0	0
			36	36		
65	AD	15	Total	O	0	0
			15	15		
65	AE	19	Total	O	0	0
			19	19		
65	AF	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	AG	3	Total 3	O 3	0	0
65	AH	1	Total 1	O 1	0	0
65	AN	2	Total 2	O 2	0	0
65	AO	1	Total 1	O 1	0	0
65	AP	15	Total 15	O 15	0	0
65	AQ	4	Total 4	O 4	0	0
65	AR	2	Total 2	O 2	0	0
65	AS	1	Total 1	O 1	0	0
65	AT	2	Total 2	O 2	0	0
65	AU	5	Total 5	O 5	0	0
65	AV	2	Total 2	O 2	0	0
65	AW	2	Total 2	O 2	0	0
65	AX	3	Total 3	O 3	0	0
65	AZ	1	Total 1	O 1	0	0
65	A0	6	Total 6	O 6	0	0
65	A1	1	Total 1	O 1	0	0
65	A3	1	Total 1	O 1	0	0
65	A5	3	Total 3	O 3	0	0
65	A6	2	Total 2	O 2	0	0
65	A7	4	Total 4	O 4	0	0
65	A8	10	Total 10	O 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	BA	212	Total 212	O 212	0	0
65	BD	2	Total 2	O 2	0	0
65	BE	2	Total 2	O 2	0	0
65	BL	1	Total 1	O 1	0	0
65	BM	1	Total 1	O 1	0	0
65	BV	2	Total 2	O 2	0	0
65	BW	3	Total 3	O 3	0	0
65	BX	8	Total 8	O 8	0	0
65	BY	1	Total 1	O 1	0	0
65	BZ	2	Total 2	O 2	0	0
65	CA	985	Total 985	O 985	0	0
65	CB	9	Total 9	O 9	0	0
65	CD	14	Total 14	O 14	0	0
65	CE	13	Total 13	O 13	0	0
65	CF	7	Total 7	O 7	0	0
65	CN	2	Total 2	O 2	0	0
65	CP	10	Total 10	O 10	0	0
65	CQ	1	Total 1	O 1	0	0
65	CR	1	Total 1	O 1	0	0
65	CT	3	Total 3	O 3	0	0
65	CU	2	Total 2	O 2	0	0

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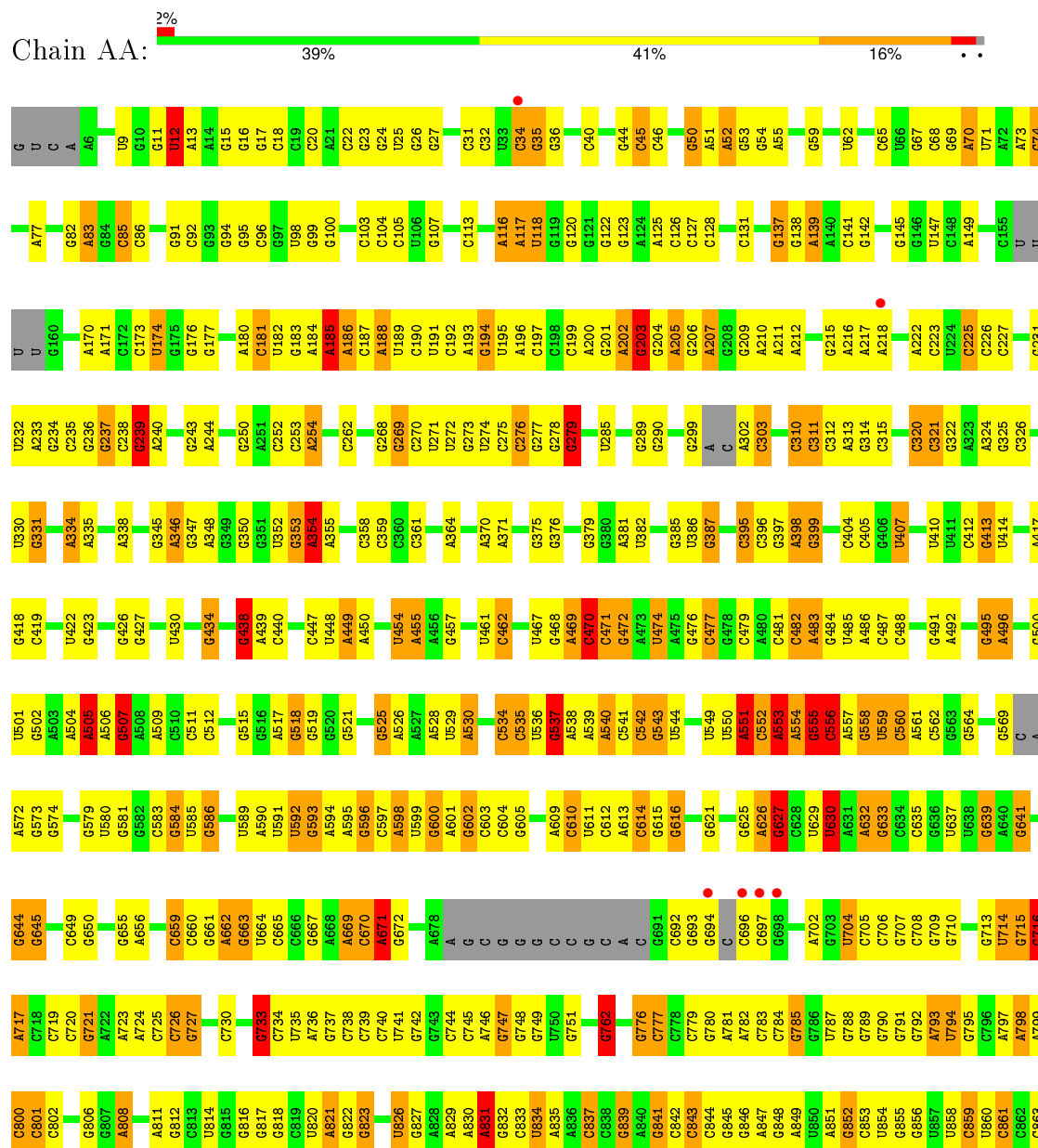
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
65	CV	1	Total	O	0	0
			1	1		
65	CY	1	Total	O	0	0
			1	1		
65	C0	6	Total	O	0	0
			6	6		
65	C1	2	Total	O	0	0
			2	2		
65	C3	2	Total	O	0	0
			2	2		
65	C6	1	Total	O	0	0
			1	1		
65	C7	1	Total	O	0	0
			1	1		
65	C8	3	Total	O	0	0
			3	3		
65	DA	155	Total	O	0	0
			155	155		
65	DE	4	Total	O	0	0
			4	4		
65	DJ	1	Total	O	0	0
			1	1		
65	DK	2	Total	O	0	0
			2	2		
65	DL	1	Total	O	0	0
			1	1		
65	DW	2	Total	O	0	0
			2	2		
65	DX	1	Total	O	0	0
			1	1		

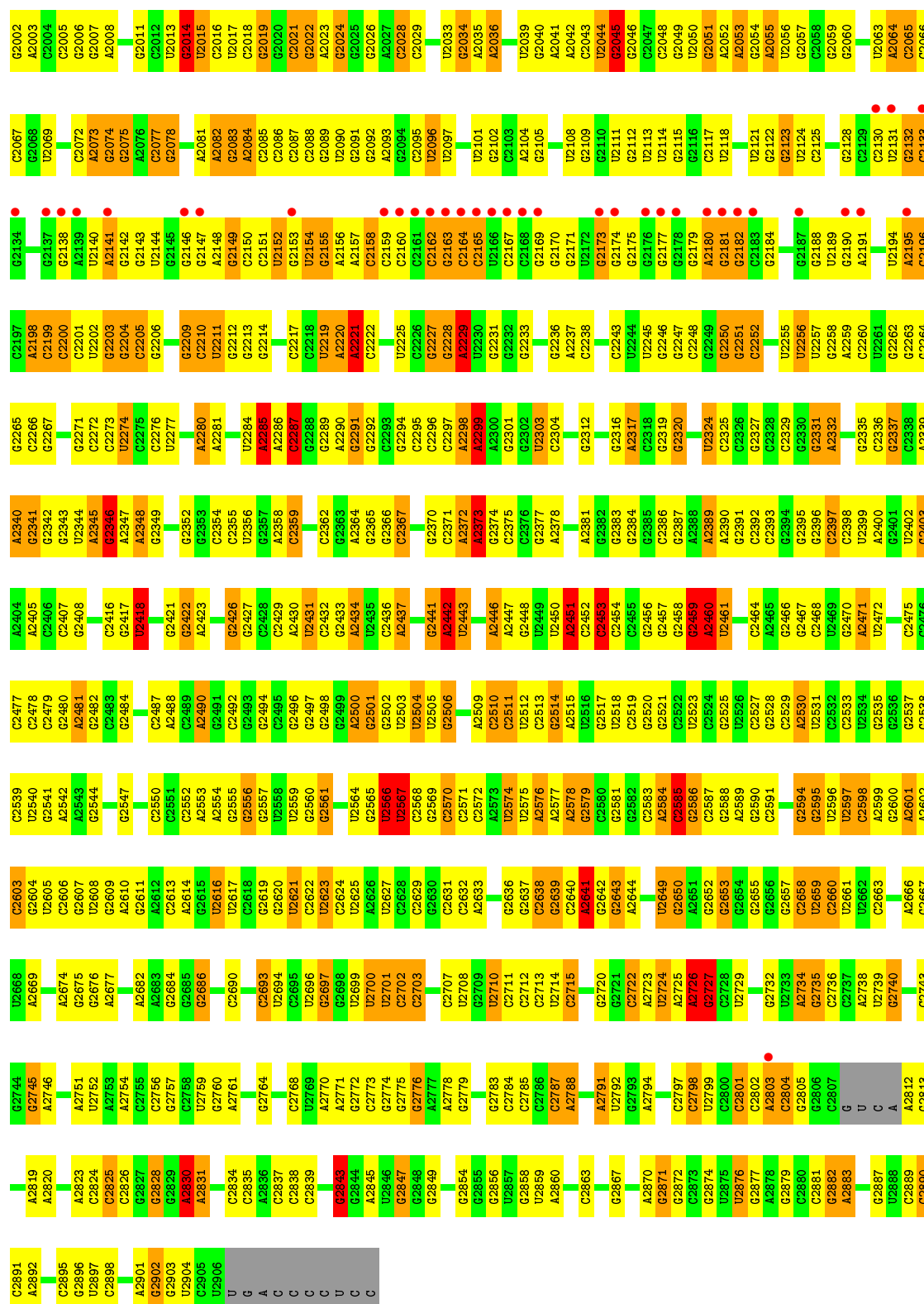
### 3 Residue-property plots

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: 23S Ribosomal RNA



U1920	A1833	G1754	A1678	C1595	G1513	U1437	G1366	G1290	G1214	G1139	A1073	G1007	C935	C984
G1921	A1834	C1755	A1679	C1596	C1514	U1438	A1367	G1291	G1217	U1140	A1074	U1008	C936	G865
A1922	C1835	U1756	C1683	C1597	C1515	A1439	U1369	A1292	G1218	A1141	A1075	C1010	A937	A866
A1923	U1836	C1757		C1598		U1440	U1370	G1294	U1219	U1143	G1076	G1011	G938	A867
C1924	U1839	G1764	U1686	C1604	A1518	A1441	G1371	U1295	U1220	A1144	A1077	U1014	C939	A868
G1925	A1840	U1765	C1687	A1605	G1522	U1442	G1374	G1296	G1221	U1147	U1078	U1015	U941	U869
G1928	A1841	U1766	A1688	G1606	G1525	U1443	U1375	G1297	C1223		G1080	C1016	A942	A871
G1929	A1842	U1767	G1689	G1607	G1526	C1444	C1376	A1299	C1222		C1084	U1017	C943	A872
C1930	A1843	U1768	G1690	C1611	G1529	C1445	A1377	A1300	G1231	C1150	C1087	U1018	A944	U873
	A1844	G1769	G1691	C1612		C1448	G1378	U1301	U1233	G1152		G1019	A945	U874
A1935	G1845	A1770	G1692	A1613		C1449	C1379	G1302	U1234	G1153		C1020	A946	U875
	A1846	G1771	G1693	A1618		G1450	G1380	C1303	A1235	U1154	G1090	G1021	U953	A876
G1938	G1847	G1772	G1694			U1451	U1381	C1304	G1237	U1155		A1027	G877	
U1939	A1848	C1775	G1695	A1616		U1452	A1382	G1305		G1156	A1091	G1022	C954	G878
U1940	A1849	G1776	G1696	A1617	C1539	C1453	G1383	C1306	G1237	G1157	A1092	G1023	A955	G879
A1941	A1850		G1697	A1618		C1454	G1384	G1306		U1158	G1093	G1024	A956	U880
G1942		C1782		U1623	A1542	G1455	G1385		G1240	U1159	A1094	G1025	A957	C881
G1943	G1855	C1783	A1701	U1624	U1543	G1456	U1386	A1311	G1241	U1160	A1096	A1026	C958	A882
G1944	A1856	C1785	A1702	C1624	C1544	C1457	U1387	G1312	G1242		G1097	G1027	U959	G883
U1945		U1786	C1703	G1625	C1545	A1458	A1388	A1313	U1243	C1169	C1098	A1029	C961	C884
	G1859	G1787	C1704	A1626	G1546			A1314	U1244	C1170	C1099	A1030	G962	U886
G1951	A1860	U1788	C1705	A1627		G1462	G1391	A1315	C1245	G1171	A1100	C1031	A963	C887
G1952	C1861			G1628	U1549	C1463	G1392	G1316	C1246	A1172	G1101	G1032		A888
U1953			C1709	G1629	C1550		G1393	G1317	C1247	U1173	G1102	G1033	C969	
A1954		A1793	C1710	A1630	C1551	U1466	C1397	A1321	A1248	A1174	A1103	A1036	C970	C891
G1955	G1870	G1794	A1711	C1631	C1552	U1467	U1398	A1322	A1249	A1175	G1104	A1037	C971	G892
C1956	U1871	G1795	A1712	A1632	C1553	G1468	G1399	G1323		U1176	G1105	C1038	A972	C893
G1957	G1872	C1796	G1713	A1554	C1555		A1399	G1324	C1252	U1177	U1106	G1039	G973	U894
	G1873		G1714	C1634	C1556	G1472	A1400	A1324	G1254	U1178	U1107	G1040	G974	G895
A1960	C1874	C1802	A1715	U1635	A1566	A1473	G1401		A1255	U1179	G1108	C1041	U975	A896
U1961		G1803	A1716	U1636	C1561	C1474	G1402	G1329	U1256	C1180	G1109	A1042	G976	U898
U1962		A1804	C1717	G1637		G1475	U1403	A1332	U1257	G1182	C1110	G1043	A977	
C1963	G1870	C1805	U1718	A1643	U1566	C1476	A1405	A1336	A1258	G1183	U1111	C1044	G978	C899
U1965	U1882	G1807	C1720	C1644	G1567	U1477	A1406	A1259	G1260	G1184	A1113	G1048	C980	U905
U1966	C1883	U1808	G1721	C1645		C1478		A1337	G1261	C1185	G1114	G1049	C981	G906
G1967		U1809	G1722	C1646	G1571	U1479	G1406	C1337		U1186	A1115	G1050	A986	U907
	U1889	U1810	A1723	C1647	G1572	A1480	G1410	U1338	G1264	U1187	A1116	C1051	A987	A908
U1968	A1890	A1811	U1724	U1648	G1573		A1411	C1339	U1265	A1188	G1117	G1052	U988	G909
	G1891	C1812	G1725		A1574	G1484	A1412		G1265	A1189	C1118	C1053	U989	
A1975	G1892	C1813		C1653	A1575	U1485	G1415	G1342	C1270	G1190		C1054	C912	U905
U1977		A1814	G1728	A1654	G1576	U1486		C1343	G1271		C1121	A1055	A913	
	A1898	A1815		A1655	G1577	G1487	U1418	C1344		C1196	C1122	A1056	G991	
C1980	A1899	A1816	U1735	A1656	C1578	G1488		G1345		C1197	A1123	A1057	G992	G916
G1981	C1901	A1817	A1736	C1657	C1579		A1419	U1346	G1272	C1198	U1124	G1058	G993	A917
C1983				C1658	G	A1491	G1420	A1347	G1273	C1199	C1125	U1058	C994	U918
C1984	G1905	C1821	C1741	G1659	U	C1492	A1248	A1348	G1274	G1200	C1126	G1059	G995	
U1985	A1906	A1822	G1742	A1660	C	G1493	G1423	G1349	G1275	A1201	U1127		C996	U924
G1986	A1907	G1823	G1743	A1664	G1584	U1495	A1424	A1354	G1278		U1128	G1062	G997	A925
C1987	C1908	U1824	G1744	G1665	G1585	A1496	A1425	G1355		C1204	U1129	U1065	A998	G926
C1988		U1825	A1745	G1666	G1586	G1497	G1426	G1356	G1281		A1130	A1066	G999	G927
G1989		G1826	G1746	U1667	U1587	G1427	G1427	G1357	G1284	C1207	A1131	A1067	C1000	G928
	A1911	U1827	A1747	A1500	G1588	A1500	A1430	U1358	G1285	G1208		G1068	G1001	G929
	G1912	C1828		U1501	A1589	U1501	A1431	U1359	G1286	G1209	A1134	A1069	A1002	G930
A1993		U1829	G1750	G1502	C1590	G1502	G1431	C1360	U1287	G1210	G1135	U1069	U1003	C931
A1994		C1831	G1751	G1673		G1508	C1432	C1361	A1288	G1212	U1136	G1070	A1004	C932
	C1917		U1753		C1593		G1434	G1365	G1289	U1213	C1138	U1072	A1005	C933
C2001					C1594								C1006	A934

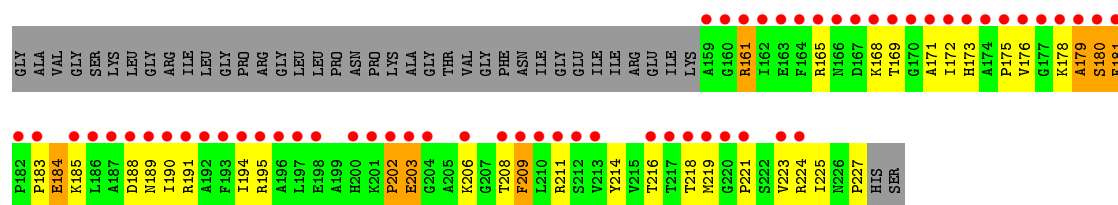


# • Molecule 1: 23S Ribosomal RNA

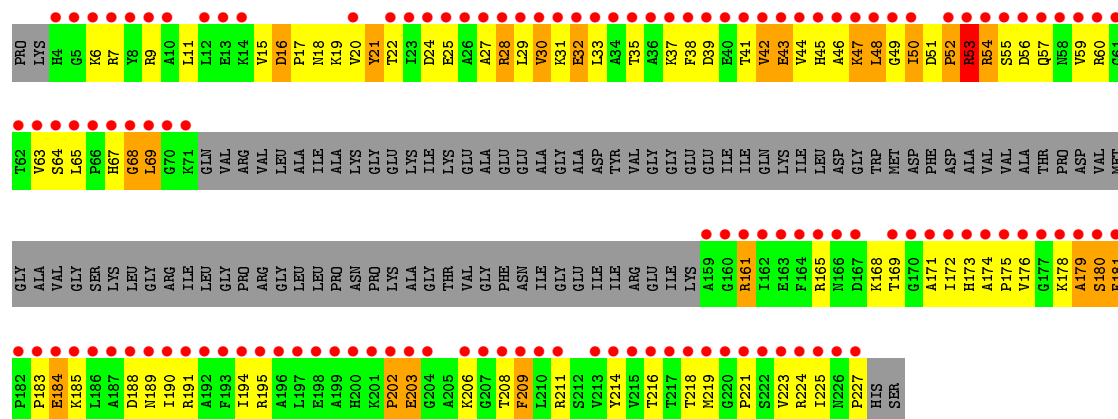
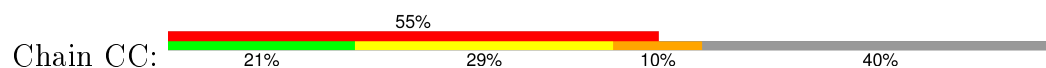




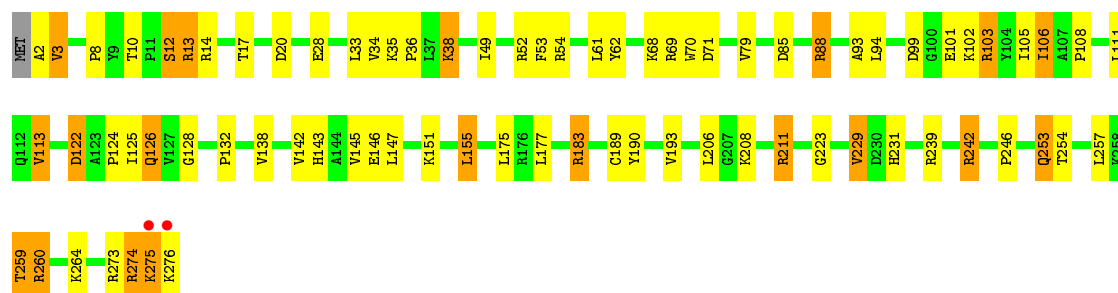
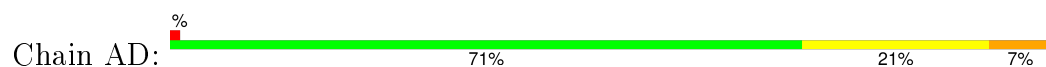




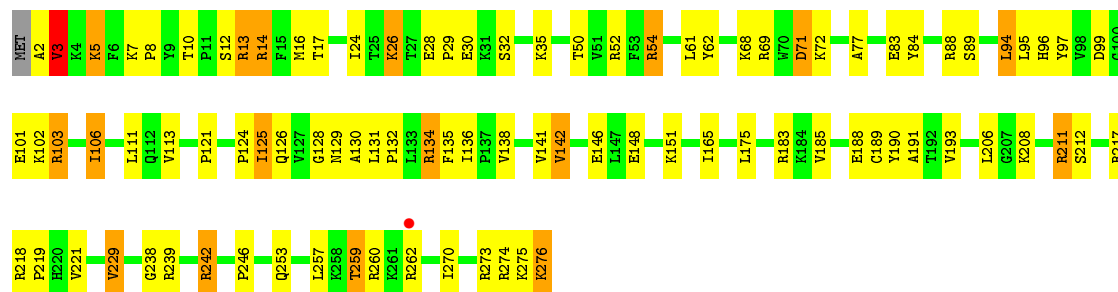
• Molecule 3: 50S ribosomal protein L1



• Molecule 4: 50S ribosomal protein L2

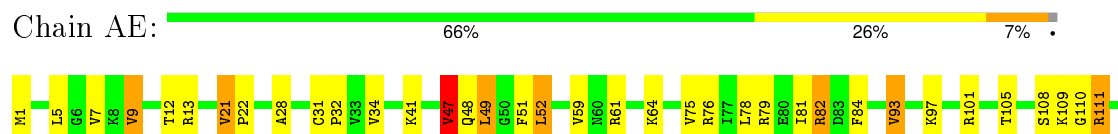


• Molecule 4: 50S ribosomal protein L2

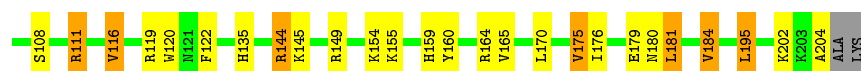
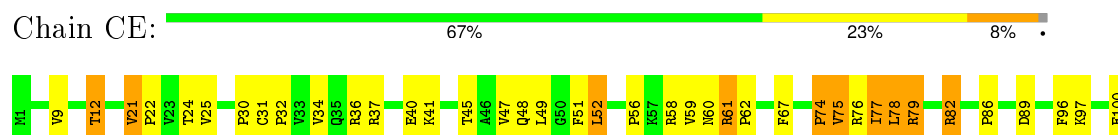


• Molecule 5: 50S ribosomal protein L3

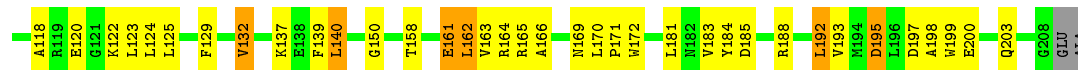
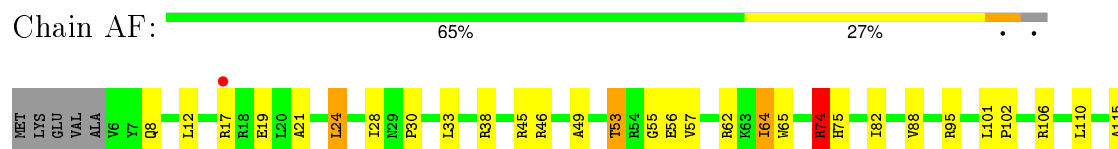




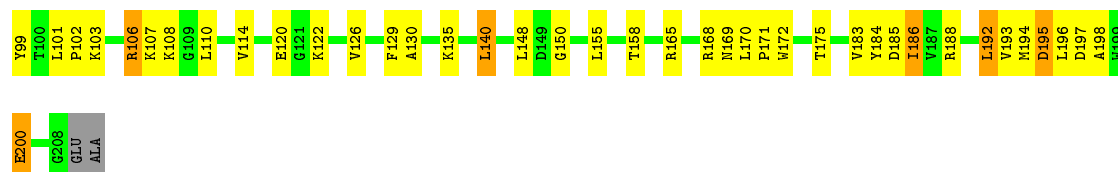
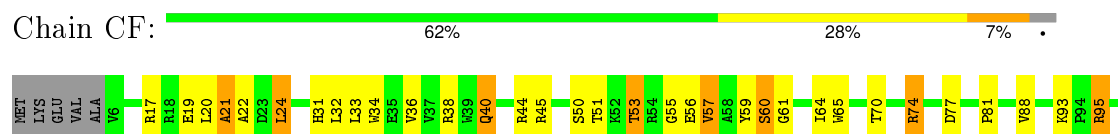
• Molecule 5: 50S ribosomal protein L3



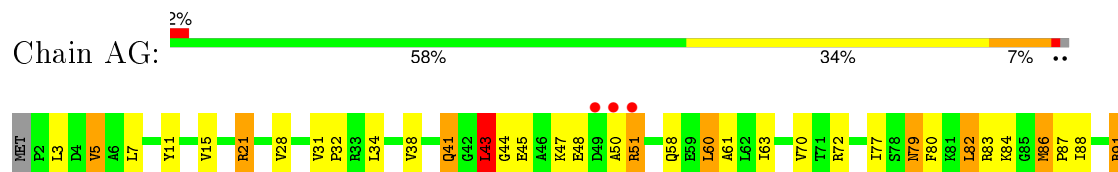
• Molecule 6: 50S ribosomal protein L4

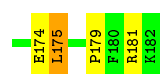


• Molecule 6: 50S ribosomal protein L4

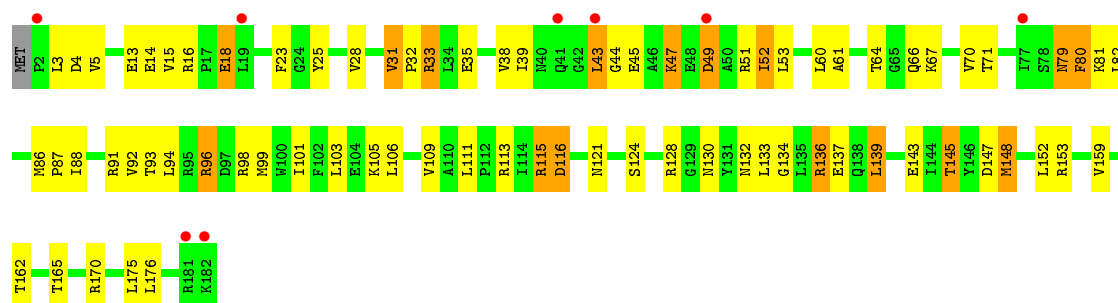


• Molecule 7: 50S ribosomal protein L5

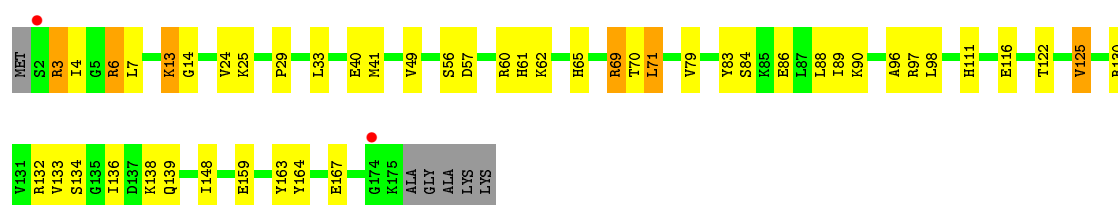




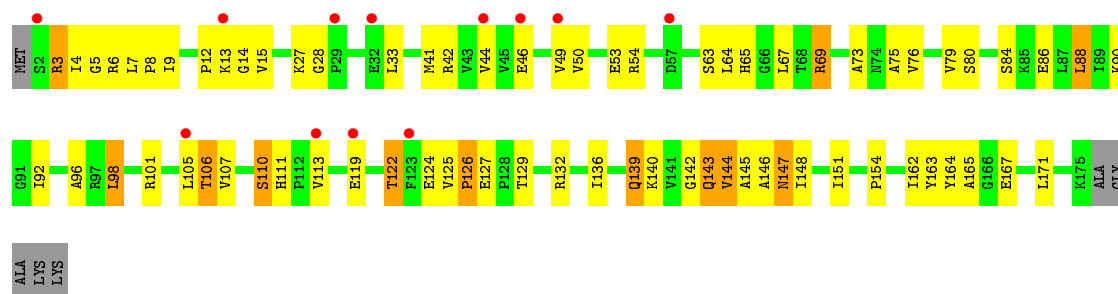
• Molecule 7: 50S ribosomal protein L5



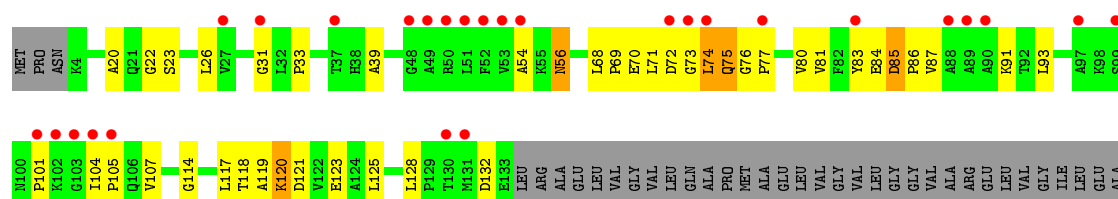
• Molecule 8: 50S ribosomal protein L6



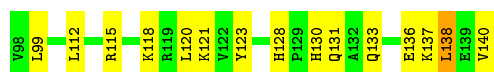
• Molecule 8: 50S ribosomal protein L6



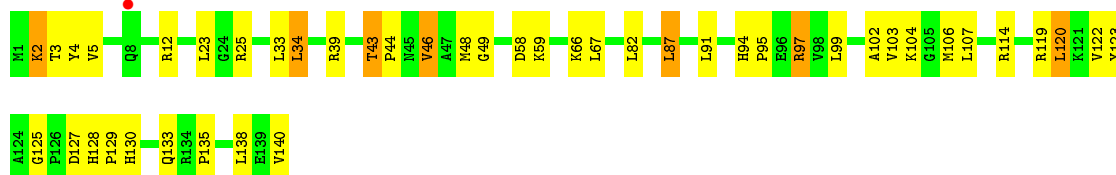
• Molecule 9: 50S ribosomal protein L10



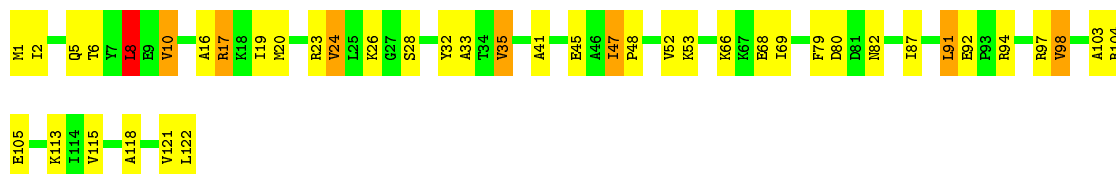




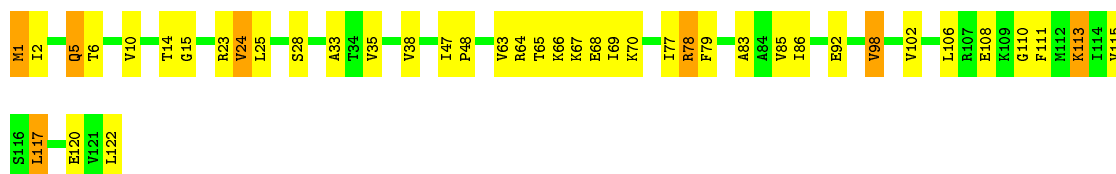
- Molecule 11: 50S ribosomal protein L13



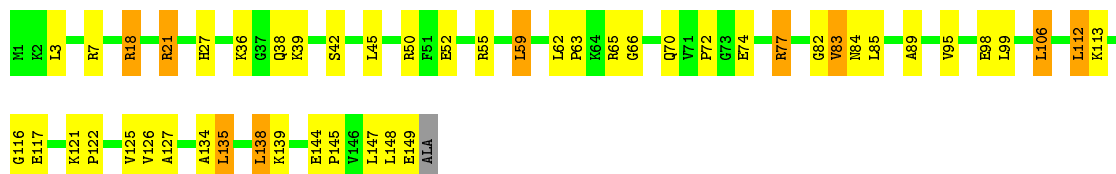
- Molecule 12: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L14



- Molecule 13: 50S ribosomal protein L15



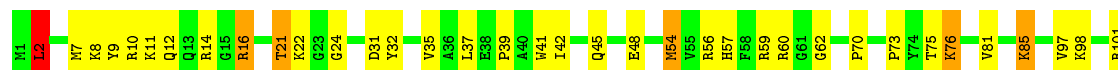
- Molecule 13: 50S ribosomal protein L15





- Molecule 14: 50S ribosomal protein L16

Chain AQ: 65% 28% 6%



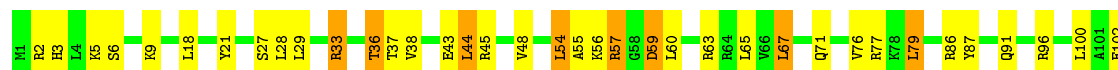
- Molecule 14: 50S ribosomal protein L16

Chain CQ: 66% 28% 6%



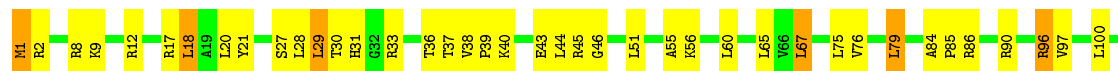
- Molecule 15: 50S ribosomal protein L17

Chain AR: 64% 29% 7%



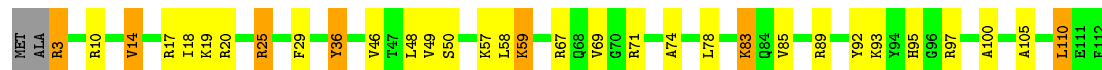
- Molecule 15: 50S ribosomal protein L17

Chain CR: 60% 34% 6%

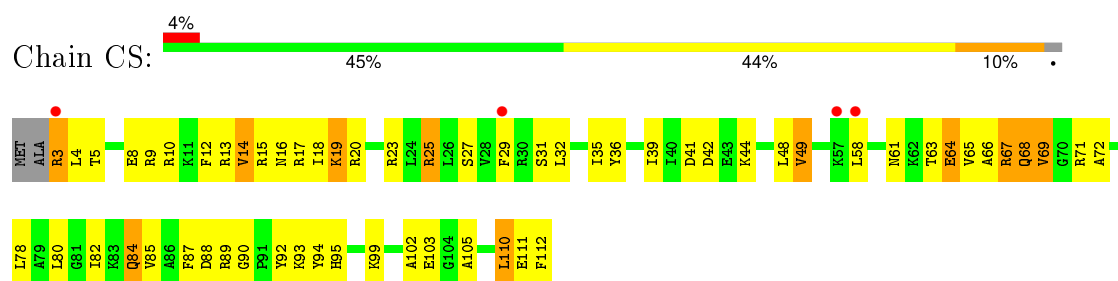


- Molecule 16: 50S ribosomal protein L18

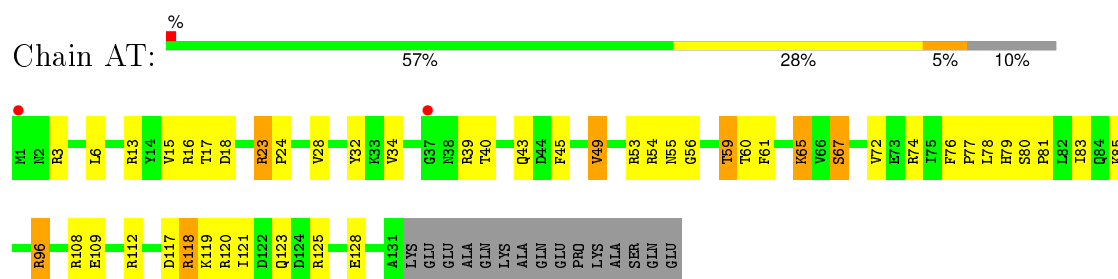
Chain AS: 70% 22% 6%



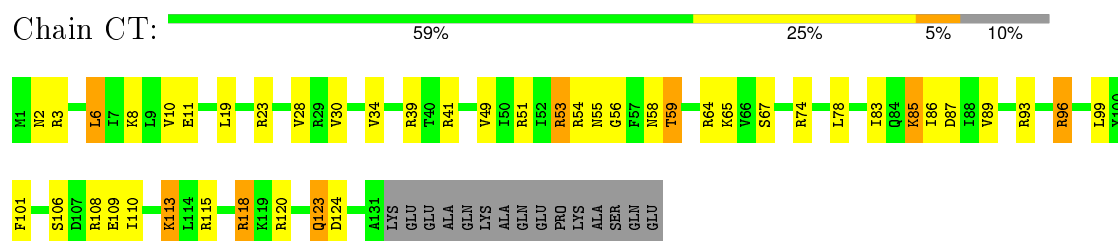
- Molecule 16: 50S ribosomal protein L18



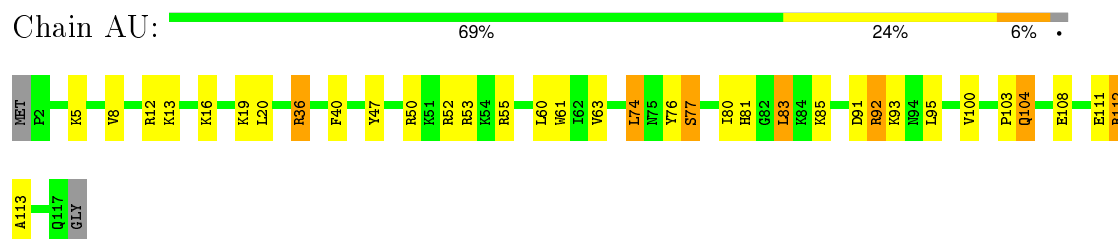
- Molecule 17: 50S ribosomal protein L19



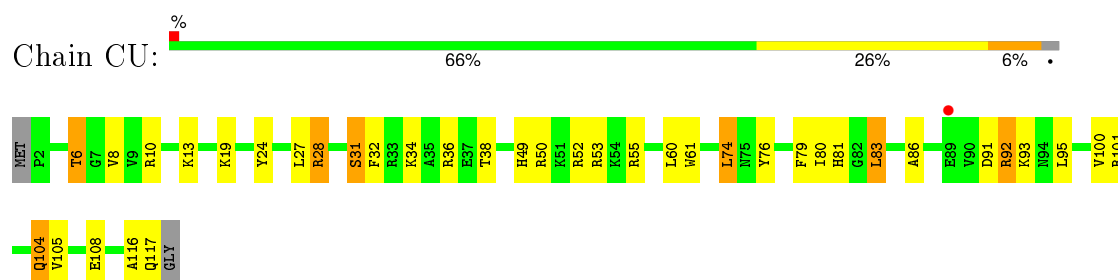
- Molecule 17: 50S ribosomal protein L19



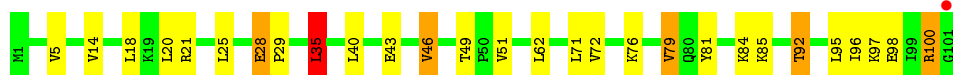
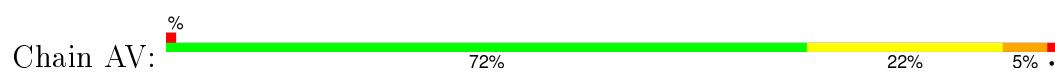
- Molecule 18: 50S ribosomal protein L20



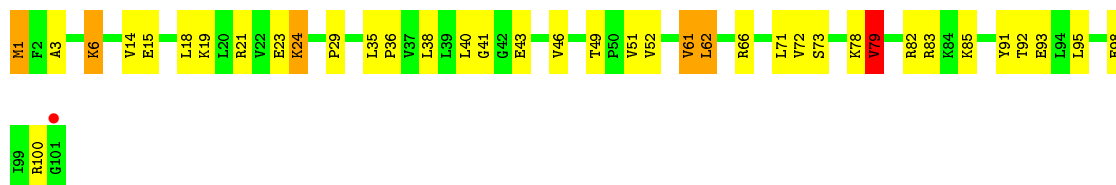
- Molecule 18: 50S ribosomal protein L20



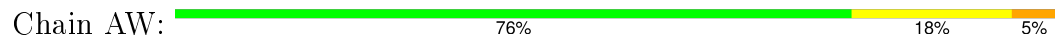
- Molecule 19: 50S ribosomal protein L21



- Molecule 19: 50S ribosomal protein L21



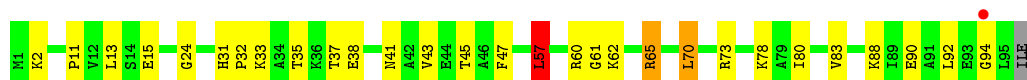
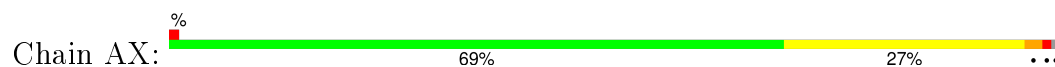
- Molecule 20: 50S ribosomal protein L22



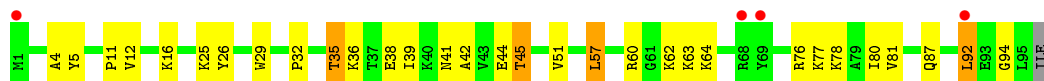
- Molecule 20: 50S ribosomal protein L22



- Molecule 21: 50S ribosomal protein L23

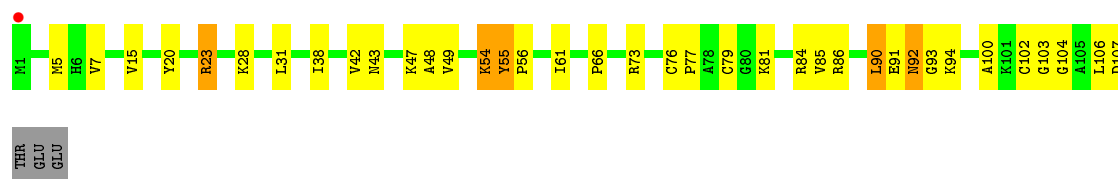


- Molecule 21: 50S ribosomal protein L23

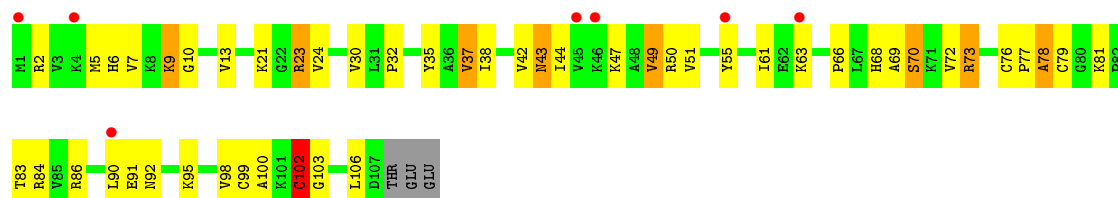


- Molecule 22: 50S ribosomal protein L24

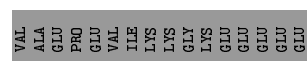
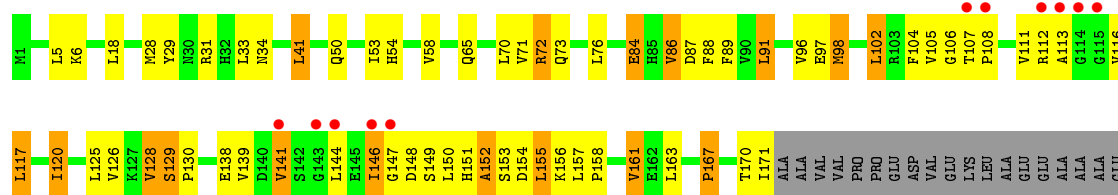




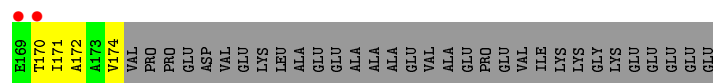
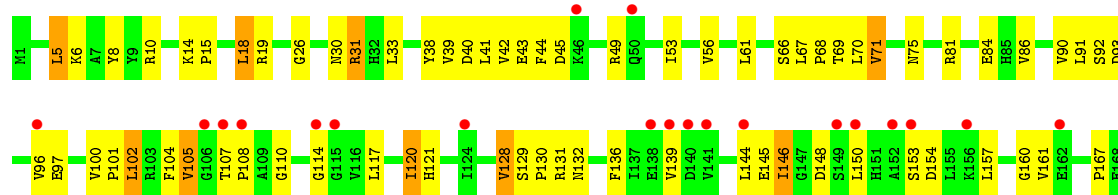
- Molecule 22: 50S ribosomal protein L24



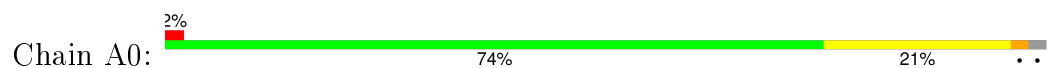
- Molecule 23: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L25

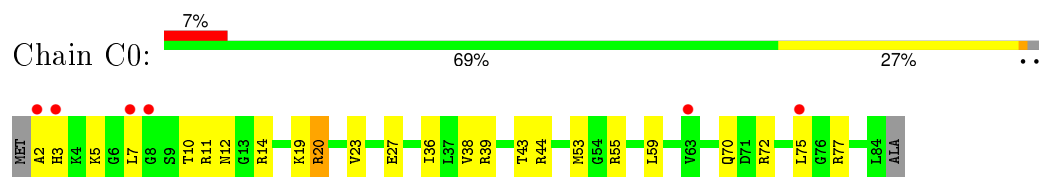


- Molecule 24: 50S ribosomal protein L27

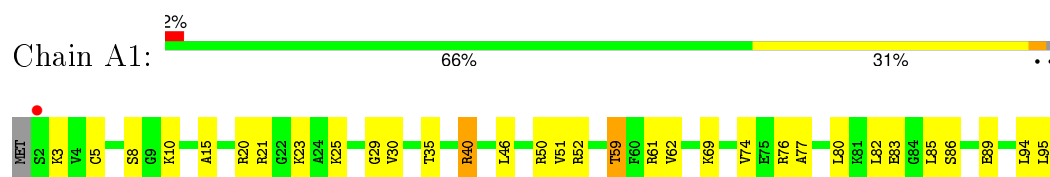




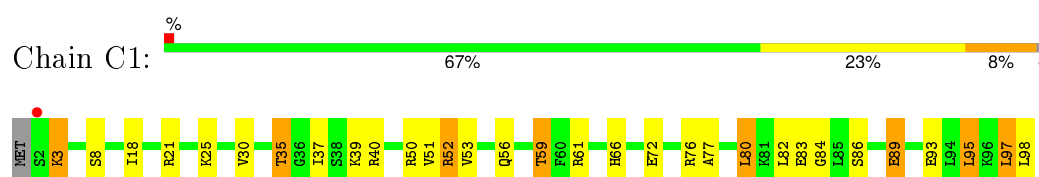
- Molecule 24: 50S ribosomal protein L27



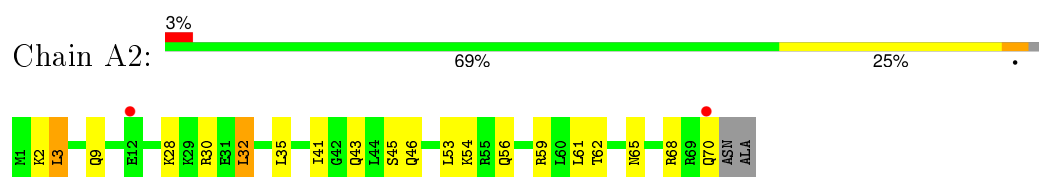
- Molecule 25: 50S ribosomal protein L28



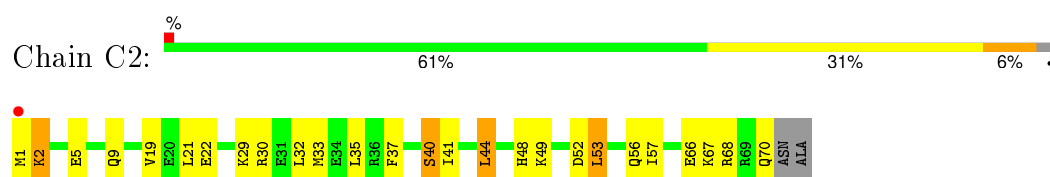
- Molecule 25: 50S ribosomal protein L28



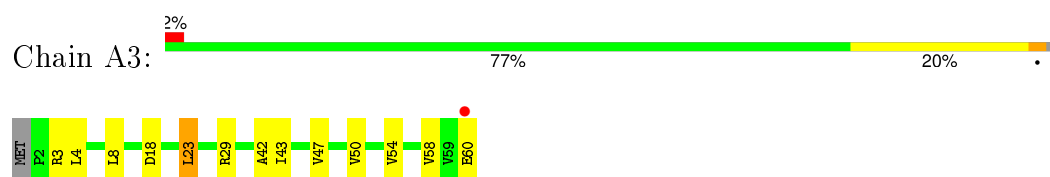
- Molecule 26: 50S ribosomal protein L29



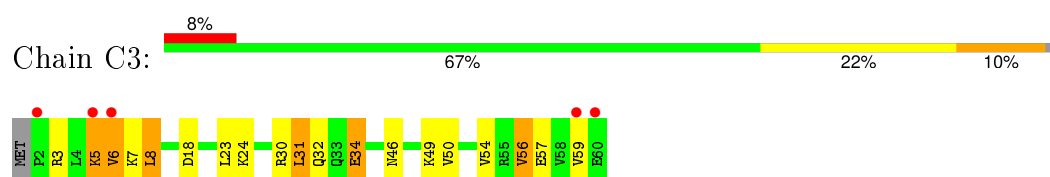
- Molecule 26: 50S ribosomal protein L29



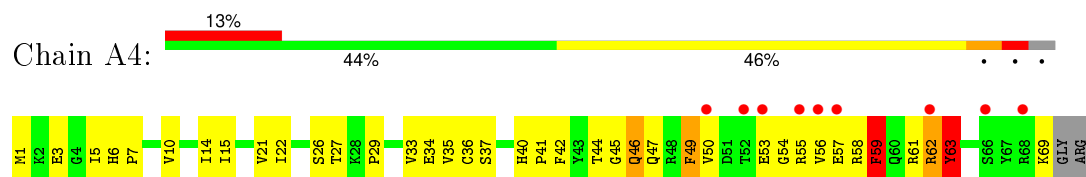
- Molecule 27: 50S ribosomal protein L30



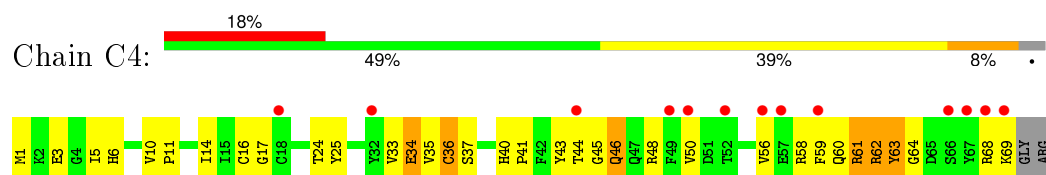
- Molecule 27: 50S ribosomal protein L30



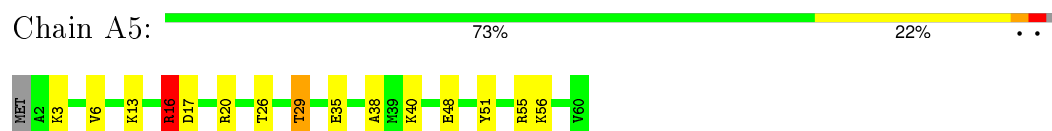
- Molecule 28: 50S ribosomal protein L31



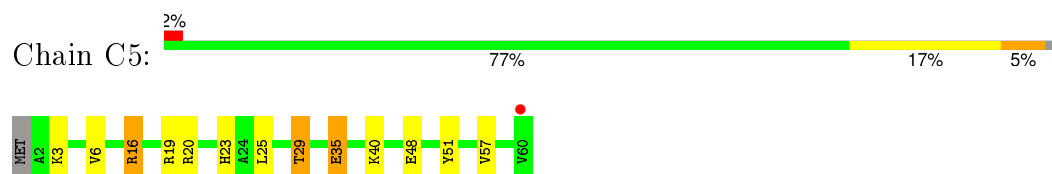
- Molecule 28: 50S ribosomal protein L31



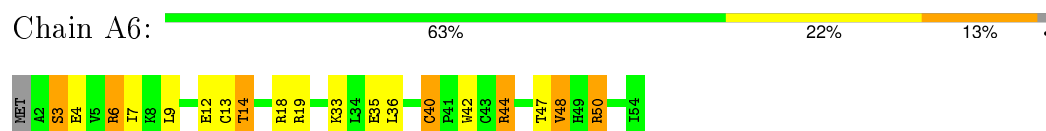
- Molecule 29: 50S ribosomal protein L32



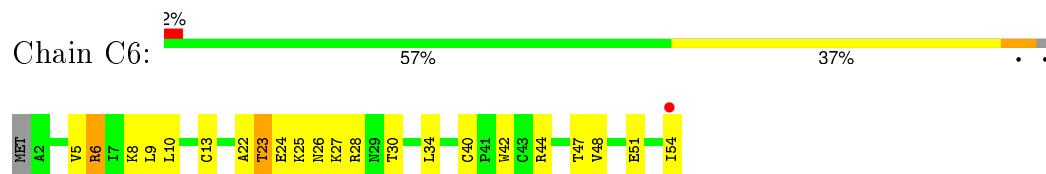
- Molecule 29: 50S ribosomal protein L32



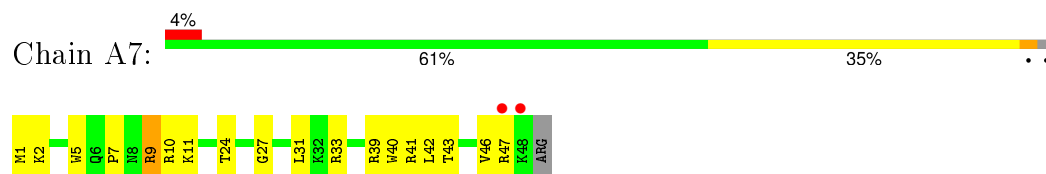
- Molecule 30: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



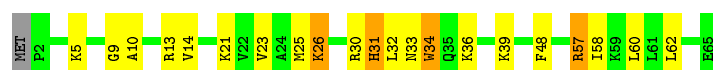
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



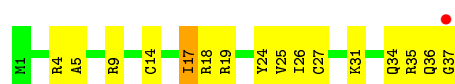
- Molecule 32: 50S ribosomal protein L35



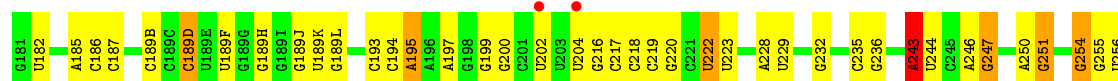
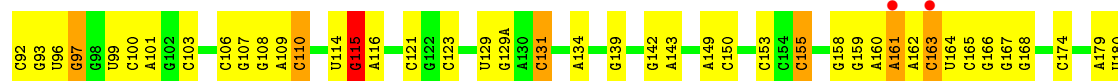
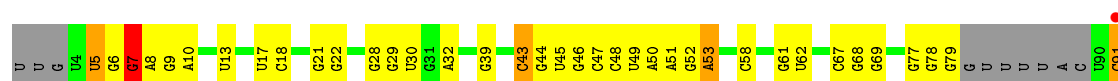
- Molecule 33: 50S ribosomal protein L36

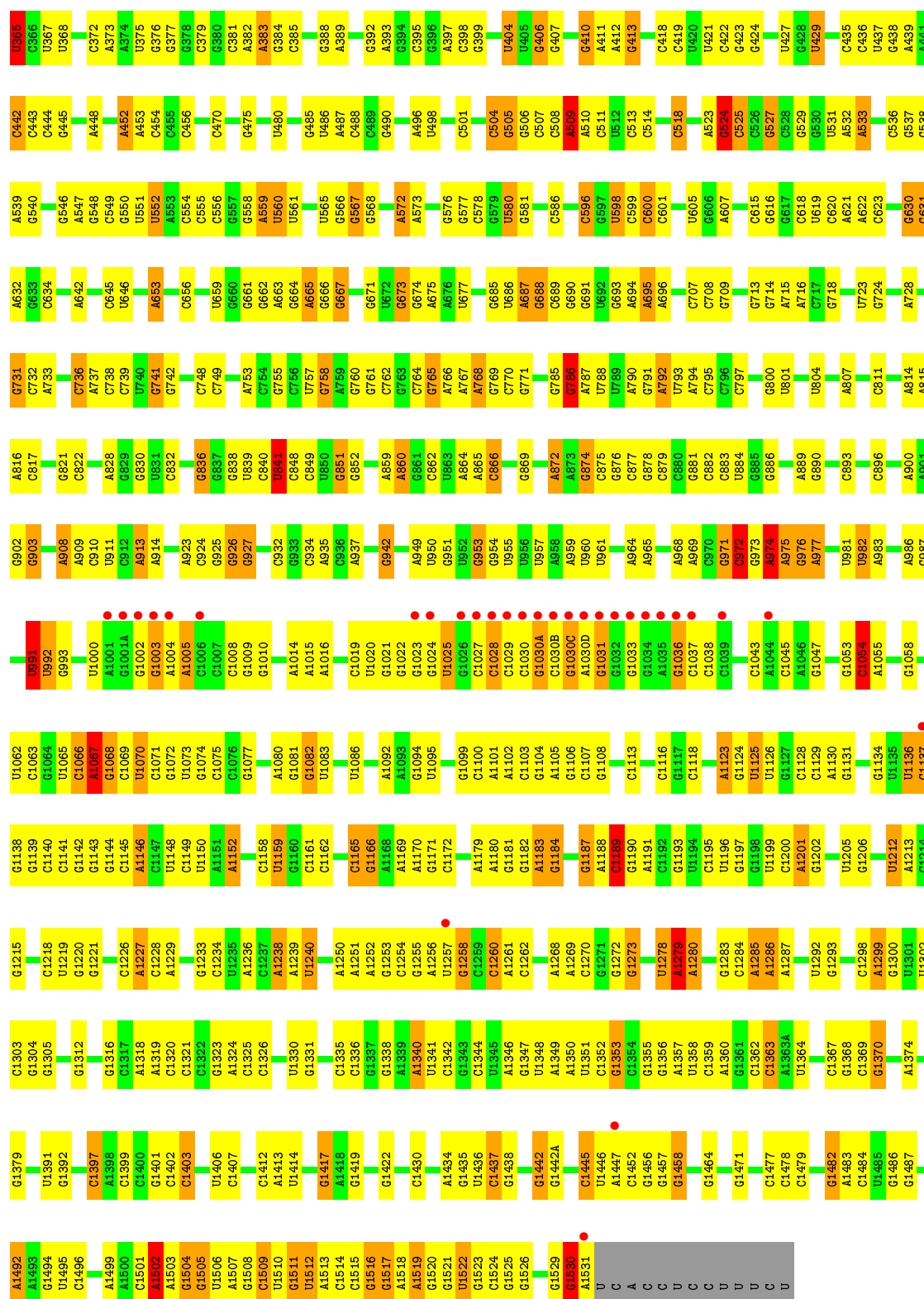


- Molecule 33: 50S ribosomal protein L36

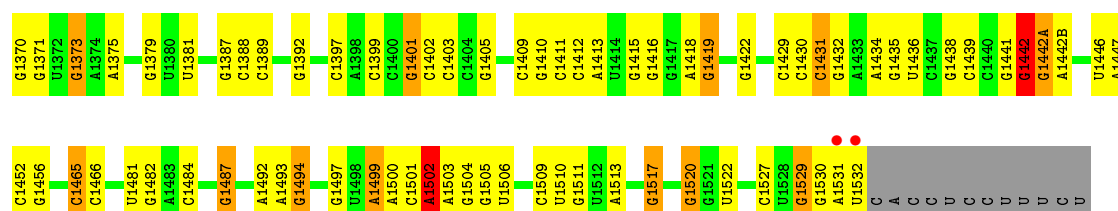


- Molecule 34: 16S Ribosomal RNA

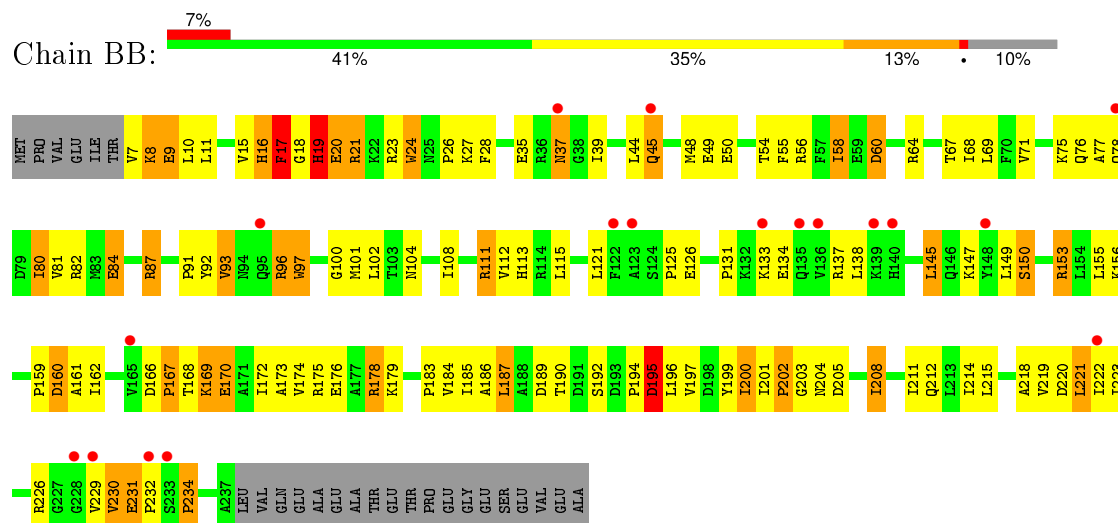




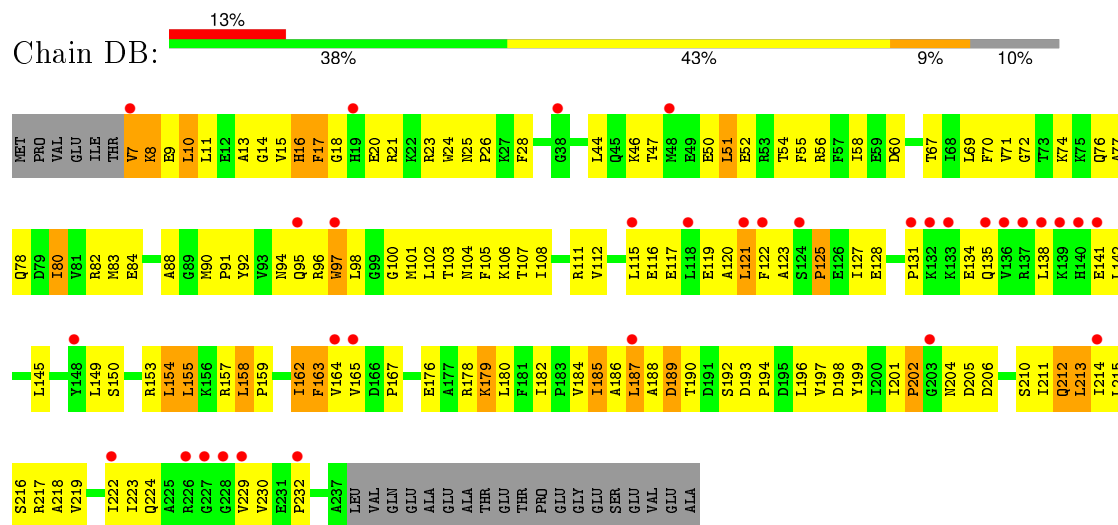
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G1241	G1241	C1158	G1084	U1025	C962	G878	A784	U686	G600	G513	C395	A300	A197	G23
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G1276	G1276		C1118	A1046	C990	C910	G828	G724	G635	G545	A439	G336	C243	A60
C1277	C1277	A1201	G1119	G1047	U991	G917	G829	G725	U636	G546	U437	C337	A161	G61
U1278	U1278	G1202	G1120	U1049	U992	A913	G830	G726	G637	G547	A438	U244	A162	G64
A1279	A1279	C1203	U1121	G1050	G993	A914	U831	A728	G638	G555	A439	C245	C163	U65
U1280	U1280	A1204	U1122	C1051	A994	A915	U832	A729	G639	C556	U441	G246	C164	G66
C1282	C1282	U1205	A1123	U1052	C998	G916	U833	G730	A640	G557	C442	G247	C165	C67
		G1206	G1124	G1053	U999	A918	C834	C732	U641	G558	G443	A344	U170	G68
A1285	A1285	G1207	U1125	C1054	C999	A919	U835	C733	A642	G559	A448	G352	A171	G70
A1286	A1286	C1208	U1126	A1055	U1000	U920	U836	G734	G644	U560	A452	G353	U172	G73
A1287	A1287	C1209	U1056	U1056	A1001	U921	G837	C735	G645	U561	A452	G354	C175	C76
A1288	A1288	G1210	G1057	G1057	G1001A	G922	G838	C736	U646	C562	G460	G355	C176	G79
A1289	A1289	U1211	G1058	G1058	G1002	A923	U839	C737	C647	A563	G461	G356	C177	G80
G1290	G1290	A1212	C1059	C1059	G1003	C924	U840	A737				A363	G257	U
G1291	G1291	A1213	C1132	C1060	A1004							A364	G258	G



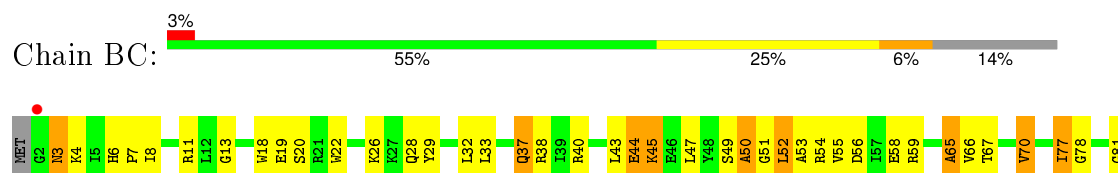
• Molecule 35: 30S ribosomal protein S2

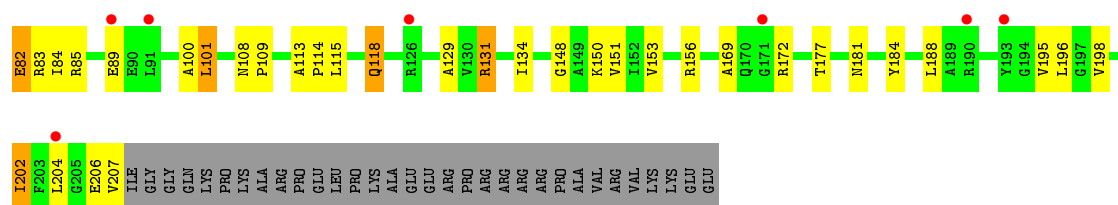


• Molecule 35: 30S ribosomal protein S2

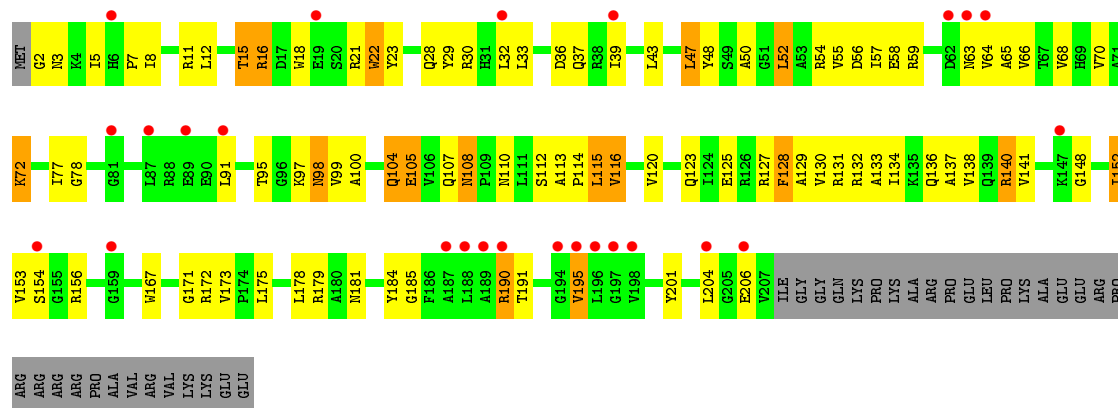


• Molecule 36: 30S ribosomal protein S3

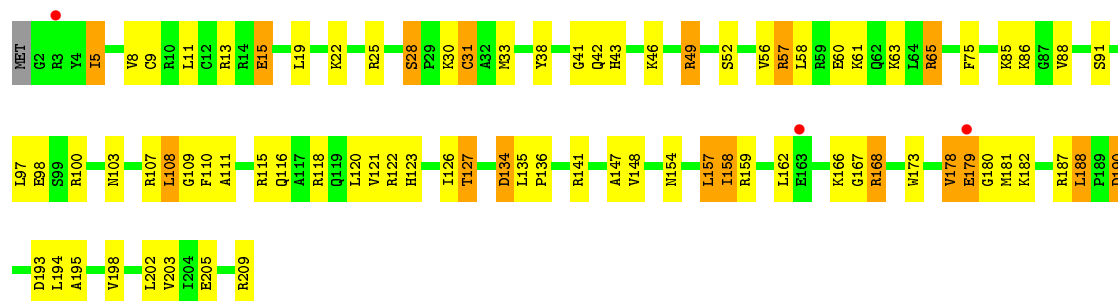




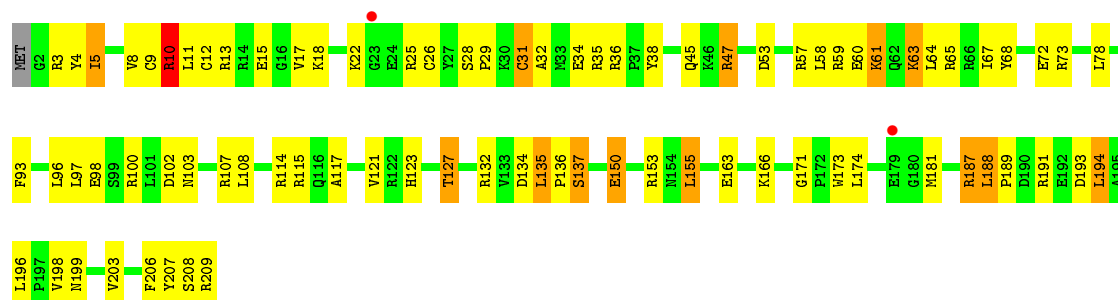
• Molecule 36: 30S ribosomal protein S3



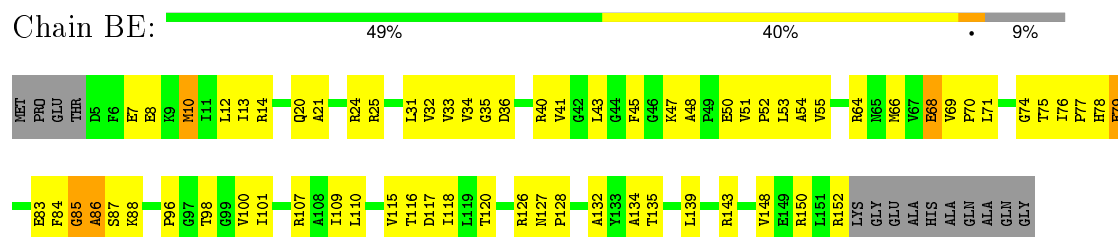
• Molecule 37: 30S ribosomal protein S4



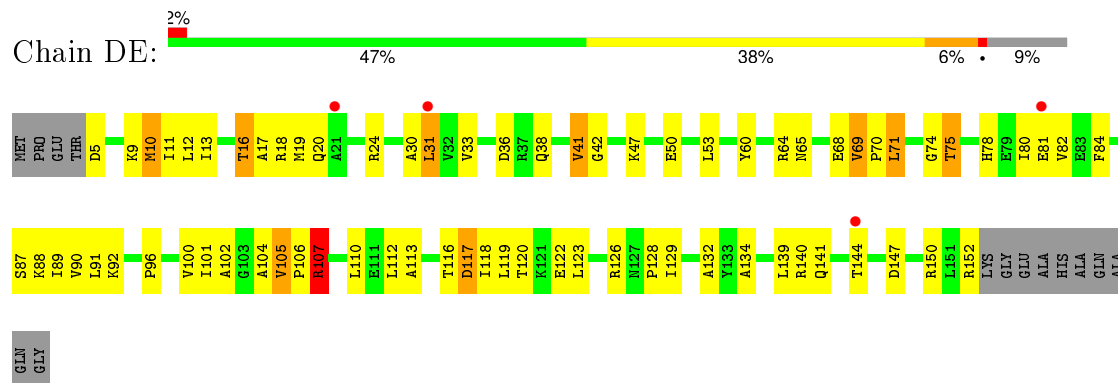
• Molecule 37: 30S ribosomal protein S4



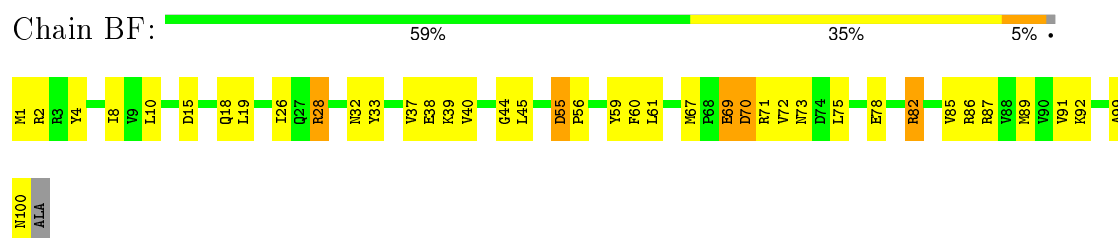
- Molecule 38: 30S ribosomal protein S5



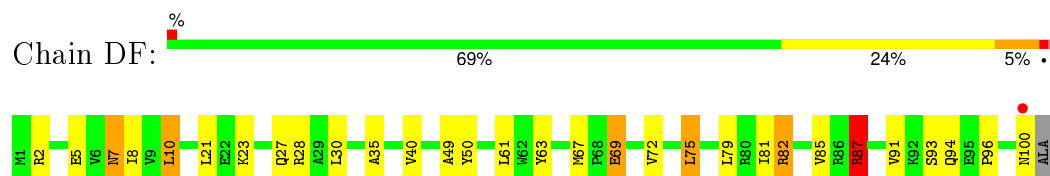
- Molecule 38: 30S ribosomal protein S5



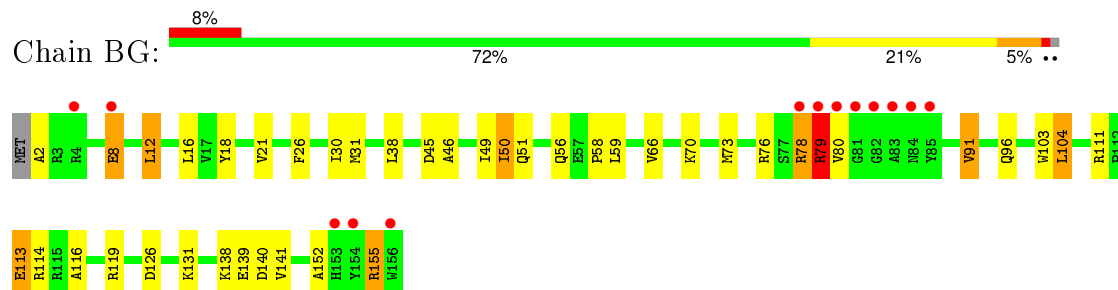
- Molecule 39: 30S ribosomal protein S6



- Molecule 39: 30S ribosomal protein S6

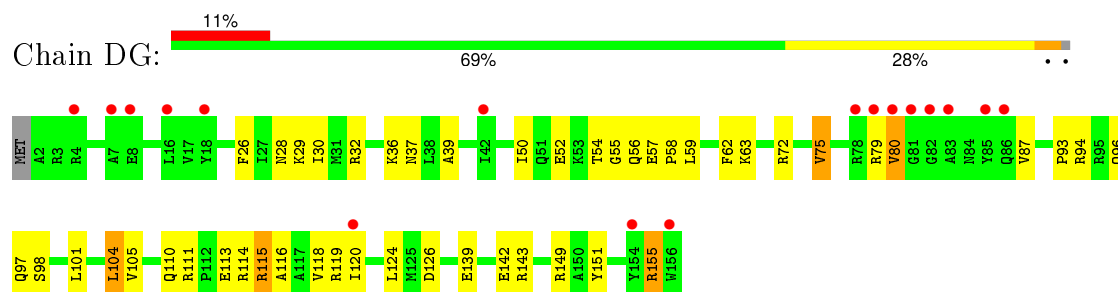


- Molecule 40: 30S ribosomal protein S7

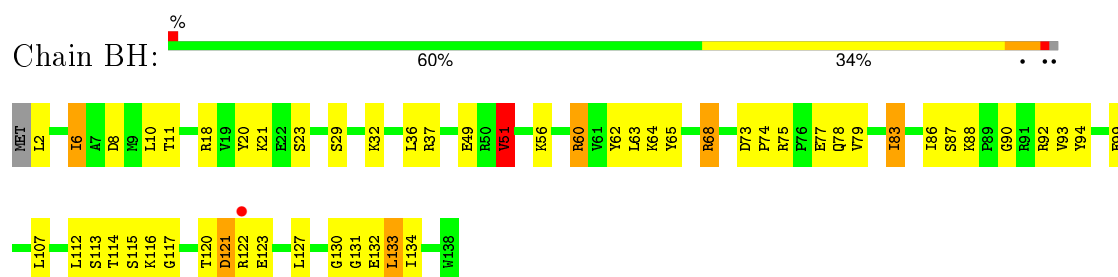




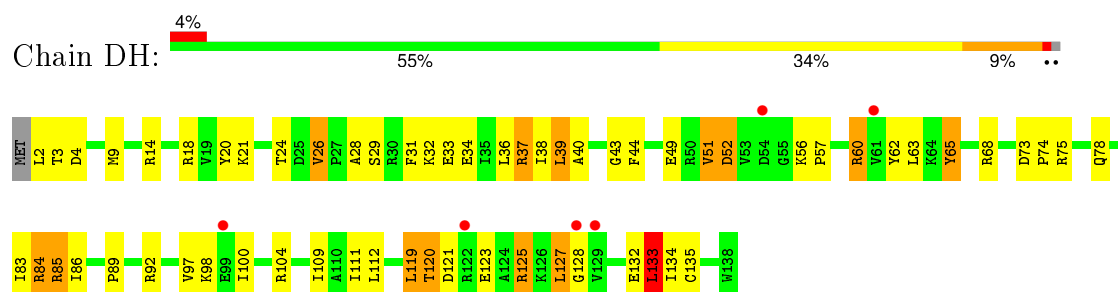
- Molecule 40: 30S ribosomal protein S7



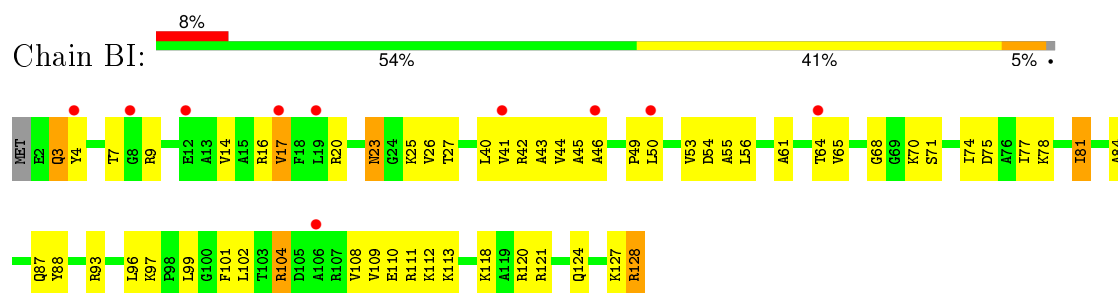
- Molecule 41: 30S ribosomal protein S8



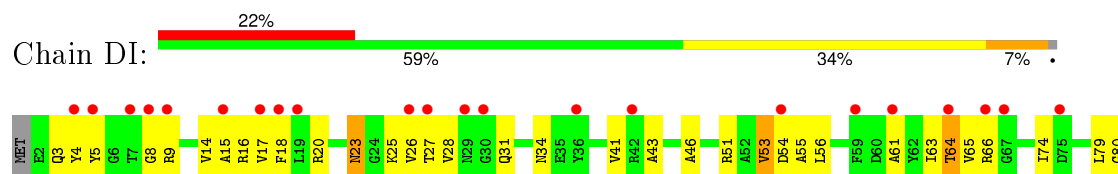
- Molecule 41: 30S ribosomal protein S8

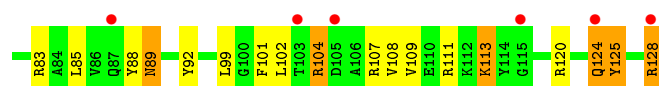


- Molecule 42: 30S ribosomal protein S9

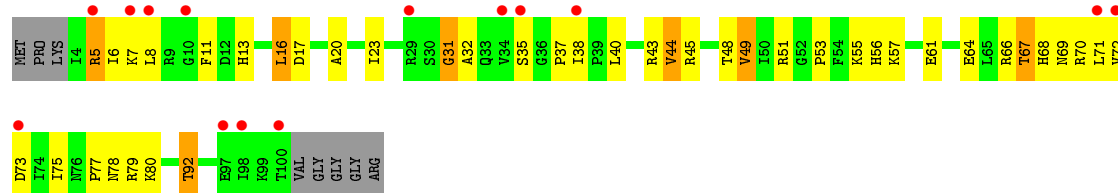


- Molecule 42: 30S ribosomal protein S9

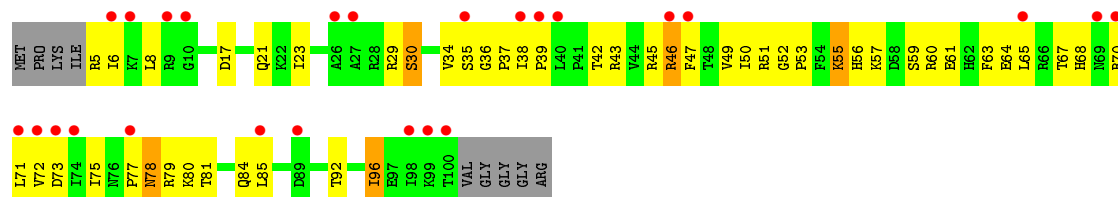




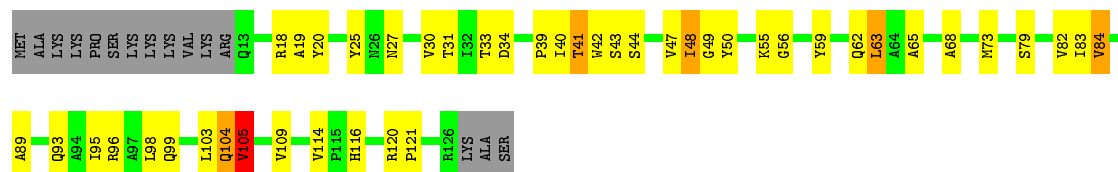
• Molecule 43: 30S ribosomal protein S10



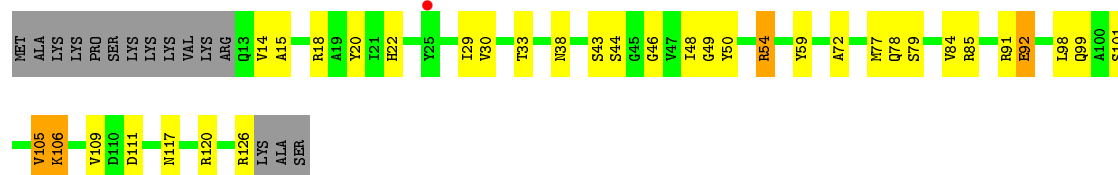
• Molecule 43: 30S ribosomal protein S10



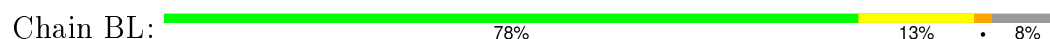
• Molecule 44: 30S ribosomal protein S11



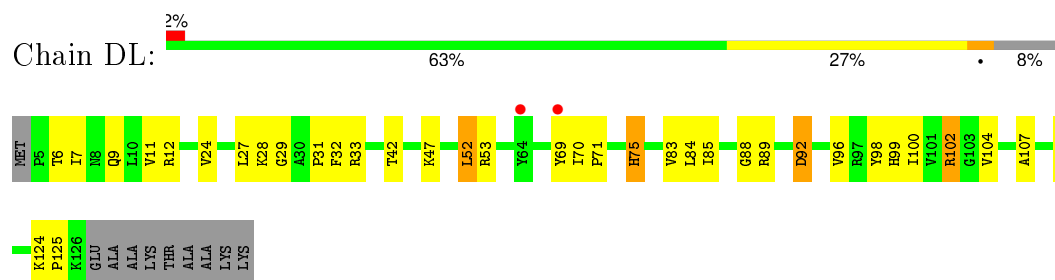
• Molecule 44: 30S ribosomal protein S11



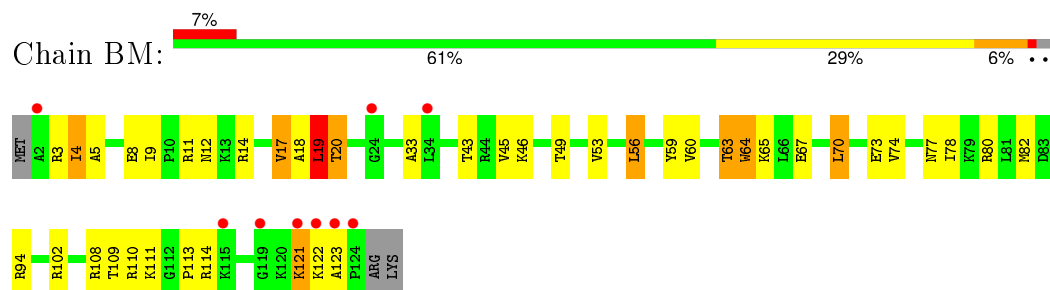
• Molecule 45: 30S ribosomal protein S12



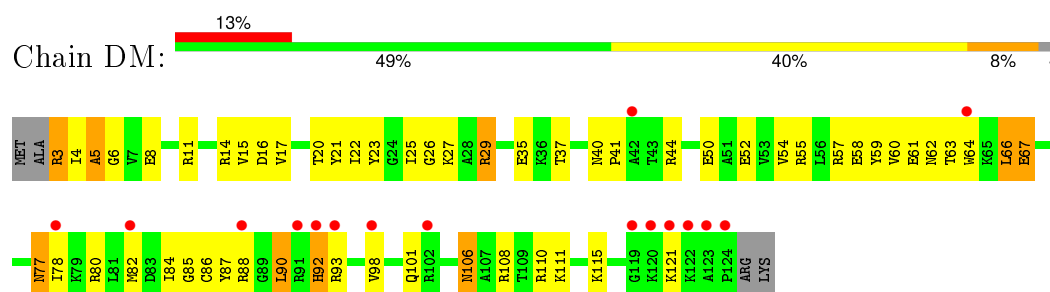
- Molecule 45: 30S ribosomal protein S12



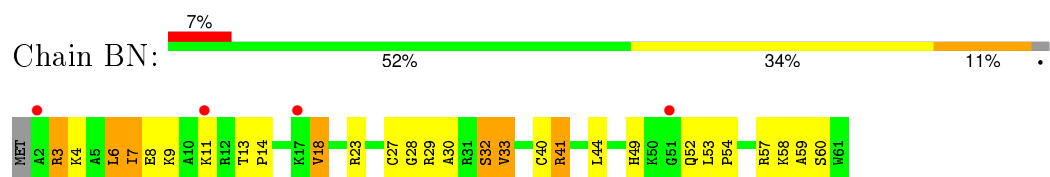
- Molecule 46: 30S ribosomal protein S13



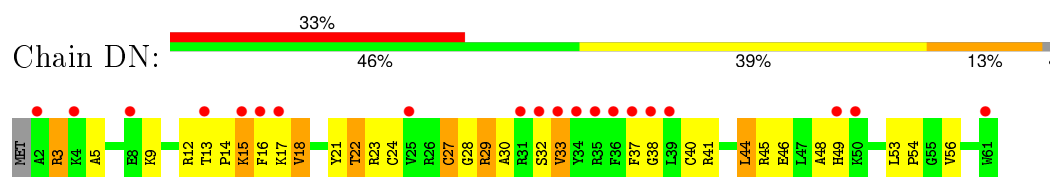
- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14 type Z

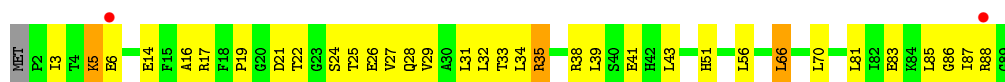


- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 48: 30S ribosomal protein S15

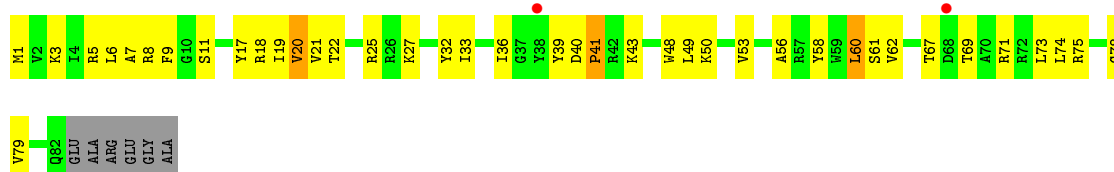




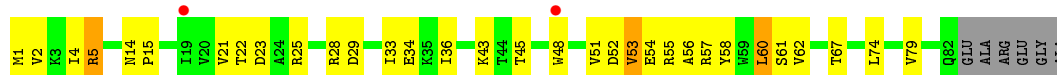
- Molecule 48: 30S ribosomal protein S15



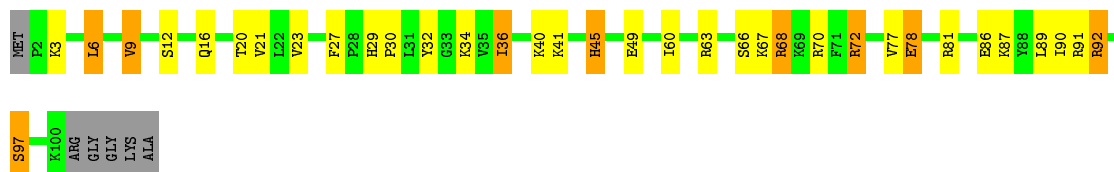
- Molecule 49: 30S ribosomal protein S16



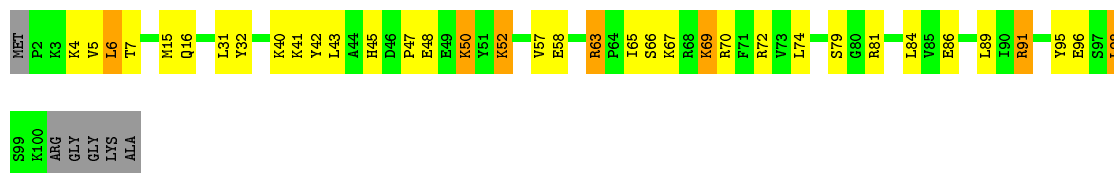
- Molecule 49: 30S ribosomal protein S16



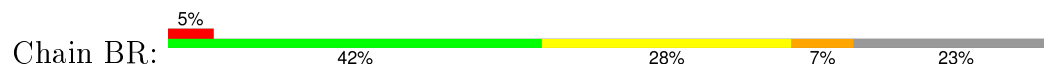
- Molecule 50: 30S ribosomal protein S17

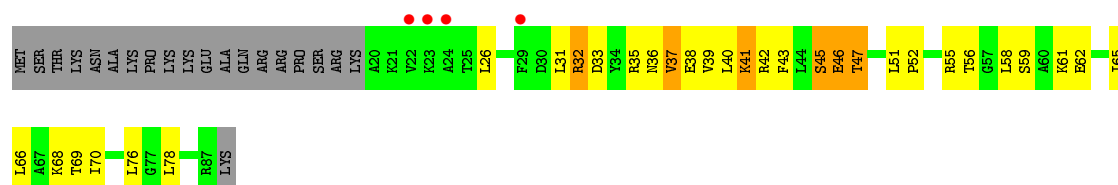


- Molecule 50: 30S ribosomal protein S17

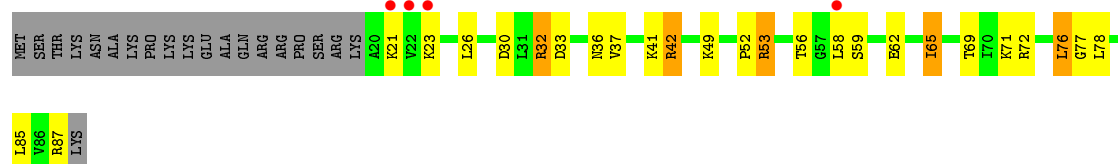


- Molecule 51: 30S ribosomal protein S18

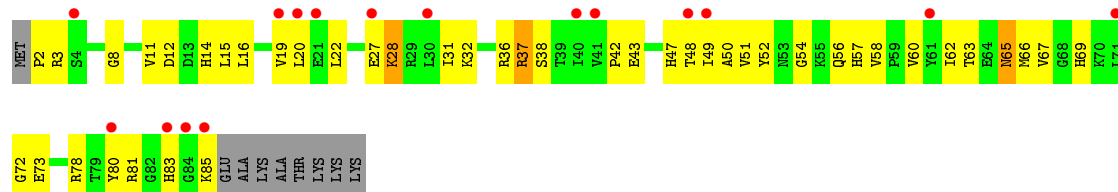




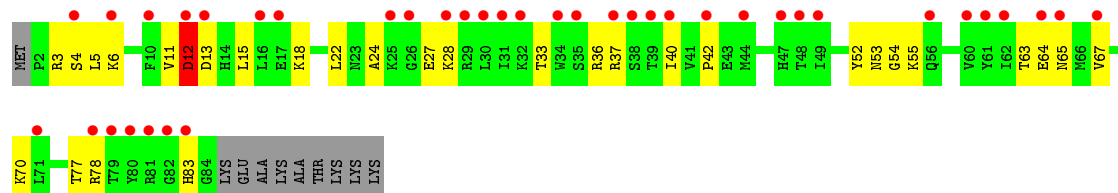
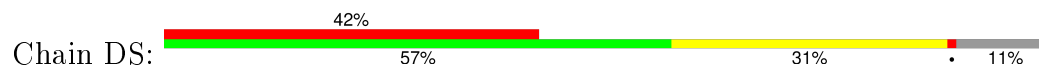
- Molecule 51: 30S ribosomal protein S18



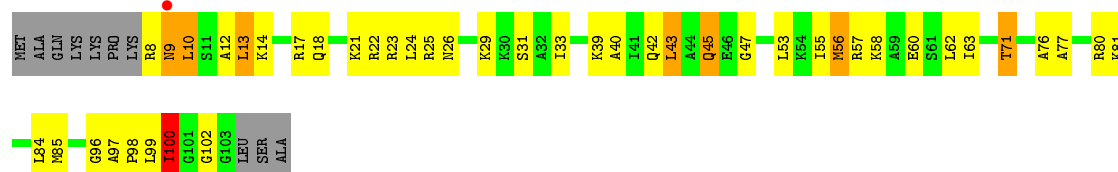
- Molecule 52: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S19

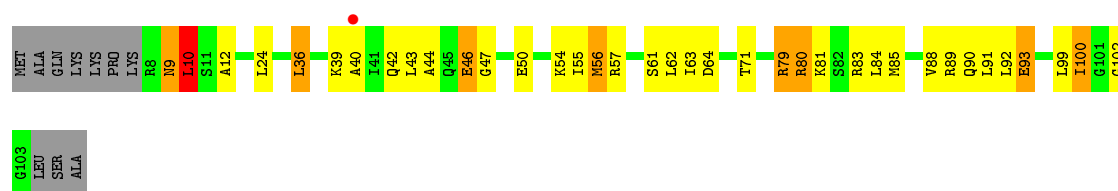


- Molecule 53: 30S ribosomal protein S20

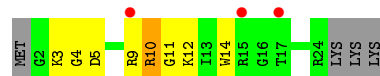


- Molecule 53: 30S ribosomal protein S20

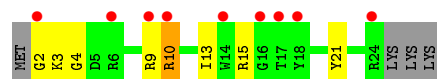




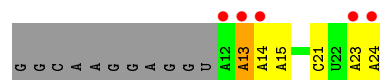
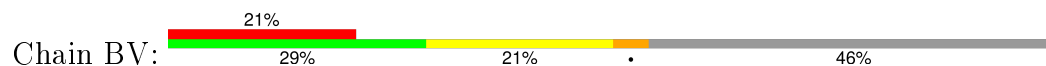
- Molecule 54: 30S ribosomal protein Thx



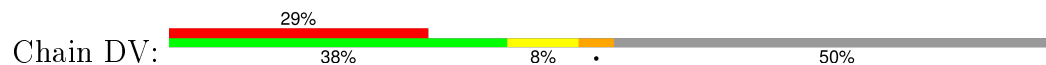
- Molecule 54: 30S ribosomal protein Thx



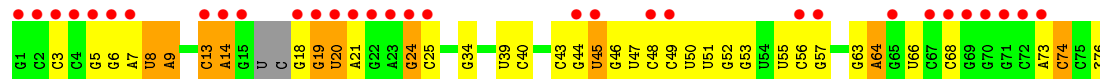
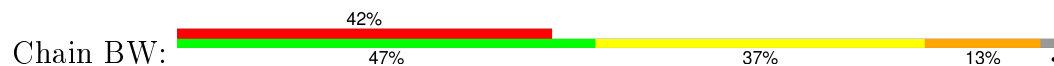
- Molecule 55: mRNA



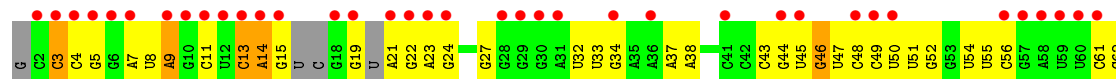
- Molecule 55: mRNA

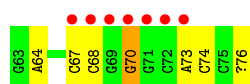


- Molecule 56: A-site tRNA



- Molecule 56: A-site tRNA





- Molecule 57: P-site tRNA

Chain BX: 62% 34% ..



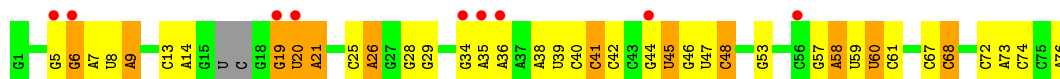
- Molecule 57: P-site tRNA

Chain DX: 3% 52% 35% 12% .



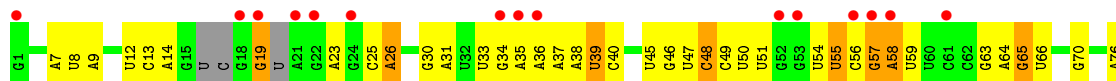
- Molecule 58: E-site tRNA

Chain BY: 12% 46% 36% 16% .



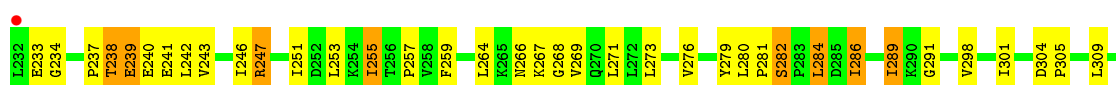
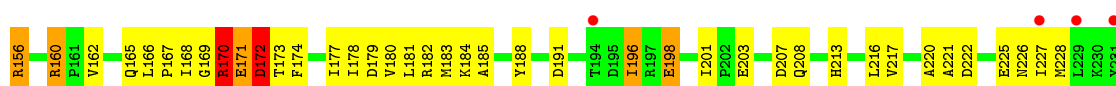
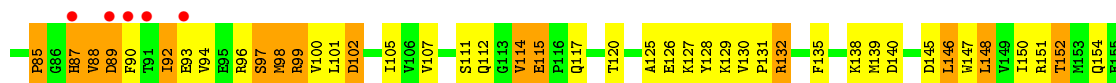
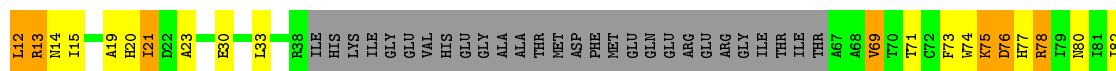
- Molecule 58: E-site tRNA

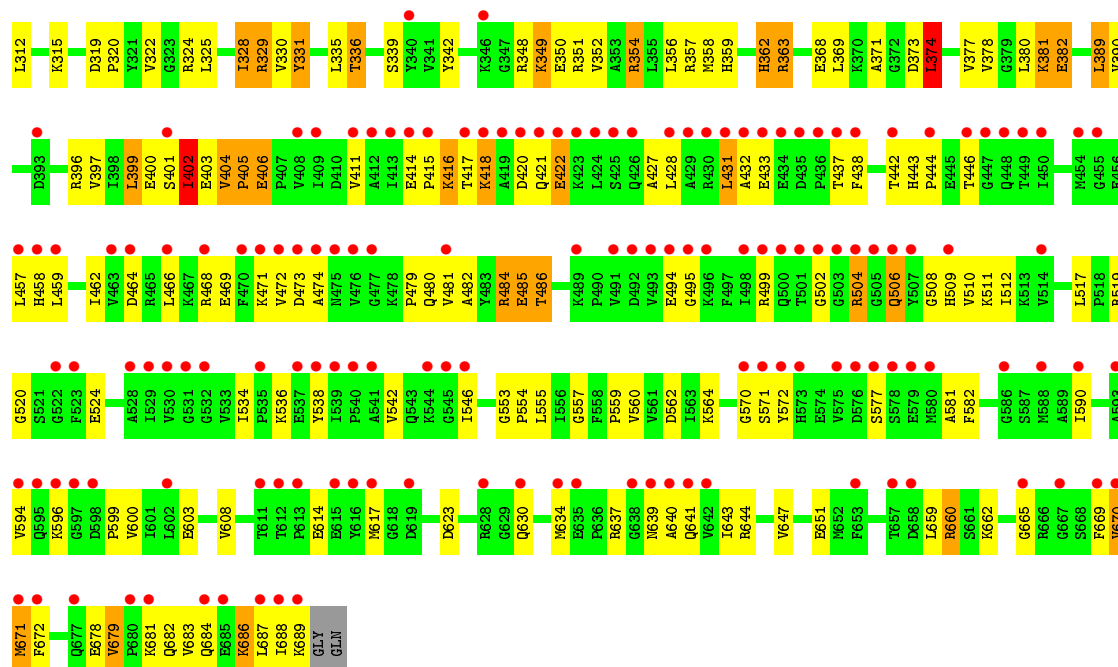
Chain DY: 20% 45% 41% 11% .



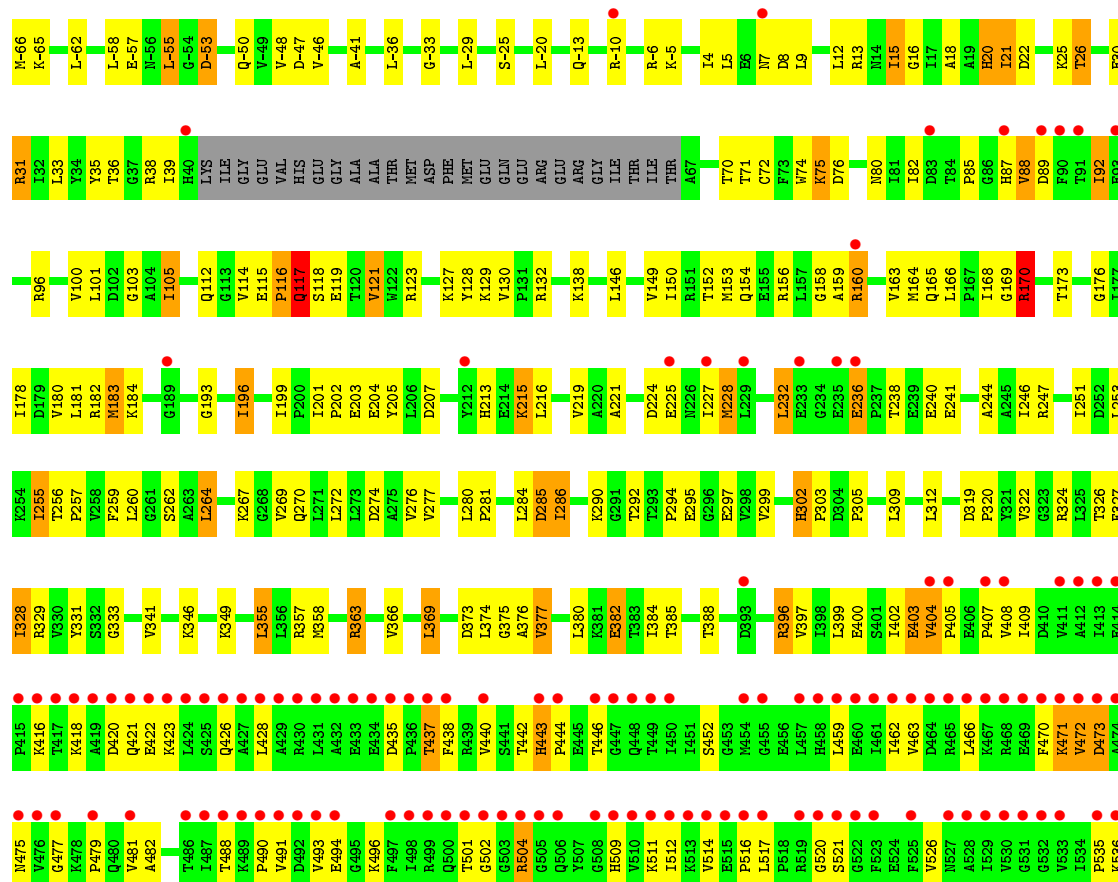
- Molecule 59: 50S ribosomal protein L9, Elongation factor G

Chain BZ: 21% 51% 35% 9% ..





- Molecule 59: 50S ribosomal protein L9, Elongation factor G







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.89 Å   449.03 Å   622.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.63 – 2.80 49.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.80) 99.0 (49.63-2.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202   ,   0.252 0.208   ,   0.255	Depositor DCC
$R_{free}$ test set	70994 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 1417809 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	313372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: 5MU, GDP, ZN, MIA, SF4, MG, F3N, 31H, 5MC, 4SU, 7MG, K, PSU

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	1.20	165/69281 (0.2%)	1.78	2173/108144 (2.0%)
1	CA	0.89	30/69179 (0.0%)	1.46	878/107984 (0.8%)
2	AB	0.97	0/2878	1.65	57/4490 (1.3%)
2	CB	0.63	0/2878	1.24	15/4490 (0.3%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.80	2/2186 (0.1%)	0.91	2/2944 (0.1%)
4	CD	0.65	0/2192	0.81	2/2951 (0.1%)
5	AE	0.81	0/1592	0.89	1/2149 (0.0%)
5	CE	0.63	0/1592	0.80	0/2149
6	AF	0.75	0/1619	0.91	2/2193 (0.1%)
6	CF	0.57	0/1615	0.74	0/2188
7	AG	0.51	0/1450	0.70	0/1959
7	CG	0.39	0/1449	0.59	0/1958
8	AH	0.67	0/1356	0.79	0/1834
8	CH	0.41	0/1356	0.62	0/1834
9	AK	0.33	0/640	0.63	0/889
9	CK	0.26	0/640	0.58	0/889
10	AL	0.31	0/503	0.53	0/673
10	CL	0.34	0/503	0.54	0/673
11	AN	0.81	0/1144	0.90	1/1543 (0.1%)
11	CN	0.57	0/1144	0.71	0/1543
12	AO	0.76	0/943	0.84	1/1269 (0.1%)
12	CO	0.68	0/943	0.75	0/1269
13	AP	0.70	0/1156	0.87	2/1537 (0.1%)
13	CP	0.51	0/1152	0.80	0/1533
14	AQ	0.77	0/1143	0.86	1/1527 (0.1%)
14	CQ	0.58	0/1143	0.69	0/1527
15	AR	0.73	0/982	0.87	0/1312
15	CR	0.58	0/982	0.77	0/1312
16	AS	0.58	0/887	0.76	1/1180 (0.1%)
16	CS	0.46	0/880	0.71	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AT	0.74	0/1105	0.88	0/1477
17	CT	0.58	0/1097	0.74	0/1468
18	AU	0.89	1/977 (0.1%)	0.92	1/1301 (0.1%)
18	CU	0.62	0/977	0.71	2/1301 (0.2%)
19	AV	0.80	0/782	0.90	1/1049 (0.1%)
19	CV	0.52	0/782	0.74	0/1049
20	AW	0.91	0/897	0.93	3/1205 (0.2%)
20	CW	0.70	0/897	0.81	0/1205
21	AX	0.82	1/764 (0.1%)	0.80	1/1025 (0.1%)
21	CX	0.62	0/764	0.75	1/1025 (0.1%)
22	AY	0.74	0/819	0.85	0/1095
22	CY	0.54	0/819	0.69	0/1095
23	AZ	0.52	0/1379	0.70	1/1873 (0.1%)
23	CZ	0.39	0/1390	0.58	0/1890
24	A0	0.67	0/662	0.88	1/881 (0.1%)
24	C0	0.56	0/662	0.68	0/881
25	A1	0.70	0/762	0.81	0/1014
25	C1	0.61	0/762	0.77	0/1014
26	A2	0.78	0/590	0.78	0/781
26	C2	0.53	0/590	0.63	0/781
27	A3	0.82	0/474	0.91	0/635
27	C3	0.49	0/469	0.69	0/630
28	A4	0.43	0/571	0.70	0/768
28	C4	0.35	0/545	0.60	0/737
29	A5	0.89	1/469 (0.2%)	1.00	2/635 (0.3%)
29	C5	0.66	0/469	0.82	0/635
30	A6	0.86	1/460 (0.2%)	0.79	0/613
30	C6	0.62	0/456	0.74	0/608
31	A7	0.84	0/426	0.99	2/561 (0.4%)
31	C7	0.70	0/426	0.78	0/561
32	A8	0.82	0/525	0.90	0/691
32	C8	0.61	0/525	0.78	0/691
33	A9	0.80	0/310	0.94	0/407
33	C9	0.60	0/310	0.73	0/407
34	BA	0.70	4/36027 (0.0%)	1.28	246/56227 (0.4%)
34	DA	0.64	1/36170 (0.0%)	1.21	131/56452 (0.2%)
35	BB	0.40	0/1881	0.67	1/2542 (0.0%)
35	DB	0.36	0/1860	0.61	0/2518
36	BC	0.38	0/1576	0.59	0/2130
36	DC	0.35	0/1568	0.57	0/2122
37	BD	0.48	0/1689	0.67	0/2267
37	DD	0.48	0/1708	0.70	1/2289 (0.0%)
38	BE	0.51	0/1145	0.69	1/1543 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DE	0.44	0/1149	0.67	0/1548
39	BF	0.52	0/825	0.70	0/1118
39	DF	0.52	0/833	0.69	1/1128 (0.1%)
40	BG	0.43	0/1250	0.58	0/1679
40	DG	0.37	0/1254	0.56	0/1683
41	BH	0.48	0/1108	0.68	0/1494
41	DH	0.42	0/1108	0.64	0/1494
42	BI	0.42	0/1005	0.62	0/1350
42	DI	0.36	0/997	0.58	0/1343
43	BJ	0.38	0/722	0.58	0/982
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.49	0/848	0.66	0/1149
44	DK	0.50	0/848	0.66	0/1149
45	BL	0.56	0/946	0.70	0/1274
45	DL	0.52	0/946	0.68	0/1274
46	BM	0.41	0/977	0.64	0/1310
46	DM	0.35	0/961	0.56	0/1291
47	BN	0.44	0/501	0.70	0/664
47	DN	0.37	0/501	0.59	1/664 (0.2%)
48	BO	0.50	0/739	0.71	0/985
48	DO	0.46	0/739	0.63	0/985
49	BP	0.53	0/697	0.69	0/939
49	DP	0.52	0/693	0.66	0/935
50	BQ	0.53	0/836	0.69	1/1117 (0.1%)
50	DQ	0.50	0/836	0.68	0/1117
51	BR	0.51	0/560	0.74	0/746
51	DR	0.52	0/560	0.66	0/746
52	BS	0.36	0/676	0.58	0/911
52	DS	0.32	0/661	0.64	0/893
53	BT	0.45	0/730	0.71	0/965
53	DT	0.46	0/733	0.69	0/969
54	BU	0.40	0/203	0.62	0/266
54	DU	0.35	0/203	0.62	0/266
55	BV	0.65	0/310	1.02	1/480 (0.2%)
55	DV	0.54	0/282	0.91	0/437
56	BW	0.43	0/1577	0.96	1/2454 (0.0%)
56	DW	0.36	0/1531	0.94	0/2379
57	BX	0.71	1/1700 (0.1%)	1.22	2/2650 (0.1%)
57	DX	0.63	1/1700 (0.1%)	1.12	4/2650 (0.2%)
58	BY	0.43	0/1602	0.98	1/2493 (0.0%)
58	DY	0.36	0/1579	0.86	0/2455
59	BZ	0.44	0/5763	0.68	2/7804 (0.0%)
59	DZ	0.41	0/5784	0.63	0/7835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.82	208/333310 (0.1%)	1.32	3545/497173 (0.7%)

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	0	1
28	A4	0	1
35	BB	0	1
53	BT	0	1
53	DT	0	1
59	DZ	0	1
All	All	0	6

The worst 5 of 208 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1188	A	N9-C4	-13.96	1.29	1.37
1	AA	354	A	N9-C4	-13.07	1.30	1.37
1	CA	528	A	N9-C4	-11.34	1.31	1.37
57	DX	74	C	O3'-P	-11.14	1.47	1.61
1	AA	2299	A	N9-C4	-10.50	1.31	1.37

The worst 5 of 3545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	990	A	N1-C6-N6	23.54	132.72	118.60
1	AA	354	A	C2-N3-C4	-21.82	99.69	110.60
1	AA	990	A	C6-C5-N7	-21.49	117.25	132.30
1	AA	1188	A	C2-N3-C4	-21.02	100.09	110.60
1	AA	990	A	C5-N7-C8	-19.83	93.98	103.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	A4	59	PHE	Peptide
1	AA	537	G	Sidechain
35	BB	8	LYS	Peptide

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Mol	Chain	Res	Type	Group
53	BT	9	ASN	Peptide
53	DT	9	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61861	0	31186	660	2
1	CA	61771	0	31146	786	0
2	AB	2573	0	1306	15	0
2	CB	2573	0	1306	26	0
3	AC	1063	0	1091	140	5
3	CC	1063	0	1089	150	10
4	AD	2136	0	2218	55	0
4	CD	2142	0	2229	67	0
5	AE	1559	0	1618	48	0
5	CE	1559	0	1618	42	0
6	AF	1584	0	1625	39	0
6	CF	1580	0	1619	50	0
7	AG	1425	0	1443	47	0
7	CG	1424	0	1434	42	0
8	AH	1330	0	1407	24	0
8	CH	1330	0	1407	42	0
9	AK	641	0	309	11	0
9	CK	641	0	309	13	0
10	AL	498	0	521	17	0
10	CL	498	0	521	21	0
11	AN	1117	0	1184	26	0
11	CN	1117	0	1184	21	0
12	AO	933	0	996	29	0
12	CO	933	0	996	22	0
13	AP	1139	0	1223	34	0
13	CP	1135	0	1212	47	0
14	AQ	1122	0	1179	36	0
14	CQ	1122	0	1179	36	0
15	AR	968	0	1033	19	0
15	CR	968	0	1033	27	0
16	AS	877	0	938	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	35	0
17	AT	1091	0	1151	31	0
17	CT	1083	0	1136	28	0
18	AU	959	0	1019	25	0
18	CU	959	0	1019	30	0
19	AV	771	0	830	13	0
19	CV	771	0	830	19	0
20	AW	886	0	940	15	0
20	CW	886	0	940	18	0
21	AX	750	0	814	20	0
21	CX	750	0	814	19	0
22	AY	806	0	881	29	0
22	CY	806	0	882	37	0
23	AZ	1349	0	1355	38	0
23	CZ	1360	0	1363	41	0
24	A0	653	0	674	20	0
24	C0	653	0	674	20	0
25	A1	755	0	826	20	0
25	C1	755	0	826	20	0
26	A2	588	0	643	9	0
26	C2	588	0	643	14	0
27	A3	469	0	518	6	0
27	C3	464	0	514	8	0
28	A4	558	0	545	22	0
28	C4	532	0	506	20	0
29	A5	455	0	465	7	0
29	C5	455	0	465	11	0
30	A6	453	0	473	13	0
30	C6	449	0	469	13	0
31	A7	418	0	467	11	0
31	C7	418	0	467	9	0
32	A8	517	0	582	23	0
32	C8	517	0	582	19	0
33	A9	307	0	335	8	0
33	C9	307	0	335	11	0
34	BA	32185	0	16245	438	0
34	DA	32312	0	16308	510	1
35	BB	1846	0	1867	80	0
35	DB	1825	0	1828	101	0
36	BC	1552	0	1546	52	0
36	DC	1544	0	1524	65	0
37	BD	1659	0	1676	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1718	53	0
38	BE	1129	0	1185	42	0
38	DE	1133	0	1191	41	0
39	BF	812	0	804	18	0
39	DF	820	0	814	23	0
40	BG	1231	0	1238	21	0
40	DG	1235	0	1249	31	0
41	BH	1088	0	1126	39	0
41	DH	1088	0	1126	37	0
42	BI	986	0	995	39	0
42	DI	978	0	966	42	0
43	BJ	709	0	650	34	0
43	DJ	714	0	672	33	0
44	BK	833	0	836	23	0
44	DK	833	0	836	16	0
45	BL	930	0	980	10	0
45	DL	930	0	980	30	0
46	BM	966	0	1024	33	0
46	DM	950	0	988	39	0
47	BN	492	0	529	22	0
47	DN	492	0	531	33	0
48	BO	728	0	760	17	0
48	DO	728	0	760	14	0
49	BP	681	0	697	27	0
49	DP	677	0	686	20	0
50	BQ	823	0	891	24	0
50	DQ	823	0	891	23	0
51	BR	555	0	618	16	0
51	DR	555	0	618	20	0
52	BS	661	0	675	39	0
52	DS	646	0	644	25	0
53	BT	728	0	798	29	0
53	DT	731	0	807	22	0
54	BU	199	0	208	7	0
54	DU	199	0	208	5	0
55	BV	277	0	140	3	0
55	DV	252	0	130	3	0
56	BW	1599	0	830	26	0
56	DW	1552	0	794	21	0
57	BX	1635	0	838	15	0
57	DX	1635	0	839	25	0
58	BY	1581	0	805	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	DY	1561	0	796	18	0
59	BZ	5663	0	5746	246	10
59	DZ	5682	0	5766	192	6
60	A0	5	0	0	0	0
60	A1	2	0	0	0	0
60	A2	1	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A7	1	0	0	0	0
60	A8	2	0	0	0	0
60	A9	1	0	0	0	0
60	AA	834	0	0	0	0
60	AB	23	0	0	0	0
60	AD	10	0	0	0	0
60	AE	5	0	0	0	0
60	AF	5	0	0	0	0
60	AG	2	0	0	0	0
60	AH	1	0	0	0	0
60	AN	3	0	0	0	0
60	AO	1	0	0	0	0
60	AP	2	0	0	0	0
60	AQ	3	0	0	0	0
60	AR	1	0	0	0	0
60	AU	4	0	0	0	0
60	AV	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	2	0	0	0	0
60	AY	1	0	0	0	0
60	AZ	1	0	0	0	0
60	BA	213	0	0	0	0
60	BB	1	0	0	0	0
60	BD	1	0	0	0	0
60	BE	1	0	0	0	0
60	BF	1	0	0	0	0
60	BK	1	0	0	0	0
60	BL	2	0	0	0	0
60	BM	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	1	0	0	0	0
60	BV	1	0	0	0	0
60	BW	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BX	15	0	0	0	0
60	BY	2	0	0	0	0
60	BZ	1	0	0	0	0
60	C0	2	0	0	0	0
60	C3	1	0	0	0	0
60	C5	1	0	0	0	0
60	C7	1	0	0	0	0
60	C8	1	0	0	0	0
60	CA	664	0	0	0	0
60	CB	13	0	0	0	0
60	CD	4	0	0	0	0
60	CE	6	0	0	0	0
60	CF	6	0	0	0	0
60	CG	1	0	0	0	0
60	CN	1	0	0	0	0
60	CO	2	0	0	0	0
60	CP	1	0	0	0	0
60	CQ	4	0	0	0	0
60	CR	2	0	0	0	0
60	CU	1	0	0	0	0
60	CV	2	0	0	0	0
60	CY	1	0	0	0	0
60	DA	168	0	0	0	0
60	DD	1	0	0	0	0
60	DE	2	0	0	0	0
60	DF	1	0	0	0	0
60	DJ	1	0	0	0	0
60	DK	2	0	0	0	0
60	DT	1	0	0	0	0
60	DW	1	0	0	0	0
60	DX	1	0	0	0	0
60	DZ	1	0	0	0	0
61	AA	1	0	0	0	0
62	A4	1	0	0	0	0
62	A5	1	0	0	0	0
62	A6	1	0	0	0	0
62	A9	1	0	0	0	0
62	AY	1	0	0	0	0
62	BN	1	0	0	0	0
62	C4	1	0	0	0	0
62	C5	1	0	0	0	0
62	C6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	C9	1	0	0	0	0
62	CY	1	0	0	0	0
62	DN	1	0	0	0	0
63	BD	8	0	0	1	0
63	DD	8	0	0	1	0
64	BZ	28	0	12	6	0
64	DZ	28	0	12	7	0
65	A0	6	0	0	0	0
65	A1	1	0	0	0	0
65	A3	1	0	0	0	0
65	A5	3	0	0	0	0
65	A6	2	0	0	0	0
65	A7	4	0	0	1	0
65	A8	10	0	0	1	0
65	AA	1408	0	0	48	0
65	AB	36	0	0	1	0
65	AD	15	0	0	1	0
65	AE	19	0	0	1	0
65	AF	7	0	0	0	0
65	AG	3	0	0	0	0
65	AH	1	0	0	0	0
65	AN	2	0	0	0	0
65	AO	1	0	0	0	0
65	AP	15	0	0	2	0
65	AQ	4	0	0	2	0
65	AR	2	0	0	2	0
65	AS	1	0	0	0	0
65	AT	2	0	0	0	0
65	AU	5	0	0	0	0
65	AV	2	0	0	0	0
65	AW	2	0	0	0	0
65	AX	3	0	0	0	0
65	AZ	1	0	0	0	0
65	BA	212	0	0	13	0
65	BD	2	0	0	0	0
65	BE	2	0	0	0	0
65	BL	1	0	0	0	0
65	BM	1	0	0	0	0
65	BV	2	0	0	0	0
65	BW	3	0	0	0	0
65	BX	8	0	0	0	0
65	BY	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BZ	2	0	0	0	0
65	C0	6	0	0	1	0
65	C1	2	0	0	0	0
65	C3	2	0	0	0	0
65	C6	1	0	0	1	0
65	C7	1	0	0	0	0
65	C8	3	0	0	0	0
65	CA	985	0	0	52	0
65	CB	9	0	0	1	0
65	CD	14	0	0	0	0
65	CE	13	0	0	1	0
65	CF	7	0	0	0	0
65	CN	2	0	0	0	0
65	CP	10	0	0	1	0
65	CQ	1	0	0	0	0
65	CR	1	0	0	0	0
65	CT	3	0	0	0	0
65	CU	2	0	0	0	0
65	CV	1	0	0	0	0
65	CY	1	0	0	0	0
65	DA	155	0	0	6	0
65	DE	4	0	0	0	0
65	DJ	1	0	0	0	0
65	DK	2	0	0	0	0
65	DL	1	0	0	0	0
65	DW	2	0	0	0	0
65	DX	1	0	0	0	0
All	All	313372	0	210866	5329	17

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 11.

The worst 5 of 5329 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1860:G:H5'	3:CC:206:LYS:CD	1.27	1.64
1:CA:1860:G:H5''	3:CC:206:LYS:CG	1.28	1.64
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.35	1.54
1:CA:1860:G:C5'	3:CC:206:LYS:HD2	1.25	1.53
1:CA:1860:G:C5'	3:CC:206:LYS:CG	1.84	1.50

The worst 5 of 17 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)
3:AC:9:ARG:NH2	59:DZ:504:ARG:NH1[3_654]	0.73	1.47
59:BZ:504:ARG:NH2	3:CC:9:ARG:NE[2_655]	1.08	1.12
59:BZ:504:ARG:NH1	3:CC:9:ARG:NH1[2_655]	1.09	1.11
3:AC:6:LYS:O	59:DZ:501:THR:O[3_654]	1.74	0.46
59:BZ:504:ARG:NH1	3:CC:9:ARG:NE[2_655]	1.80	0.40

## 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	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	1
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	1
4	AD	273/276 (99%)	248 (91%)	22 (8%)	3 (1%)	17	50
4	CD	273/276 (99%)	245 (90%)	25 (9%)	3 (1%)	17	50
5	AE	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	34	69
5	CE	202/206 (98%)	189 (94%)	10 (5%)	3 (2%)	13	40
6	AF	201/210 (96%)	185 (92%)	16 (8%)	0	100	100
6	CF	201/210 (96%)	189 (94%)	8 (4%)	4 (2%)	9	30
7	AG	179/182 (98%)	159 (89%)	14 (8%)	6 (3%)	5	16
7	CG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	5	16
8	AH	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	30	65
8	CH	172/180 (96%)	153 (89%)	13 (8%)	6 (4%)	4	15
9	AK	128/173 (74%)	74 (58%)	26 (20%)	28 (22%)	0	0
9	CK	128/173 (74%)	80 (62%)	28 (22%)	20 (16%)	0	0
10	AL	64/147 (44%)	47 (73%)	13 (20%)	4 (6%)	2	4
10	CL	64/147 (44%)	44 (69%)	17 (27%)	3 (5%)	3	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AN	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
11	CN	138/140 (99%)	126 (91%)	10 (7%)	2 (1%)	14	42
12	AO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	24	58
12	CO	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	24	58
13	AP	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	14	42
13	CP	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	9	30
14	AQ	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
14	CQ	139/141 (99%)	123 (88%)	13 (9%)	3 (2%)	8	28
15	AR	116/118 (98%)	109 (94%)	6 (5%)	1 (1%)	21	55
15	CR	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	21	55
16	AS	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	21	55
16	CS	108/112 (96%)	89 (82%)	17 (16%)	2 (2%)	10	32
17	AT	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
17	CT	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
18	AU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
18	CU	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
19	AV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	19	52
19	CV	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	9	30
20	AW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
20	CW	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
21	AX	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	17	50
21	CX	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	17	50
22	AY	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	19	52
22	CY	105/110 (96%)	90 (86%)	11 (10%)	4 (4%)	4	13
23	AZ	169/206 (82%)	136 (80%)	28 (17%)	5 (3%)	5	18
23	CZ	172/206 (84%)	144 (84%)	25 (14%)	3 (2%)	11	36
24	A0	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	16	47
24	C0	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	9 (10%)	0	100	100
25	C1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	17	50
26	A2	68/72 (94%)	66 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	C2	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	11	34
28	A4	67/71 (94%)	44 (66%)	16 (24%)	7 (10%)	1	1
28	C4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	3
29	A5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	C5	57/60 (95%)	57 (100%)	0	0	100	100
30	A6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
30	C6	51/54 (94%)	45 (88%)	6 (12%)	0	100	100
31	A7	46/49 (94%)	46 (100%)	0	0	100	100
31	C7	46/49 (94%)	44 (96%)	0	2 (4%)	3	10
32	A8	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	C8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	5	17
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	35 (100%)	0	0	100	100
35	BB	229/256 (90%)	187 (82%)	29 (13%)	13 (6%)	2	6
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	4
36	BC	204/239 (85%)	171 (84%)	25 (12%)	8 (4%)	4	12
36	DC	204/239 (85%)	171 (84%)	30 (15%)	3 (2%)	13	40
37	BD	206/209 (99%)	186 (90%)	16 (8%)	4 (2%)	10	32
37	DD	206/209 (99%)	180 (87%)	20 (10%)	6 (3%)	6	19
38	BE	146/162 (90%)	128 (88%)	13 (9%)	5 (3%)	5	16
38	DE	146/162 (90%)	128 (88%)	12 (8%)	6 (4%)	3	11
39	BF	98/101 (97%)	89 (91%)	7 (7%)	2 (2%)	9	30
39	DF	98/101 (97%)	91 (93%)	6 (6%)	1 (1%)	19	52
40	BG	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	15	44
40	DG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	15	44
41	BH	135/138 (98%)	120 (89%)	12 (9%)	3 (2%)	8	28
41	DH	135/138 (98%)	121 (90%)	12 (9%)	2 (2%)	13	40
42	BI	125/128 (98%)	111 (89%)	10 (8%)	4 (3%)	5	17
42	DI	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	12	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BJ	95/105 (90%)	81 (85%)	9 (10%)	5 (5%)	2	7
43	DJ	94/105 (90%)	77 (82%)	10 (11%)	7 (7%)	1	3
44	BK	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	11	34
44	DK	112/129 (87%)	98 (88%)	10 (9%)	4 (4%)	4	14
45	BL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	24	58
45	DL	120/132 (91%)	109 (91%)	11 (9%)	0	100	100
46	BM	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	7	24
46	DM	120/126 (95%)	98 (82%)	13 (11%)	9 (8%)	1	3
47	BN	58/61 (95%)	49 (84%)	8 (14%)	1 (2%)	11	36
47	DN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	11	36
48	BO	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	8	26
48	DO	86/89 (97%)	72 (84%)	12 (14%)	2 (2%)	8	26
49	BP	80/88 (91%)	66 (82%)	12 (15%)	2 (2%)	7	24
49	DP	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	15	44
50	BQ	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	19	52
50	DQ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
51	BR	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	13	40
51	DR	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
52	BS	82/93 (88%)	73 (89%)	9 (11%)	0	100	100
52	DS	81/93 (87%)	67 (83%)	12 (15%)	2 (2%)	7	24
53	BT	94/106 (89%)	78 (83%)	10 (11%)	6 (6%)	2	4
53	DT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	3	10
54	BU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	3	9
59	BZ	722/758 (95%)	598 (83%)	92 (13%)	32 (4%)	3	10
59	DZ	726/758 (96%)	594 (82%)	97 (13%)	35 (5%)	3	9
All	All	13220/14444 (92%)	11544 (87%)	1298 (10%)	378 (3%)	6	19

5 of 378 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS

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Mol	Chain	Res	Type
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	18	45
3	CC	111/180 (62%)	103 (93%)	8 (7%)	18	45
4	AD	215/218 (99%)	189 (88%)	26 (12%)	6	18
4	CD	216/218 (99%)	181 (84%)	35 (16%)	3	8
5	AE	164/166 (99%)	140 (85%)	24 (15%)	4	11
5	CE	164/166 (99%)	139 (85%)	25 (15%)	3	10
6	AF	160/166 (96%)	134 (84%)	26 (16%)	3	8
6	CF	159/166 (96%)	135 (85%)	24 (15%)	3	10
7	AG	143/156 (92%)	119 (83%)	24 (17%)	2	8
7	CG	142/156 (91%)	108 (76%)	34 (24%)	1	2
8	AH	144/148 (97%)	128 (89%)	16 (11%)	8	23
8	CH	144/148 (97%)	125 (87%)	19 (13%)	5	14
10	AL	50/111 (45%)	45 (90%)	5 (10%)	9	27
10	CL	50/111 (45%)	45 (90%)	5 (10%)	9	27
11	AN	118/119 (99%)	94 (80%)	24 (20%)	1	4
11	CN	118/119 (99%)	98 (83%)	20 (17%)	2	7
12	AO	100/100 (100%)	83 (83%)	17 (17%)	2	7
12	CO	100/100 (100%)	83 (83%)	17 (17%)	2	7
13	AP	116/116 (100%)	97 (84%)	19 (16%)	3	8
13	CP	115/116 (99%)	99 (86%)	16 (14%)	4	13
14	AQ	111/111 (100%)	90 (81%)	21 (19%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	95 (86%)	16 (14%)	4	12
15	AR	101/101 (100%)	79 (78%)	22 (22%)	1	3
15	CR	101/101 (100%)	84 (83%)	17 (17%)	2	8
16	AS	87/88 (99%)	71 (82%)	16 (18%)	2	6
16	CS	85/88 (97%)	67 (79%)	18 (21%)	1	4
17	AT	115/127 (91%)	97 (84%)	18 (16%)	3	9
17	CT	113/127 (89%)	93 (82%)	20 (18%)	2	7
18	AU	93/94 (99%)	77 (83%)	16 (17%)	2	7
18	CU	93/94 (99%)	82 (88%)	11 (12%)	6	19
19	AV	80/82 (98%)	65 (81%)	15 (19%)	2	6
19	CV	80/82 (98%)	67 (84%)	13 (16%)	3	8
20	AW	90/92 (98%)	80 (89%)	10 (11%)	8	23
20	CW	90/92 (98%)	79 (88%)	11 (12%)	6	18
21	AX	77/78 (99%)	73 (95%)	4 (5%)	29	62
21	CX	77/78 (99%)	70 (91%)	7 (9%)	12	33
22	AY	85/91 (93%)	73 (86%)	12 (14%)	4	12
22	CY	85/91 (93%)	70 (82%)	15 (18%)	2	7
23	AZ	145/179 (81%)	117 (81%)	28 (19%)	2	5
23	CZ	145/179 (81%)	125 (86%)	20 (14%)	4	13
24	A0	65/67 (97%)	63 (97%)	2 (3%)	47	81
24	C0	65/67 (97%)	60 (92%)	5 (8%)	16	41
25	A1	80/83 (96%)	72 (90%)	8 (10%)	9	27
25	C1	80/83 (96%)	69 (86%)	11 (14%)	4	13
26	A2	65/67 (97%)	54 (83%)	11 (17%)	2	7
26	C2	65/67 (97%)	55 (85%)	10 (15%)	3	10
27	A3	51/52 (98%)	44 (86%)	7 (14%)	4	13
27	C3	50/52 (96%)	38 (76%)	12 (24%)	1	2
28	A4	60/63 (95%)	49 (82%)	11 (18%)	2	6
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	4	13
29	C5	50/52 (96%)	44 (88%)	6 (12%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	40 (78%)	11 (22%)	1	3
30	C6	50/52 (96%)	43 (86%)	7 (14%)	4	13
31	A7	41/42 (98%)	35 (85%)	6 (15%)	4	11
31	C7	41/42 (98%)	36 (88%)	5 (12%)	6	18
32	A8	54/55 (98%)	47 (87%)	7 (13%)	5	15
32	C8	54/55 (98%)	49 (91%)	5 (9%)	11	32
33	A9	34/34 (100%)	31 (91%)	3 (9%)	12	35
33	C9	34/34 (100%)	29 (85%)	5 (15%)	4	11
35	BB	192/220 (87%)	144 (75%)	48 (25%)	1	2
35	DB	187/220 (85%)	157 (84%)	30 (16%)	3	9
36	BC	143/188 (76%)	124 (87%)	19 (13%)	5	14
36	DC	141/188 (75%)	115 (82%)	26 (18%)	2	6
37	BD	170/181 (94%)	146 (86%)	24 (14%)	4	12
37	DD	174/181 (96%)	148 (85%)	26 (15%)	4	11
38	BE	113/123 (92%)	104 (92%)	9 (8%)	15	40
38	DE	114/123 (93%)	96 (84%)	18 (16%)	3	9
39	BF	84/90 (93%)	71 (84%)	13 (16%)	3	10
39	DF	86/90 (96%)	75 (87%)	11 (13%)	5	16
40	BG	119/127 (94%)	98 (82%)	21 (18%)	2	7
40	DG	120/127 (94%)	112 (93%)	8 (7%)	20	50
41	BH	114/119 (96%)	98 (86%)	16 (14%)	4	13
41	DH	114/119 (96%)	92 (81%)	22 (19%)	2	5
42	BI	91/99 (92%)	72 (79%)	19 (21%)	1	4
42	DI	89/99 (90%)	71 (80%)	18 (20%)	1	4
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	6	18
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	3	9
44	BK	83/99 (84%)	71 (86%)	12 (14%)	4	11
44	DK	83/99 (84%)	74 (89%)	9 (11%)	8	23
45	BL	97/109 (89%)	90 (93%)	7 (7%)	18	45
45	DL	97/109 (89%)	86 (89%)	11 (11%)	7	22
46	BM	95/101 (94%)	82 (86%)	13 (14%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	92/101 (91%)	76 (83%)	16 (17%)	2	7
47	BN	49/50 (98%)	39 (80%)	10 (20%)	1	4
47	DN	49/50 (98%)	40 (82%)	9 (18%)	2	6
48	BO	78/80 (98%)	64 (82%)	14 (18%)	2	6
48	DO	78/80 (98%)	68 (87%)	10 (13%)	5	16
49	BP	69/74 (93%)	56 (81%)	13 (19%)	2	6
49	DP	68/74 (92%)	61 (90%)	7 (10%)	9	26
50	BQ	94/97 (97%)	81 (86%)	13 (14%)	4	13
50	DQ	94/97 (97%)	82 (87%)	12 (13%)	5	16
51	BR	59/77 (77%)	47 (80%)	12 (20%)	1	4
51	DR	59/77 (77%)	51 (86%)	8 (14%)	5	14
52	BS	70/80 (88%)	61 (87%)	9 (13%)	5	16
52	DS	67/80 (84%)	60 (90%)	7 (10%)	9	25
53	BT	70/82 (85%)	59 (84%)	11 (16%)	3	9
53	DT	71/82 (87%)	58 (82%)	13 (18%)	2	6
54	BU	18/22 (82%)	16 (89%)	2 (11%)	8	23
54	DU	18/22 (82%)	16 (89%)	2 (11%)	8	23
59	BZ	604/636 (95%)	489 (81%)	115 (19%)	2	5
59	DZ	607/636 (95%)	505 (83%)	102 (17%)	2	8
All	All	10652/11672 (91%)	9013 (85%)	1639 (15%)	3	10

5 of 1639 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	BZ	89	ASP
6	CF	140	LEU
51	DR	85	LEU
59	BZ	222	ASP
3	CC	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
59	BZ	573	HIS

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Mol	Chain	Res	Type
10	CL	116	ASN
59	DZ	-50	GLN
59	BZ	675	HIS
4	CD	96	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2866/2915 (98%)	477 (16%)	41 (1%)
1	CA	2860/2915 (98%)	517 (18%)	37 (1%)
2	AB	119/121 (98%)	11 (9%)	0
2	CB	119/121 (98%)	19 (15%)	0
34	BA	1494/1521 (98%)	265 (17%)	21 (1%)
34	DA	1501/1521 (98%)	284 (18%)	23 (1%)
55	BV	12/24 (50%)	3 (25%)	0
55	DV	11/24 (45%)	1 (9%)	0
56	BW	70/76 (92%)	18 (25%)	1 (1%)
56	DW	67/76 (88%)	22 (32%)	2 (2%)
57	BX	74/77 (96%)	10 (13%)	0
57	DX	74/77 (96%)	13 (17%)	0
58	BY	71/76 (93%)	20 (28%)	2 (2%)
58	DY	69/76 (90%)	19 (27%)	0
All	All	9407/9620 (97%)	1679 (17%)	127 (1%)

5 of 1679 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C
1	AA	62	U

5 of 127 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	1201	A
1	CA	310	A
34	DA	991	U
34	BA	1335	C
58	BY	58	A

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

40 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$
56	PSU	BW	32	60,56	13,21,22	1.25	1 (7%)	18,30,33	3.35	6 (33%)
56	MIA	BW	37	56	21,31,32	1.88	2 (9%)	26,44,47	1.92	7 (26%)
56	PSU	BW	39	56	13,21,22	0.74	0	18,30,33	3.50	5 (27%)
56	7MG	BW	46	56	19,26,27	1.00	1 (5%)	24,39,42	2.92	7 (29%)
56	5MU	BW	54	56	12,22,23	0.50	0	14,32,35	2.57	2 (14%)
56	PSU	BW	55	56	13,21,22	0.66	0	18,30,33	3.46	6 (33%)
56	F3N	BW	76	1,56	27,36,37	1.34	5 (18%)	31,51,54	2.34	3 (9%)
56	4SU	BW	8	56	11,21,22	1.25	1 (9%)	13,30,33	1.17	1 (7%)
57	5MC	BX	32	57	13,22,23	1.14	1 (7%)	15,32,35	1.51	3 (20%)
57	5MU	BX	54	60,57	12,22,23	0.47	0	14,32,35	2.53	2 (14%)
57	PSU	BX	55	57	13,21,22	1.46	1 (7%)	18,30,33	3.41	6 (33%)
57	31H	BX	76	60,57	25,34,35	1.25	4 (16%)	26,47,50	3.08	5 (19%)
57	4SU	BX	8	57	11,21,22	1.18	1 (9%)	13,30,33	1.31	1 (7%)
58	PSU	BY	32	58	13,21,22	0.77	0	18,30,33	3.46	5 (27%)
58	MIA	BY	37	58	15,24,32	1.27	2 (13%)	16,35,47	2.23	3 (18%)
58	PSU	BY	39	58	13,21,22	1.23	1 (7%)	18,30,33	3.33	6 (33%)
58	7MG	BY	46	58	19,26,27	1.02	1 (5%)	24,39,42	3.07	6 (25%)
58	5MU	BY	54	58	12,22,23	0.36	0	14,32,35	2.43	2 (14%)
58	PSU	BY	55	58	13,21,22	1.27	1 (7%)	18,30,33	3.38	6 (33%)
58	4SU	BY	8	58	11,21,22	1.27	1 (9%)	13,30,33	1.24	1 (7%)
56	PSU	DW	32	56	13,21,22	0.84	1 (7%)	18,30,33	3.35	6 (33%)
56	MIA	DW	37	56	15,24,32	1.20	2 (13%)	16,35,47	2.10	2 (12%)
56	PSU	DW	39	56	13,21,22	1.32	1 (7%)	18,30,33	3.55	6 (33%)
56	7MG	DW	46	56	19,26,27	0.96	1 (5%)	24,39,42	2.89	6 (25%)
56	5MU	DW	54	56	12,22,23	0.34	0	14,32,35	2.42	2 (14%)
56	PSU	DW	55	56	13,21,22	0.99	1 (7%)	18,30,33	3.53	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	F3N	DW	76	1,56	27,36,37	1.46	5 (18%)	31,51,54	2.46	5 (16%)
56	4SU	DW	8	56	11,21,22	1.24	1 (9%)	13,30,33	1.30	1 (7%)
57	5MC	DX	32	57	13,22,23	1.51	1 (7%)	15,32,35	1.01	2 (13%)
57	5MU	DX	54	57	12,22,23	0.42	0	14,32,35	2.12	2 (14%)
57	PSU	DX	55	57	13,21,22	1.01	1 (7%)	18,30,33	3.41	5 (27%)
57	31H	DX	76	60,57	25,34,35	1.24	4 (16%)	26,47,50	3.07	5 (19%)
57	4SU	DX	8	57	11,21,22	1.30	1 (9%)	13,30,33	1.00	1 (7%)
58	PSU	DY	32	58	13,21,22	1.15	1 (7%)	18,30,33	3.42	6 (33%)
58	MIA	DY	37	58	15,24,32	1.17	2 (13%)	16,35,47	2.12	2 (12%)
58	PSU	DY	39	58	13,21,22	1.17	2 (15%)	18,30,33	3.39	5 (27%)
58	7MG	DY	46	58	19,26,27	1.07	1 (5%)	24,39,42	3.29	8 (33%)
58	5MU	DY	54	58	12,22,23	0.36	0	14,32,35	2.35	2 (14%)
58	PSU	DY	55	58	13,21,22	1.20	1 (7%)	18,30,33	3.34	6 (33%)
58	4SU	DY	8	58	11,21,22	1.28	1 (9%)	13,30,33	1.25	1 (7%)

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
56	PSU	BW	32	60,56	-	0/7/25/26	0/2/2/2
56	MIA	BW	37	56	-	0/11/33/34	0/3/3/3
56	PSU	BW	39	56	-	0/7/25/26	0/2/2/2
56	7MG	BW	46	56	-	0/7/37/38	0/3/3/3
56	5MU	BW	54	56	-	0/3/25/26	0/2/2/2
56	PSU	BW	55	56	-	0/7/25/26	0/2/2/2
56	F3N	BW	76	1,56	-	0/15/37/38	0/4/4/4
56	4SU	BW	8	56	-	0/3/25/26	0/2/2/2
57	5MC	BX	32	57	-	0/3/25/26	0/2/2/2
57	5MU	BX	54	60,57	-	0/3/25/26	0/2/2/2
57	PSU	BX	55	57	-	0/7/25/26	0/2/2/2
57	31H	BX	76	60,57	-	1/18/40/41	0/3/3/3
57	4SU	BX	8	57	-	0/3/25/26	0/2/2/2
58	PSU	BY	32	58	-	0/7/25/26	0/2/2/2
58	MIA	BY	37	58	-	0/3/25/34	0/3/3/3
58	PSU	BY	39	58	-	0/7/25/26	0/2/2/2
58	7MG	BY	46	58	-	0/7/37/38	0/3/3/3
58	5MU	BY	54	58	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PSU	BY	55	58	-	0/7/25/26	0/2/2/2
58	4SU	BY	8	58	-	0/3/25/26	0/2/2/2
56	PSU	DW	32	56	-	0/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/3/25/34	0/3/3/3
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	0/7/37/38	0/3/3/3
56	5MU	DW	54	56	-	0/3/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	F3N	DW	76	1,56	-	0/15/37/38	0/4/4/4
56	4SU	DW	8	56	-	0/3/25/26	0/2/2/2
57	5MC	DX	32	57	-	0/3/25/26	0/2/2/2
57	5MU	DX	54	57	-	0/3/25/26	0/2/2/2
57	PSU	DX	55	57	-	0/7/25/26	0/2/2/2
57	31H	DX	76	60,57	-	1/18/40/41	0/3/3/3
57	4SU	DX	8	57	-	0/3/25/26	0/2/2/2
58	PSU	DY	32	58	-	0/7/25/26	0/2/2/2
58	MIA	DY	37	58	-	0/3/25/34	0/3/3/3
58	PSU	DY	39	58	-	0/7/25/26	0/2/2/2
58	7MG	DY	46	58	-	0/7/37/38	0/3/3/3
58	5MU	DY	54	58	-	0/3/25/26	0/2/2/2
58	PSU	DY	55	58	-	0/7/25/26	0/2/2/2
58	4SU	DY	8	58	-	0/3/25/26	0/2/2/2

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-7.59	1.69	1.75
57	BX	55	PSU	C5-C1'	-4.74	1.48	1.52
56	DW	39	PSU	C5-C1'	-4.33	1.48	1.52
58	BY	55	PSU	C5-C1'	-4.06	1.48	1.52
57	DX	8	4SU	C4-S4	-4.04	1.59	1.67

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DW	76	F3N	N3-C2-N1	-11.79	119.87	128.89
56	BW	76	F3N	N3-C2-N1	-11.78	119.87	128.89
57	BX	76	31H	N3-C2-N1	-11.65	119.97	128.89
57	DX	76	31H	N3-C2-N1	-11.61	120.00	128.89
56	BW	39	PSU	N1-C2-N3	-11.47	121.02	128.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	DX	76	31H	OCN-CN-N-CA
57	BX	76	31H	OCN-CN-N-CA

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	39	PSU	1	0
56	BW	55	PSU	1	0
56	BW	76	F3N	2	0
56	BW	8	4SU	1	0
57	BX	32	5MC	2	0
57	BX	55	PSU	1	0
58	BY	39	PSU	1	0
58	BY	8	4SU	1	0
56	DW	32	PSU	1	0
56	DW	37	MIA	1	0
56	DW	46	7MG	2	0
56	DW	54	5MU	1	0
56	DW	55	PSU	1	0
56	DW	76	F3N	4	0
57	DX	55	PSU	1	0
57	DX	76	31H	3	0
57	DX	8	4SU	1	0
58	DY	37	MIA	2	0
58	DY	39	PSU	1	0
58	DY	55	PSU	3	0
58	DY	8	4SU	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 2073 ligands modelled in this entry, 2069 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
63	SF4	BD	501	37	0,12,12	0.00	-	0,24,24	0.00	-
64	GDP	BZ	702	60	23,30,30	1.15	2 (8%)	30,47,47	2.01	7 (23%)
63	SF4	DD	501	37	0,12,12	0.00	-	0,24,24	0.00	-
64	GDP	DZ	702	60	23,30,30	1.08	2 (8%)	30,47,47	1.85	8 (26%)

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
63	SF4	BD	501	37	-	0/0/48/48	0/6/5/5
64	GDP	BZ	702	60	-	0/12/32/32	0/3/3/3
63	SF4	DD	501	37	-	0/0/48/48	0/6/5/5
64	GDP	DZ	702	60	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	BZ	702	GDP	C6-C5	2.67	1.46	1.41
64	DZ	702	GDP	C5-C4	2.96	1.47	1.40
64	DZ	702	GDP	C6-C5	3.10	1.47	1.41
64	BZ	702	GDP	C5-C4	3.13	1.47	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	BZ	702	GDP	C5-C6-N1	-5.06	116.67	123.59
64	BZ	702	GDP	C2'-C1'-N9	-4.63	107.22	114.29
64	DZ	702	GDP	C5-C6-N1	-4.40	117.57	123.59
64	DZ	702	GDP	PA-O3A-PB	-3.38	121.33	132.67
64	DZ	702	GDP	C2'-C1'-N9	-3.25	109.32	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	BD	501	SF4	1	0
64	BZ	702	GDP	6	0
63	DD	501	SF4	1	0
64	DZ	702	GDP	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	2872/2915 (98%)	-0.13	60 (2%) 67 56	16, 36, 153, 292	0
1	CA	2868/2915 (98%)	-0.01	112 (3%) 43 31	25, 54, 187, 320	0
2	AB	120/121 (99%)	-0.38	0 100 100	26, 52, 72, 110	0
2	CB	120/121 (99%)	-0.08	0 100 100	55, 87, 110, 177	0
3	AC	137/228 (60%)	4.05	114 (83%) 0 0	95, 162, 210, 232	0
3	CC	137/228 (60%)	5.81	126 (91%) 0 0	115, 183, 225, 239	0
4	AD	275/276 (99%)	-0.47	2 (0%) 89 84	16, 35, 59, 113	0
4	CD	275/276 (99%)	-0.33	1 (0%) 93 90	19, 46, 73, 142	0
5	AE	204/206 (99%)	-0.47	0 100 100	8, 36, 67, 101	0
5	CE	204/206 (99%)	-0.27	0 100 100	25, 53, 88, 136	0
6	AF	203/210 (96%)	-0.41	1 (0%) 91 88	12, 37, 91, 175	0
6	CF	203/210 (96%)	-0.29	0 100 100	23, 63, 114, 164	0
7	AG	181/182 (99%)	-0.22	3 (1%) 73 63	41, 71, 110, 179	0
7	CG	181/182 (99%)	0.32	8 (4%) 38 26	74, 106, 143, 190	0
8	AH	174/180 (96%)	-0.35	2 (1%) 82 74	30, 51, 81, 174	0
8	CH	174/180 (96%)	0.63	12 (6%) 20 11	45, 94, 139, 208	0
9	AK	130/173 (75%)	1.30	27 (20%) 1 1	62, 125, 191, 235	0
9	CK	130/173 (75%)	2.94	73 (56%) 0 0	104, 173, 211, 231	0
10	AL	66/147 (44%)	4.22	51 (77%) 0 0	134, 182, 226, 242	0
10	CL	66/147 (44%)	5.96	53 (80%) 0 0	115, 198, 249, 257	0
11	AN	140/140 (100%)	-0.52	0 100 100	17, 34, 76, 106	0
11	CN	140/140 (100%)	-0.09	1 (0%) 89 84	33, 59, 97, 139	0
12	AO	122/122 (100%)	-0.32	0 100 100	20, 40, 67, 95	0
12	CO	122/122 (100%)	-0.29	0 100 100	33, 52, 83, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AP	149/150 (99%)	-0.29	0 100 100	14, 44, 83, 127	0
13	CP	149/150 (99%)	0.23	4 (2%) 58 45	29, 66, 112, 154	0
14	AQ	141/141 (100%)	-0.37	0 100 100	17, 39, 66, 97	0
14	CQ	141/141 (100%)	-0.32	0 100 100	33, 62, 91, 156	0
15	AR	118/118 (100%)	-0.47	0 100 100	17, 32, 57, 96	0
15	CR	118/118 (100%)	-0.26	0 100 100	29, 52, 78, 97	0
16	AS	110/112 (98%)	-0.15	0 100 100	32, 54, 81, 102	0
16	CS	110/112 (98%)	0.28	4 (3%) 46 34	53, 82, 112, 143	0
17	AT	131/146 (89%)	-0.29	2 (1%) 76 68	23, 44, 94, 160	0
17	CT	131/146 (89%)	-0.31	0 100 100	37, 58, 99, 155	0
18	AU	116/118 (98%)	-0.56	0 100 100	15, 28, 48, 110	0
18	CU	116/118 (98%)	-0.27	1 (0%) 85 79	36, 52, 82, 123	0
19	AV	101/101 (100%)	-0.56	1 (0%) 84 77	19, 34, 63, 119	0
19	CV	101/101 (100%)	-0.03	1 (0%) 84 77	33, 72, 108, 138	0
20	AW	112/113 (99%)	-0.44	0 100 100	15, 29, 56, 134	0
20	CW	112/113 (99%)	-0.23	1 (0%) 85 79	27, 48, 86, 149	0
21	AX	95/96 (98%)	-0.44	1 (1%) 82 74	22, 38, 69, 125	0
21	CX	95/96 (98%)	0.04	4 (4%) 40 28	40, 61, 93, 134	0
22	AY	107/110 (97%)	-0.28	1 (0%) 85 79	25, 48, 92, 129	0
22	CY	107/110 (97%)	0.69	7 (6%) 22 13	43, 78, 114, 172	0
23	AZ	171/206 (83%)	0.08	11 (6%) 23 14	33, 73, 144, 235	0
23	CZ	174/206 (84%)	0.85	22 (12%) 5 2	60, 107, 174, 243	0
24	A0	83/85 (97%)	-0.30	2 (2%) 62 50	18, 38, 68, 147	0
24	C0	83/85 (97%)	0.32	6 (7%) 18 10	37, 62, 96, 135	0
25	A1	97/98 (98%)	-0.21	2 (2%) 67 56	23, 44, 85, 108	0
25	C1	97/98 (98%)	-0.09	1 (1%) 84 77	33, 54, 107, 119	0
26	A2	70/72 (97%)	-0.27	2 (2%) 55 43	22, 47, 74, 149	0
26	C2	70/72 (97%)	0.04	1 (1%) 78 69	51, 78, 99, 121	0
27	A3	59/60 (98%)	-0.28	1 (1%) 73 63	18, 34, 63, 112	0
27	C3	59/60 (98%)	0.61	5 (8%) 13 6	43, 62, 108, 167	0
28	A4	69/71 (97%)	0.49	9 (13%) 5 2	60, 100, 186, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	C4	69/71 (97%)	0.98	13 (18%) 2 1	89, 138, 197, 212	0
29	A5	59/60 (98%)	-0.56	0 100 100	15, 30, 55, 84	0
29	C5	59/60 (98%)	-0.22	1 (1%) 73 63	29, 46, 77, 112	0
30	A6	53/54 (98%)	-0.38	0 100 100	24, 42, 67, 91	0
30	C6	53/54 (98%)	-0.08	1 (1%) 70 59	43, 63, 88, 103	0
31	A7	48/49 (97%)	-0.26	2 (4%) 40 28	14, 26, 63, 126	0
31	C7	48/49 (97%)	-0.08	1 (2%) 67 56	26, 38, 83, 105	0
32	A8	64/65 (98%)	-0.43	0 100 100	17, 32, 46, 72	0
32	C8	64/65 (98%)	-0.23	0 100 100	36, 51, 70, 101	0
33	A9	37/37 (100%)	-0.11	0 100 100	23, 39, 60, 80	0
33	C9	37/37 (100%)	0.25	1 (2%) 58 45	42, 66, 96, 108	0
34	BA	1497/1521 (98%)	0.05	35 (2%) 64 52	32, 76, 169, 302	0
34	DA	1503/1521 (98%)	0.13	37 (2%) 61 48	40, 83, 174, 317	0
35	BB	231/256 (90%)	0.49	18 (7%) 16 8	61, 108, 167, 197	0
35	DB	231/256 (90%)	0.84	33 (14%) 4 2	77, 129, 184, 232	0
36	BC	206/239 (86%)	0.33	8 (3%) 43 31	60, 103, 138, 194	0
36	DC	206/239 (86%)	0.91	25 (12%) 6 3	77, 127, 170, 196	0
37	BD	208/209 (99%)	0.07	3 (1%) 78 69	51, 82, 121, 168	0
37	DD	208/209 (99%)	-0.01	2 (0%) 84 77	47, 80, 112, 165	0
38	BE	148/162 (91%)	-0.08	0 100 100	48, 73, 111, 140	0
38	DE	148/162 (91%)	0.20	4 (2%) 58 45	46, 89, 128, 151	0
39	BF	100/101 (99%)	-0.21	0 100 100	45, 80, 116, 137	0
39	DF	100/101 (99%)	-0.17	1 (1%) 84 77	49, 80, 104, 121	0
40	BG	155/156 (99%)	0.28	13 (8%) 14 6	59, 88, 132, 174	0
40	DG	155/156 (99%)	0.68	17 (10%) 7 3	67, 103, 142, 192	0
41	BH	137/138 (99%)	0.09	1 (0%) 89 84	45, 76, 106, 135	0
41	DH	137/138 (99%)	0.38	6 (4%) 38 26	55, 88, 127, 170	0
42	BI	127/128 (99%)	0.61	10 (7%) 15 8	50, 101, 140, 166	0
42	DI	127/128 (99%)	1.32	28 (22%) 1 1	66, 118, 159, 201	0
43	BJ	97/105 (92%)	0.82	14 (14%) 3 2	53, 113, 158, 199	0
43	DJ	96/105 (91%)	1.47	25 (26%) 1 0	70, 134, 181, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	BK	114/129 (88%)	-0.26	0 100 100	45, 72, 112, 129	0
44	DK	114/129 (88%)	-0.01	1 (0%) 85 79	44, 80, 118, 139	0
45	BL	122/132 (92%)	-0.22	0 100 100	38, 63, 88, 113	0
45	DL	122/132 (92%)	-0.01	2 (1%) 74 66	37, 72, 94, 141	0
46	BM	123/126 (97%)	0.54	9 (7%) 18 10	55, 95, 129, 222	0
46	DM	122/126 (96%)	0.90	16 (13%) 5 2	71, 125, 153, 188	0
47	BN	60/61 (98%)	0.57	4 (6%) 21 12	65, 95, 123, 138	0
47	DN	60/61 (98%)	1.71	20 (33%) 0 0	84, 123, 166, 208	0
48	BO	88/89 (98%)	-0.04	2 (2%) 64 52	39, 68, 110, 142	0
48	DO	88/89 (98%)	0.26	0 100 100	43, 78, 112, 127	0
49	BP	82/88 (93%)	0.35	2 (2%) 62 50	54, 76, 109, 134	0
49	DP	82/88 (93%)	0.19	2 (2%) 62 50	53, 70, 96, 131	0
50	BQ	99/105 (94%)	-0.07	0 100 100	43, 69, 97, 110	0
50	DQ	99/105 (94%)	0.10	0 100 100	51, 74, 103, 123	0
51	BR	68/88 (77%)	0.48	4 (5%) 26 16	48, 73, 112, 135	0
51	DR	68/88 (77%)	0.48	4 (5%) 26 16	46, 78, 116, 135	0
52	BS	84/93 (90%)	1.07	16 (19%) 2 1	67, 110, 163, 180	0
52	DS	83/93 (89%)	1.89	39 (46%) 0 0	92, 141, 187, 229	0
53	BT	96/106 (90%)	0.25	1 (1%) 84 77	53, 77, 115, 169	0
53	DT	96/106 (90%)	0.29	1 (1%) 84 77	52, 77, 117, 132	0
54	BU	23/27 (85%)	0.78	3 (13%) 5 2	56, 89, 104, 114	0
54	DU	23/27 (85%)	1.73	9 (39%) 0 0	79, 109, 130, 142	0
55	BV	13/24 (54%)	1.63	5 (38%) 0 0	49, 87, 172, 178	0
55	DV	12/24 (50%)	2.51	7 (58%) 0 0	63, 120, 171, 199	0
56	BW	66/76 (86%)	2.49	32 (48%) 0 0	64, 169, 230, 256	0
56	DW	64/76 (84%)	3.51	44 (68%) 0 0	92, 197, 239, 263	0
57	BX	71/77 (92%)	-0.02	0 100 100	34, 78, 124, 188	0
57	DX	71/77 (92%)	0.21	2 (2%) 56 44	34, 100, 148, 162	0
58	BY	67/76 (88%)	0.88	9 (13%) 4 2	39, 159, 224, 266	0
58	DY	66/76 (86%)	1.30	15 (22%) 1 1	57, 178, 229, 251	0
59	BZ	728/758 (96%)	1.11	156 (21%) 1 1	41, 107, 195, 257	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
59	DZ	730/758 (96%)	1.56	230 (31%) <b>1</b> <b>0</b>	38, 116, 213, 248	0
All	All	22848/24064 (94%)	0.26	1669 (7%) <b>18</b> <b>10</b>	8, 68, 177, 320	0

The worst 5 of 1669 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
59	BZ	503	GLY	25.7
10	CL	137	GLU	19.6
3	CC	174	ALA	18.4
10	CL	138	VAL	16.2
59	BZ	502	GLY	15.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
56	PSU	BW	39	20/21	0.90	0.23	-	96,96,96,96	0
58	MIA	BY	37	22/30	0.85	0.18	-	118,118,118,118	0
56	4SU	BW	8	20/21	0.64	0.28	-	200,200,200,200	0
58	5MU	DY	54	21/22	0.73	0.36	-	200,200,200,200	0
56	PSU	BW	55	20/21	0.73	0.31	-	113,113,113,113	0
58	4SU	BY	8	20/21	0.71	0.21	-	191,191,191,191	0
58	PSU	DY	32	20/21	0.82	0.20	-	154,154,154,154	0
57	PSU	BX	55	20/21	0.94	0.13	-	74,74,74,74	0
58	PSU	BY	55	20/21	0.64	0.24	-	205,205,205,205	0
58	MIA	DY	37	22/30	0.68	0.29	-	156,156,156,156	0
57	5MU	DX	54	21/22	0.94	0.18	-	108,108,108,108	0
57	31H	BX	76	32/33	0.94	0.26	-	58,58,58,58	4
56	5MU	BW	54	21/22	0.89	0.25	-	89,89,89,89	0
58	PSU	DY	55	20/21	0.51	0.53	-	222,222,222,222	0
58	7MG	BY	46	24/25	0.71	0.21	-	200,200,200,200	0
57	5MC	BX	32	21/22	0.95	0.17	-	65,65,65,65	0
56	7MG	DW	46	24/25	0.65	0.34	-	244,244,244,244	0
56	PSU	BW	32	20/21	0.92	0.21	-	110,110,110,110	0
57	31H	DX	76	32/33	0.87	0.31	-	58,58,58,58	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	PSU	DW	32	20/21	0.89	0.36	-	139,139,139,139	0
56	PSU	DW	55	20/21	0.52	0.44	-	190,190,190,190	0
58	PSU	BY	32	20/21	0.84	0.20	-	126,126,126,126	0
56	5MU	DW	54	21/22	0.87	0.22	-	118,118,118,118	0
58	4SU	DY	8	20/21	0.62	0.21	-	193,193,193,193	0
56	MIA	DW	37	22/30	0.90	0.27	-	116,116,116,116	0
57	4SU	BX	8	20/21	0.93	0.14	-	70,70,70,70	1
56	F3N	BW	76	33/34	0.96	0.25	-	54,54,54,54	1
58	7MG	DY	46	24/25	0.64	0.24	-	206,206,206,206	0
56	7MG	BW	46	24/25	0.72	0.27	-	203,203,203,203	0
56	4SU	DW	8	20/21	0.58	0.49	-	225,225,225,225	0
56	PSU	DW	39	20/21	0.89	0.24	-	118,118,118,118	0
57	5MU	BX	54	21/22	0.93	0.17	-	85,85,85,85	0
58	PSU	DY	39	20/21	0.84	0.21	-	138,138,138,138	0
57	4SU	DX	8	20/21	0.90	0.14	-	96,96,96,96	0
56	MIA	BW	37	29/30	0.90	0.30	-	95,95,95,95	1
56	F3N	DW	76	33/34	0.91	0.35	-	75,75,75,75	1
58	5MU	BY	54	21/22	0.30	0.33	-	217,217,217,217	0
57	5MC	DX	32	21/22	0.93	0.20	-	86,86,86,86	0
58	PSU	BY	39	20/21	0.91	0.17	-	106,106,106,106	0
57	PSU	DX	55	20/21	0.91	0.13	-	95,95,95,95	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3110	1/1	0.80	0.49	130.27	57,57,57,57	0
60	MG	CE	304	1/1	0.86	0.75	95.16	74,74,74,74	0
60	MG	CA	3182	1/1	0.97	0.58	89.51	45,45,45,45	0
60	MG	AA	3183	1/1	0.72	0.97	88.23	89,89,89,89	0
60	MG	AA	3240	1/1	0.91	0.51	83.99	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3170	1/1	0.91	0.57	77.69	44,44,44,44	1
60	MG	AA	3770	1/1	0.45	0.80	73.21	57,57,57,57	1
60	MG	AA	3671	1/1	0.86	0.58	65.39	31,31,31,31	1
60	MG	AA	3121	1/1	0.85	0.30	61.99	63,63,63,63	0
60	MG	AA	3806	1/1	0.86	0.55	46.27	56,56,56,56	0
60	MG	AA	3115	1/1	0.97	0.47	45.73	44,44,44,44	0
60	MG	AA	3018	1/1	0.81	0.66	45.66	55,55,55,55	0
60	MG	AA	3196	1/1	0.97	0.34	45.12	48,48,48,48	0
60	MG	AA	3134	1/1	0.94	0.52	45.11	49,49,49,49	0
60	MG	AA	3705	1/1	0.91	0.44	44.42	29,29,29,29	1
60	MG	CA	3218	1/1	0.83	0.88	43.83	63,63,63,63	0
60	MG	AA	3817	1/1	0.96	0.46	41.72	40,40,40,40	0
60	MG	AA	3739	1/1	0.60	0.42	40.61	90,90,90,90	0
60	MG	AH	201	1/1	0.83	1.24	40.42	83,83,83,83	0
60	MG	AA	3101	1/1	0.89	0.47	38.58	68,68,68,68	0
60	MG	C5	101	1/1	0.90	0.43	36.58	64,64,64,64	0
60	MG	CA	3641	1/1	0.95	0.54	35.93	59,59,59,59	0
60	MG	CF	302	1/1	0.91	0.32	33.58	64,64,64,64	0
60	MG	CF	306	1/1	0.74	0.94	33.26	85,85,85,85	0
60	MG	CA	3595	1/1	0.92	0.26	32.98	67,67,67,67	0
60	MG	AA	3160	1/1	0.85	0.48	32.92	96,96,96,96	0
60	MG	AA	3213	1/1	0.93	0.61	32.67	49,49,49,49	0
60	MG	DA	1667	1/1	0.89	0.43	32.45	70,70,70,70	0
60	MG	AA	3060	1/1	0.94	0.34	31.97	23,23,23,23	0
60	MG	CA	3099	1/1	0.97	0.46	30.72	55,55,55,55	0
60	MG	AA	3044	1/1	0.95	0.36	30.69	62,62,62,62	0
60	MG	CA	3022	1/1	0.92	0.62	30.67	76,76,76,76	0
60	MG	AA	3822	1/1	0.90	0.60	30.59	67,67,67,67	0
60	MG	CA	3165	1/1	0.92	0.52	30.20	58,58,58,58	0
60	MG	CA	3496	1/1	0.82	0.55	30.19	58,58,58,58	0
60	MG	AA	3231	1/1	0.92	0.49	29.73	87,87,87,87	0
60	MG	CE	301	1/1	0.86	0.60	29.57	54,54,54,54	0
60	MG	AA	3038	1/1	0.93	0.40	29.24	42,42,42,42	0
60	MG	AA	3082	1/1	0.98	0.58	28.14	57,57,57,57	1
60	MG	AA	3818	1/1	0.98	0.36	27.88	46,46,46,46	0
60	MG	AA	3302	1/1	0.95	0.34	27.53	58,58,58,58	0
60	MG	CA	3312	1/1	0.89	0.38	27.15	52,52,52,52	0
60	MG	CF	301	1/1	0.83	0.45	27.00	61,61,61,61	0
60	MG	AA	3133	1/1	0.95	0.47	26.48	92,92,92,92	1
60	MG	AA	3772	1/1	0.93	0.53	26.40	37,37,37,37	0
60	MG	AA	3803	1/1	0.95	0.33	26.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3500	1/1	0.88	0.47	25.81	56,56,56,56	0
60	MG	AA	3144	1/1	0.97	0.49	25.72	48,48,48,48	0
60	MG	AA	3769	1/1	0.88	0.45	25.71	48,48,48,48	1
60	MG	CA	3655	1/1	0.91	0.47	25.45	69,69,69,69	0
60	MG	CE	303	1/1	0.73	0.39	25.27	55,55,55,55	0
60	MG	AU	201	1/1	0.89	0.53	25.21	72,72,72,72	0
60	MG	AA	3300	1/1	0.81	0.30	25.14	43,43,43,43	0
60	MG	CA	3656	1/1	0.92	0.54	25.05	75,75,75,75	0
60	MG	AA	3829	1/1	0.82	0.39	25.01	89,89,89,89	0
60	MG	BA	1687	1/1	0.92	0.59	24.67	73,73,73,73	0
60	MG	AA	3043	1/1	0.92	0.29	24.61	39,39,39,39	0
60	MG	AA	3178	1/1	0.99	0.43	24.24	50,50,50,50	0
60	MG	AF	303	1/1	0.87	0.56	23.85	54,54,54,54	0
60	MG	AA	3167	1/1	0.91	0.29	23.74	69,69,69,69	0
60	MG	CA	3282	1/1	0.73	0.38	22.31	75,75,75,75	0
60	MG	AA	3211	1/1	0.93	0.59	21.98	53,53,53,53	0
60	MG	AA	3706	1/1	0.99	0.35	21.68	26,26,26,26	1
60	MG	AA	3034	1/1	0.94	0.34	21.60	84,84,84,84	0
60	MG	CA	3035	1/1	0.87	0.36	21.53	47,47,47,47	0
60	MG	CA	3662	1/1	0.90	0.37	21.52	60,60,60,60	0
60	MG	AB	3008	1/1	0.95	0.39	21.39	46,46,46,46	0
60	MG	CA	3463	1/1	0.95	0.43	21.07	75,75,75,75	0
60	MG	CA	3115	1/1	0.84	0.54	20.69	71,71,71,71	0
60	MG	CA	3464	1/1	0.87	0.61	20.51	78,78,78,78	0
60	MG	CU	201	1/1	0.95	0.51	20.51	62,62,62,62	0
60	MG	CA	3028	1/1	0.97	0.64	20.12	60,60,60,60	0
60	MG	AA	3129	1/1	0.95	0.26	20.00	52,52,52,52	0
60	MG	CA	3026	1/1	0.96	0.47	19.94	55,55,55,55	0
60	MG	AA	3354	1/1	0.93	0.29	19.84	56,56,56,56	0
60	MG	AA	3033	1/1	0.88	0.41	19.83	48,48,48,48	0
60	MG	AA	3692	1/1	0.67	0.48	19.80	86,86,86,86	0
60	MG	AA	3250	1/1	0.86	0.45	19.51	46,46,46,46	1
60	MG	AA	3212	1/1	0.99	0.40	19.29	43,43,43,43	0
60	MG	CD	301	1/1	0.92	0.35	18.88	61,61,61,61	0
60	MG	AA	3662	1/1	0.95	0.33	18.83	60,60,60,60	0
60	MG	AU	204	1/1	0.95	0.45	18.69	55,55,55,55	0
60	MG	CA	3084	1/1	0.93	0.39	18.69	73,73,73,73	0
60	MG	BA	1757	1/1	0.79	0.35	18.61	63,63,63,63	0
60	MG	CA	3102	1/1	0.92	0.34	18.51	50,50,50,50	0
60	MG	AE	305	1/1	0.88	0.42	18.43	44,44,44,44	0
60	MG	AA	3116	1/1	0.97	0.32	18.32	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3702	1/1	0.80	0.45	18.27	45,45,45,45	1
60	MG	AD	310	1/1	0.92	0.49	18.20	63,63,63,63	0
60	MG	CA	3438	1/1	0.97	0.29	18.15	45,45,45,45	0
60	MG	AA	3347	1/1	0.74	0.32	18.07	63,63,63,63	0
60	MG	DA	1686	1/1	0.21	0.36	18.06	102,102,102,102	0
60	MG	CA	3460	1/1	0.90	0.28	18.05	57,57,57,57	0
60	MG	AA	3698	1/1	0.90	0.31	17.97	51,51,51,51	1
60	MG	AA	3810	1/1	0.92	0.34	17.94	49,49,49,49	0
60	MG	AA	3210	1/1	0.79	0.55	17.48	106,106,106,106	0
60	MG	CQ	201	1/1	0.58	0.76	17.37	85,85,85,85	0
60	MG	CA	3121	1/1	0.95	0.32	17.22	78,78,78,78	0
60	MG	AA	3460	1/1	0.90	0.30	17.19	81,81,81,81	0
60	MG	AA	3339	1/1	0.94	0.29	17.12	18,18,18,18	0
60	MG	AA	3824	1/1	0.88	0.33	17.01	53,53,53,53	0
60	MG	CA	3541	1/1	0.97	0.34	16.99	58,58,58,58	0
60	MG	CA	3215	1/1	0.91	0.43	16.78	50,50,50,50	0
60	MG	CA	3653	1/1	0.40	0.52	16.76	102,102,102,102	0
60	MG	BA	1724	1/1	0.88	0.31	16.59	60,60,60,60	0
60	MG	AA	3281	1/1	0.96	0.43	16.45	38,38,38,38	0
60	MG	CA	3226	1/1	0.82	0.37	16.37	56,56,56,56	0
60	MG	CA	3220	1/1	0.90	0.50	16.33	89,89,89,89	0
60	MG	CA	3156	1/1	0.81	1.42	16.19	92,92,92,92	0
60	MG	AA	3581	1/1	0.92	0.26	16.10	48,48,48,48	0
60	MG	AA	3507	1/1	0.91	0.25	16.04	53,53,53,53	0
60	MG	BA	1804	1/1	0.75	0.47	15.74	94,94,94,94	0
60	MG	AA	3050	1/1	0.94	0.25	15.59	29,29,29,29	0
60	MG	AA	3767	1/1	0.83	0.29	15.51	75,75,75,75	0
60	MG	CA	3601	1/1	0.92	0.36	15.19	61,61,61,61	0
60	MG	CA	3346	1/1	0.92	0.31	15.13	48,48,48,48	0
60	MG	CA	3576	1/1	0.81	0.35	15.13	91,91,91,91	0
60	MG	AA	3740	1/1	0.89	0.26	15.11	54,54,54,54	0
60	MG	C7	101	1/1	0.91	0.43	14.99	47,47,47,47	0
60	MG	AA	3596	1/1	0.93	0.21	14.95	39,39,39,39	0
60	MG	AA	3461	1/1	0.92	0.22	14.94	57,57,57,57	0
60	MG	AA	3127	1/1	0.83	0.45	14.93	83,83,83,83	0
60	MG	AA	3258	1/1	0.87	0.26	14.92	32,32,32,32	0
60	MG	CA	3418	1/1	0.89	0.31	14.73	53,53,53,53	0
60	MG	AA	3828	1/1	0.71	0.55	14.71	68,68,68,68	0
60	MG	AX	102	1/1	0.77	0.37	14.48	78,78,78,78	0
60	MG	CA	3233	1/1	0.97	0.30	14.24	52,52,52,52	0
60	MG	AA	3200	1/1	0.87	0.28	14.19	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
60	MG	AA	3181	1/1	0.83	0.40	14.19	55,55,55,55	0
60	MG	CA	3163	1/1	0.94	0.31	14.05	41,41,41,41	0
60	MG	AD	305	1/1	0.92	0.55	14.03	75,75,75,75	0
60	MG	AA	3296	1/1	0.98	0.27	14.01	40,40,40,40	0
60	MG	AA	3228	1/1	0.88	0.32	14.01	63,63,63,63	0
60	MG	AP	201	1/1	0.97	0.31	13.63	35,35,35,35	0
60	MG	CA	3439	1/1	0.97	0.23	13.58	47,47,47,47	0
60	MG	CA	3181	1/1	0.88	0.31	13.47	68,68,68,68	0
60	MG	CA	3619	1/1	0.75	0.35	13.19	78,78,78,78	0
60	MG	CA	3122	1/1	0.79	0.33	13.09	95,95,95,95	0
60	MG	CA	3320	1/1	0.97	0.25	13.07	47,47,47,47	0
60	MG	AA	3137	1/1	0.92	0.36	13.03	55,55,55,55	0
60	MG	AA	3036	1/1	0.83	0.20	13.02	63,63,63,63	0
60	MG	CA	3110	1/1	0.96	0.33	12.80	35,35,35,35	0
60	MG	AA	3819	1/1	0.97	0.37	12.77	46,46,46,46	0
60	MG	AA	3112	1/1	0.98	0.36	12.74	44,44,44,44	0
60	MG	BA	1705	1/1	0.95	0.30	12.67	61,61,61,61	0
60	MG	AA	3039	1/1	0.96	0.25	12.66	34,34,34,34	0
60	MG	DA	1767	1/1	0.84	0.56	12.51	88,88,88,88	0
60	MG	AA	3376	1/1	0.95	0.21	12.41	39,39,39,39	0
60	MG	CA	3032	1/1	0.77	0.43	12.40	67,67,67,67	0
60	MG	BA	1629	1/1	0.78	0.25	12.30	71,71,71,71	0
60	MG	AA	3525	1/1	0.92	0.21	11.87	45,45,45,45	0
60	MG	CA	3279	1/1	0.97	0.26	11.79	46,46,46,46	0
60	MG	AA	3047	1/1	0.94	0.30	11.58	40,40,40,40	0
60	MG	AA	3510	1/1	0.96	0.22	11.56	13,13,13,13	0
60	MG	AA	3589	1/1	0.87	0.33	11.53	31,31,31,31	1
60	MG	AA	3131	1/1	0.96	0.29	11.46	39,39,39,39	0
60	MG	CA	3529	1/1	0.73	0.31	11.40	69,69,69,69	0
60	MG	AA	3248	1/1	0.88	0.49	10.92	79,79,79,79	0
60	MG	CA	3154	1/1	0.92	0.22	10.90	68,68,68,68	0
60	MG	AA	3582	1/1	0.76	0.35	10.87	78,78,78,78	0
60	MG	AA	3289	1/1	0.91	0.19	10.79	47,47,47,47	0
60	MG	BA	1671	1/1	0.80	0.36	10.78	71,71,71,71	0
60	MG	CA	3179	1/1	0.95	0.27	10.78	27,27,27,27	0
60	MG	AA	3717	1/1	0.97	0.23	10.74	47,47,47,47	0
60	MG	AA	3714	1/1	0.94	0.24	10.73	44,44,44,44	0
60	MG	AA	3120	1/1	0.89	0.26	10.63	54,54,54,54	0
60	MG	AA	3564	1/1	0.97	0.23	10.61	17,17,17,17	0
60	MG	CA	3288	1/1	0.90	0.34	10.53	39,39,39,39	0
60	MG	DA	1619	1/1	0.93	0.36	10.48	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3214	1/1	0.91	0.28	10.41	50,50,50,50	0
60	MG	BA	1686	1/1	0.98	0.25	10.38	58,58,58,58	0
60	MG	CA	3106	1/1	0.93	0.27	10.21	45,45,45,45	0
60	MG	AD	302	1/1	0.94	0.39	10.18	31,31,31,31	0
60	MG	AA	3206	1/1	0.96	0.19	9.95	55,55,55,55	0
60	MG	AA	3109	1/1	0.84	0.35	9.81	75,75,75,75	0
60	MG	AA	3797	1/1	0.91	0.31	9.79	60,60,60,60	0
60	MG	AA	3825	1/1	0.96	0.29	9.74	45,45,45,45	0
60	MG	AA	3524	1/1	0.85	0.30	9.72	41,41,41,41	0
60	MG	CA	3408	1/1	0.94	0.27	9.32	35,35,35,35	0
60	MG	CA	3160	1/1	0.95	0.27	9.21	33,33,33,33	0
60	MG	AA	3830	1/1	0.94	0.30	9.02	75,75,75,75	0
60	MG	CA	3209	1/1	0.91	0.27	9.01	101,101,101,101	0
60	MG	CA	3184	1/1	0.87	0.26	8.92	43,43,43,43	0
60	MG	CA	3311	1/1	0.72	0.29	8.85	54,54,54,54	0
60	MG	AA	3827	1/1	0.91	0.29	8.75	39,39,39,39	0
60	MG	AA	3604	1/1	0.89	0.23	8.73	44,44,44,44	1
60	MG	AA	3823	1/1	0.94	0.34	8.70	51,51,51,51	0
60	MG	CA	3293	1/1	0.85	0.31	8.64	82,82,82,82	0
60	MG	DA	1638	1/1	0.81	0.28	8.48	60,60,60,60	0
60	MG	AA	3019	1/1	0.89	0.26	8.42	53,53,53,53	0
60	MG	AA	3708	1/1	0.86	0.30	8.40	71,71,71,71	0
60	MG	AD	301	1/1	0.97	0.34	8.33	46,46,46,46	0
60	MG	DA	1650	1/1	0.92	0.31	8.22	48,48,48,48	0
60	MG	AA	3686	1/1	0.96	0.24	8.18	62,62,62,62	0
60	MG	CV	202	1/1	0.95	0.35	8.16	82,82,82,82	0
60	MG	CA	3236	1/1	0.85	0.30	8.11	80,80,80,80	0
60	MG	CA	3366	1/1	0.85	0.24	8.10	60,60,60,60	0
60	MG	CA	3330	1/1	0.92	0.27	8.03	37,37,37,37	0
60	MG	CA	3450	1/1	0.98	0.24	8.01	38,38,38,38	0
60	MG	AA	3149	1/1	0.98	0.25	7.95	15,15,15,15	0
60	MG	BA	1658	1/1	0.91	0.55	7.88	68,68,68,68	0
60	MG	DA	1637	1/1	0.94	0.37	7.87	61,61,61,61	0
60	MG	CA	3157	1/1	0.97	0.23	7.84	56,56,56,56	0
60	MG	AA	3539	1/1	0.95	0.23	7.82	42,42,42,42	0
60	MG	CA	3083	1/1	0.76	0.22	7.79	80,80,80,80	0
60	MG	CA	3227	1/1	0.95	0.25	7.73	30,30,30,30	0
60	MG	AD	304	1/1	0.97	0.34	7.68	49,49,49,49	0
60	MG	AA	3173	1/1	0.94	0.26	7.52	74,74,74,74	0
60	MG	DA	1696	1/1	0.95	0.26	7.49	65,65,65,65	0
60	MG	AA	3517	1/1	0.96	0.31	7.44	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3430	1/1	0.94	0.22	7.37	38,38,38,38	0
60	MG	CA	3407	1/1	0.80	0.28	7.36	41,41,41,41	0
60	MG	AA	3711	1/1	0.95	0.37	7.34	41,41,41,41	0
60	MG	AA	3020	1/1	0.96	0.18	7.29	25,25,25,25	0
60	MG	AA	3654	1/1	0.84	0.25	7.27	81,81,81,81	0
60	MG	DA	1646	1/1	0.96	0.30	7.24	51,51,51,51	0
60	MG	CA	3659	1/1	0.80	0.35	7.21	72,72,72,72	0
60	MG	CA	3187	1/1	0.78	0.32	7.18	70,70,70,70	0
60	MG	AA	3721	1/1	0.90	0.20	7.08	21,21,21,21	0
60	MG	CA	3143	1/1	0.90	0.23	7.02	62,62,62,62	0
60	MG	AA	3119	1/1	0.89	0.22	7.01	41,41,41,41	0
60	MG	AA	3514	1/1	0.97	0.21	7.00	32,32,32,32	0
60	MG	AA	3669	1/1	0.97	0.21	6.98	36,36,36,36	0
60	MG	AA	3516	1/1	0.90	0.27	6.98	38,38,38,38	0
60	MG	AA	3251	1/1	0.93	0.26	6.94	50,50,50,50	0
60	MG	AW	3003	1/1	0.95	0.33	6.93	38,38,38,38	0
60	MG	CA	3455	1/1	0.97	0.27	6.82	37,37,37,37	0
60	MG	AA	3602	1/1	0.95	0.21	6.82	39,39,39,39	0
60	MG	AA	3834	1/1	0.93	0.29	6.70	49,49,49,49	0
60	MG	AA	3102	1/1	0.95	0.24	6.66	38,38,38,38	0
60	MG	A0	101	1/1	0.79	0.23	6.65	88,88,88,88	0
60	MG	AA	3816	1/1	0.96	0.24	6.65	64,64,64,64	0
60	MG	AA	3001	1/1	0.94	0.21	6.58	39,39,39,39	0
60	MG	AA	3833	1/1	0.97	0.24	6.58	39,39,39,39	0
60	MG	CA	3013	1/1	0.87	0.32	6.57	52,52,52,52	0
60	MG	AD	309	1/1	0.80	0.34	6.52	58,58,58,58	0
60	MG	BA	1615	1/1	0.94	0.30	6.52	65,65,65,65	0
60	MG	CA	3324	1/1	0.97	0.22	6.45	31,31,31,31	0
60	MG	AA	3220	1/1	0.95	0.19	6.32	65,65,65,65	0
60	MG	AA	3408	1/1	0.82	0.26	6.29	41,41,41,41	0
60	MG	AA	3369	1/1	0.84	0.19	6.24	59,59,59,59	0
60	MG	AA	3023	1/1	0.98	0.46	6.22	40,40,40,40	1
60	MG	AA	3310	1/1	0.92	0.17	6.21	37,37,37,37	0
60	MG	CA	3413	1/1	0.94	0.25	6.21	38,38,38,38	0
60	MG	CA	3087	1/1	0.79	0.41	6.16	107,107,107,107	0
60	MG	AA	3315	1/1	0.95	0.21	6.10	56,56,56,56	0
60	MG	DA	1694	1/1	0.92	0.27	6.08	60,60,60,60	0
60	MG	AA	3417	1/1	0.93	0.19	6.04	16,16,16,16	0
60	MG	BA	1662	1/1	0.90	0.17	6.01	45,45,45,45	0
60	MG	AA	3222	1/1	0.92	0.26	5.97	58,58,58,58	0
60	MG	AA	3141	1/1	0.91	0.20	5.96	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3356	1/1	0.95	0.24	5.95	28,28,28,28	0
60	MG	AB	3014	1/1	0.72	0.23	5.92	70,70,70,70	0
60	MG	CA	3598	1/1	0.88	0.21	5.87	66,66,66,66	0
60	MG	AU	202	1/1	0.92	0.27	5.84	65,65,65,65	0
60	MG	BA	1626	1/1	0.92	0.25	5.80	72,72,72,72	0
60	MG	AA	3451	1/1	0.96	0.18	5.80	43,43,43,43	0
60	MG	AA	3415	1/1	0.99	0.20	5.68	29,29,29,29	0
60	MG	AA	3185	1/1	0.97	0.20	5.65	35,35,35,35	0
60	MG	AA	3257	1/1	0.91	0.22	5.63	18,18,18,18	0
60	MG	AQ	3001	1/1	0.86	0.26	5.60	56,56,56,56	0
60	MG	CA	3129	1/1	0.83	0.30	5.58	76,76,76,76	0
60	MG	AA	3035	1/1	0.96	0.22	5.56	69,69,69,69	0
60	MG	AA	3735	1/1	0.92	0.27	5.46	30,30,30,30	0
60	MG	CA	3549	1/1	0.89	0.18	5.42	29,29,29,29	0
60	MG	AA	3352	1/1	0.92	0.18	5.29	64,64,64,64	0
60	MG	AA	3790	1/1	0.97	0.23	5.28	11,11,11,11	0
60	MG	CA	3411	1/1	0.73	0.24	5.26	49,49,49,49	0
60	MG	AA	3021	1/1	0.90	0.20	5.24	49,49,49,49	0
60	MG	CA	3652	1/1	0.75	0.23	5.22	79,79,79,79	0
60	MG	DA	1742	1/1	0.88	0.25	5.17	52,52,52,52	0
60	MG	AA	3218	1/1	0.98	0.20	5.16	10,10,10,10	0
60	MG	AA	3274	1/1	0.92	0.49	5.13	48,48,48,48	1
60	MG	AA	3529	1/1	0.94	0.19	5.13	12,12,12,12	1
60	MG	AA	3045	1/1	0.97	0.33	5.09	58,58,58,58	0
60	MG	AA	3309	1/1	0.91	0.18	5.07	72,72,72,72	0
60	MG	AA	3387	1/1	0.96	0.21	5.03	34,34,34,34	0
60	MG	AN	3002	1/1	0.90	0.20	5.01	76,76,76,76	0
60	MG	CA	3264	1/1	0.96	0.20	4.96	54,54,54,54	0
60	MG	AA	3241	1/1	0.96	0.26	4.93	29,29,29,29	0
60	MG	DA	1651	1/1	0.65	0.26	4.92	86,86,86,86	0
60	MG	CA	3002	1/1	0.93	0.24	4.88	32,32,32,32	0
60	MG	CA	3210	1/1	0.88	0.23	4.87	44,44,44,44	0
60	MG	AA	3528	1/1	0.96	0.19	4.87	26,26,26,26	0
60	MG	BA	1683	1/1	0.91	0.24	4.83	50,50,50,50	0
60	MG	CA	3558	1/1	0.96	0.20	4.82	49,49,49,49	1
60	MG	BA	1765	1/1	0.98	0.30	4.82	67,67,67,67	0
60	MG	AA	3437	1/1	0.91	0.20	4.77	25,25,25,25	0
60	MG	CA	3307	1/1	0.98	0.21	4.75	31,31,31,31	0
60	MG	CA	3315	1/1	0.91	0.21	4.71	44,44,44,44	0
60	MG	CA	3274	1/1	0.95	0.18	4.68	64,64,64,64	0
60	MG	AA	3401	1/1	0.92	0.22	4.66	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3323	1/1	0.97	0.18	4.65	42,42,42,42	0
60	MG	DA	1679	1/1	0.95	0.38	4.64	70,70,70,70	0
60	MG	AA	3398	1/1	0.95	0.19	4.62	29,29,29,29	0
60	MG	C3	101	1/1	0.84	0.46	4.60	91,91,91,91	0
60	MG	AA	3486	1/1	0.80	0.21	4.60	34,34,34,34	0
60	MG	CA	3446	1/1	0.97	0.24	4.60	37,37,37,37	0
60	MG	AA	3385	1/1	0.96	0.20	4.59	24,24,24,24	0
60	MG	CA	3198	1/1	0.96	0.25	4.58	49,49,49,49	0
60	MG	AA	3826	1/1	0.98	0.22	4.58	56,56,56,56	0
60	MG	AA	3357	1/1	0.96	0.18	4.53	52,52,52,52	0
60	MG	AA	3741	1/1	0.95	0.27	4.48	47,47,47,47	0
60	MG	AN	3001	1/1	0.86	0.47	4.47	64,64,64,64	0
60	MG	CA	3166	1/1	0.98	0.20	4.46	31,31,31,31	0
60	MG	AA	3559	1/1	0.90	0.21	4.45	37,37,37,37	0
60	MG	CA	3265	1/1	0.86	0.20	4.44	66,66,66,66	0
60	MG	AA	3430	1/1	0.97	0.24	4.37	23,23,23,23	0
60	MG	AA	3454	1/1	0.95	0.16	4.27	27,27,27,27	0
60	MG	DE	201	1/1	0.78	0.31	4.25	93,93,93,93	0
60	MG	DA	1714	1/1	0.90	0.39	4.24	82,82,82,82	0
60	MG	AA	3792	1/1	0.95	0.26	4.21	35,35,35,35	0
60	MG	AA	3513	1/1	0.93	0.22	4.20	37,37,37,37	0
60	MG	CA	3449	1/1	0.97	0.21	4.16	52,52,52,52	0
60	MG	CA	3082	1/1	0.96	0.21	4.12	31,31,31,31	0
60	MG	AA	3438	1/1	0.86	0.21	4.11	75,75,75,75	0
60	MG	CA	3359	1/1	0.97	0.22	4.06	44,44,44,44	0
60	MG	AA	3378	1/1	0.86	0.21	4.04	24,24,24,24	0
60	MG	BA	1655	1/1	0.95	0.26	4.04	65,65,65,65	0
60	MG	BA	1630	1/1	0.80	0.19	3.89	61,61,61,61	0
60	MG	DA	1674	1/1	0.93	0.28	3.86	60,60,60,60	0
60	MG	DA	1611	1/1	0.74	0.23	3.86	80,80,80,80	0
60	MG	AA	3180	1/1	0.86	0.25	3.84	53,53,53,53	0
60	MG	AA	3518	1/1	0.94	0.18	3.82	28,28,28,28	0
60	MG	CA	3381	1/1	0.97	0.22	3.82	37,37,37,37	0
60	MG	AA	3565	1/1	0.97	0.21	3.78	26,26,26,26	0
60	MG	AA	3541	1/1	0.78	0.20	3.77	61,61,61,61	0
60	MG	AA	3712	1/1	0.92	0.20	3.73	50,50,50,50	0
60	MG	AA	3052	1/1	0.96	0.20	3.68	15,15,15,15	0
60	MG	AA	3556	1/1	0.94	0.17	3.67	54,54,54,54	0
60	MG	DA	1631	1/1	0.77	0.22	3.65	55,55,55,55	0
60	MG	AA	3386	1/1	0.97	0.21	3.63	19,19,19,19	0
60	MG	AA	3506	1/1	0.97	0.20	3.59	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3505	1/1	0.97	0.23	3.55	29,29,29,29	0
60	MG	BA	1749	1/1	0.99	0.27	3.53	52,52,52,52	0
60	MG	BA	1778	1/1	0.98	0.26	3.53	52,52,52,52	0
60	MG	CA	3114	1/1	0.86	0.20	3.50	59,59,59,59	0
60	MG	DA	1719	1/1	0.85	0.22	3.49	87,87,87,87	0
60	MG	AA	3523	1/1	0.98	0.17	3.42	35,35,35,35	0
60	MG	CA	3617	1/1	0.86	0.38	3.42	41,41,41,41	0
60	MG	AA	3042	1/1	0.97	0.20	3.39	43,43,43,43	0
60	MG	AA	3184	1/1	0.95	0.20	3.39	39,39,39,39	0
60	MG	CA	3249	1/1	0.80	0.18	3.32	67,67,67,67	0
60	MG	AA	3551	1/1	0.95	0.17	3.28	58,58,58,58	0
60	MG	AA	3832	1/1	0.96	0.21	3.26	52,52,52,52	0
60	MG	CV	201	1/1	0.95	0.36	3.25	84,84,84,84	0
60	MG	AU	203	1/1	0.89	0.24	3.17	55,55,55,55	0
60	MG	CA	3038	1/1	0.96	0.21	3.13	26,26,26,26	0
60	MG	AA	3313	1/1	0.92	0.17	3.13	31,31,31,31	0
60	MG	AA	3330	1/1	0.97	0.21	3.13	33,33,33,33	0
60	MG	BA	1785	1/1	0.89	0.19	3.12	69,69,69,69	0
60	MG	BA	1675	1/1	0.93	0.19	3.12	50,50,50,50	0
60	MG	CA	3068	1/1	0.84	0.19	3.08	73,73,73,73	0
60	MG	AD	308	1/1	0.97	0.36	3.08	49,49,49,49	0
60	MG	AA	3253	1/1	0.95	0.19	3.07	42,42,42,42	0
60	MG	BA	1601	1/1	0.82	0.19	3.06	66,66,66,66	0
60	MG	BA	1701	1/1	0.94	0.21	3.05	47,47,47,47	0
60	MG	AA	3217	1/1	0.92	0.16	3.04	50,50,50,50	0
60	MG	DA	1688	1/1	0.88	0.20	2.99	46,46,46,46	0
60	MG	AA	3172	1/1	0.97	0.18	2.95	50,50,50,50	0
60	MG	AA	3294	1/1	0.90	0.19	2.92	56,56,56,56	0
60	MG	AA	3277	1/1	0.91	0.19	2.92	48,48,48,48	0
60	MG	CQ	202	1/1	0.92	0.25	2.85	56,56,56,56	0
60	MG	DA	1706	1/1	0.94	0.19	2.81	70,70,70,70	0
60	MG	AA	3535	1/1	0.94	0.18	2.79	37,37,37,37	0
60	MG	CA	3423	1/1	0.96	0.17	2.79	57,57,57,57	0
60	MG	AA	3187	1/1	0.89	0.17	2.79	29,29,29,29	0
60	MG	AA	3540	1/1	0.92	0.20	2.77	28,28,28,28	0
60	MG	CA	3018	1/1	0.78	0.18	2.72	59,59,59,59	0
60	MG	AF	301	1/1	0.85	0.20	2.68	49,49,49,49	0
60	MG	CA	3473	1/1	0.93	0.24	2.67	48,48,48,48	0
60	MG	AA	3272	1/1	0.93	0.41	2.64	74,74,74,74	0
60	MG	BB	3001	1/1	0.96	0.23	2.63	67,67,67,67	0
60	MG	CA	3431	1/1	0.78	0.17	2.61	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1679	1/1	0.92	0.20	2.59	51,51,51,51	0
60	MG	AA	3532	1/1	0.97	0.18	2.55	20,20,20,20	0
60	MG	CA	3625	1/1	0.98	0.23	2.49	46,46,46,46	0
60	MG	AA	3168	1/1	0.93	0.20	2.47	60,60,60,60	0
60	MG	CA	3100	1/1	0.96	0.17	2.46	75,75,75,75	0
60	MG	DA	1602	1/1	0.80	0.22	2.45	65,65,65,65	0
60	MG	AA	3471	1/1	0.99	0.18	2.33	24,24,24,24	0
60	MG	CA	3454	1/1	0.98	0.23	2.31	43,43,43,43	0
60	MG	AA	3190	1/1	0.95	0.18	2.27	51,51,51,51	0
60	MG	CA	3004	1/1	0.97	0.18	2.25	43,43,43,43	0
60	MG	AA	3008	1/1	0.98	0.17	2.22	28,28,28,28	0
60	MG	AB	3016	1/1	0.87	0.14	2.21	47,47,47,47	0
60	MG	AA	3384	1/1	0.95	0.16	2.20	26,26,26,26	0
60	MG	CA	3103	1/1	0.77	0.19	2.18	80,80,80,80	0
60	MG	BA	1648	1/1	0.95	0.18	2.15	28,28,28,28	0
60	MG	AA	3796	1/1	0.99	0.24	2.11	45,45,45,45	0
60	MG	CA	3488	1/1	0.94	0.17	2.11	58,58,58,58	0
60	MG	AA	3572	1/1	0.90	0.16	2.07	51,51,51,51	0
60	MG	AD	306	1/1	0.80	0.22	1.99	108,108,108,108	0
60	MG	CA	3661	1/1	0.93	0.18	1.95	78,78,78,78	0
60	MG	CA	3224	1/1	0.97	0.18	1.94	32,32,32,32	0
60	MG	CA	3426	1/1	0.95	0.16	1.94	46,46,46,46	0
60	MG	DA	1763	1/1	0.86	0.15	1.92	61,61,61,61	0
60	MG	CA	3134	1/1	0.94	0.18	1.91	64,64,64,64	0
60	MG	BA	1678	1/1	0.95	0.22	1.89	52,52,52,52	0
60	MG	CA	3452	1/1	0.94	0.17	1.79	37,37,37,37	0
60	MG	AA	3723	1/1	0.98	0.16	1.79	30,30,30,30	0
60	MG	BA	1791	1/1	0.92	0.18	1.78	58,58,58,58	0
60	MG	CA	3297	1/1	0.96	0.16	1.77	55,55,55,55	0
60	MG	CA	3316	1/1	0.97	0.19	1.72	34,34,34,34	0
60	MG	AA	3484	1/1	0.92	0.23	1.65	48,48,48,48	0
60	MG	AA	3407	1/1	0.96	0.19	1.64	22,22,22,22	0
60	MG	AA	3835	1/1	0.94	0.23	1.63	34,34,34,34	1
60	MG	AA	3809	1/1	0.96	0.25	1.63	46,46,46,46	0
60	MG	CA	3650	1/1	0.91	0.17	1.57	42,42,42,42	0
60	MG	CA	3495	1/1	0.91	0.18	1.52	64,64,64,64	0
60	MG	AA	3457	1/1	0.96	0.17	1.45	18,18,18,18	0
60	MG	AA	3501	1/1	0.92	0.16	1.40	45,45,45,45	0
60	MG	AA	3801	1/1	0.95	0.16	1.29	39,39,39,39	0
60	MG	CA	3040	1/1	0.94	0.18	1.24	63,63,63,63	0
60	MG	AA	3432	1/1	0.99	0.16	1.24	24,24,24,24	0
60	MG	AA	3527	1/1	0.97	0.16	1.24	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CB	3007	1/1	0.90	0.14	1.22	57,57,57,57	0
60	MG	A9	502	1/1	0.93	0.28	1.20	52,52,52,52	0
60	MG	AA	3820	1/1	0.94	0.21	1.19	31,31,31,31	0
60	MG	CA	3657	1/1	0.94	0.24	1.16	34,34,34,34	0
60	MG	CA	3422	1/1	0.98	0.18	1.15	43,43,43,43	0
60	MG	CA	3344	1/1	0.96	0.18	1.15	27,27,27,27	0
60	MG	DA	1740	1/1	0.98	0.17	1.13	56,56,56,56	0
60	MG	AA	3328	1/1	0.98	0.22	1.12	21,21,21,21	0
60	MG	DA	1685	1/1	0.96	0.20	1.10	49,49,49,49	0
60	MG	DA	1668	1/1	0.87	0.27	1.07	68,68,68,68	0
60	MG	AA	3606	1/1	0.96	0.18	1.07	62,62,62,62	0
60	MG	BA	1640	1/1	0.90	0.19	1.02	56,56,56,56	0
60	MG	DA	1601	1/1	0.93	0.17	0.99	59,59,59,59	0
60	MG	AA	3791	1/1	0.94	0.23	0.99	48,48,48,48	0
60	MG	BA	1690	1/1	0.93	0.19	0.96	59,59,59,59	0
60	MG	AA	3012	1/1	0.94	0.17	0.96	38,38,38,38	0
60	MG	AA	3298	1/1	0.94	0.15	0.95	28,28,28,28	0
60	MG	CA	3328	1/1	0.95	0.17	0.95	40,40,40,40	0
60	MG	CA	3361	1/1	0.87	0.14	0.93	70,70,70,70	0
60	MG	CA	3357	1/1	0.85	0.17	0.92	34,34,34,34	0
60	MG	CA	3425	1/1	0.93	0.15	0.92	45,45,45,45	0
60	MG	CA	3223	1/1	0.98	0.18	0.85	46,46,46,46	0
60	MG	BA	1775	1/1	0.99	0.22	0.83	47,47,47,47	0
60	MG	DA	1657	1/1	0.87	0.14	0.81	75,75,75,75	0
60	MG	DA	1644	1/1	0.96	0.18	0.77	49,49,49,49	0
60	MG	BA	1603	1/1	0.85	0.20	0.75	65,65,65,65	0
60	MG	AA	3224	1/1	0.98	0.19	0.74	26,26,26,26	0
60	MG	CA	3589	1/1	0.85	0.16	0.73	67,67,67,67	0
60	MG	AA	3393	1/1	0.93	0.17	0.72	18,18,18,18	0
60	MG	CA	3304	1/1	0.95	0.15	0.69	48,48,48,48	0
60	MG	CA	3390	1/1	0.87	0.21	0.66	42,42,42,42	0
60	MG	CA	3097	1/1	0.88	0.17	0.66	79,79,79,79	0
60	MG	CA	3280	1/1	0.82	0.17	0.63	43,43,43,43	0
60	MG	BA	1684	1/1	0.91	0.21	0.62	64,64,64,64	0
60	MG	CD	304	1/1	0.94	0.23	0.58	32,32,32,32	0
60	MG	CA	3651	1/1	0.97	0.17	0.57	41,41,41,41	0
60	MG	CA	3615	1/1	0.95	0.15	0.52	33,33,33,33	0
60	MG	DA	1765	1/1	0.72	0.26	0.50	66,66,66,66	0
60	MG	DT	3001	1/1	0.83	0.25	0.48	59,59,59,59	0
60	MG	CA	3417	1/1	0.93	0.18	0.47	58,58,58,58	0
60	MG	AA	3053	1/1	0.98	0.15	0.47	21,21,21,21	0
60	MG	DA	1642	1/1	0.85	0.17	0.46	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
60	MG	CA	3649	1/1	0.97	0.19	0.45	15,15,15,15	0
60	MG	BT	3001	1/1	0.92	0.27	0.41	47,47,47,47	0
60	MG	AA	3504	1/1	0.90	0.13	0.32	44,44,44,44	0
60	MG	AA	3585	1/1	0.82	0.15	0.31	60,60,60,60	0
60	MG	CA	3554	1/1	0.94	0.16	0.24	60,60,60,60	0
60	MG	CA	3318	1/1	0.97	0.16	0.21	31,31,31,31	0
60	MG	CF	305	1/1	0.96	0.20	0.20	45,45,45,45	0
60	MG	AA	3312	1/1	0.95	0.14	0.19	25,25,25,25	0
60	MG	BN	503	1/1	0.78	0.22	0.17	61,61,61,61	0
60	MG	AA	3574	1/1	0.98	0.15	0.16	26,26,26,26	0
60	MG	AA	3483	1/1	0.90	0.18	0.13	21,21,21,21	0
60	MG	DA	1693	1/1	0.94	0.15	0.11	50,50,50,50	0
60	MG	CA	3266	1/1	0.95	0.15	0.11	67,67,67,67	0
62	ZN	A5	101	1/1	1.00	0.13	0.08	40,40,40,40	0
60	MG	CA	3518	1/1	0.95	0.18	0.03	72,72,72,72	0
60	MG	AA	3333	1/1	0.93	0.15	0.03	33,33,33,33	0
60	MG	AA	3380	1/1	0.91	0.18	-0.01	75,75,75,75	0
60	MG	CA	3211	1/1	0.98	0.14	-0.17	19,19,19,19	0
60	MG	CA	3415	1/1	0.97	0.18	-0.19	43,43,43,43	0
60	MG	CA	3044	1/1	0.93	0.14	-0.26	64,64,64,64	0
60	MG	CA	3017	1/1	0.98	0.15	-0.26	28,28,28,28	0
60	MG	CG	3001	1/1	0.93	0.19	-0.28	66,66,66,66	0
60	MG	CA	3335	1/1	0.91	0.16	-0.30	38,38,38,38	0
60	MG	AA	3620	1/1	0.96	0.14	-0.31	49,49,49,49	0
60	MG	CA	3660	1/1	0.83	0.14	-0.32	65,65,65,65	0
60	MG	CA	3300	1/1	0.94	0.15	-0.33	56,56,56,56	0
60	MG	BA	1813	1/1	0.88	0.17	-0.38	66,66,66,66	0
60	MG	BA	1741	1/1	0.96	0.15	-0.38	49,49,49,49	0
60	MG	BA	1759	1/1	0.85	0.14	-0.42	60,60,60,60	0
60	MG	CA	3034	1/1	0.94	0.15	-0.45	51,51,51,51	0
60	MG	AA	3622	1/1	0.89	0.13	-0.46	52,52,52,52	0
60	MG	AA	3617	1/1	0.97	0.12	-0.47	32,32,32,32	0
60	MG	AA	3405	1/1	0.97	0.15	-0.49	27,27,27,27	0
60	MG	CA	3486	1/1	0.86	0.14	-0.54	48,48,48,48	0
64	GDP	BZ	702	28/28	0.97	0.14	-0.55	57,57,57,57	1
60	MG	CA	3313	1/1	0.98	0.14	-0.55	54,54,54,54	0
60	MG	AD	303	1/1	0.90	0.13	-0.58	46,46,46,46	0
60	MG	AA	3759	1/1	0.94	0.13	-0.60	29,29,29,29	0
60	MG	DE	202	1/1	0.83	0.17	-0.70	92,92,92,92	0
60	MG	AA	3799	1/1	0.94	0.12	-0.70	45,45,45,45	0
60	MG	DA	1681	1/1	0.96	0.14	-0.71	44,44,44,44	0
60	MG	CA	3208	1/1	0.94	0.12	-0.71	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3374	1/1	0.97	0.15	-0.71	22,22,22,22	0
60	MG	AA	3058	1/1	0.91	0.12	-0.71	38,38,38,38	0
60	MG	BA	1617	1/1	0.86	0.16	-0.74	64,64,64,64	0
60	MG	AA	3355	1/1	0.97	0.14	-0.83	19,19,19,19	0
60	MG	CA	3351	1/1	0.92	0.13	-0.84	50,50,50,50	0
62	ZN	A6	102	1/1	0.99	0.10	-0.84	47,47,47,47	0
60	MG	AA	3390	1/1	0.96	0.14	-0.89	23,23,23,23	0
60	MG	CA	3337	1/1	0.99	0.13	-0.91	27,27,27,27	0
60	MG	DA	1665	1/1	0.93	0.15	-0.93	57,57,57,57	0
60	MG	BA	1717	1/1	0.92	0.15	-0.94	77,77,77,77	0
60	MG	AA	3382	1/1	0.93	0.13	-0.94	29,29,29,29	0
62	ZN	A9	501	1/1	0.99	0.11	-0.98	45,45,45,45	0
60	MG	AA	3395	1/1	0.98	0.14	-0.99	21,21,21,21	0
60	MG	CA	3175	1/1	0.89	0.14	-1.00	59,59,59,59	0
60	MG	CA	3101	1/1	0.64	0.11	-1.00	86,86,86,86	0
60	MG	AA	3202	1/1	0.85	0.12	-1.02	46,46,46,46	0
64	GDP	DZ	702	28/28	0.96	0.13	-1.09	69,69,69,69	0
60	MG	BA	1811	1/1	0.94	0.14	-1.09	52,52,52,52	0
60	MG	DA	1606	1/1	0.94	0.17	-1.10	66,66,66,66	0
60	MG	DA	1768	1/1	0.90	0.10	-1.11	57,57,57,57	0
60	MG	CA	3436	1/1	0.96	0.15	-1.11	34,34,34,34	0
60	MG	CA	3368	1/1	0.97	0.12	-1.15	45,45,45,45	0
60	MG	CA	3459	1/1	0.82	0.12	-1.22	46,46,46,46	0
60	MG	DA	1720	1/1	0.87	0.12	-1.25	61,61,61,61	0
60	MG	CO	202	1/1	0.97	0.13	-1.26	53,53,53,53	0
60	MG	CA	3559	1/1	0.96	0.14	-1.26	30,30,30,30	0
60	MG	BA	1810	1/1	0.97	0.13	-1.27	39,39,39,39	0
60	MG	AX	101	1/1	0.97	0.11	-1.29	37,37,37,37	0
60	MG	BX	102	1/1	0.84	0.10	-1.31	78,78,78,78	0
60	MG	CA	3309	1/1	0.88	0.11	-1.31	50,50,50,50	0
62	ZN	C9	501	1/1	0.99	0.07	-1.32	70,70,70,70	0
60	MG	AA	3084	1/1	0.95	0.10	-1.34	27,27,27,27	0
60	MG	DA	1622	1/1	0.91	0.15	-1.36	43,43,43,43	0
60	MG	AA	3776	1/1	0.96	0.12	-1.41	21,21,21,21	0
60	MG	BA	1729	1/1	0.97	0.13	-1.43	38,38,38,38	0
60	MG	CA	3358	1/1	0.95	0.13	-1.44	41,41,41,41	0
60	MG	AA	3345	1/1	0.94	0.10	-1.47	34,34,34,34	0
60	MG	BA	1619	1/1	0.90	0.13	-1.50	54,54,54,54	0
60	MG	DA	1766	1/1	0.98	0.07	-1.53	41,41,41,41	0
60	MG	CE	302	1/1	0.94	0.13	-1.55	31,31,31,31	0
60	MG	CA	3054	1/1	0.89	0.13	-1.56	50,50,50,50	0
60	MG	AA	3037	1/1	0.98	0.12	-1.63	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
62	ZN	C6	501	1/1	0.98	0.09	-1.65	66,66,66,66	0
60	MG	CA	3395	1/1	0.95	0.12	-1.70	60,60,60,60	0
62	ZN	BN	501	1/1	0.98	0.09	-1.75	83,83,83,83	0
63	SF4	DD	501	8/8	0.98	0.11	-1.75	71,71,71,71	0
60	MG	BA	1753	1/1	0.96	0.14	-1.75	48,48,48,48	0
60	MG	CA	3263	1/1	0.91	0.12	-1.76	50,50,50,50	0
60	MG	A1	101	1/1	0.93	0.10	-1.77	58,58,58,58	0
60	MG	BA	1696	1/1	0.84	0.14	-1.79	84,84,84,84	0
60	MG	AA	3375	1/1	0.96	0.13	-1.82	16,16,16,16	0
60	MG	BM	201	1/1	0.89	0.06	-1.83	60,60,60,60	0
60	MG	CA	3105	1/1	0.92	0.12	-1.85	47,47,47,47	0
60	MG	AA	3049	1/1	0.92	0.14	-1.85	35,35,35,35	0
62	ZN	A4	501	1/1	0.95	0.08	-1.88	120,120,120,120	0
63	SF4	BD	501	8/8	0.99	0.11	-1.90	67,67,67,67	0
60	MG	AA	3492	1/1	0.92	0.12	-1.92	41,41,41,41	0
60	MG	AA	3391	1/1	0.96	0.13	-1.95	27,27,27,27	0
62	ZN	C4	501	1/1	0.95	0.07	-1.95	163,163,163,163	0
60	MG	BA	1612	1/1	0.89	0.14	-1.96	79,79,79,79	0
60	MG	CA	3010	1/1	0.94	0.13	-1.96	49,49,49,49	0
60	MG	AG	201	1/1	0.98	0.05	-2.02	41,41,41,41	0
60	MG	CA	3186	1/1	0.98	0.07	-2.03	49,49,49,49	0
60	MG	CB	3004	1/1	0.94	0.13	-2.04	70,70,70,70	0
60	MG	AB	3003	1/1	0.93	0.12	-2.08	40,40,40,40	0
60	MG	CA	3261	1/1	0.84	0.12	-2.10	50,50,50,50	0
60	MG	CA	3019	1/1	0.94	0.14	-2.12	23,23,23,23	0
60	MG	AA	3613	1/1	0.91	0.12	-2.15	96,96,96,96	0
60	MG	CA	3567	1/1	0.98	0.12	-2.18	42,42,42,42	0
60	MG	DA	1625	1/1	0.97	0.12	-2.20	38,38,38,38	0
60	MG	AA	3342	1/1	0.89	0.11	-2.24	77,77,77,77	0
60	MG	AG	202	1/1	0.86	0.08	-2.25	69,69,69,69	0
60	MG	CA	3271	1/1	0.90	0.12	-2.42	59,59,59,59	0
62	ZN	AY	501	1/1	0.99	0.06	-2.45	68,68,68,68	0
60	MG	CA	3520	1/1	0.92	0.10	-2.46	27,27,27,27	0
60	MG	CA	3340	1/1	0.98	0.13	-2.47	38,38,38,38	0
60	MG	CA	3120	1/1	0.97	0.12	-2.47	47,47,47,47	0
62	ZN	CY	501	1/1	0.98	0.05	-2.52	92,92,92,92	0
60	MG	AA	3007	1/1	0.98	0.10	-2.55	18,18,18,18	0
60	MG	AA	3734	1/1	0.96	0.12	-2.56	23,23,23,23	0
60	MG	CA	3370	1/1	0.99	0.13	-2.59	31,31,31,31	0
60	MG	CA	3240	1/1	0.83	0.14	-2.65	49,49,49,49	0
62	ZN	C5	102	1/1	0.99	0.07	-2.74	66,66,66,66	0
60	MG	AF	302	1/1	0.95	0.09	-2.80	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
62	ZN	DN	501	1/1	0.97	0.07	-2.82	120,120,120,120	0
60	MG	AA	3009	1/1	0.96	0.09	-2.85	26,26,26,26	0
60	MG	AA	3754	1/1	0.96	0.09	-2.95	25,25,25,25	0
60	MG	AB	3020	1/1	0.93	0.09	-2.95	66,66,66,66	0
60	MG	AB	3007	1/1	0.98	0.07	-2.97	37,37,37,37	0
60	MG	BA	1616	1/1	0.95	0.11	-3.05	69,69,69,69	0
60	MG	CA	3523	1/1	0.89	0.09	-3.12	77,77,77,77	0
60	MG	BX	105	1/1	0.85	0.09	-3.14	87,87,87,87	0
60	MG	CA	3189	1/1	0.96	0.07	-3.16	40,40,40,40	0
60	MG	BA	1654	1/1	0.95	0.12	-3.21	45,45,45,45	0
60	MG	CA	3602	1/1	0.93	0.07	-3.21	49,49,49,49	0
60	MG	BA	1607	1/1	0.86	0.11	-3.27	64,64,64,64	0
60	MG	AA	3623	1/1	0.93	0.10	-3.30	58,58,58,58	0
60	MG	CA	3174	1/1	0.98	0.12	-3.30	31,31,31,31	0
60	MG	CA	3047	1/1	0.96	0.06	-3.37	54,54,54,54	0
60	MG	AA	3542	1/1	0.87	0.10	-3.38	47,47,47,47	0
60	MG	AA	3306	1/1	0.98	0.15	-3.47	3,3,3,3	0
60	MG	AA	3069	1/1	0.91	0.08	-3.52	32,32,32,32	0
60	MG	BA	1734	1/1	0.97	0.13	-3.53	35,35,35,35	0
60	MG	AA	3079	1/1	0.90	0.10	-3.59	27,27,27,27	0
60	MG	AA	3750	1/1	0.99	0.10	-3.73	26,26,26,26	0
60	MG	AA	3099	1/1	0.92	0.08	-3.78	48,48,48,48	0
60	MG	AA	3616	1/1	0.98	0.10	-3.78	33,33,33,33	0
60	MG	BA	1685	1/1	0.93	0.11	-3.79	41,41,41,41	0
60	MG	BA	1736	1/1	0.92	0.10	-3.83	66,66,66,66	0
60	MG	AA	3410	1/1	0.98	0.13	-3.85	19,19,19,19	0
60	MG	AA	3571	1/1	0.72	0.11	-3.86	53,53,53,53	0
60	MG	AA	3446	1/1	0.93	0.11	-3.91	25,25,25,25	0
60	MG	AA	3583	1/1	0.98	0.12	-3.94	18,18,18,18	0
60	MG	AB	3017	1/1	0.95	0.07	-3.97	76,76,76,76	0
60	MG	DA	1653	1/1	0.97	0.08	-4.09	29,29,29,29	0
60	MG	CA	3289	1/1	0.96	0.13	-4.12	23,23,23,23	0
60	MG	CA	3461	1/1	0.98	0.10	-4.17	46,46,46,46	0
60	MG	AA	3683	1/1	0.91	0.10	-4.28	40,40,40,40	0
60	MG	AA	3668	1/1	0.97	0.10	-4.30	25,25,25,25	0
60	MG	CA	3135	1/1	0.88	0.11	-4.30	73,73,73,73	0
60	MG	CA	3626	1/1	0.90	0.09	-4.46	52,52,52,52	0
60	MG	AA	3308	1/1	0.95	0.11	-4.65	45,45,45,45	0
60	MG	AA	3774	1/1	0.96	0.10	-4.66	44,44,44,44	0
60	MG	BA	1680	1/1	0.94	0.08	-4.73	50,50,50,50	0
60	MG	BA	1620	1/1	0.92	0.09	-4.74	60,60,60,60	0
60	MG	CA	3062	1/1	0.90	0.09	-5.04	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1674	1/1	0.68	0.08	-5.07	78,78,78,78	0
60	MG	AA	3236	1/1	0.88	0.10	-5.13	61,61,61,61	0
60	MG	AA	3381	1/1	0.89	0.12	-5.14	34,34,34,34	0
60	MG	AA	3619	1/1	0.92	0.12	-5.18	39,39,39,39	0
60	MG	AA	3497	1/1	0.92	0.10	-5.31	36,36,36,36	0
60	MG	CA	3012	1/1	0.93	0.09	-5.32	41,41,41,41	0
60	MG	DA	1618	1/1	0.88	0.08	-5.38	51,51,51,51	0
60	MG	CA	3574	1/1	0.94	0.11	-5.48	31,31,31,31	0
60	MG	CA	3525	1/1	0.92	0.07	-5.49	30,30,30,30	0
60	MG	AA	3214	1/1	0.94	0.08	-5.80	47,47,47,47	0
60	MG	CA	3272	1/1	0.94	0.05	-6.22	56,56,56,56	0
60	MG	BA	1643	1/1	0.91	0.09	-6.35	56,56,56,56	0
60	MG	BA	1742	1/1	0.96	0.09	-6.45	45,45,45,45	0
60	MG	AA	3340	1/1	0.99	0.10	-6.50	3,3,3,3	0
60	MG	CA	3577	1/1	0.96	0.12	-6.86	52,52,52,52	0
60	MG	CA	3362	1/1	0.95	0.11	-7.14	20,20,20,20	0
60	MG	AA	3400	1/1	0.97	0.07	-7.23	19,19,19,19	0
60	MG	AA	3072	1/1	0.92	0.08	-7.39	20,20,20,20	0
60	MG	AA	3371	1/1	0.98	0.07	-7.44	21,21,21,21	0
60	MG	CA	3027	1/1	0.98	0.05	-7.88	29,29,29,29	0
60	MG	AA	3547	1/1	0.93	0.06	-8.12	50,50,50,50	0
60	MG	CA	3009	1/1	0.95	0.05	-8.50	24,24,24,24	0
60	MG	BA	1792	1/1	0.92	0.07	-8.55	61,61,61,61	0
60	MG	AA	3011	1/1	0.97	0.10	-9.47	27,27,27,27	0
60	MG	BA	1611	1/1	0.97	0.09	-10.17	31,31,31,31	0
60	MG	AA	3022	1/1	0.96	0.09	-12.93	19,19,19,19	0
60	MG	BA	1613	1/1	0.88	0.07	-13.74	92,92,92,92	0
60	MG	CA	3319	1/1	0.95	0.07	-15.86	32,32,32,32	0
60	MG	CA	3479	1/1	0.95	0.16	-	67,67,67,67	0
60	MG	AA	3199	1/1	0.88	0.22	-	61,61,61,61	0
60	MG	AA	3169	1/1	0.97	0.26	-	36,36,36,36	0
60	MG	BA	1739	1/1	0.88	0.18	-	52,52,52,52	0
60	MG	CA	3061	1/1	0.95	0.15	-	36,36,36,36	0
60	MG	AA	3356	1/1	0.94	0.12	-	51,51,51,51	0
60	MG	AA	3146	1/1	0.79	0.20	-	53,53,53,53	0
60	MG	CA	3585	1/1	0.96	0.11	-	44,44,44,44	0
60	MG	AA	3597	1/1	0.97	0.12	-	58,58,58,58	0
60	MG	BA	1660	1/1	0.92	0.32	-	55,55,55,55	0
60	MG	CA	3080	1/1	0.79	0.58	-	78,78,78,78	0
60	MG	AA	3325	1/1	0.92	0.11	-	78,78,78,78	0
60	MG	AA	3232	1/1	0.97	0.22	-	58,58,58,58	0
60	MG	AA	3481	1/1	0.90	0.06	-	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
60	MG	AA	3111	1/1	0.87	0.31	-	47,47,47,47	0
60	MG	CA	3112	1/1	0.82	0.47	-	76,76,76,76	0
60	MG	CA	3136	1/1	0.89	0.20	-	112,112,112,112	0
60	MG	AA	3068	1/1	0.93	0.34	-	52,52,52,52	0
60	MG	AA	3422	1/1	0.96	0.19	-	22,22,22,22	0
60	MG	CA	3624	1/1	0.94	0.22	-	76,76,76,76	0
60	MG	AA	3459	1/1	0.95	0.47	-	65,65,65,65	0
60	MG	DD	502	1/1	0.82	0.50	-	64,64,64,64	0
60	MG	AA	3442	1/1	0.84	0.13	-	73,73,73,73	0
60	MG	AA	3522	1/1	0.96	0.16	-	31,31,31,31	0
60	MG	CA	3089	1/1	0.69	0.71	-	78,78,78,78	0
60	MG	AA	3468	1/1	0.95	0.12	-	34,34,34,34	0
60	MG	AA	3488	1/1	0.90	0.09	-	56,56,56,56	0
60	MG	AA	3531	1/1	0.93	0.15	-	61,61,61,61	0
60	MG	AA	3675	1/1	0.94	0.16	-	67,67,67,67	0
60	MG	CA	3059	1/1	0.73	0.38	-	66,66,66,66	0
60	MG	AA	3447	1/1	0.87	0.19	-	44,44,44,44	0
60	MG	CA	3033	1/1	0.89	0.12	-	47,47,47,47	0
60	MG	AA	3618	1/1	0.91	0.13	-	39,39,39,39	0
60	MG	CA	3497	1/1	0.86	0.18	-	85,85,85,85	0
60	MG	CA	3338	1/1	0.86	0.15	-	58,58,58,58	0
60	MG	CB	3010	1/1	0.80	0.16	-	67,67,67,67	0
60	MG	AA	3365	1/1	0.93	0.40	-	55,55,55,55	0
60	MG	AA	3713	1/1	0.75	0.52	-	48,48,48,48	0
60	MG	A8	5001	1/1	0.88	0.31	-	66,66,66,66	0
60	MG	BA	1714	1/1	0.99	0.16	-	44,44,44,44	0
60	MG	DA	1735	1/1	0.78	0.10	-	75,75,75,75	0
60	MG	DX	3001	1/1	0.59	0.41	-	75,75,75,75	0
60	MG	DA	1691	1/1	0.90	0.18	-	66,66,66,66	0
60	MG	DA	1628	1/1	0.87	0.20	-	69,69,69,69	0
60	MG	AA	3219	1/1	0.93	0.22	-	38,38,38,38	0
60	MG	CA	3648	1/1	0.88	0.60	-	78,78,78,78	0
60	MG	CA	3302	1/1	0.89	0.11	-	67,67,67,67	0
60	MG	CA	3153	1/1	0.89	0.31	-	54,54,54,54	0
60	MG	CA	3245	1/1	0.71	0.30	-	53,53,53,53	0
60	MG	CA	3043	1/1	0.81	0.19	-	75,75,75,75	0
60	MG	CA	3231	1/1	0.94	0.26	-	56,56,56,56	0
60	MG	CA	3190	1/1	0.92	0.30	-	77,77,77,77	0
60	MG	AA	3242	1/1	0.62	0.20	-	69,69,69,69	0
60	MG	CA	3633	1/1	0.79	0.19	-	85,85,85,85	0
60	MG	CA	3334	1/1	0.92	0.09	-	56,56,56,56	0
60	MG	DA	1709	1/1	0.96	0.22	-	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
60	MG	CA	3075	1/1	0.86	0.15	-	51,51,51,51	0
60	MG	AB	3006	1/1	0.86	0.21	-	84,84,84,84	0
60	MG	AA	3189	1/1	0.97	0.26	-	31,31,31,31	0
60	MG	BA	1625	1/1	0.90	0.24	-	53,53,53,53	0
60	MG	AA	3764	1/1	0.84	0.37	-	48,48,48,48	0
60	MG	CA	3530	1/1	0.89	0.15	-	68,68,68,68	0
60	MG	C8	5001	1/1	0.94	0.29	-	43,43,43,43	0
60	MG	AA	3720	1/1	0.94	0.35	-	78,78,78,78	0
60	MG	AA	3191	1/1	0.89	0.29	-	57,57,57,57	0
60	MG	AA	3473	1/1	0.88	0.14	-	57,57,57,57	0
60	MG	CN	5001	1/1	0.98	0.10	-	64,64,64,64	0
60	MG	CA	3618	1/1	0.95	0.21	-	79,79,79,79	0
60	MG	BA	1735	1/1	0.93	0.14	-	58,58,58,58	0
60	MG	AA	3738	1/1	0.87	0.14	-	73,73,73,73	0
60	MG	CA	3515	1/1	0.91	0.11	-	72,72,72,72	0
60	MG	DA	1658	1/1	0.86	0.13	-	89,89,89,89	0
60	MG	AA	3661	1/1	0.85	0.17	-	78,78,78,78	0
60	MG	AA	3667	1/1	0.91	0.14	-	45,45,45,45	0
60	MG	AB	3001	1/1	0.88	0.18	-	80,80,80,80	0
60	MG	CA	3251	1/1	0.97	0.15	-	62,62,62,62	0
60	MG	CA	3081	1/1	0.85	0.40	-	69,69,69,69	0
60	MG	AA	3329	1/1	0.88	0.23	-	82,82,82,82	0
60	MG	CA	3587	1/1	0.88	0.14	-	72,72,72,72	0
60	MG	DA	1705	1/1	0.91	0.17	-	61,61,61,61	0
60	MG	CA	3348	1/1	0.69	0.15	-	78,78,78,78	0
60	MG	CA	3531	1/1	0.93	0.13	-	67,67,67,67	0
60	MG	BA	1691	1/1	0.67	0.34	-	98,98,98,98	0
60	MG	AA	3107	1/1	0.88	0.17	-	51,51,51,51	0
60	MG	CA	3550	1/1	0.39	0.36	-	88,88,88,88	0
60	MG	AA	3320	1/1	0.94	0.24	-	65,65,65,65	0
60	MG	CA	3203	1/1	0.94	0.32	-	45,45,45,45	0
60	MG	CA	3085	1/1	0.62	0.53	-	82,82,82,82	0
60	MG	CA	3256	1/1	0.96	0.29	-	73,73,73,73	0
60	MG	CA	3572	1/1	0.92	0.22	-	82,82,82,82	0
60	MG	AB	3021	1/1	0.85	0.14	-	75,75,75,75	0
60	MG	AA	3802	1/1	0.88	0.27	-	55,55,55,55	0
60	MG	BA	1755	1/1	0.83	0.18	-	92,92,92,92	0
60	MG	AA	3123	1/1	0.93	0.48	-	55,55,55,55	0
60	MG	CA	3246	1/1	0.91	0.28	-	79,79,79,79	0
60	MG	DA	1702	1/1	0.78	0.27	-	58,58,58,58	0
60	MG	AA	3746	1/1	0.93	0.43	-	62,62,62,62	0
60	MG	AA	3798	1/1	0.92	0.10	-	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
60	MG	CA	3126	1/1	0.91	0.54	-	71,71,71,71	0
60	MG	AA	3758	1/1	0.81	0.35	-	70,70,70,70	0
60	MG	AA	3601	1/1	0.93	0.28	-	44,44,44,44	0
60	MG	BF	3001	1/1	0.91	0.15	-	49,49,49,49	0
60	MG	AA	3243	1/1	0.83	0.29	-	79,79,79,79	0
60	MG	AA	3025	1/1	0.86	0.44	-	60,60,60,60	0
60	MG	CA	3571	1/1	0.93	0.15	-	52,52,52,52	0
60	MG	AA	3485	1/1	0.98	0.17	-	34,34,34,34	0
60	MG	CA	3560	1/1	0.83	0.16	-	103,103,103,103	0
60	MG	CA	3508	1/1	0.94	0.14	-	74,74,74,74	0
60	MG	CD	302	1/1	0.89	0.43	-	51,51,51,51	0
60	MG	CA	3130	1/1	0.96	0.17	-	57,57,57,57	0
60	MG	CA	3588	1/1	0.57	0.19	-	78,78,78,78	0
60	MG	AA	3261	1/1	0.92	0.27	-	53,53,53,53	0
60	MG	AA	3679	1/1	0.91	0.18	-	64,64,64,64	0
60	MG	CB	3013	1/1	0.90	0.12	-	90,90,90,90	0
60	MG	AA	3140	1/1	0.87	0.90	-	66,66,66,66	0
60	MG	CA	3079	1/1	0.52	0.57	-	82,82,82,82	0
60	MG	AA	3815	1/1	0.95	0.46	-	72,72,72,72	0
60	MG	AA	3502	1/1	0.96	0.09	-	41,41,41,41	0
60	MG	AA	3783	1/1	0.71	0.39	-	68,68,68,68	0
60	MG	AA	3727	1/1	0.86	0.16	-	64,64,64,64	0
60	MG	DA	1675	1/1	0.91	0.13	-	61,61,61,61	0
60	MG	BA	1628	1/1	0.91	0.30	-	59,59,59,59	0
60	MG	CA	3090	1/1	0.60	0.46	-	98,98,98,98	0
60	MG	CA	3332	1/1	0.97	0.24	-	47,47,47,47	0
60	MG	CA	3145	1/1	0.94	0.33	-	65,65,65,65	0
60	MG	DA	1684	1/1	0.93	0.29	-	54,54,54,54	0
60	MG	CA	3118	1/1	0.93	0.11	-	67,67,67,67	0
60	MG	CA	3278	1/1	0.92	0.24	-	38,38,38,38	0
60	MG	CA	3467	1/1	0.78	0.45	-	99,99,99,99	0
60	MG	AA	3570	1/1	0.93	0.14	-	22,22,22,22	0
60	MG	CA	3663	1/1	0.88	0.26	-	74,74,74,74	0
60	MG	BA	1799	1/1	0.88	0.07	-	69,69,69,69	0
60	MG	AA	3659	1/1	0.92	0.10	-	56,56,56,56	0
60	MG	CA	3195	1/1	0.74	0.18	-	36,36,36,36	0
60	MG	AA	3425	1/1	0.86	0.17	-	40,40,40,40	0
60	MG	BA	1621	1/1	0.78	0.66	-	78,78,78,78	0
60	MG	DA	1680	1/1	0.95	0.17	-	40,40,40,40	0
60	MG	DA	1728	1/1	0.96	0.09	-	53,53,53,53	0
60	MG	CA	3609	1/1	0.95	0.21	-	62,62,62,62	0
60	MG	AA	3017	1/1	0.87	0.11	-	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
60	MG	CY	502	1/1	0.97	0.14	-	53,53,53,53	0
60	MG	AA	3074	1/1	0.96	0.37	-	26,26,26,26	0
60	MG	AA	3279	1/1	0.82	0.55	-	62,62,62,62	0
60	MG	AA	3676	1/1	0.95	0.17	-	46,46,46,46	0
60	MG	AA	3428	1/1	0.93	0.14	-	36,36,36,36	0
60	MG	CA	3643	1/1	0.88	0.33	-	83,83,83,83	0
60	MG	AA	3321	1/1	0.81	0.08	-	45,45,45,45	0
60	MG	AA	3373	1/1	0.95	0.22	-	23,23,23,23	0
60	MG	CA	3582	1/1	0.93	0.15	-	60,60,60,60	0
60	MG	AA	3681	1/1	0.93	0.21	-	52,52,52,52	0
60	MG	CQ	204	1/1	0.93	0.28	-	74,74,74,74	0
60	MG	DA	1727	1/1	0.95	0.17	-	65,65,65,65	0
60	MG	AA	3646	1/1	0.87	0.28	-	82,82,82,82	0
60	MG	BA	1709	1/1	0.59	0.27	-	96,96,96,96	0
60	MG	AA	3080	1/1	0.89	0.36	-	54,54,54,54	0
60	MG	DA	1643	1/1	0.98	0.14	-	51,51,51,51	0
60	MG	AA	3448	1/1	0.93	0.27	-	74,74,74,74	0
60	MG	DA	1614	1/1	0.82	0.15	-	71,71,71,71	0
60	MG	AA	3097	1/1	0.99	0.26	-	29,29,29,29	0
60	MG	CA	3354	1/1	0.94	0.18	-	40,40,40,40	0
60	MG	AA	3487	1/1	0.76	0.10	-	66,66,66,66	0
60	MG	DA	1672	1/1	0.90	0.16	-	61,61,61,61	0
60	MG	CA	3050	1/1	0.91	0.65	-	55,55,55,55	0
60	MG	CA	3485	1/1	0.87	0.24	-	76,76,76,76	0
60	MG	CA	3242	1/1	0.89	0.33	-	48,48,48,48	0
60	MG	DA	1753	1/1	0.61	0.26	-	85,85,85,85	0
60	MG	AA	3731	1/1	0.98	0.14	-	34,34,34,34	0
60	MG	BA	1704	1/1	0.95	0.26	-	68,68,68,68	0
60	MG	CA	3172	1/1	0.96	0.17	-	41,41,41,41	0
60	MG	DA	1612	1/1	0.98	0.13	-	46,46,46,46	0
60	MG	AA	3087	1/1	0.88	0.31	-	62,62,62,62	0
60	MG	CA	3605	1/1	0.95	0.19	-	72,72,72,72	0
60	MG	AA	3106	1/1	0.85	0.19	-	43,43,43,43	0
60	MG	CA	3622	1/1	0.64	0.17	-	106,106,106,106	0
60	MG	AA	3245	1/1	0.75	0.22	-	79,79,79,79	0
60	MG	AA	3538	1/1	0.82	0.20	-	62,62,62,62	0
60	MG	AA	3595	1/1	0.86	0.18	-	60,60,60,60	0
60	MG	DA	1692	1/1	0.94	0.26	-	49,49,49,49	0
60	MG	CA	3171	1/1	0.97	0.43	-	48,48,48,48	0
60	MG	AA	3268	1/1	0.87	0.23	-	80,80,80,80	0
60	MG	AW	3002	1/1	0.89	0.19	-	59,59,59,59	0
60	MG	DA	1722	1/1	0.87	0.19	-	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
60	MG	AA	3282	1/1	0.96	0.39	-	65,65,65,65	0
60	MG	CA	3441	1/1	0.93	0.16	-	37,37,37,37	0
60	MG	CA	3132	1/1	0.83	0.19	-	67,67,67,67	0
60	MG	DA	1738	1/1	0.85	0.25	-	100,100,100,100	0
60	MG	AN	3003	1/1	0.89	0.07	-	52,52,52,52	0
60	MG	CA	3065	1/1	0.90	0.15	-	56,56,56,56	0
60	MG	CA	3339	1/1	0.93	0.33	-	75,75,75,75	0
60	MG	CA	3545	1/1	0.84	0.11	-	93,93,93,93	0
60	MG	CA	3158	1/1	0.99	0.33	-	54,54,54,54	0
60	MG	BA	1768	1/1	0.97	0.18	-	64,64,64,64	0
60	MG	CA	3384	1/1	0.87	0.20	-	52,52,52,52	0
60	MG	CA	3379	1/1	0.88	0.22	-	62,62,62,62	0
60	MG	CA	3036	1/1	0.89	0.26	-	65,65,65,65	0
60	MG	BE	3001	1/1	0.97	0.08	-	83,83,83,83	0
60	MG	A1	102	1/1	0.95	0.16	-	46,46,46,46	0
60	MG	CA	3470	1/1	0.91	0.11	-	55,55,55,55	0
60	MG	AA	3360	1/1	0.89	0.44	-	72,72,72,72	0
60	MG	CA	3493	1/1	0.94	0.22	-	66,66,66,66	0
60	MG	CA	3553	1/1	0.97	0.14	-	77,77,77,77	0
60	MG	AA	3475	1/1	0.94	0.15	-	73,73,73,73	0
60	MG	DA	1682	1/1	0.94	0.30	-	60,60,60,60	0
60	MG	BA	1786	1/1	0.78	0.33	-	79,79,79,79	0
60	MG	AA	3318	1/1	0.97	0.16	-	64,64,64,64	0
60	MG	DA	1613	1/1	0.90	0.25	-	50,50,50,50	0
60	MG	AA	3469	1/1	0.95	0.20	-	37,37,37,37	0
60	MG	CA	3021	1/1	0.86	0.33	-	91,91,91,91	0
60	MG	BA	1746	1/1	0.96	0.16	-	70,70,70,70	0
60	MG	AA	3552	1/1	0.93	0.14	-	73,73,73,73	0
60	MG	AA	3633	1/1	0.96	0.25	-	51,51,51,51	0
60	MG	DA	1708	1/1	0.97	0.10	-	67,67,67,67	0
60	MG	AA	3780	1/1	0.87	0.35	-	51,51,51,51	1
60	MG	CA	3453	1/1	0.93	0.08	-	43,43,43,43	0
60	MG	AA	3733	1/1	0.97	0.13	-	40,40,40,40	0
60	MG	CA	3092	1/1	0.66	0.49	-	74,74,74,74	0
60	MG	AA	3760	1/1	0.95	0.34	-	50,50,50,50	0
60	MG	AQ	3003	1/1	0.98	0.34	-	37,37,37,37	0
60	MG	BA	1805	1/1	0.95	0.10	-	55,55,55,55	0
60	MG	CA	3611	1/1	0.89	0.30	-	64,64,64,64	0
60	MG	DA	1695	1/1	0.87	0.18	-	79,79,79,79	0
60	MG	DA	1689	1/1	0.91	0.24	-	68,68,68,68	0
60	MG	AA	3612	1/1	0.84	0.20	-	60,60,60,60	0
60	MG	AA	3650	1/1	0.83	0.29	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3491	1/1	0.27	0.61	-	99,99,99,99	0
60	MG	AB	3023	1/1	0.92	0.26	-	63,63,63,63	0
60	MG	CA	3401	1/1	0.86	0.07	-	75,75,75,75	0
60	MG	AA	3725	1/1	0.62	0.27	-	42,42,42,42	0
60	MG	CA	3088	1/1	0.90	0.43	-	85,85,85,85	0
60	MG	AA	3794	1/1	0.91	0.20	-	47,47,47,47	0
60	MG	CA	3394	1/1	0.86	0.26	-	54,54,54,54	0
60	MG	AD	307	1/1	0.74	0.20	-	54,54,54,54	0
60	MG	CA	3041	1/1	0.88	0.47	-	67,67,67,67	0
60	MG	DA	1656	1/1	0.95	0.07	-	67,67,67,67	0
60	MG	AA	3143	1/1	0.96	0.05	-	37,37,37,37	0
60	MG	CA	3094	1/1	0.76	0.35	-	92,92,92,92	0
60	MG	BA	1783	1/1	0.94	0.15	-	61,61,61,61	0
60	MG	DA	1729	1/1	0.86	0.10	-	82,82,82,82	0
60	MG	AA	3685	1/1	0.96	0.15	-	58,58,58,58	0
60	MG	AA	3673	1/1	0.97	0.24	-	58,58,58,58	0
60	MG	CA	3342	1/1	0.92	0.17	-	84,84,84,84	0
60	MG	CA	3489	1/1	0.93	0.18	-	64,64,64,64	0
60	MG	CA	3386	1/1	0.86	0.14	-	79,79,79,79	0
60	MG	CA	3014	1/1	0.96	0.14	-	58,58,58,58	0
60	MG	AA	3046	1/1	0.91	0.36	-	47,47,47,47	0
60	MG	AA	3249	1/1	0.71	0.45	-	64,64,64,64	0
60	MG	BA	1807	1/1	0.89	0.21	-	72,72,72,72	0
60	MG	AA	3409	1/1	0.97	0.19	-	51,51,51,51	0
60	MG	CA	3555	1/1	0.81	0.08	-	59,59,59,59	0
60	MG	AA	3812	1/1	0.90	0.20	-	78,78,78,78	0
60	MG	CA	3301	1/1	0.94	0.43	-	56,56,56,56	0
60	MG	CA	3404	1/1	0.90	0.11	-	46,46,46,46	0
60	MG	CA	3107	1/1	0.95	0.11	-	64,64,64,64	0
60	MG	AA	3188	1/1	0.96	0.16	-	15,15,15,15	0
60	MG	BA	1681	1/1	0.87	0.65	-	69,69,69,69	0
60	MG	CA	3285	1/1	0.97	0.07	-	41,41,41,41	0
60	MG	BA	1706	1/1	0.65	0.25	-	82,82,82,82	0
60	MG	AA	3057	1/1	0.96	0.29	-	56,56,56,56	0
60	MG	AA	3607	1/1	0.95	0.15	-	39,39,39,39	0
60	MG	AA	3207	1/1	0.94	0.34	-	67,67,67,67	0
60	MG	BA	1737	1/1	0.72	0.28	-	87,87,87,87	0
60	MG	AA	3394	1/1	0.91	0.13	-	22,22,22,22	0
60	MG	AA	3349	1/1	0.94	0.13	-	34,34,34,34	0
60	MG	AA	3230	1/1	0.83	0.34	-	55,55,55,55	0
60	MG	CA	3290	1/1	0.94	0.15	-	61,61,61,61	0
60	MG	AV	201	1/1	0.97	0.27	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3358	1/1	0.96	0.06	-	72,72,72,72	0
60	MG	CA	3503	1/1	0.85	0.09	-	67,67,67,67	0
60	MG	CA	3023	1/1	0.92	0.20	-	56,56,56,56	0
60	MG	DA	1629	1/1	0.90	0.80	-	79,79,79,79	0
60	MG	DA	1627	1/1	0.95	0.36	-	48,48,48,48	0
60	MG	AA	3458	1/1	0.92	0.20	-	79,79,79,79	0
60	MG	CA	3573	1/1	0.85	0.12	-	82,82,82,82	0
60	MG	AA	3299	1/1	0.82	0.18	-	64,64,64,64	0
60	MG	BA	1798	1/1	0.92	0.38	-	62,62,62,62	0
60	MG	AB	3018	1/1	0.85	0.14	-	76,76,76,76	0
60	MG	CA	3658	1/1	0.88	0.19	-	62,62,62,62	0
60	MG	AA	3194	1/1	0.88	0.35	-	58,58,58,58	0
60	MG	AA	3449	1/1	0.95	0.20	-	46,46,46,46	0
60	MG	CA	3104	1/1	0.93	0.15	-	64,64,64,64	0
60	MG	AA	3709	1/1	0.99	0.47	-	39,39,39,39	0
60	MG	AA	3465	1/1	0.99	0.05	-	49,49,49,49	0
60	MG	AA	3024	1/1	0.86	0.13	-	60,60,60,60	0
60	MG	BA	1793	1/1	0.88	0.10	-	68,68,68,68	0
60	MG	CA	3331	1/1	0.96	0.47	-	62,62,62,62	0
60	MG	AA	3687	1/1	0.91	0.11	-	48,48,48,48	0
60	MG	AA	3660	1/1	0.98	0.34	-	58,58,58,58	0
60	MG	AB	3011	1/1	0.88	0.17	-	47,47,47,47	0
60	MG	BA	1682	1/1	0.93	0.11	-	71,71,71,71	0
60	MG	DA	1659	1/1	0.94	0.35	-	79,79,79,79	0
60	MG	BA	1651	1/1	0.94	0.12	-	69,69,69,69	0
60	MG	DA	1761	1/1	0.86	0.08	-	68,68,68,68	0
60	MG	CA	3526	1/1	0.67	0.13	-	69,69,69,69	0
60	MG	AA	3130	1/1	0.87	0.33	-	59,59,59,59	0
60	MG	AA	3678	1/1	0.87	0.13	-	62,62,62,62	0
60	MG	CB	3005	1/1	0.94	0.23	-	65,65,65,65	0
60	MG	CA	3628	1/1	0.81	0.11	-	76,76,76,76	0
60	MG	CA	3569	1/1	0.88	0.16	-	71,71,71,71	0
60	MG	CA	3260	1/1	0.91	0.13	-	59,59,59,59	0
60	MG	CA	3149	1/1	0.92	0.22	-	58,58,58,58	0
60	MG	AA	3512	1/1	0.91	0.13	-	32,32,32,32	0
60	MG	CA	3552	1/1	0.87	0.09	-	60,60,60,60	0
60	MG	CA	3419	1/1	0.93	0.18	-	55,55,55,55	0
60	MG	CA	3069	1/1	0.84	0.28	-	66,66,66,66	0
60	MG	CA	3360	1/1	0.94	0.17	-	52,52,52,52	0
60	MG	CA	3447	1/1	0.96	0.12	-	44,44,44,44	0
60	MG	AA	3695	1/1	0.94	0.29	-	50,50,50,50	0
60	MG	AA	3059	1/1	0.73	0.52	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3389	1/1	0.91	0.09	-	55,55,55,55	0
60	MG	DA	1617	1/1	0.88	0.18	-	47,47,47,47	0
60	MG	BA	1609	1/1	0.85	0.20	-	77,77,77,77	0
60	MG	BA	1647	1/1	0.91	0.09	-	57,57,57,57	0
60	MG	CA	3443	1/1	0.96	0.31	-	40,40,40,40	0
60	MG	AA	3132	1/1	0.86	0.45	-	43,43,43,43	0
60	MG	CA	3270	1/1	0.96	0.33	-	69,69,69,69	0
60	MG	CA	3111	1/1	0.64	0.20	-	82,82,82,82	0
60	MG	AA	3205	1/1	0.96	0.31	-	45,45,45,45	0
60	MG	BA	1645	1/1	0.88	0.76	-	58,58,58,58	0
60	MG	DA	1609	1/1	0.86	0.18	-	49,49,49,49	0
60	MG	AA	3290	1/1	0.97	0.16	-	78,78,78,78	0
60	MG	AA	3367	1/1	0.95	0.11	-	52,52,52,52	0
60	MG	CA	3353	1/1	0.93	0.13	-	48,48,48,48	0
60	MG	AA	3773	1/1	0.71	0.20	-	77,77,77,77	0
60	MG	AA	3789	1/1	0.85	0.21	-	71,71,71,71	0
60	MG	AA	3397	1/1	0.97	0.36	-	41,41,41,41	0
60	MG	DA	1747	1/1	0.88	0.11	-	67,67,67,67	0
60	MG	CA	3637	1/1	0.87	0.24	-	78,78,78,78	0
60	MG	AA	3788	1/1	0.91	0.17	-	64,64,64,64	0
60	MG	CA	3631	1/1	0.75	0.29	-	88,88,88,88	0
60	MG	CA	3213	1/1	0.83	0.34	-	62,62,62,62	0
60	MG	CA	3563	1/1	0.93	0.29	-	30,30,30,30	0
60	MG	CA	3512	1/1	0.93	0.12	-	58,58,58,58	0
60	MG	AA	3680	1/1	0.94	0.12	-	70,70,70,70	0
60	MG	CA	3398	1/1	0.94	0.20	-	57,57,57,57	0
60	MG	AA	3267	1/1	0.95	0.31	-	43,43,43,43	0
60	MG	AA	3694	1/1	0.61	0.17	-	49,49,49,49	0
60	MG	AA	3090	1/1	0.94	0.27	-	52,52,52,52	0
60	MG	CA	3037	1/1	0.91	0.19	-	65,65,65,65	0
60	MG	CA	3064	1/1	0.88	0.20	-	72,72,72,72	0
60	MG	CA	3275	1/1	0.84	0.13	-	73,73,73,73	0
60	MG	BA	1740	1/1	0.52	0.12	-	89,89,89,89	0
60	MG	CA	3363	1/1	0.91	0.18	-	55,55,55,55	0
60	MG	DA	1624	1/1	0.87	0.07	-	83,83,83,83	0
60	MG	DA	1639	1/1	0.91	0.10	-	59,59,59,59	0
60	MG	DA	1630	1/1	0.87	0.27	-	51,51,51,51	0
60	MG	AA	3259	1/1	0.96	0.36	-	27,27,27,27	0
60	MG	AA	3337	1/1	0.84	0.22	-	52,52,52,52	0
60	MG	BA	1794	1/1	0.93	0.15	-	63,63,63,63	0
60	MG	CA	3349	1/1	0.92	0.15	-	36,36,36,36	0
60	MG	AA	3377	1/1	0.90	0.15	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3549	1/1	0.94	0.12	-	53,53,53,53	0
60	MG	AA	3491	1/1	0.89	0.30	-	40,40,40,40	0
60	MG	AA	3563	1/1	0.89	0.07	-	37,37,37,37	1
60	MG	CA	3176	1/1	0.95	0.35	-	60,60,60,60	0
60	MG	AA	3591	1/1	0.93	0.23	-	61,61,61,61	0
60	MG	DK	201	1/1	0.93	0.23	-	55,55,55,55	0
60	MG	BA	1669	1/1	0.86	0.18	-	70,70,70,70	0
60	MG	BA	1673	1/1	0.90	0.72	-	63,63,63,63	0
60	MG	CA	3284	1/1	0.93	0.22	-	49,49,49,49	0
60	MG	CA	3127	1/1	0.90	0.16	-	68,68,68,68	0
60	MG	AA	3691	1/1	0.96	0.09	-	51,51,51,51	0
60	MG	CA	3193	1/1	0.98	0.36	-	47,47,47,47	0
60	MG	CA	3519	1/1	0.90	0.20	-	68,68,68,68	0
60	MG	AA	3051	1/1	0.59	0.69	-	84,84,84,84	0
60	MG	AA	3420	1/1	0.91	0.13	-	26,26,26,26	0
60	MG	AA	3346	1/1	0.83	0.23	-	32,32,32,32	0
60	MG	BA	1767	1/1	0.72	0.27	-	73,73,73,73	0
60	MG	AA	3747	1/1	0.84	0.33	-	65,65,65,65	0
60	MG	CA	3327	1/1	0.94	0.22	-	37,37,37,37	0
60	MG	DA	1610	1/1	0.66	0.29	-	59,59,59,59	0
60	MG	AA	3577	1/1	0.93	0.13	-	65,65,65,65	0
60	MG	CA	3074	1/1	0.90	0.31	-	64,64,64,64	0
60	MG	CA	3159	1/1	0.98	0.42	-	42,42,42,42	0
60	MG	AA	3590	1/1	0.93	0.19	-	71,71,71,71	0
60	MG	AA	3297	1/1	0.87	0.08	-	56,56,56,56	0
60	MG	AA	3753	1/1	0.81	0.15	-	59,59,59,59	0
60	MG	AA	3682	1/1	0.95	0.20	-	58,58,58,58	0
60	MG	AA	3653	1/1	0.96	0.12	-	47,47,47,47	0
60	MG	CA	3409	1/1	0.88	0.32	-	63,63,63,63	0
60	MG	CA	3259	1/1	0.98	0.17	-	19,19,19,19	0
60	MG	AA	3136	1/1	0.42	0.46	-	74,74,74,74	0
60	MG	AA	3238	1/1	0.86	0.13	-	68,68,68,68	0
60	MG	AA	3361	1/1	0.99	0.17	-	33,33,33,33	0
60	MG	BA	1722	1/1	0.67	0.29	-	86,86,86,86	0
60	MG	CA	3474	1/1	0.79	0.14	-	72,72,72,72	0
60	MG	CA	3540	1/1	0.86	0.24	-	71,71,71,71	0
60	MG	DA	1699	1/1	0.93	0.20	-	79,79,79,79	0
60	MG	BA	1790	1/1	0.73	0.32	-	87,87,87,87	0
60	MG	CA	3424	1/1	0.95	0.25	-	40,40,40,40	0
60	MG	BA	1699	1/1	0.73	0.19	-	70,70,70,70	0
60	MG	AA	3658	1/1	0.94	0.22	-	25,25,25,25	0
60	MG	DA	1669	1/1	0.98	0.20	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1713	1/1	0.95	0.15	-	59,59,59,59	0
60	MG	BA	1637	1/1	0.94	0.19	-	64,64,64,64	0
60	MG	AA	3427	1/1	0.98	0.12	-	34,34,34,34	0
60	MG	BX	112	1/1	0.68	0.21	-	78,78,78,78	0
60	MG	DA	1711	1/1	0.96	0.10	-	64,64,64,64	0
60	MG	CA	3116	1/1	0.94	0.45	-	57,57,57,57	0
60	MG	CA	3341	1/1	0.84	0.19	-	35,35,35,35	0
60	MG	CA	3621	1/1	0.94	0.22	-	55,55,55,55	0
60	MG	CA	3167	1/1	0.82	0.32	-	68,68,68,68	0
60	MG	CA	3456	1/1	0.96	0.15	-	37,37,37,37	0
60	MG	AA	3472	1/1	0.95	0.23	-	37,37,37,37	0
60	MG	BA	1663	1/1	0.96	0.13	-	66,66,66,66	0
60	MG	BA	1672	1/1	0.83	0.22	-	61,61,61,61	0
60	MG	AA	3423	1/1	0.97	0.22	-	53,53,53,53	0
60	MG	CA	3131	1/1	0.95	0.28	-	61,61,61,61	0
60	MG	CA	3451	1/1	0.97	0.12	-	78,78,78,78	0
60	MG	BA	1730	1/1	0.93	0.21	-	68,68,68,68	0
60	MG	CA	3377	1/1	0.83	0.14	-	53,53,53,53	0
60	MG	DA	1707	1/1	0.90	0.09	-	79,79,79,79	0
60	MG	BA	1636	1/1	0.92	0.27	-	66,66,66,66	0
60	MG	A0	102	1/1	0.97	0.06	-	41,41,41,41	0
60	MG	AA	3334	1/1	0.96	0.21	-	62,62,62,62	0
60	MG	AA	3614	1/1	0.91	0.14	-	66,66,66,66	0
60	MG	BA	1707	1/1	0.93	0.24	-	57,57,57,57	0
60	MG	AA	3155	1/1	0.96	0.24	-	31,31,31,31	0
60	MG	AA	3441	1/1	0.85	0.18	-	62,62,62,62	0
60	MG	AA	3005	1/1	0.82	0.20	-	63,63,63,63	0
60	MG	BA	1634	1/1	0.91	0.21	-	71,71,71,71	0
60	MG	DA	1745	1/1	0.96	0.23	-	54,54,54,54	0
60	MG	AA	3781	1/1	0.95	0.17	-	49,49,49,49	0
60	MG	CA	3402	1/1	0.91	0.16	-	46,46,46,46	0
60	MG	AA	3048	1/1	0.82	0.16	-	39,39,39,39	0
60	MG	CA	3627	1/1	0.95	0.07	-	59,59,59,59	0
60	MG	AA	3696	1/1	0.95	0.20	-	62,62,62,62	0
60	MG	BA	1716	1/1	0.96	0.27	-	71,71,71,71	0
60	MG	CA	3269	1/1	0.94	0.40	-	64,64,64,64	0
60	MG	CA	3388	1/1	0.86	0.18	-	97,97,97,97	0
60	MG	CA	3646	1/1	0.83	0.10	-	90,90,90,90	0
60	MG	BA	1693	1/1	0.94	0.14	-	69,69,69,69	0
60	MG	AA	3503	1/1	0.94	0.14	-	41,41,41,41	0
60	MG	CA	3299	1/1	0.95	0.23	-	42,42,42,42	0
60	MG	CA	3565	1/1	0.95	0.14	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3104	1/1	0.91	0.25	-	55,55,55,55	0
60	MG	BN	502	1/1	0.94	0.29	-	64,64,64,64	0
60	MG	CA	3636	1/1	0.91	0.32	-	60,60,60,60	0
60	MG	AA	3478	1/1	0.95	0.07	-	70,70,70,70	0
60	MG	CA	3537	1/1	0.94	0.10	-	64,64,64,64	0
60	MG	CA	3108	1/1	0.90	0.18	-	84,84,84,84	0
60	MG	AA	3763	1/1	0.75	0.26	-	66,66,66,66	0
60	MG	CA	3142	1/1	0.85	0.26	-	73,73,73,73	0
60	MG	AA	3029	1/1	0.86	0.20	-	50,50,50,50	0
60	MG	AA	3233	1/1	0.92	0.28	-	85,85,85,85	0
60	MG	CA	3535	1/1	0.73	0.19	-	74,74,74,74	0
60	MG	CA	3180	1/1	0.95	0.17	-	46,46,46,46	0
60	MG	DA	1764	1/1	0.58	0.41	-	94,94,94,94	0
60	MG	BA	1800	1/1	0.09	0.56	-	116,116,116,116	0
60	MG	AA	3399	1/1	0.97	0.24	-	51,51,51,51	0
60	MG	BY	3001	1/1	0.88	0.06	-	78,78,78,78	0
60	MG	CA	3373	1/1	0.96	0.38	-	71,71,71,71	0
60	MG	BA	1602	1/1	0.84	0.20	-	75,75,75,75	0
60	MG	CA	3238	1/1	0.91	0.34	-	73,73,73,73	0
60	MG	DA	1655	1/1	0.84	0.22	-	72,72,72,72	0
60	MG	CA	3235	1/1	0.80	0.37	-	78,78,78,78	0
60	MG	AA	3500	1/1	0.89	0.14	-	27,27,27,27	0
60	MG	AA	3156	1/1	0.88	0.23	-	46,46,46,46	0
60	MG	AA	3113	1/1	0.92	0.23	-	41,41,41,41	0
60	MG	AF	305	1/1	0.97	0.09	-	48,48,48,48	0
60	MG	AA	3509	1/1	0.87	0.26	-	51,51,51,51	0
60	MG	A4	502	1/1	0.86	0.18	-	81,81,81,81	0
60	MG	AA	3576	1/1	0.97	0.29	-	49,49,49,49	0
60	MG	AA	3343	1/1	0.94	0.07	-	60,60,60,60	0
60	MG	CA	3039	1/1	0.88	0.39	-	76,76,76,76	0
60	MG	AA	3175	1/1	0.84	0.33	-	50,50,50,50	1
60	MG	CO	201	1/1	0.87	0.16	-	72,72,72,72	0
60	MG	CA	3178	1/1	0.98	0.21	-	54,54,54,54	0
60	MG	AA	3566	1/1	0.96	0.19	-	26,26,26,26	0
60	MG	AA	3700	1/1	0.76	0.21	-	48,48,48,48	0
60	MG	AA	3317	1/1	0.94	0.19	-	56,56,56,56	0
60	MG	BA	1788	1/1	0.81	0.17	-	79,79,79,79	0
60	MG	DA	1677	1/1	0.82	0.38	-	67,67,67,67	0
60	MG	AA	3636	1/1	0.94	0.21	-	71,71,71,71	0
60	MG	AA	3640	1/1	0.79	0.49	-	74,74,74,74	0
60	MG	AA	3455	1/1	0.88	0.23	-	80,80,80,80	0
60	MG	BX	107	1/1	0.87	0.11	-	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
60	MG	DA	1662	1/1	0.86	0.10	-	51,51,51,51	0
60	MG	DA	1671	1/1	0.60	0.65	-	77,77,77,77	0
60	MG	CA	3647	1/1	0.94	0.38	-	61,61,61,61	0
60	MG	BA	1763	1/1	0.70	0.08	-	75,75,75,75	0
60	MG	AA	3730	1/1	0.96	0.27	-	34,34,34,34	0
60	MG	AA	3624	1/1	0.84	0.27	-	56,56,56,56	0
60	MG	CA	3546	1/1	0.95	0.17	-	59,59,59,59	0
60	MG	AZ	5001	1/1	0.79	0.11	-	67,67,67,67	0
60	MG	CA	3355	1/1	0.84	0.12	-	71,71,71,71	0
60	MG	AA	3338	1/1	0.95	0.12	-	49,49,49,49	0
60	MG	AA	3341	1/1	0.93	0.14	-	74,74,74,74	0
60	MG	AA	3490	1/1	0.43	0.52	-	87,87,87,87	0
60	MG	A7	101	1/1	0.96	0.10	-	57,57,57,57	0
60	MG	BA	1751	1/1	0.94	0.30	-	49,49,49,49	0
60	MG	CA	3221	1/1	0.92	0.56	-	60,60,60,60	0
60	MG	CA	3584	1/1	0.84	0.27	-	91,91,91,91	0
60	MG	CA	3133	1/1	0.89	0.20	-	72,72,72,72	0
60	MG	BA	1758	1/1	0.83	0.18	-	56,56,56,56	0
60	MG	CA	3060	1/1	0.94	0.28	-	50,50,50,50	0
60	MG	AA	3177	1/1	0.86	0.21	-	43,43,43,43	0
60	MG	DA	1733	1/1	0.92	0.09	-	73,73,73,73	0
60	MG	AA	3464	1/1	0.95	0.09	-	69,69,69,69	0
60	MG	AA	3634	1/1	0.95	0.25	-	63,63,63,63	0
60	MG	AA	3075	1/1	0.96	0.28	-	47,47,47,47	0
60	MG	CA	3306	1/1	0.99	0.11	-	39,39,39,39	0
60	MG	CA	3607	1/1	0.85	0.18	-	76,76,76,76	0
60	MG	AA	3693	1/1	0.92	0.19	-	47,47,47,47	0
60	MG	CA	3216	1/1	0.96	0.25	-	32,32,32,32	0
60	MG	AB	3009	1/1	0.94	0.10	-	62,62,62,62	0
60	MG	CA	3583	1/1	0.83	0.28	-	114,114,114,114	0
60	MG	CA	3568	1/1	0.94	0.24	-	71,71,71,71	0
60	MG	CA	3086	1/1	0.84	0.15	-	65,65,65,65	0
60	MG	AA	3103	1/1	0.97	0.12	-	11,11,11,11	0
60	MG	AA	3065	1/1	0.97	0.41	-	51,51,51,51	0
60	MG	BA	1649	1/1	0.87	0.34	-	56,56,56,56	0
60	MG	A0	103	1/1	0.94	0.12	-	67,67,67,67	0
60	MG	AA	3521	1/1	0.97	0.19	-	30,30,30,30	0
60	MG	CA	3664	1/1	0.70	0.31	-	69,69,69,69	0
60	MG	BA	1720	1/1	0.91	0.14	-	51,51,51,51	0
60	MG	CA	3482	1/1	0.67	0.29	-	89,89,89,89	0
60	MG	BW	102	1/1	0.79	0.20	-	75,75,75,75	0
60	MG	AA	3031	1/1	0.98	0.25	-	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3368	1/1	0.96	0.30	-	54,54,54,54	0
60	MG	CA	3336	1/1	0.99	0.12	-	64,64,64,64	0
60	MG	AA	3225	1/1	0.56	0.89	-	91,91,91,91	0
60	MG	CA	3049	1/1	0.63	0.29	-	63,63,63,63	0
60	MG	AA	3652	1/1	0.86	0.44	-	87,87,87,87	0
60	MG	AA	3688	1/1	0.83	0.16	-	76,76,76,76	0
60	MG	AA	3587	1/1	0.91	0.17	-	44,44,44,44	0
60	MG	A6	101	1/1	0.90	0.20	-	69,69,69,69	0
60	MG	CA	3222	1/1	0.79	0.70	-	81,81,81,81	0
60	MG	CA	3173	1/1	0.94	0.53	-	72,72,72,72	0
60	MG	CB	3012	1/1	0.78	0.16	-	74,74,74,74	0
60	MG	CA	3437	1/1	0.90	0.25	-	41,41,41,41	0
60	MG	AA	3412	1/1	0.85	0.16	-	58,58,58,58	0
60	MG	AA	3737	1/1	0.98	0.15	-	25,25,25,25	0
60	MG	DA	1704	1/1	0.68	0.31	-	83,83,83,83	0
60	MG	BA	1692	1/1	0.95	0.31	-	69,69,69,69	0
60	MG	AY	502	1/1	0.89	0.24	-	54,54,54,54	0
60	MG	DA	1721	1/1	0.89	0.32	-	60,60,60,60	0
60	MG	BA	1779	1/1	0.55	0.33	-	82,82,82,82	0
60	MG	A2	3001	1/1	0.78	0.25	-	62,62,62,62	0
60	MG	BA	1719	1/1	0.90	0.27	-	75,75,75,75	0
60	MG	AA	3777	1/1	0.90	0.32	-	58,58,58,58	0
60	MG	AA	3626	1/1	0.96	0.23	-	59,59,59,59	0
60	MG	CA	3155	1/1	0.79	0.48	-	69,69,69,69	0
60	MG	AA	3561	1/1	0.90	0.17	-	64,64,64,64	0
60	MG	AA	3635	1/1	0.94	0.15	-	33,33,33,33	0
60	MG	AA	3093	1/1	0.79	0.85	-	81,81,81,81	0
60	MG	DA	1623	1/1	0.65	0.38	-	70,70,70,70	0
60	MG	CA	3197	1/1	0.93	0.28	-	48,48,48,48	0
60	MG	BA	1710	1/1	0.92	0.10	-	83,83,83,83	0
60	MG	CB	3001	1/1	0.91	0.21	-	68,68,68,68	0
60	MG	AA	3276	1/1	0.95	0.18	-	64,64,64,64	0
60	MG	BX	111	1/1	0.86	0.14	-	67,67,67,67	0
60	MG	AB	3012	1/1	0.97	0.14	-	24,24,24,24	1
60	MG	CA	3536	1/1	0.87	0.13	-	95,95,95,95	0
60	MG	CA	3468	1/1	0.96	0.17	-	37,37,37,37	0
60	MG	AA	3748	1/1	0.96	0.18	-	62,62,62,62	0
60	MG	AA	3273	1/1	0.91	0.27	-	57,57,57,57	0
60	MG	CA	3067	1/1	0.75	0.60	-	82,82,82,82	0
60	MG	CA	3253	1/1	0.96	0.38	-	61,61,61,61	0
60	MG	CA	3070	1/1	0.57	0.57	-	78,78,78,78	0
60	MG	CA	3123	1/1	0.89	0.26	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3654	1/1	0.93	0.63	-	76,76,76,76	0
60	MG	BA	1713	1/1	0.94	0.24	-	61,61,61,61	0
60	MG	AA	3003	1/1	0.96	0.07	-	14,14,14,14	0
60	MG	CA	3207	1/1	0.94	0.48	-	62,62,62,62	0
60	MG	AA	3808	1/1	0.93	0.16	-	47,47,47,47	0
60	MG	CA	3113	1/1	0.76	0.47	-	75,75,75,75	0
60	MG	CA	3229	1/1	0.93	0.21	-	48,48,48,48	0
60	MG	BA	1752	1/1	0.78	0.07	-	48,48,48,48	0
60	MG	AA	3778	1/1	0.90	0.10	-	68,68,68,68	0
60	MG	AB	3015	1/1	0.87	0.12	-	51,51,51,51	0
60	MG	CA	3367	1/1	0.96	0.13	-	39,39,39,39	0
60	MG	CA	3117	1/1	0.96	0.13	-	46,46,46,46	0
60	MG	AA	3768	1/1	0.84	0.35	-	67,67,67,67	0
60	MG	CA	3616	1/1	0.73	0.34	-	62,62,62,62	0
60	MG	AA	3429	1/1	0.86	0.22	-	58,58,58,58	0
60	MG	BX	113	1/1	0.87	0.20	-	78,78,78,78	0
60	MG	CA	3369	1/1	0.96	0.17	-	65,65,65,65	0
60	MG	AA	3689	1/1	0.72	0.16	-	84,84,84,84	0
60	MG	AA	3766	1/1	0.71	0.22	-	69,69,69,69	0
60	MG	AE	302	1/1	0.96	0.18	-	62,62,62,62	0
60	MG	AA	3672	1/1	0.93	0.07	-	71,71,71,71	0
60	MG	CA	3071	1/1	0.82	0.31	-	53,53,53,53	0
60	MG	AA	3761	1/1	0.95	0.19	-	72,72,72,72	0
60	MG	AA	3718	1/1	0.97	0.14	-	40,40,40,40	0
60	MG	AB	3019	1/1	0.77	0.18	-	61,61,61,61	0
60	MG	CA	3057	1/1	0.78	0.71	-	77,77,77,77	0
60	MG	AA	3494	1/1	0.90	0.14	-	66,66,66,66	0
60	MG	CA	3534	1/1	0.90	0.12	-	58,58,58,58	0
60	MG	AA	3592	1/1	0.89	0.26	-	67,67,67,67	0
60	MG	BA	1624	1/1	0.59	0.21	-	75,75,75,75	0
60	MG	BK	3101	1/1	0.51	0.56	-	95,95,95,95	0
60	MG	CA	3630	1/1	0.88	0.21	-	91,91,91,91	0
60	MG	CA	3562	1/1	0.87	0.17	-	69,69,69,69	0
60	MG	CA	3291	1/1	0.79	0.17	-	74,74,74,74	0
60	MG	AA	3440	1/1	0.82	0.18	-	63,63,63,63	0
60	MG	CA	3509	1/1	0.78	0.19	-	52,52,52,52	0
60	MG	CA	3138	1/1	0.88	0.28	-	67,67,67,67	0
60	MG	CA	3501	1/1	0.96	0.17	-	78,78,78,78	0
60	MG	BV	101	1/1	0.81	0.16	-	78,78,78,78	0
60	MG	BA	1677	1/1	0.95	0.32	-	57,57,57,57	0
60	MG	CB	3011	1/1	0.88	0.27	-	51,51,51,51	0
60	MG	AA	3331	1/1	0.95	0.20	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3151	1/1	0.85	0.32	-	63,63,63,63	0
60	MG	BA	1604	1/1	0.91	0.16	-	85,85,85,85	0
60	MG	CA	3188	1/1	0.92	0.27	-	55,55,55,55	0
60	MG	DA	1750	1/1	0.89	0.18	-	86,86,86,86	0
60	MG	AA	3445	1/1	0.90	0.06	-	59,59,59,59	0
60	MG	AA	3664	1/1	0.66	0.21	-	94,94,94,94	0
60	MG	BX	115	1/1	0.93	0.20	-	44,44,44,44	0
60	MG	CR	202	1/1	0.88	0.39	-	61,61,61,61	0
60	MG	AA	3081	1/1	0.90	0.20	-	38,38,38,38	0
60	MG	AA	3729	1/1	0.92	0.07	-	40,40,40,40	0
60	MG	CA	3325	1/1	0.94	0.25	-	42,42,42,42	0
60	MG	AA	3608	1/1	0.89	0.15	-	66,66,66,66	0
60	MG	AA	3062	1/1	0.87	0.36	-	60,60,60,60	0
60	MG	CA	3499	1/1	0.92	0.21	-	68,68,68,68	0
60	MG	AA	3431	1/1	0.95	0.15	-	25,25,25,25	0
60	MG	A5	102	1/1	0.92	0.25	-	46,46,46,46	0
60	MG	AA	3067	1/1	0.94	0.62	-	82,82,82,82	0
60	MG	AA	3216	1/1	0.97	0.17	-	68,68,68,68	0
60	MG	CA	3140	1/1	0.93	0.55	-	54,54,54,54	0
60	MG	CA	3268	1/1	0.91	0.21	-	46,46,46,46	0
60	MG	AA	3550	1/1	0.90	0.21	-	47,47,47,47	0
60	MG	CA	3273	1/1	0.77	0.21	-	42,42,42,42	0
60	MG	AA	3027	1/1	0.82	0.55	-	85,85,85,85	0
60	MG	CA	3376	1/1	0.62	0.17	-	94,94,94,94	0
60	MG	CA	3579	1/1	0.96	0.07	-	58,58,58,58	0
60	MG	DA	1603	1/1	0.97	0.07	-	52,52,52,52	0
60	MG	CA	3329	1/1	0.81	0.22	-	59,59,59,59	0
60	MG	CA	3374	1/1	0.72	0.15	-	74,74,74,74	0
60	MG	AF	304	1/1	0.76	0.43	-	69,69,69,69	0
60	MG	CA	3164	1/1	0.95	0.13	-	38,38,38,38	0
60	MG	BA	1773	1/1	0.92	0.24	-	69,69,69,69	0
60	MG	CA	3416	1/1	0.97	0.28	-	33,33,33,33	0
60	MG	DA	1621	1/1	0.84	0.08	-	69,69,69,69	0
60	MG	AA	3600	1/1	0.93	0.39	-	70,70,70,70	0
60	MG	CA	3551	1/1	0.91	0.15	-	76,76,76,76	0
60	MG	CA	3248	1/1	0.96	0.08	-	58,58,58,58	0
60	MG	BA	1633	1/1	0.88	0.36	-	65,65,65,65	0
60	MG	CA	3613	1/1	0.64	0.31	-	42,42,42,42	0
60	MG	AA	3244	1/1	0.98	0.39	-	42,42,42,42	0
60	MG	DA	1616	1/1	0.98	0.41	-	44,44,44,44	0
60	MG	AA	3016	1/1	0.87	0.31	-	44,44,44,44	0
60	MG	AA	3765	1/1	0.91	0.20	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3096	1/1	0.90	0.22	-	54,54,54,54	0
60	MG	DA	1645	1/1	0.98	0.34	-	58,58,58,58	0
60	MG	CA	3521	1/1	0.80	0.34	-	59,59,59,59	0
60	MG	AA	3530	1/1	0.90	0.10	-	60,60,60,60	0
60	MG	C0	102	1/1	0.86	0.08	-	56,56,56,56	0
60	MG	BA	1727	1/1	0.97	0.28	-	53,53,53,53	0
60	MG	BA	1652	1/1	0.92	0.10	-	65,65,65,65	0
60	MG	CA	3296	1/1	0.81	0.14	-	61,61,61,61	0
60	MG	CA	3124	1/1	0.93	0.38	-	68,68,68,68	0
60	MG	AA	3176	1/1	0.93	0.21	-	70,70,70,70	0
60	MG	CA	3052	1/1	0.94	0.33	-	46,46,46,46	0
60	MG	AA	3350	1/1	0.97	0.16	-	54,54,54,54	0
60	MG	AA	3364	1/1	0.88	0.24	-	57,57,57,57	0
60	MG	CA	3326	1/1	0.93	0.21	-	54,54,54,54	0
60	MG	CE	306	1/1	0.88	0.09	-	69,69,69,69	0
60	MG	DA	1758	1/1	0.85	0.35	-	80,80,80,80	0
60	MG	AA	3477	1/1	0.89	0.15	-	47,47,47,47	0
60	MG	CA	3343	1/1	0.94	0.15	-	37,37,37,37	0
60	MG	CA	3492	1/1	0.93	0.26	-	60,60,60,60	0
60	MG	CA	3294	1/1	0.98	0.31	-	40,40,40,40	0
60	MG	AA	3322	1/1	0.94	0.19	-	37,37,37,37	0
60	MG	BA	1697	1/1	0.94	0.47	-	80,80,80,80	0
60	MG	CA	3465	1/1	0.94	0.08	-	64,64,64,64	0
60	MG	CA	3472	1/1	0.95	0.28	-	49,49,49,49	0
60	MG	AA	3757	1/1	0.93	0.29	-	67,67,67,67	0
60	MG	DA	1731	1/1	0.97	0.19	-	51,51,51,51	0
60	MG	BA	1635	1/1	0.93	0.29	-	62,62,62,62	0
60	MG	AA	3545	1/1	0.93	0.06	-	64,64,64,64	0
60	MG	BA	1688	1/1	0.86	0.29	-	71,71,71,71	0
60	MG	AA	3284	1/1	0.97	0.39	-	45,45,45,45	0
60	MG	CA	3237	1/1	0.94	0.34	-	70,70,70,70	0
60	MG	AA	3235	1/1	0.90	0.27	-	42,42,42,42	0
60	MG	AA	3336	1/1	0.96	0.27	-	52,52,52,52	0
60	MG	CA	3502	1/1	0.55	0.14	-	66,66,66,66	0
60	MG	CA	3644	1/1	0.92	0.17	-	60,60,60,60	0
60	MG	BA	1650	1/1	0.92	0.22	-	49,49,49,49	0
60	MG	AA	3139	1/1	0.92	0.25	-	64,64,64,64	0
60	MG	CA	3128	1/1	0.95	0.22	-	31,31,31,31	0
60	MG	AA	3118	1/1	0.95	0.30	-	59,59,59,59	0
60	MG	CA	3547	1/1	0.97	0.06	-	57,57,57,57	1
60	MG	AA	3264	1/1	0.96	0.09	-	54,54,54,54	0
60	MG	AA	3285	1/1	0.88	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
60	MG	BA	1808	1/1	0.80	0.16	-	80,80,80,80	0
60	MG	BA	1750	1/1	0.97	0.10	-	54,54,54,54	0
60	MG	BA	1698	1/1	0.90	0.31	-	57,57,57,57	0
60	MG	CA	3548	1/1	0.85	0.12	-	53,53,53,53	0
60	MG	CA	3480	1/1	0.89	0.14	-	61,61,61,61	0
60	MG	BA	1644	1/1	0.91	0.27	-	72,72,72,72	0
60	MG	CA	3095	1/1	0.91	0.09	-	92,92,92,92	0
60	MG	CA	3011	1/1	0.84	0.25	-	75,75,75,75	0
60	MG	CA	3212	1/1	0.67	0.10	-	78,78,78,78	0
60	MG	AA	3088	1/1	0.75	0.53	-	42,42,42,42	0
60	MG	AA	3208	1/1	0.83	0.27	-	55,55,55,55	0
60	MG	AA	3732	1/1	0.78	0.18	-	63,63,63,63	0
60	MG	AA	3076	1/1	0.97	0.13	-	6,6,6,6	0
60	MG	CB	3008	1/1	0.47	0.26	-	87,87,87,87	0
60	MG	CA	3639	1/1	0.97	0.31	-	54,54,54,54	0
60	MG	AA	3246	1/1	0.54	0.60	-	86,86,86,86	0
60	MG	BA	1627	1/1	0.77	0.21	-	63,63,63,63	0
60	MG	CA	3024	1/1	0.96	0.62	-	67,67,67,67	0
60	MG	CA	3015	1/1	0.79	0.49	-	66,66,66,66	0
60	MG	AA	3745	1/1	0.85	0.28	-	42,42,42,42	0
60	MG	BA	1731	1/1	0.92	0.06	-	65,65,65,65	0
60	MG	AA	3283	1/1	0.93	0.31	-	48,48,48,48	0
60	MG	DA	1703	1/1	0.98	0.06	-	59,59,59,59	0
60	MG	DA	1701	1/1	0.94	0.14	-	61,61,61,61	0
60	MG	AA	3122	1/1	0.94	0.29	-	39,39,39,39	0
60	MG	AA	3089	1/1	0.81	0.39	-	58,58,58,58	0
60	MG	CA	3490	1/1	0.85	0.41	-	81,81,81,81	0
60	MG	AA	3656	1/1	0.87	0.24	-	62,62,62,62	1
60	MG	AA	3637	1/1	0.88	0.19	-	54,54,54,54	0
60	MG	AA	3201	1/1	0.91	0.31	-	71,71,71,71	0
60	MG	AA	3752	1/1	0.90	0.63	-	75,75,75,75	0
60	MG	DK	202	1/1	0.89	0.23	-	80,80,80,80	0
60	MG	CA	3510	1/1	0.88	0.17	-	71,71,71,71	0
60	MG	CA	3243	1/1	0.92	0.35	-	55,55,55,55	0
60	MG	CA	3333	1/1	0.90	0.20	-	64,64,64,64	0
60	MG	AA	3588	1/1	0.97	0.15	-	33,33,33,33	0
60	MG	AA	3091	1/1	0.95	0.48	-	62,62,62,62	0
60	MG	CA	3042	1/1	0.52	0.89	-	84,84,84,84	0
60	MG	CA	3191	1/1	0.86	0.27	-	61,61,61,61	0
60	MG	AA	3154	1/1	0.89	0.16	-	64,64,64,64	0
60	MG	AA	3305	1/1	0.92	0.16	-	38,38,38,38	0
60	MG	CA	3614	1/1	0.89	0.28	-	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
60	MG	CA	3109	1/1	0.95	0.18	-	65,65,65,65	0
60	MG	AA	3666	1/1	0.95	0.29	-	28,28,28,28	0
60	MG	AA	3663	1/1	0.97	0.20	-	61,61,61,61	0
60	MG	AA	3015	1/1	0.71	0.46	-	74,74,74,74	0
60	MG	BA	1664	1/1	0.93	0.57	-	64,64,64,64	0
60	MG	AA	3030	1/1	0.97	0.34	-	44,44,44,44	1
60	MG	CA	3252	1/1	0.96	0.25	-	30,30,30,30	0
60	MG	AA	3291	1/1	0.87	0.13	-	84,84,84,84	0
60	MG	CA	3487	1/1	0.82	0.29	-	64,64,64,64	0
60	MG	BA	1657	1/1	0.77	0.47	-	72,72,72,72	0
60	MG	CA	3498	1/1	0.85	0.33	-	68,68,68,68	0
60	MG	AA	3793	1/1	0.79	0.35	-	76,76,76,76	0
60	MG	BA	1711	1/1	0.94	0.37	-	63,63,63,63	0
60	MG	AA	3533	1/1	0.94	0.12	-	20,20,20,20	0
60	MG	BL	202	1/1	0.97	0.14	-	56,56,56,56	0
60	MG	BA	1762	1/1	0.90	0.07	-	57,57,57,57	0
60	MG	CA	3323	1/1	0.90	0.16	-	32,32,32,32	0
60	MG	AA	3493	1/1	0.94	0.22	-	56,56,56,56	0
60	MG	CA	3119	1/1	0.92	0.69	-	63,63,63,63	0
60	MG	DA	1739	1/1	0.67	0.43	-	85,85,85,85	0
60	MG	AA	3782	1/1	0.91	0.17	-	70,70,70,70	0
60	MG	AA	3114	1/1	0.93	0.34	-	55,55,55,55	0
60	MG	AA	3125	1/1	0.91	0.35	-	74,74,74,74	0
60	MG	AA	3326	1/1	0.96	0.14	-	22,22,22,22	0
60	MG	BA	1789	1/1	0.88	0.11	-	68,68,68,68	0
60	MG	AA	3645	1/1	0.96	0.10	-	57,57,57,57	0
60	MG	CA	3298	1/1	0.76	0.21	-	68,68,68,68	0
60	MG	AA	3142	1/1	0.90	0.27	-	50,50,50,50	0
60	MG	CA	3152	1/1	0.70	0.16	-	67,67,67,67	0
60	MG	CA	3591	1/1	0.95	0.14	-	69,69,69,69	0
60	MG	AA	3554	1/1	0.95	0.07	-	48,48,48,48	0
60	MG	AA	3234	1/1	0.75	0.41	-	58,58,58,58	0
60	MG	AA	3066	1/1	0.91	0.19	-	63,63,63,63	0
60	MG	CA	3185	1/1	0.93	0.32	-	47,47,47,47	0
60	MG	CA	3557	1/1	0.89	0.25	-	76,76,76,76	0
60	MG	CA	3006	1/1	0.97	0.09	-	24,24,24,24	0
60	MG	CA	3305	1/1	0.88	0.31	-	64,64,64,64	0
60	MG	CA	3440	1/1	0.94	0.41	-	69,69,69,69	0
60	MG	DA	1752	1/1	0.92	0.32	-	73,73,73,73	0
60	MG	AA	3605	1/1	0.80	0.11	-	66,66,66,66	0
60	MG	CA	3228	1/1	0.90	0.71	-	68,68,68,68	0
60	MG	BA	1642	1/1	0.86	0.18	-	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
60	MG	DZ	701	1/1	0.97	0.24	-	47,47,47,47	0
60	MG	AA	3456	1/1	0.99	0.12	-	64,64,64,64	0
60	MG	AA	3303	1/1	0.89	0.21	-	30,30,30,30	0
60	MG	AB	3002	1/1	0.98	0.22	-	55,55,55,55	0
60	MG	CA	3147	1/1	0.96	0.12	-	51,51,51,51	0
60	MG	DA	1717	1/1	0.94	0.16	-	70,70,70,70	0
60	MG	AA	3784	1/1	0.90	0.15	-	69,69,69,69	0
60	MG	DA	1734	1/1	0.70	0.28	-	75,75,75,75	0
60	MG	BA	1667	1/1	0.91	0.15	-	69,69,69,69	0
60	MG	AA	3388	1/1	0.88	0.16	-	55,55,55,55	0
60	MG	BA	1797	1/1	0.96	0.15	-	75,75,75,75	0
60	MG	CA	3202	1/1	0.78	0.32	-	67,67,67,67	0
60	MG	CA	3596	1/1	0.89	0.10	-	75,75,75,75	0
60	MG	DA	1710	1/1	0.92	0.23	-	56,56,56,56	0
60	MG	CA	3634	1/1	0.85	0.21	-	82,82,82,82	0
60	MG	AA	3690	1/1	0.91	0.11	-	58,58,58,58	0
60	MG	BA	1638	1/1	0.84	0.64	-	83,83,83,83	0
60	MG	DA	1670	1/1	0.87	0.25	-	74,74,74,74	0
60	MG	BA	1641	1/1	0.95	0.29	-	56,56,56,56	0
60	MG	CA	3586	1/1	0.94	0.25	-	75,75,75,75	0
60	MG	CA	3005	1/1	0.86	0.18	-	69,69,69,69	0
60	MG	CA	3025	1/1	0.95	0.50	-	32,32,32,32	1
60	MG	C0	101	1/1	0.92	0.07	-	50,50,50,50	0
60	MG	AA	3742	1/1	0.95	0.20	-	68,68,68,68	0
60	MG	AA	3061	1/1	0.81	0.77	-	64,64,64,64	0
60	MG	CA	3580	1/1	0.96	0.12	-	37,37,37,37	0
60	MG	CA	3053	1/1	0.93	0.19	-	71,71,71,71	0
60	MG	AA	3426	1/1	0.94	0.20	-	47,47,47,47	0
60	MG	CA	3250	1/1	0.83	0.17	-	69,69,69,69	0
60	MG	AA	3628	1/1	0.97	0.18	-	62,62,62,62	0
60	MG	DA	1741	1/1	0.92	0.32	-	81,81,81,81	0
60	MG	CA	3542	1/1	0.74	0.20	-	82,82,82,82	0
60	MG	BA	1689	1/1	0.80	0.29	-	65,65,65,65	0
60	MG	CA	3314	1/1	0.90	0.15	-	41,41,41,41	0
60	MG	BA	1756	1/1	0.95	0.25	-	43,43,43,43	0
60	MG	AA	3179	1/1	0.91	0.23	-	62,62,62,62	0
60	MG	AA	3002	1/1	0.77	0.24	-	53,53,53,53	0
60	MG	AA	3055	1/1	0.90	0.17	-	61,61,61,61	0
60	MG	AA	3642	1/1	0.94	0.23	-	60,60,60,60	0
60	MG	AA	3041	1/1	0.93	0.33	-	41,41,41,41	0
60	MG	BA	1606	1/1	0.97	0.28	-	74,74,74,74	0
60	MG	AA	3785	1/1	0.91	0.21	-	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
60	MG	AA	3599	1/1	0.66	0.43	-	113,113,113,113	0
60	MG	AB	3005	1/1	0.81	0.17	-	70,70,70,70	0
60	MG	DA	1726	1/1	0.93	0.16	-	58,58,58,58	0
60	MG	BA	1670	1/1	0.76	0.30	-	76,76,76,76	0
60	MG	AA	3192	1/1	0.69	0.42	-	69,69,69,69	0
60	MG	CA	3308	1/1	0.93	0.19	-	35,35,35,35	0
60	MG	CA	3638	1/1	0.94	0.48	-	68,68,68,68	0
60	MG	AA	3070	1/1	0.66	0.35	-	68,68,68,68	0
60	MG	BX	106	1/1	0.80	0.17	-	85,85,85,85	0
60	MG	CA	3405	1/1	0.96	0.15	-	50,50,50,50	0
60	MG	AA	3648	1/1	0.70	0.17	-	80,80,80,80	0
60	MG	BA	1780	1/1	0.97	0.07	-	44,44,44,44	0
60	MG	AA	3463	1/1	0.95	0.19	-	41,41,41,41	0
60	MG	AA	3161	1/1	0.79	0.57	-	89,89,89,89	0
60	MG	AA	3078	1/1	0.88	0.26	-	54,54,54,54	0
60	MG	CA	3428	1/1	0.93	0.36	-	50,50,50,50	0
60	MG	A0	104	1/1	0.73	0.80	-	81,81,81,81	0
60	MG	AA	3553	1/1	0.94	0.17	-	47,47,47,47	0
60	MG	CA	3200	1/1	0.89	0.15	-	65,65,65,65	0
60	MG	BA	1760	1/1	0.93	0.18	-	68,68,68,68	0
60	MG	AB	3022	1/1	0.94	0.06	-	79,79,79,79	0
60	MG	BA	1721	1/1	0.98	0.26	-	60,60,60,60	0
60	MG	BX	114	1/1	0.93	0.26	-	57,57,57,57	0
60	MG	CA	3146	1/1	0.83	0.31	-	79,79,79,79	0
60	MG	CB	3009	1/1	0.92	0.16	-	66,66,66,66	0
60	MG	CA	3645	1/1	0.78	0.13	-	78,78,78,78	0
60	MG	DA	1716	1/1	0.91	0.27	-	56,56,56,56	0
60	MG	AA	3171	1/1	0.86	0.51	-	71,71,71,71	0
60	MG	AA	3174	1/1	0.94	0.27	-	39,39,39,39	0
60	MG	CA	3051	1/1	0.82	0.18	-	52,52,52,52	0
60	MG	BA	1776	1/1	0.83	0.10	-	64,64,64,64	0
60	MG	AA	3610	1/1	0.95	0.10	-	66,66,66,66	0
60	MG	AA	3476	1/1	0.89	0.10	-	50,50,50,50	0
60	MG	CA	3183	1/1	0.75	0.43	-	83,83,83,83	0
60	MG	AA	3804	1/1	0.91	0.38	-	70,70,70,70	0
60	MG	AA	3562	1/1	0.91	0.06	-	45,45,45,45	0
60	MG	BA	1732	1/1	0.88	0.25	-	65,65,65,65	0
60	MG	DA	1751	1/1	0.88	0.25	-	84,84,84,84	0
60	MG	CA	3392	1/1	0.96	0.09	-	66,66,66,66	0
60	MG	DA	1636	1/1	0.90	0.32	-	77,77,77,77	0
60	MG	AA	3795	1/1	0.85	0.28	-	26,26,26,26	1
60	MG	CE	305	1/1	0.81	0.26	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BA	1676	1/1	0.93	0.24	-	39,39,39,39	0
60	MG	AA	3152	1/1	0.78	0.41	-	80,80,80,80	0
60	MG	AA	3787	1/1	0.94	0.27	-	55,55,55,55	0
60	MG	AA	3598	1/1	0.88	0.20	-	57,57,57,57	0
60	MG	AA	3403	1/1	0.97	0.14	-	55,55,55,55	0
60	MG	CA	3539	1/1	0.89	0.31	-	72,72,72,72	0
60	MG	DA	1615	1/1	0.51	0.52	-	87,87,87,87	0
60	MG	CA	3597	1/1	0.50	0.47	-	108,108,108,108	0
60	MG	DA	1737	1/1	0.82	0.40	-	73,73,73,73	0
60	MG	AA	3744	1/1	0.79	0.15	-	79,79,79,79	0
60	MG	AA	3579	1/1	0.65	0.14	-	66,66,66,66	0
60	MG	CA	3635	1/1	0.92	0.30	-	77,77,77,77	0
60	MG	AA	3813	1/1	0.91	0.21	-	68,68,68,68	0
60	MG	AA	3643	1/1	0.97	0.14	-	56,56,56,56	0
60	MG	CA	3169	1/1	0.82	0.28	-	65,65,65,65	0
60	MG	CA	3310	1/1	0.95	0.21	-	45,45,45,45	0
60	MG	CA	3434	1/1	0.93	0.17	-	67,67,67,67	0
60	MG	BA	1656	1/1	0.84	0.19	-	83,83,83,83	0
60	MG	CA	3148	1/1	0.92	0.15	-	41,41,41,41	0
60	MG	AA	3467	1/1	0.96	0.13	-	54,54,54,54	0
60	MG	CA	3295	1/1	0.90	0.29	-	55,55,55,55	0
60	MG	AA	3286	1/1	0.98	0.25	-	48,48,48,48	0
60	MG	AA	3756	1/1	0.86	0.24	-	57,57,57,57	0
60	MG	DA	1698	1/1	0.92	0.15	-	75,75,75,75	0
60	MG	AE	304	1/1	0.86	0.53	-	70,70,70,70	0
60	MG	CA	3347	1/1	0.98	0.14	-	37,37,37,37	0
60	MG	BA	1694	1/1	0.87	0.23	-	78,78,78,78	0
60	MG	AA	3418	1/1	0.95	0.17	-	22,22,22,22	0
60	MG	AR	5001	1/1	0.97	0.14	-	34,34,34,34	0
60	MG	AA	3166	1/1	0.98	0.12	-	52,52,52,52	0
60	MG	AA	3359	1/1	0.97	0.18	-	31,31,31,31	0
60	MG	AA	3396	1/1	0.99	0.14	-	22,22,22,22	0
60	MG	CA	3283	1/1	0.90	0.23	-	57,57,57,57	0
60	MG	AA	3707	1/1	0.94	0.43	-	59,59,59,59	0
60	MG	AA	3186	1/1	0.95	0.24	-	53,53,53,53	0
60	MG	CA	3623	1/1	0.93	0.58	-	71,71,71,71	0
60	MG	AA	3575	1/1	0.87	0.16	-	63,63,63,63	0
60	MG	CA	3254	1/1	0.89	0.15	-	35,35,35,35	0
60	MG	AA	3135	1/1	0.95	0.16	-	53,53,53,53	0
60	MG	CA	3382	1/1	0.86	0.18	-	70,70,70,70	0
60	MG	DA	1757	1/1	0.81	0.13	-	77,77,77,77	0
60	MG	AE	301	1/1	0.85	0.40	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	BD	502	1/1	0.87	0.42	-	56,56,56,56	0
60	MG	CA	3629	1/1	0.86	0.14	-	74,74,74,74	0
60	MG	AA	3270	1/1	0.88	0.20	-	92,92,92,92	0
60	MG	BX	103	1/1	0.82	0.08	-	88,88,88,88	0
60	MG	CA	3098	1/1	0.45	1.04	-	90,90,90,90	0
60	MG	CA	3475	1/1	0.73	0.17	-	55,55,55,55	0
60	MG	AA	3275	1/1	0.96	0.39	-	56,56,56,56	0
60	MG	BA	1700	1/1	0.94	0.11	-	62,62,62,62	0
60	MG	CP	201	1/1	0.96	0.13	-	57,57,57,57	0
60	MG	CQ	203	1/1	0.86	0.28	-	62,62,62,62	0
60	MG	DA	1664	1/1	0.87	0.24	-	49,49,49,49	0
60	MG	AA	3749	1/1	0.94	0.14	-	30,30,30,30	0
60	MG	CA	3196	1/1	0.95	0.28	-	57,57,57,57	0
60	MG	AA	3703	1/1	0.97	0.07	-	76,76,76,76	0
60	MG	AA	3586	1/1	0.94	0.19	-	75,75,75,75	0
60	MG	CA	3599	1/1	0.80	0.09	-	75,75,75,75	0
60	MG	AA	3280	1/1	0.91	0.20	-	63,63,63,63	0
60	MG	AA	3638	1/1	0.76	0.36	-	72,72,72,72	0
60	MG	BA	1608	1/1	0.92	0.35	-	52,52,52,52	0
60	MG	CA	3400	1/1	0.98	0.10	-	48,48,48,48	0
60	MG	CA	3528	1/1	0.87	0.07	-	51,51,51,51	1
60	MG	AA	3470	1/1	0.98	0.13	-	24,24,24,24	0
60	MG	CA	3524	1/1	0.75	0.29	-	87,87,87,87	0
60	MG	AA	3153	1/1	0.93	0.27	-	47,47,47,47	0
60	MG	BA	1708	1/1	0.90	0.27	-	55,55,55,55	0
60	MG	CA	3592	1/1	0.66	0.23	-	87,87,87,87	0
60	MG	CB	3002	1/1	0.92	0.13	-	78,78,78,78	0
60	MG	DA	1723	1/1	0.94	0.28	-	53,53,53,53	0
60	MG	BA	1771	1/1	0.97	0.13	-	48,48,48,48	0
60	MG	BA	1618	1/1	0.85	0.52	-	54,54,54,54	0
60	MG	CA	3556	1/1	0.95	0.05	-	77,77,77,77	0
60	MG	DA	1678	1/1	0.92	0.40	-	66,66,66,66	0
60	MG	DA	1640	1/1	0.91	0.35	-	73,73,73,73	0
60	MG	AA	3223	1/1	0.93	0.17	-	21,21,21,21	0
60	MG	CA	3578	1/1	0.57	0.12	-	96,96,96,96	0
60	MG	BA	1623	1/1	0.90	0.25	-	67,67,67,67	0
60	MG	AA	3269	1/1	0.91	0.54	-	78,78,78,78	0
60	MG	CA	3380	1/1	0.94	0.16	-	37,37,37,37	0
60	MG	BA	1781	1/1	0.93	0.14	-	63,63,63,63	0
60	MG	CA	3137	1/1	0.97	0.18	-	64,64,64,64	0
60	MG	CA	3076	1/1	0.91	0.32	-	48,48,48,48	0
60	MG	CA	3511	1/1	0.76	0.34	-	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
60	MG	AA	3288	1/1	0.90	0.13	-	39,39,39,39	0
60	MG	CA	3139	1/1	0.49	0.53	-	83,83,83,83	0
60	MG	CA	3620	1/1	0.92	0.22	-	41,41,41,41	0
60	MG	AA	3404	1/1	0.97	0.10	-	50,50,50,50	0
60	MG	BA	1796	1/1	0.94	0.18	-	75,75,75,75	0
60	MG	BA	1801	1/1	0.91	0.12	-	55,55,55,55	0
60	MG	DA	1673	1/1	0.83	0.40	-	68,68,68,68	0
60	MG	BA	1712	1/1	0.83	0.60	-	68,68,68,68	0
60	MG	CA	3219	1/1	0.85	0.32	-	57,57,57,57	0
60	MG	AA	3701	1/1	0.95	0.56	-	62,62,62,62	0
60	MG	AA	3508	1/1	0.98	0.13	-	42,42,42,42	0
60	MG	AA	3543	1/1	0.84	0.17	-	84,84,84,84	0
60	MG	AA	3807	1/1	0.95	0.20	-	62,62,62,62	0
60	MG	DA	1647	1/1	0.97	0.14	-	39,39,39,39	0
60	MG	AA	3496	1/1	0.97	0.05	-	43,43,43,43	0
60	MG	AA	3719	1/1	0.95	0.09	-	62,62,62,62	0
60	MG	AA	3138	1/1	0.93	0.14	-	58,58,58,58	0
60	MG	AA	3316	1/1	0.85	0.20	-	64,64,64,64	0
60	MG	BA	1718	1/1	0.93	0.16	-	48,48,48,48	0
60	MG	AA	3762	1/1	0.96	0.26	-	63,63,63,63	0
60	MG	AA	3578	1/1	0.74	0.37	-	71,71,71,71	0
60	MG	DA	1755	1/1	0.96	0.14	-	69,69,69,69	0
60	MG	AA	3406	1/1	0.93	0.14	-	52,52,52,52	0
60	MG	AA	3434	1/1	0.86	0.27	-	58,58,58,58	0
60	MG	AA	3197	1/1	0.94	0.32	-	42,42,42,42	0
60	MG	CA	3317	1/1	0.90	0.16	-	61,61,61,61	0
60	MG	AE	303	1/1	0.97	0.19	-	23,23,23,23	0
60	MG	AA	3073	1/1	0.93	0.22	-	61,61,61,61	0
60	MG	CA	3287	1/1	0.89	0.35	-	43,43,43,43	0
60	MG	CA	3205	1/1	0.92	0.31	-	66,66,66,66	0
60	MG	DF	3001	1/1	0.93	0.12	-	53,53,53,53	0
60	MG	BA	1754	1/1	0.94	0.05	-	75,75,75,75	0
60	MG	AA	3278	1/1	0.92	0.35	-	58,58,58,58	0
60	MG	BA	1605	1/1	0.91	0.11	-	76,76,76,76	0
60	MG	AA	3548	1/1	0.77	0.13	-	69,69,69,69	0
60	MG	CA	3073	1/1	0.38	0.73	-	94,94,94,94	0
60	MG	BA	1726	1/1	0.94	0.17	-	59,59,59,59	0
60	MG	BW	101	1/1	0.64	0.47	-	82,82,82,82	0
60	MG	AA	3771	1/1	0.94	0.18	-	40,40,40,40	0
60	MG	AA	3071	1/1	0.94	0.73	-	55,55,55,55	0
60	MG	AA	3227	1/1	0.99	0.25	-	75,75,75,75	0
60	MG	AA	3443	1/1	0.83	0.21	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AB	3013	1/1	0.94	0.13	-	55,55,55,55	0
60	MG	BA	1770	1/1	0.73	0.12	-	62,62,62,62	0
60	MG	CA	3277	1/1	0.98	0.18	-	43,43,43,43	0
60	MG	BL	201	1/1	0.89	0.20	-	104,104,104,104	0
60	MG	BA	1806	1/1	0.92	0.17	-	63,63,63,63	0
60	MG	CA	3435	1/1	0.93	0.16	-	55,55,55,55	0
60	MG	AA	3148	1/1	0.99	0.24	-	48,48,48,48	0
60	MG	AA	3775	1/1	0.95	0.18	-	52,52,52,52	0
60	MG	AA	3715	1/1	0.91	0.09	-	62,62,62,62	0
60	MG	AA	3092	1/1	0.90	0.23	-	41,41,41,41	0
60	MG	BX	101	1/1	0.93	0.30	-	63,63,63,63	0
60	MG	AA	3433	1/1	0.95	0.28	-	50,50,50,50	0
60	MG	CA	3003	1/1	0.97	0.31	-	49,49,49,49	0
60	MG	CA	3544	1/1	0.90	0.18	-	74,74,74,74	0
60	MG	BA	1803	1/1	0.58	0.22	-	79,79,79,79	0
60	MG	DA	1743	1/1	0.73	0.13	-	83,83,83,83	0
60	MG	A0	105	1/1	0.87	0.08	-	52,52,52,52	0
60	MG	AA	3499	1/1	0.91	0.11	-	46,46,46,46	0
60	MG	DA	1604	1/1	0.95	0.12	-	90,90,90,90	0
60	MG	BA	1653	1/1	0.93	0.23	-	62,62,62,62	0
60	MG	AA	3609	1/1	0.92	0.21	-	57,57,57,57	0
60	MG	AA	3014	1/1	0.91	0.17	-	45,45,45,45	0
60	MG	BA	1745	1/1	0.93	0.09	-	46,46,46,46	0
60	MG	AA	3677	1/1	0.99	0.20	-	26,26,26,26	0
60	MG	AA	3335	1/1	0.97	0.19	-	14,14,14,14	0
60	MG	CA	3483	1/1	0.79	0.17	-	67,67,67,67	0
60	MG	AA	3419	1/1	0.89	0.05	-	88,88,88,88	0
60	MG	AA	3670	1/1	0.94	0.17	-	66,66,66,66	0
60	MG	BA	1782	1/1	0.88	0.29	-	72,72,72,72	0
60	MG	DA	1620	1/1	0.77	0.23	-	68,68,68,68	0
60	MG	AA	3424	1/1	0.95	0.11	-	48,48,48,48	0
60	MG	AA	3265	1/1	0.83	0.36	-	64,64,64,64	0
60	MG	AA	3247	1/1	0.87	0.42	-	75,75,75,75	0
60	MG	AA	3831	1/1	0.95	0.38	-	41,41,41,41	0
60	MG	AA	3704	1/1	0.95	0.17	-	57,57,57,57	0
60	MG	AA	3641	1/1	0.98	0.14	-	45,45,45,45	0
60	MG	DA	1712	1/1	0.88	0.17	-	67,67,67,67	0
60	MG	AA	3004	1/1	0.92	0.14	-	30,30,30,30	0
60	MG	CA	3077	1/1	0.82	0.28	-	62,62,62,62	0
60	MG	BA	1728	1/1	0.94	0.18	-	53,53,53,53	0
60	MG	AA	3584	1/1	0.97	0.12	-	63,63,63,63	0
60	MG	CA	3640	1/1	0.86	0.24	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3096	1/1	0.77	0.28	-	75,75,75,75	0
60	MG	CA	3286	1/1	0.89	0.21	-	62,62,62,62	0
60	MG	CA	3462	1/1	0.81	0.34	-	63,63,63,63	0
60	MG	AA	3450	1/1	0.92	0.27	-	71,71,71,71	0
60	MG	CA	3007	1/1	0.88	0.24	-	75,75,75,75	0
60	MG	AA	3010	1/1	0.87	0.29	-	68,68,68,68	0
60	MG	BA	1777	1/1	0.95	0.12	-	76,76,76,76	0
60	MG	AA	3226	1/1	0.90	0.27	-	51,51,51,51	0
60	MG	BA	1646	1/1	0.75	0.52	-	71,71,71,71	0
60	MG	AA	3558	1/1	0.94	0.14	-	72,72,72,72	0
60	MG	DA	1746	1/1	0.87	0.28	-	67,67,67,67	0
60	MG	CR	201	1/1	0.89	0.36	-	63,63,63,63	0
60	MG	AA	3462	1/1	0.95	0.06	-	73,73,73,73	0
60	MG	AA	3630	1/1	0.90	0.15	-	66,66,66,66	0
60	MG	AA	3255	1/1	0.95	0.28	-	64,64,64,64	0
60	MG	BA	1661	1/1	0.88	0.45	-	59,59,59,59	0
60	MG	AA	3534	1/1	0.96	0.20	-	34,34,34,34	0
60	MG	DA	1663	1/1	0.95	0.10	-	53,53,53,53	0
60	MG	CA	3399	1/1	0.97	0.18	-	45,45,45,45	0
60	MG	BA	1703	1/1	0.67	0.22	-	65,65,65,65	0
60	MG	CA	3372	1/1	0.91	0.29	-	63,63,63,63	0
60	MG	DA	1654	1/1	0.92	0.40	-	48,48,48,48	0
60	MG	AA	3444	1/1	0.80	0.09	-	52,52,52,52	0
60	MG	CA	3469	1/1	0.94	0.58	-	76,76,76,76	0
60	MG	DA	1759	1/1	0.96	0.42	-	64,64,64,64	0
60	MG	CA	3321	1/1	0.95	0.13	-	65,65,65,65	0
60	MG	CA	3281	1/1	0.82	0.20	-	74,74,74,74	0
60	MG	AA	3389	1/1	0.95	0.18	-	46,46,46,46	0
60	MG	AA	3649	1/1	0.80	0.07	-	78,78,78,78	0
60	MG	CA	3543	1/1	0.16	0.55	-	114,114,114,114	0
60	MG	DA	1744	1/1	0.96	0.14	-	57,57,57,57	0
60	MG	CF	303	1/1	0.90	0.28	-	63,63,63,63	0
60	MG	AB	3004	1/1	0.90	0.29	-	69,69,69,69	0
60	MG	CA	3144	1/1	0.89	0.29	-	84,84,84,84	0
60	MG	CF	304	1/1	0.97	0.15	-	46,46,46,46	0
60	MG	AA	3631	1/1	0.86	0.39	-	74,74,74,74	0
60	MG	AA	3414	1/1	0.95	0.17	-	43,43,43,43	0
60	MG	BA	1631	1/1	0.92	0.09	-	44,44,44,44	0
60	MG	AA	3147	1/1	0.92	0.51	-	52,52,52,52	0
60	MG	CA	3504	1/1	0.96	0.11	-	77,77,77,77	0
60	MG	A8	5002	1/1	0.95	0.25	-	45,45,45,45	0
60	MG	CA	3258	1/1	0.97	0.17	-	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
60	MG	AA	3779	1/1	0.95	0.28	-	41,41,41,41	0
60	MG	AA	3593	1/1	0.94	0.14	-	49,49,49,49	0
60	MG	DA	1648	1/1	0.84	0.46	-	66,66,66,66	0
60	MG	CA	3478	1/1	0.41	0.29	-	91,91,91,91	0
60	MG	AA	3126	1/1	0.97	0.24	-	68,68,68,68	0
60	MG	CA	3410	1/1	0.85	0.19	-	72,72,72,72	0
60	MG	AA	3026	1/1	0.64	0.38	-	69,69,69,69	0
60	MG	CA	3420	1/1	0.93	0.26	-	50,50,50,50	0
60	MG	CA	3230	1/1	0.88	0.11	-	64,64,64,64	0
60	MG	AA	3366	1/1	0.94	0.18	-	35,35,35,35	0
60	MG	CA	3217	1/1	0.94	0.13	-	52,52,52,52	0
60	MG	AA	3621	1/1	0.86	0.12	-	34,34,34,34	0
60	MG	AA	3453	1/1	0.97	0.11	-	51,51,51,51	0
60	MG	BA	1665	1/1	0.94	0.41	-	68,68,68,68	0
60	MG	AA	3098	1/1	0.81	0.29	-	65,65,65,65	0
60	MG	CA	3267	1/1	0.91	0.24	-	110,110,110,110	0
60	MG	CA	3371	1/1	0.81	0.61	-	70,70,70,70	0
60	MG	CA	3471	1/1	0.95	0.21	-	59,59,59,59	0
60	MG	DA	1635	1/1	0.91	0.44	-	61,61,61,61	0
60	MG	BA	1723	1/1	0.91	0.27	-	61,61,61,61	0
60	MG	CA	3393	1/1	0.92	0.35	-	47,47,47,47	0
60	MG	CA	3403	1/1	0.94	0.19	-	70,70,70,70	0
60	MG	CA	3484	1/1	0.91	0.26	-	56,56,56,56	0
60	MG	CA	3352	1/1	0.98	0.23	-	40,40,40,40	0
60	MG	CA	3029	1/1	0.93	0.11	-	68,68,68,68	0
60	MG	CA	3001	1/1	0.86	0.17	-	81,81,81,81	0
60	MG	DA	1641	1/1	0.94	0.13	-	55,55,55,55	0
60	MG	CA	3466	1/1	0.98	0.14	-	56,56,56,56	0
60	MG	AA	3751	1/1	0.75	0.20	-	76,76,76,76	0
60	MG	AA	3755	1/1	0.74	0.23	-	77,77,77,77	0
60	MG	CA	3365	1/1	0.94	0.18	-	69,69,69,69	0
60	MG	AA	3266	1/1	0.84	0.28	-	55,55,55,55	0
60	MG	CB	3006	1/1	0.67	0.19	-	82,82,82,82	0
60	MG	BA	1747	1/1	0.97	0.14	-	53,53,53,53	0
60	MG	AA	3498	1/1	0.90	0.17	-	56,56,56,56	0
60	MG	AA	3229	1/1	0.96	0.13	-	33,33,33,33	0
60	MG	AA	3697	1/1	0.96	0.15	-	71,71,71,71	0
60	MG	AO	5001	1/1	0.99	0.10	-	43,43,43,43	0
60	MG	CA	3458	1/1	0.91	0.14	-	28,28,28,28	0
60	MG	CA	3517	1/1	0.86	0.21	-	75,75,75,75	0
60	MG	AP	202	1/1	0.93	0.26	-	70,70,70,70	0
60	MG	AA	3526	1/1	0.94	0.15	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	DA	1724	1/1	0.90	0.19	-	74,74,74,74	0
60	MG	CA	3262	1/1	0.97	0.28	-	59,59,59,59	0
60	MG	AA	3332	1/1	0.92	0.18	-	55,55,55,55	0
60	MG	CA	3391	1/1	0.93	0.10	-	67,67,67,67	0
60	MG	AA	3145	1/1	0.92	0.32	-	41,41,41,41	1
60	MG	AA	3627	1/1	0.93	0.14	-	53,53,53,53	0
60	MG	AA	3736	1/1	0.53	0.37	-	74,74,74,74	0
60	MG	CA	3031	1/1	0.48	0.72	-	102,102,102,102	0
60	MG	AA	3544	1/1	0.85	0.18	-	16,16,16,16	0
60	MG	CA	3594	1/1	0.96	0.16	-	62,62,62,62	0
60	MG	AA	3293	1/1	0.95	0.14	-	68,68,68,68	0
60	MG	AA	3287	1/1	0.88	0.20	-	25,25,25,25	0
60	MG	AA	3162	1/1	0.95	0.32	-	35,35,35,35	0
60	MG	AA	3262	1/1	0.92	0.58	-	70,70,70,70	0
60	MG	DA	1700	1/1	0.82	0.21	-	66,66,66,66	0
60	MG	CA	3444	1/1	0.96	0.24	-	70,70,70,70	0
60	MG	DJ	5001	1/1	0.88	0.17	-	94,94,94,94	0
60	MG	BA	1748	1/1	0.95	0.34	-	75,75,75,75	0
60	MG	CA	3513	1/1	0.94	0.24	-	109,109,109,109	0
60	MG	AA	3800	1/1	0.89	0.28	-	59,59,59,59	0
60	MG	DA	1748	1/1	0.85	0.18	-	78,78,78,78	0
60	MG	BY	3002	1/1	0.71	0.17	-	83,83,83,83	0
60	MG	AA	3105	1/1	0.83	0.18	-	77,77,77,77	0
60	MG	CA	3151	1/1	0.82	0.21	-	66,66,66,66	0
60	MG	CA	3201	1/1	0.86	0.32	-	70,70,70,70	0
60	MG	CA	3642	1/1	0.74	0.11	-	75,75,75,75	0
60	MG	BA	1772	1/1	0.94	0.33	-	51,51,51,51	0
60	MG	AA	3363	1/1	0.98	0.24	-	47,47,47,47	0
60	MG	CA	3396	1/1	0.91	0.14	-	59,59,59,59	0
60	MG	CA	3414	1/1	0.93	0.18	-	50,50,50,50	0
60	MG	AA	3150	1/1	0.65	0.32	-	63,63,63,63	0
60	MG	DA	1725	1/1	0.90	0.13	-	78,78,78,78	0
60	MG	CA	3421	1/1	0.95	0.19	-	39,39,39,39	0
60	MG	AA	3198	1/1	0.89	0.09	-	47,47,47,47	0
60	MG	DA	1608	1/1	0.70	0.50	-	79,79,79,79	0
60	MG	CA	3162	1/1	0.91	0.27	-	57,57,57,57	0
60	MG	AA	3260	1/1	0.92	0.43	-	67,67,67,67	0
60	MG	AB	3010	1/1	0.85	0.09	-	56,56,56,56	1
60	MG	CA	3514	1/1	0.46	0.16	-	68,68,68,68	0
60	MG	BA	1715	1/1	0.84	0.21	-	90,90,90,90	0
60	MG	AA	3040	1/1	0.47	0.13	-	93,93,93,93	0
60	MG	BA	1702	1/1	0.89	0.45	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3046	1/1	0.94	0.07	-	72,72,72,72	0
60	MG	CA	3387	1/1	0.82	0.39	-	73,73,73,73	0
60	MG	AA	3083	1/1	0.93	0.68	-	48,48,48,48	1
60	MG	DA	1652	1/1	0.98	0.09	-	68,68,68,68	0
60	MG	AA	3495	1/1	0.91	0.20	-	58,58,58,58	0
60	MG	CA	3507	1/1	0.92	0.14	-	99,99,99,99	0
60	MG	AA	3651	1/1	0.94	0.23	-	66,66,66,66	0
60	MG	CA	3072	1/1	0.92	0.43	-	54,54,54,54	0
60	MG	AA	3032	1/1	0.93	0.54	-	62,62,62,62	0
60	MG	BA	1784	1/1	0.85	0.18	-	59,59,59,59	0
60	MG	AA	3086	1/1	0.96	0.35	-	43,43,43,43	1
60	MG	AA	3722	1/1	0.95	0.17	-	31,31,31,31	0
60	MG	DA	1634	1/1	0.78	0.34	-	66,66,66,66	0
60	MG	AA	3379	1/1	0.89	0.14	-	40,40,40,40	1
60	MG	AA	3568	1/1	0.89	0.22	-	23,23,23,23	0
60	MG	AA	3124	1/1	0.98	0.24	-	39,39,39,39	1
60	MG	DA	1760	1/1	0.96	0.27	-	53,53,53,53	0
60	MG	AA	3439	1/1	0.88	0.18	-	43,43,43,43	0
60	MG	DA	1697	1/1	0.93	0.21	-	67,67,67,67	0
60	MG	CA	3255	1/1	0.94	0.35	-	61,61,61,61	0
60	MG	CA	3093	1/1	0.89	0.34	-	77,77,77,77	0
60	MG	AA	3436	1/1	0.96	0.13	-	31,31,31,31	0
60	MG	AA	3716	1/1	0.82	0.20	-	63,63,63,63	0
60	MG	AA	3351	1/1	0.81	0.10	-	80,80,80,80	0
60	MG	AA	3724	1/1	0.90	0.31	-	37,37,37,37	0
60	MG	DA	1633	1/1	0.93	0.58	-	67,67,67,67	0
60	MG	BX	109	1/1	0.96	0.22	-	55,55,55,55	0
60	MG	CA	3378	1/1	0.95	0.15	-	63,63,63,63	0
60	MG	AA	3611	1/1	0.96	0.26	-	57,57,57,57	0
60	MG	CA	3608	1/1	0.89	0.11	-	69,69,69,69	0
60	MG	CA	3008	1/1	0.97	0.39	-	52,52,52,52	0
60	MG	AA	3674	1/1	0.92	0.09	-	56,56,56,56	0
60	MG	DA	1676	1/1	0.68	0.29	-	69,69,69,69	0
60	MG	CA	3612	1/1	0.95	0.13	-	59,59,59,59	0
60	MG	BA	1733	1/1	0.85	0.09	-	57,57,57,57	0
60	MG	AA	3452	1/1	0.92	0.07	-	53,53,53,53	0
60	MG	CA	3522	1/1	0.97	0.24	-	25,25,25,25	0
60	MG	AA	3307	1/1	0.90	0.12	-	35,35,35,35	0
60	MG	CA	3604	1/1	0.93	0.19	-	54,54,54,54	0
60	MG	AA	3182	1/1	0.81	0.27	-	73,73,73,73	0
60	MG	AA	3165	1/1	0.80	0.41	-	64,64,64,64	0
60	MG	CA	3412	1/1	0.85	0.21	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3743	1/1	0.89	0.20	-	66,66,66,66	0
60	MG	BA	1725	1/1	0.96	0.31	-	52,52,52,52	0
60	MG	AA	3684	1/1	0.93	0.17	-	47,47,47,47	0
60	MG	DA	1683	1/1	0.96	0.42	-	60,60,60,60	0
60	MG	AA	3580	1/1	0.85	0.14	-	26,26,26,26	0
60	MG	AA	3520	1/1	0.99	0.15	-	34,34,34,34	0
60	MG	AA	3311	1/1	0.96	0.21	-	46,46,46,46	0
60	MG	AA	3221	1/1	0.74	0.16	-	72,72,72,72	0
60	MG	AA	3372	1/1	0.95	0.27	-	59,59,59,59	0
60	MG	CA	3170	1/1	0.89	0.36	-	68,68,68,68	0
60	MG	CA	3232	1/1	0.92	0.24	-	69,69,69,69	0
60	MG	AA	3655	1/1	0.85	0.20	-	55,55,55,55	0
60	MG	CA	3538	1/1	0.82	0.31	-	58,58,58,58	0
60	MG	CA	3055	1/1	0.85	0.29	-	77,77,77,77	0
60	MG	CA	3206	1/1	0.37	0.66	-	109,109,109,109	0
60	MG	CA	3448	1/1	0.96	0.09	-	64,64,64,64	0
60	MG	BA	1787	1/1	0.82	0.13	-	64,64,64,64	0
60	MG	CA	3141	1/1	0.94	0.32	-	51,51,51,51	0
60	MG	CA	3177	1/1	0.48	0.65	-	98,98,98,98	0
60	MG	AA	3370	1/1	0.92	0.16	-	43,43,43,43	0
60	MG	CA	3192	1/1	0.97	0.26	-	47,47,47,47	0
60	MG	AA	3159	1/1	0.80	0.41	-	66,66,66,66	0
60	MG	BA	1744	1/1	0.96	0.13	-	48,48,48,48	0
60	MG	AA	3292	1/1	0.95	0.18	-	31,31,31,31	0
60	MG	AA	3479	1/1	0.83	0.14	-	66,66,66,66	0
60	MG	DA	1607	1/1	0.92	0.83	-	63,63,63,63	0
60	MG	BA	1632	1/1	0.87	0.23	-	60,60,60,60	0
60	MG	AA	3163	1/1	0.84	0.27	-	73,73,73,73	0
60	MG	AA	3064	1/1	0.94	0.22	-	31,31,31,31	0
60	MG	DA	1718	1/1	0.83	0.11	-	66,66,66,66	0
60	MG	AA	3295	1/1	0.92	0.16	-	24,24,24,24	0
60	MG	CA	3445	1/1	0.81	0.36	-	70,70,70,70	0
60	MG	AA	3215	1/1	0.92	0.18	-	48,48,48,48	0
60	MG	BA	1622	1/1	0.80	0.63	-	64,64,64,64	0
60	MG	CA	3161	1/1	0.97	0.44	-	45,45,45,45	0
60	MG	DA	1626	1/1	0.90	0.41	-	63,63,63,63	0
60	MG	CA	3383	1/1	0.84	0.34	-	66,66,66,66	0
60	MG	CA	3476	1/1	0.98	0.22	-	60,60,60,60	0
60	MG	AA	3710	1/1	0.94	0.17	-	55,55,55,55	0
60	MG	AA	3028	1/1	0.85	0.30	-	40,40,40,40	1
60	MG	AA	3603	1/1	0.97	0.10	-	68,68,68,68	0
60	MG	DA	1661	1/1	0.82	0.14	-	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
60	MG	AA	3108	1/1	0.31	0.41	-	88,88,88,88	0
60	MG	AW	3001	1/1	0.93	0.19	-	46,46,46,46	0
60	MG	CA	3432	1/1	0.98	0.13	-	29,29,29,29	0
60	MG	AA	3006	1/1	0.93	0.28	-	56,56,56,56	0
60	MG	AA	3164	1/1	0.78	0.21	-	106,106,106,106	0
60	MG	CA	3241	1/1	0.74	0.19	-	69,69,69,69	0
60	MG	AA	3482	1/1	0.89	0.26	-	46,46,46,46	0
60	MG	CA	3561	1/1	0.96	0.12	-	62,62,62,62	0
60	MG	BA	1795	1/1	0.98	0.15	-	64,64,64,64	0
60	MG	CA	3593	1/1	0.93	0.11	-	62,62,62,62	0
60	MG	CA	3125	1/1	0.93	0.48	-	58,58,58,58	0
60	MG	AA	3537	1/1	0.70	0.12	-	90,90,90,90	0
60	MG	BX	104	1/1	0.91	0.20	-	67,67,67,67	0
60	MG	CA	3397	1/1	0.85	0.10	-	80,80,80,80	0
60	MG	AA	3786	1/1	0.97	0.19	-	57,57,57,57	0
60	MG	CA	3168	1/1	0.91	0.23	-	65,65,65,65	0
60	MG	DA	1749	1/1	0.83	0.23	-	72,72,72,72	0
60	MG	BA	1764	1/1	0.97	0.16	-	55,55,55,55	0
60	MG	AQ	3002	1/1	0.72	0.31	-	79,79,79,79	0
60	MG	CA	3532	1/1	0.82	0.16	-	59,59,59,59	0
60	MG	CA	3276	1/1	0.87	0.17	-	32,32,32,32	0
60	MG	AA	3158	1/1	0.87	0.37	-	50,50,50,50	0
60	MG	AA	3515	1/1	0.94	0.14	-	27,27,27,27	0
60	MG	BA	1766	1/1	0.83	0.16	-	81,81,81,81	0
60	MG	AA	3639	1/1	0.82	0.23	-	74,74,74,74	0
60	MG	AA	3557	1/1	0.97	0.17	-	21,21,21,21	0
60	MG	CA	3603	1/1	0.90	0.28	-	93,93,93,93	0
60	MG	BX	110	1/1	0.89	0.14	-	67,67,67,67	0
60	MG	CA	3078	1/1	0.94	0.14	-	49,49,49,49	0
60	MG	BA	1809	1/1	0.91	0.18	-	74,74,74,74	0
60	MG	AA	3629	1/1	0.96	0.11	-	51,51,51,51	0
60	MG	DA	1649	1/1	0.94	0.30	-	53,53,53,53	0
60	MG	AA	3195	1/1	0.86	0.20	-	55,55,55,55	0
60	MG	BA	1639	1/1	0.98	0.37	-	42,42,42,42	0
60	MG	AA	3193	1/1	0.97	0.20	-	63,63,63,63	0
60	MG	AA	3699	1/1	0.96	0.22	-	61,61,61,61	0
60	MG	BZ	701	1/1	0.97	0.20	-	58,58,58,58	0
60	MG	CA	3610	1/1	0.92	0.45	-	94,94,94,94	0
60	MG	AA	3344	1/1	0.95	0.18	-	65,65,65,65	0
60	MG	AA	3466	1/1	0.91	0.17	-	48,48,48,48	0
60	MG	BA	1774	1/1	0.88	0.09	-	79,79,79,79	0
60	MG	AA	3536	1/1	0.96	0.09	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3632	1/1	0.70	0.27	-	97,97,97,97	0
60	MG	AA	3013	1/1	0.97	0.14	-	38,38,38,38	0
60	MG	AA	3821	1/1	0.93	0.13	-	59,59,59,59	0
60	MG	CA	3527	1/1	0.34	0.38	-	83,83,83,83	0
60	MG	AA	3625	1/1	0.66	0.30	-	88,88,88,88	0
60	MG	AA	3314	1/1	0.95	0.20	-	43,43,43,43	0
60	MG	AA	3644	1/1	0.87	0.21	-	74,74,74,74	0
60	MG	BA	1668	1/1	0.91	0.18	-	72,72,72,72	0
60	MG	DA	1756	1/1	0.94	0.24	-	60,60,60,60	0
60	MG	BA	1695	1/1	0.96	0.06	-	64,64,64,64	0
60	MG	AA	3480	1/1	0.77	0.13	-	78,78,78,78	0
60	MG	AA	3811	1/1	0.91	0.59	-	65,65,65,65	0
60	MG	AA	3474	1/1	0.94	0.14	-	74,74,74,74	0
60	MG	CA	3345	1/1	0.96	0.19	-	41,41,41,41	0
60	MG	CA	3350	1/1	0.92	0.07	-	74,74,74,74	0
60	MG	CA	3016	1/1	0.66	0.48	-	69,69,69,69	0
60	MG	CA	3481	1/1	0.51	0.24	-	86,86,86,86	0
60	MG	CA	3150	1/1	0.92	0.12	-	52,52,52,52	0
60	MG	CA	3056	1/1	0.93	0.34	-	83,83,83,83	0
60	MG	CA	3385	1/1	0.99	0.26	-	48,48,48,48	0
60	MG	CA	3234	1/1	0.70	0.36	-	96,96,96,96	0
60	MG	AA	3489	1/1	0.83	0.32	-	39,39,39,39	0
60	MG	CA	3566	1/1	0.92	0.24	-	47,47,47,47	0
60	MG	CA	3442	1/1	0.88	0.13	-	70,70,70,70	0
60	MG	AW	3004	1/1	0.96	0.14	-	45,45,45,45	0
60	MG	DA	1762	1/1	0.69	0.16	-	86,86,86,86	0
60	MG	AA	3392	1/1	0.93	0.17	-	31,31,31,31	0
60	MG	CA	3505	1/1	0.76	0.25	-	66,66,66,66	0
60	MG	BX	108	1/1	0.96	0.10	-	78,78,78,78	0
60	MG	CA	3632	1/1	0.98	0.15	-	55,55,55,55	0
60	MG	CA	3204	1/1	0.89	0.25	-	88,88,88,88	0
60	MG	DA	1715	1/1	0.42	0.46	-	87,87,87,87	0
60	MG	AA	3411	1/1	0.97	0.15	-	21,21,21,21	0
60	MG	AA	3555	1/1	0.97	0.16	-	57,57,57,57	0
60	MG	AA	3327	1/1	0.55	0.23	-	36,36,36,36	0
60	MG	CA	3091	1/1	0.77	0.40	-	60,60,60,60	0
60	MG	AA	3567	1/1	0.92	0.14	-	69,69,69,69	0
60	MG	CA	3506	1/1	0.65	0.25	-	120,120,120,120	0
60	MG	CA	3433	1/1	0.95	0.15	-	45,45,45,45	0
60	MG	BA	1743	1/1	0.97	0.08	-	60,60,60,60	0
60	MG	AA	3077	1/1	0.94	0.26	-	44,44,44,44	0
60	MG	AA	3383	1/1	0.93	0.21	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3519	1/1	0.97	0.13	-	39,39,39,39	0
60	MG	AA	3560	1/1	0.97	0.20	-	49,49,49,49	0
60	MG	CB	3003	1/1	0.98	0.13	-	61,61,61,61	0
60	MG	DA	1605	1/1	0.91	0.29	-	59,59,59,59	0
60	MG	CA	3590	1/1	0.70	0.53	-	78,78,78,78	0
60	MG	CA	3257	1/1	0.90	0.14	-	45,45,45,45	0
60	MG	AA	3117	1/1	0.95	0.17	-	64,64,64,64	0
60	MG	CA	3030	1/1	0.82	0.43	-	52,52,52,52	0
60	MG	AA	3304	1/1	0.99	0.17	-	44,44,44,44	0
60	MG	AA	3204	1/1	0.81	0.45	-	83,83,83,83	0
60	MG	BA	1610	1/1	0.95	0.14	-	112,112,112,112	0
60	MG	AA	3271	1/1	0.58	0.28	-	81,81,81,81	0
60	MG	AA	3435	1/1	0.91	0.27	-	54,54,54,54	0
60	MG	AA	3324	1/1	0.67	0.10	-	69,69,69,69	0
60	MG	AA	3348	1/1	0.95	0.30	-	39,39,39,39	0
60	MG	AA	3256	1/1	0.94	0.18	-	24,24,24,24	0
60	MG	CA	3564	1/1	0.94	0.28	-	33,33,33,33	0
60	MG	CA	3292	1/1	0.93	0.15	-	56,56,56,56	0
60	MG	AA	3569	1/1	0.96	0.19	-	17,17,17,17	0
60	MG	CA	3600	1/1	0.98	0.12	-	60,60,60,60	0
60	MG	AA	3203	1/1	0.35	1.03	-	125,125,125,125	0
60	MG	CA	3477	1/1	0.89	0.24	-	65,65,65,65	0
60	MG	AA	3254	1/1	0.91	0.29	-	47,47,47,47	0
60	MG	AA	3319	1/1	0.98	0.17	-	28,28,28,28	0
60	MG	BA	1659	1/1	0.92	0.32	-	68,68,68,68	0
60	MG	DA	1660	1/1	0.95	0.29	-	81,81,81,81	0
60	MG	CA	3045	1/1	0.87	0.23	-	68,68,68,68	0
60	MG	AA	3594	1/1	0.96	0.26	-	48,48,48,48	0
60	MG	AA	3511	1/1	0.93	0.26	-	84,84,84,84	0
60	MG	AA	3413	1/1	0.83	0.15	-	34,34,34,34	0
60	MG	BA	1812	1/1	0.93	0.16	-	47,47,47,47	0
60	MG	CA	3247	1/1	0.75	0.16	-	45,45,45,45	0
60	MG	AA	3100	1/1	0.96	0.21	-	34,34,34,34	0
60	MG	AA	3085	1/1	0.96	0.25	-	80,80,80,80	0
60	MG	AA	3728	1/1	0.90	0.27	-	75,75,75,75	0
60	MG	AA	3301	1/1	0.98	0.17	-	59,59,59,59	0
60	MG	CA	3303	1/1	0.72	0.28	-	52,52,52,52	0
60	MG	DA	1754	1/1	0.92	0.23	-	77,77,77,77	0
60	MG	BA	1769	1/1	0.98	0.26	-	80,80,80,80	0
60	MG	DW	3001	1/1	0.75	0.80	-	90,90,90,90	0
60	MG	AA	3362	1/1	0.88	0.21	-	69,69,69,69	0
60	MG	CA	3199	1/1	0.67	0.57	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	AA	3805	1/1	0.38	1.55	-	117,117,117,117	0
60	MG	CA	3244	1/1	0.69	0.32	-	70,70,70,70	0
60	MG	CA	3516	1/1	0.95	0.20	-	58,58,58,58	0
60	MG	AA	3128	1/1	0.97	0.47	-	53,53,53,53	1
60	MG	DA	1687	1/1	0.93	0.25	-	60,60,60,60	0
60	MG	AA	3209	1/1	0.91	0.26	-	64,64,64,64	0
60	MG	AA	3263	1/1	0.68	0.44	-	75,75,75,75	0
60	MG	AA	3402	1/1	0.90	0.33	-	53,53,53,53	0
60	MG	AA	3615	1/1	0.84	0.39	-	65,65,65,65	0
60	MG	CA	3194	1/1	0.74	0.55	-	87,87,87,87	0
60	MG	CA	3606	1/1	0.89	0.27	-	58,58,58,58	0
60	MG	AA	3726	1/1	0.96	0.13	-	74,74,74,74	0
60	MG	DA	1666	1/1	0.89	0.19	-	45,45,45,45	0
60	MG	CA	3063	1/1	0.66	0.71	-	74,74,74,74	0
60	MG	CA	3020	1/1	0.96	0.18	-	38,38,38,38	0
60	MG	AA	3157	1/1	0.89	0.33	-	93,93,93,93	0
60	MG	AA	3657	1/1	0.80	0.11	-	73,73,73,73	0
60	MG	CA	3225	1/1	0.95	0.24	-	73,73,73,73	0
60	MG	BA	1802	1/1	0.94	0.13	-	58,58,58,58	0
60	MG	AA	3237	1/1	0.85	0.08	-	51,51,51,51	0
60	MG	AA	3573	1/1	0.94	0.09	-	47,47,47,47	0
60	MG	BA	1666	1/1	0.87	0.33	-	70,70,70,70	0
60	MG	CA	3457	1/1	0.88	0.21	-	60,60,60,60	0
60	MG	CA	3429	1/1	0.93	0.23	-	80,80,80,80	0
60	MG	AA	3647	1/1	0.96	0.14	-	35,35,35,35	0
60	MG	DA	1736	1/1	0.96	0.17	-	63,63,63,63	0
60	MG	DA	1690	1/1	0.95	0.20	-	74,74,74,74	0
60	MG	CA	3058	1/1	0.85	0.44	-	74,74,74,74	0
60	MG	AA	3095	1/1	0.89	0.16	-	58,58,58,58	0
60	MG	CA	3375	1/1	0.96	0.09	-	65,65,65,65	0
60	MG	AA	3063	1/1	0.89	0.17	-	46,46,46,46	0
60	MG	CA	3406	1/1	0.93	0.08	-	54,54,54,54	0
60	MG	AA	3421	1/1	0.91	0.12	-	73,73,73,73	0
60	MG	AA	3665	1/1	0.96	0.06	-	63,63,63,63	0
60	MG	CA	3364	1/1	0.94	0.18	-	64,64,64,64	0
60	MG	CA	3494	1/1	0.87	0.17	-	58,58,58,58	0
60	MG	CA	3048	1/1	0.92	0.30	-	48,48,48,48	0
60	MG	CA	3570	1/1	0.94	0.09	-	61,61,61,61	0
60	MG	BA	1761	1/1	0.92	0.18	-	74,74,74,74	0
60	MG	DA	1632	1/1	0.93	0.20	-	77,77,77,77	0
60	MG	CA	3066	1/1	0.92	0.42	-	69,69,69,69	0
60	MG	CA	3322	1/1	0.90	0.28	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
60	MG	CA	3575	1/1	0.62	0.47	-	77,77,77,77	0
60	MG	DA	1732	1/1	0.96	0.11	-	54,54,54,54	0
60	MG	AA	3054	1/1	0.93	0.28	-	26,26,26,26	0
60	MG	CA	3581	1/1	0.54	0.22	-	100,100,100,100	0
61	K	AA	3814	1/1	0.91	0.27	-	87,87,87,87	0
60	MG	BA	1614	1/1	0.92	0.18	-	70,70,70,70	0
60	MG	AA	3252	1/1	0.83	0.37	-	76,76,76,76	0
60	MG	DA	1730	1/1	0.93	0.39	-	65,65,65,65	0
60	MG	CA	3427	1/1	0.95	0.29	-	69,69,69,69	0
60	MG	CA	3239	1/1	0.65	0.32	-	76,76,76,76	0
60	MG	CD	303	1/1	0.90	0.14	-	70,70,70,70	0
60	MG	CA	3533	1/1	0.84	0.14	-	63,63,63,63	0
60	MG	AA	3546	1/1	0.95	0.17	-	36,36,36,36	0
60	MG	AA	3056	1/1	0.82	0.49	-	72,72,72,72	0
60	MG	AA	3094	1/1	0.96	0.31	-	82,82,82,82	0
60	MG	AA	3239	1/1	0.96	0.21	-	63,63,63,63	0
60	MG	BA	1738	1/1	0.91	0.23	-	55,55,55,55	0
60	MG	AA	3353	1/1	0.88	0.11	-	68,68,68,68	0
60	MG	AA	3416	1/1	0.95	0.19	-	31,31,31,31	0

## 6.5 Other polymers

There are no such residues in this entry.