



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:10 am GMT

PDB ID : 4WQU
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-22
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28972

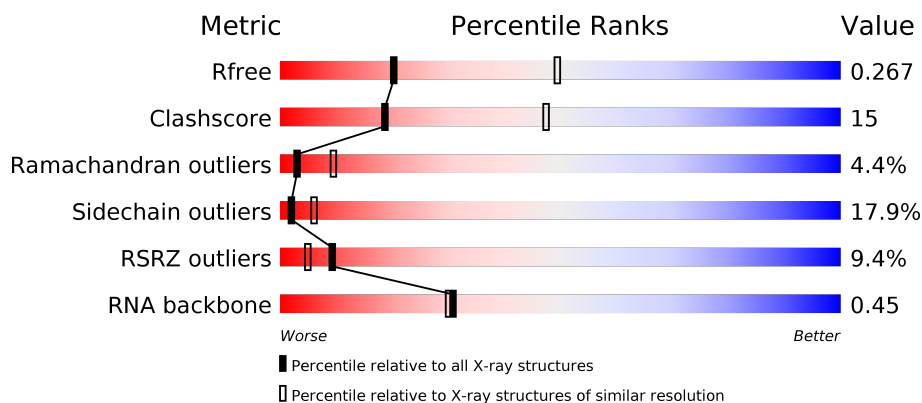
1 Overall quality at a glance

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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)
RNA backbone	2435	1007 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>3%</div> <div>24% 47% 23%</div> <div>• •</div> </div>
1	CA	2915	<div> <div>4%</div> <div>32% 44% 19%</div> <div>• •</div> </div>
2	AB	121	<div> <div>28% 55% 14%</div> <div>• •</div> </div>
2	CB	121	<div> <div>0%</div> <div>36% 47% 17%</div> <div>•</div> </div>




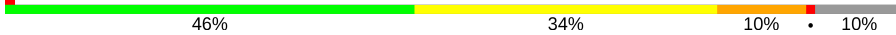





















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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150	
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	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
57	BZ	758	
57	DZ	758	
58	BX	10	
58	DX	10	

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
58	2QY	DX	10	-	-	X	-
59	MG	A0	101	-	-	-	X
59	MG	AA	3012	-	-	-	X
59	MG	AA	3018	-	-	-	X
59	MG	AA	3023	-	-	-	X
59	MG	AA	3033	-	-	-	X
59	MG	AA	3034	-	-	-	X
59	MG	AA	3036	-	-	-	X
59	MG	AA	3038	-	-	-	X
59	MG	AA	3039	-	-	-	X
59	MG	AA	3042	-	-	-	X
59	MG	AA	3043	-	-	-	X
59	MG	AA	3044	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3045	-	-	-	X
59	MG	AA	3047	-	-	-	X
59	MG	AA	3050	-	-	-	X
59	MG	AA	3053	-	-	-	X
59	MG	AA	3060	-	-	-	X
59	MG	AA	3081	-	-	-	X
59	MG	AA	3082	-	-	-	X
59	MG	AA	3101	-	-	-	X
59	MG	AA	3102	-	-	-	X
59	MG	AA	3109	-	-	-	X
59	MG	AA	3110	-	-	-	X
59	MG	AA	3113	-	-	-	X
59	MG	AA	3117	-	-	-	X
59	MG	AA	3120	-	-	-	X
59	MG	AA	3128	-	-	-	X
59	MG	AA	3130	-	-	-	X
59	MG	AA	3131	-	-	-	X
59	MG	AA	3133	-	-	-	X
59	MG	AA	3134	-	-	-	X
59	MG	AA	3136	-	-	-	X
59	MG	AA	3137	-	-	-	X
59	MG	AA	3140	-	-	-	X
59	MG	AA	3144	-	-	-	X
59	MG	AA	3147	-	-	-	X
59	MG	AA	3152	-	-	-	X
59	MG	AA	3158	-	-	-	X
59	MG	AA	3161	-	-	-	X
59	MG	AA	3171	-	-	-	X
59	MG	AA	3172	-	-	-	X
59	MG	AA	3174	-	-	-	X
59	MG	AA	3176	-	-	-	X
59	MG	AA	3177	-	-	-	X
59	MG	AA	3179	-	-	-	X
59	MG	AA	3182	-	-	-	X
59	MG	AA	3184	-	-	-	X
59	MG	AA	3186	-	-	-	X
59	MG	AA	3188	-	-	-	X
59	MG	AA	3193	-	-	-	X
59	MG	AA	3199	-	-	-	X
59	MG	AA	3209	-	-	-	X
59	MG	AA	3213	-	-	-	X
59	MG	AA	3214	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3215	-	-	-	X
59	MG	AA	3216	-	-	-	X
59	MG	AA	3217	-	-	-	X
59	MG	AA	3224	-	-	-	X
59	MG	AA	3226	-	-	-	X
59	MG	AA	3228	-	-	-	X
59	MG	AA	3235	-	-	-	X
59	MG	AA	3241	-	-	-	X
59	MG	AA	3244	-	-	-	X
59	MG	AA	3250	-	-	-	X
59	MG	AA	3253	-	-	-	X
59	MG	AA	3254	-	-	-	X
59	MG	AA	3255	-	-	-	X
59	MG	AA	3257	-	-	-	X
59	MG	AA	3261	-	-	-	X
59	MG	AA	3280	-	-	-	X
59	MG	AA	3286	-	-	-	X
59	MG	AA	3294	-	-	-	X
59	MG	AA	3301	-	-	-	X
59	MG	AA	3307	-	-	-	X
59	MG	AA	3315	-	-	-	X
59	MG	AA	3317	-	-	-	X
59	MG	AA	3335	-	-	-	X
59	MG	AA	3344	-	-	-	X
59	MG	AA	3360	-	-	-	X
59	MG	AA	3384	-	-	-	X
59	MG	AA	3391	-	-	-	X
59	MG	AA	3392	-	-	-	X
59	MG	AA	3393	-	-	-	X
59	MG	AA	3398	-	-	-	X
59	MG	AA	3403	-	-	-	X
59	MG	AA	3404	-	-	-	X
59	MG	AA	3413	-	-	-	X
59	MG	AA	3421	-	-	-	X
59	MG	AA	3423	-	-	-	X
59	MG	AA	3429	-	-	-	X
59	MG	AA	3443	-	-	-	X
59	MG	AA	3466	-	-	-	X
59	MG	AA	3509	-	-	-	X
59	MG	AA	3510	-	-	-	X
59	MG	AA	3511	-	-	-	X
59	MG	AA	3515	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3519	-	-	-	X
59	MG	AA	3529	-	-	-	X
59	MG	AA	3532	-	-	-	X
59	MG	AA	3534	-	-	-	X
59	MG	AA	3543	-	-	-	X
59	MG	AA	3547	-	-	-	X
59	MG	AA	3561	-	-	-	X
59	MG	AA	3563	-	-	-	X
59	MG	AA	3565	-	-	-	X
59	MG	AA	3569	-	-	-	X
59	MG	AA	3576	-	-	-	X
59	MG	AA	3593	-	-	-	X
59	MG	AA	3606	-	-	-	X
59	MG	AA	3608	-	-	-	X
59	MG	AA	3625	-	-	-	X
59	MG	AA	3653	-	-	-	X
59	MG	AA	3659	-	-	-	X
59	MG	AA	3667	-	-	-	X
59	MG	AA	3682	-	-	-	X
59	MG	AA	3688	-	-	-	X
59	MG	AA	3690	-	-	-	X
59	MG	AA	3691	-	-	-	X
59	MG	AA	3702	-	-	-	X
59	MG	AA	3706	-	-	-	X
59	MG	AA	3708	-	-	-	X
59	MG	AA	3710	-	-	-	X
59	MG	AA	3712	-	-	-	X
59	MG	AA	3718	-	-	-	X
59	MG	AA	3721	-	-	-	X
59	MG	AA	3730	-	-	-	X
59	MG	AA	3740	-	-	-	X
59	MG	AA	3766	-	-	-	X
59	MG	AA	3771	-	-	-	X
59	MG	AA	3772	-	-	-	X
59	MG	AA	3775	-	-	-	X
59	MG	AA	3793	-	-	-	X
59	MG	AA	3794	-	-	-	X
59	MG	AA	3795	-	-	-	X
59	MG	AA	3799	-	-	-	X
59	MG	AA	3803	-	-	-	X
59	MG	AA	3806	-	-	-	X
59	MG	AA	3809	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3813	-	-	-	X
59	MG	AA	3814	-	-	-	X
59	MG	AA	3818	-	-	-	X
59	MG	AA	3820	-	-	-	X
59	MG	AA	3822	-	-	-	X
59	MG	AA	3823	-	-	-	X
59	MG	AA	3824	-	-	-	X
59	MG	AA	3825	-	-	-	X
59	MG	AA	3826	-	-	-	X
59	MG	AA	3827	-	-	-	X
59	MG	AA	3828	-	-	-	X
59	MG	AA	3829	-	-	-	X
59	MG	AA	3830	-	-	-	X
59	MG	AA	3832	-	-	-	X
59	MG	AB	3003	-	-	-	X
59	MG	AB	3020	-	-	-	X
59	MG	AD	301	-	-	-	X
59	MG	AD	304	-	-	-	X
59	MG	AD	305	-	-	-	X
59	MG	AD	307	-	-	-	X
59	MG	AD	308	-	-	-	X
59	MG	AD	309	-	-	-	X
59	MG	AD	310	-	-	-	X
59	MG	AE	305	-	-	-	X
59	MG	AF	301	-	-	-	X
59	MG	AF	304	-	-	-	X
59	MG	AH	201	-	-	-	X
59	MG	AP	201	-	-	-	X
59	MG	AQ	202	-	-	-	X
59	MG	AU	202	-	-	-	X
59	MG	AU	204	-	-	-	X
59	MG	AU	205	-	-	-	X
59	MG	AV	201	-	-	-	X
59	MG	AW	3003	-	-	-	X
59	MG	AX	3001	-	-	-	X
59	MG	BA	1607	-	-	-	X
59	MG	BA	1612	-	-	-	X
59	MG	BA	1615	-	-	-	X
59	MG	BA	1616	-	-	-	X
59	MG	BA	1627	-	-	-	X
59	MG	BA	1628	-	-	-	X
59	MG	BA	1630	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	1631	-	-	-	X
59	MG	BA	1641	-	-	-	X
59	MG	BA	1656	-	-	-	X
59	MG	BA	1663	-	-	-	X
59	MG	BA	1665	-	-	-	X
59	MG	BA	1672	-	-	-	X
59	MG	BA	1676	-	-	-	X
59	MG	BA	1679	-	-	-	X
59	MG	BA	1684	-	-	-	X
59	MG	BA	1687	-	-	-	X
59	MG	BA	1691	-	-	-	X
59	MG	BA	1714	-	-	-	X
59	MG	BA	1723	-	-	-	X
59	MG	BA	1725	-	-	-	X
59	MG	BA	1735	-	-	-	X
59	MG	BA	1740	-	-	-	X
59	MG	BA	1757	-	-	-	X
59	MG	BA	1758	-	-	-	X
59	MG	BA	1780	-	-	-	X
59	MG	BA	1787	-	-	-	X
59	MG	BA	1788	-	-	-	X
59	MG	C3	3001	-	-	-	X
59	MG	C5	101	-	-	-	X
59	MG	C7	101	-	-	-	X
59	MG	CA	3002	-	-	-	X
59	MG	CA	3010	-	-	-	X
59	MG	CA	3025	-	-	-	X
59	MG	CA	3026	-	-	-	X
59	MG	CA	3028	-	-	-	X
59	MG	CA	3033	-	-	-	X
59	MG	CA	3035	-	-	-	X
59	MG	CA	3036	-	-	-	X
59	MG	CA	3039	-	-	-	X
59	MG	CA	3041	-	-	-	X
59	MG	CA	3045	-	-	-	X
59	MG	CA	3054	-	-	-	X
59	MG	CA	3058	-	-	-	X
59	MG	CA	3068	-	-	-	X
59	MG	CA	3087	-	-	-	X
59	MG	CA	3090	-	-	-	X
59	MG	CA	3100	-	-	-	X
59	MG	CA	3103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3105	-	-	-	X
59	MG	CA	3108	-	-	-	X
59	MG	CA	3113	-	-	-	X
59	MG	CA	3137	-	-	-	X
59	MG	CA	3140	-	-	-	X
59	MG	CA	3146	-	-	-	X
59	MG	CA	3157	-	-	-	X
59	MG	CA	3159	-	-	-	X
59	MG	CA	3160	-	-	-	X
59	MG	CA	3162	-	-	-	X
59	MG	CA	3163	-	-	-	X
59	MG	CA	3166	-	-	-	X
59	MG	CA	3168	-	-	-	X
59	MG	CA	3169	-	-	-	X
59	MG	CA	3182	-	-	-	X
59	MG	CA	3201	-	-	-	X
59	MG	CA	3207	-	-	-	X
59	MG	CA	3210	-	-	-	X
59	MG	CA	3212	-	-	-	X
59	MG	CA	3213	-	-	-	X
59	MG	CA	3217	-	-	-	X
59	MG	CA	3218	-	-	-	X
59	MG	CA	3221	-	-	-	X
59	MG	CA	3225	-	-	-	X
59	MG	CA	3226	-	-	-	X
59	MG	CA	3227	-	-	-	X
59	MG	CA	3229	-	-	-	X
59	MG	CA	3230	-	-	-	X
59	MG	CA	3243	-	-	-	X
59	MG	CA	3252	-	-	-	X
59	MG	CA	3277	-	-	-	X
59	MG	CA	3285	-	-	-	X
59	MG	CA	3291	-	-	-	X
59	MG	CA	3309	-	-	-	X
59	MG	CA	3314	-	-	-	X
59	MG	CA	3318	-	-	-	X
59	MG	CA	3322	-	-	-	X
59	MG	CA	3326	-	-	-	X
59	MG	CA	3330	-	-	-	X
59	MG	CA	3332	-	-	-	X
59	MG	CA	3333	-	-	-	X
59	MG	CA	3346	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3348	-	-	-	X
59	MG	CA	3353	-	-	-	X
59	MG	CA	3358	-	-	-	X
59	MG	CA	3361	-	-	-	X
59	MG	CA	3372	-	-	-	X
59	MG	CA	3375	-	-	-	X
59	MG	CA	3383	-	-	-	X
59	MG	CA	3409	-	-	-	X
59	MG	CA	3410	-	-	-	X
59	MG	CA	3413	-	-	-	X
59	MG	CA	3415	-	-	-	X
59	MG	CA	3420	-	-	-	X
59	MG	CA	3427	-	-	-	X
59	MG	CA	3428	-	-	-	X
59	MG	CA	3432	-	-	-	X
59	MG	CA	3440	-	-	-	X
59	MG	CA	3441	-	-	-	X
59	MG	CA	3442	-	-	-	X
59	MG	CA	3452	-	-	-	X
59	MG	CA	3455	-	-	-	X
59	MG	CA	3457	-	-	-	X
59	MG	CA	3458	-	-	-	X
59	MG	CA	3463	-	-	-	X
59	MG	CA	3486	-	-	-	X
59	MG	CA	3492	-	-	-	X
59	MG	CA	3499	-	-	-	X
59	MG	CA	3500	-	-	-	X
59	MG	CA	3502	-	-	-	X
59	MG	CA	3503	-	-	-	X
59	MG	CA	3526	-	-	-	X
59	MG	CA	3532	-	-	-	X
59	MG	CA	3544	-	-	-	X
59	MG	CA	3552	-	-	-	X
59	MG	CA	3557	-	-	-	X
59	MG	CA	3589	-	-	-	X
59	MG	CA	3603	-	-	-	X
59	MG	CA	3618	-	-	-	X
59	MG	CA	3619	-	-	-	X
59	MG	CA	3635	-	-	-	X
59	MG	CA	3636	-	-	-	X
59	MG	CA	3642	-	-	-	X
59	MG	CA	3650	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3653	-	-	-	X
59	MG	CA	3655	-	-	-	X
59	MG	CA	3657	-	-	-	X
59	MG	CA	3658	-	-	-	X
59	MG	CA	3660	-	-	-	X
59	MG	CA	3661	-	-	-	X
59	MG	CB	3007	-	-	-	X
59	MG	CE	301	-	-	-	X
59	MG	CE	303	-	-	-	X
59	MG	CF	301	-	-	-	X
59	MG	CQ	202	-	-	-	X
59	MG	CU	201	-	-	-	X
59	MG	CV	201	-	-	-	X
59	MG	CW	201	-	-	-	X
59	MG	DA	1601	-	-	-	X
59	MG	DA	1609	-	-	-	X
59	MG	DA	1622	-	-	-	X
59	MG	DA	1634	-	-	-	X
59	MG	DA	1640	-	-	-	X
59	MG	DA	1642	-	-	-	X
59	MG	DA	1650	-	-	-	X
59	MG	DA	1652	-	-	-	X
59	MG	DA	1655	-	-	-	X
59	MG	DA	1665	-	-	-	X
59	MG	DA	1671	-	-	-	X
59	MG	DA	1683	-	-	-	X
59	MG	DA	1745	-	-	-	X
59	MG	DA	1769	-	-	-	X
59	MG	DT	3001	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310038 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	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			
23	CZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
24	C0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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	1495	Total	C	N	O	P	0	0	0
			32141	14304	5958	10384	1495			
34	DA	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

- 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	117	Total	C	N	O	S	0	0	0
			923	570	191	160	2			
46	DM	116	Total	C	N	O	S	0	0	0
			907	558	188	159	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	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	BY	74	Total	C	N	O	P	S	0	0
			1581	707	285	515	73	1		
56	DW	76	Total	C	N	O	P	S	0	0
			1631	731	290	532	76	2		
56	DY	73	Total	C	N	O	P	S	0	0
			1561	698	283	507	72	1		

- Molecule 57 is a protein called 50S ribosomal protein L9,Elongation factor G.

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

- Molecule 58 is a protein called Dityromycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	BX	10	Total	C	N	O	0	0	0
			93	67	10	16			
58	DX	10	Total	C	N	O	0	0	0
			93	67	10	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AP	3	Total	Mg	0	0
			3	3		
59	CR	1	Total	Mg	0	0
			1	1		
59	BA	215	Total	Mg	0	0
			215	215		
59	CA	664	Total	Mg	0	0
			664	664		
59	C5	1	Total	Mg	0	0
			1	1		
59	AB	23	Total	Mg	0	0
			23	23		
59	BL	2	Total	Mg	0	0
			2	2		
59	CV	2	Total	Mg	0	0
			2	2		
59	A6	2	Total	Mg	0	0
			2	2		
59	BE	1	Total	Mg	0	0
			1	1		
59	AW	3	Total	Mg	0	0
			3	3		
59	C1	1	Total	Mg	0	0
			1	1		
59	AN	3	Total	Mg	0	0
			3	3		
59	DZ	2	Total	Mg	0	0
			2	2		
59	AX	1	Total	Mg	0	0
			1	1		
59	CN	1	Total	Mg	0	0
			1	1		
59	A2	1	Total	Mg	0	0
			1	1		
59	C8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DD	1	Total 1	Mg 1	0	0
59	BB	1	Total 1	Mg 1	0	0
59	BT	1	Total 1	Mg 1	0	0
59	AE	5	Total 5	Mg 5	0	0
59	BM	1	Total 1	Mg 1	0	0
59	CU	1	Total 1	Mg 1	0	0
59	BF	1	Total 1	Mg 1	0	0
59	AV	2	Total 2	Mg 2	0	0
59	DA	171	Total 171	Mg 171	0	0
59	CB	13	Total 13	Mg 13	0	0
59	C0	1	Total 1	Mg 1	0	0
59	AA	832	Total 832	Mg 832	0	0
59	CQ	4	Total 4	Mg 4	0	0
59	A5	1	Total 1	Mg 1	0	0
59	AR	1	Total 1	Mg 1	0	0
59	CG	1	Total 1	Mg 1	0	0
59	DK	1	Total 1	Mg 1	0	0
59	DF	1	Total 1	Mg 1	0	0
59	AD	10	Total 10	Mg 10	0	0
59	BN	2	Total 2	Mg 2	0	0
59	DJ	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	C7	1	Total 1	Mg 1	0	0
59	C3	1	Total 1	Mg 1	0	0
59	AZ	1	Total 1	Mg 1	0	0
59	BK	1	Total 1	Mg 1	0	0
59	AU	5	Total 5	Mg 5	0	0
59	DW	3	Total 3	Mg 3	0	0
59	A9	1	Total 1	Mg 1	0	0
59	CF	4	Total 4	Mg 4	0	0
59	CX	1	Total 1	Mg 1	0	0
59	A0	5	Total 5	Mg 5	0	0
59	AG	2	Total 2	Mg 2	0	0
59	DE	2	Total 2	Mg 2	0	0
59	AQ	4	Total 4	Mg 4	0	0
59	CE	5	Total 5	Mg 5	0	0
59	AH	1	Total 1	Mg 1	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	CO	1	Total 1	Mg 1	0	0
59	CP	1	Total 1	Mg 1	0	0
59	BS	1	Total 1	Mg 1	0	0
59	CW	1	Total 1	Mg 1	0	0
59	A7	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CD	4	Total 4	Mg 4	0	0
59	BD	1	Total 1	Mg 1	0	0
59	DT	1	Total 1	Mg 1	0	0
59	A8	1	Total 1	Mg 1	0	0
59	AO	1	Total 1	Mg 1	0	0
59	BW	3	Total 3	Mg 3	0	0
59	AY	1	Total 1	Mg 1	0	0
59	AF	6	Total 6	Mg 6	0	0

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

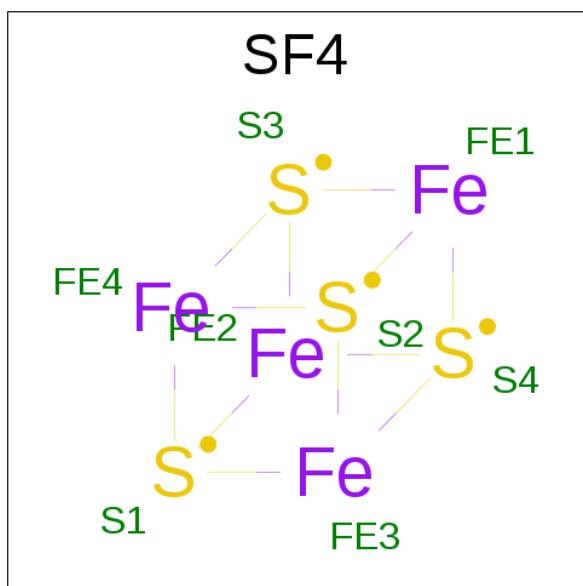
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total 1	Zn 1	0	0
60	BN	1	Total 1	Zn 1	0	0
60	C4	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0
60	C6	1	Total 1	Zn 1	0	0
60	A6	1	Total 1	Zn 1	0	0
60	C9	1	Total 1	Zn 1	0	0
60	DN	1	Total 1	Zn 1	0	0
60	A4	1	Total 1	Zn 1	0	0
60	A5	1	Total 1	Zn 1	0	0
60	A9	1	Total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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CY	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AA	1413	Total 1413	O 1413	0	0
63	AB	38	Total 38	O 38	0	0
63	AD	10	Total 10	O 10	0	0
63	AE	17	Total 17	O 17	0	0
63	AF	11	Total 11	O 11	0	0
63	AG	3	Total 3	O 3	0	0
63	AH	1	Total 1	O 1	0	0
63	AN	1	Total 1	O 1	0	0
63	AO	3	Total 3	O 3	0	0
63	AP	16	Total 16	O 16	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AQ	4	Total 4	O 4	0	0
63	AR	2	Total 2	O 2	0	0
63	AS	1	Total 1	O 1	0	0
63	AT	1	Total 1	O 1	0	0
63	AU	4	Total 4	O 4	0	0
63	AV	1	Total 1	O 1	0	0
63	AW	1	Total 1	O 1	0	0
63	AX	3	Total 3	O 3	0	0
63	AZ	1	Total 1	O 1	0	0
63	A0	6	Total 6	O 6	0	0
63	A1	2	Total 2	O 2	0	0
63	A3	2	Total 2	O 2	0	0
63	A5	3	Total 3	O 3	0	0
63	A6	1	Total 1	O 1	0	0
63	A7	2	Total 2	O 2	0	0
63	A8	10	Total 10	O 10	0	0
63	A9	1	Total 1	O 1	0	0
63	BA	213	Total 213	O 213	0	0
63	BD	1	Total 1	O 1	0	0
63	BM	1	Total 1	O 1	0	0
63	BO	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BP	1	Total 1	O 1	0	0
63	BV	1	Total 1	O 1	0	0
63	BW	1	Total 1	O 1	0	0
63	BZ	2	Total 2	O 2	0	0
63	CA	983	Total 983	O 983	0	0
63	CB	9	Total 9	O 9	0	0
63	CD	15	Total 15	O 15	0	0
63	CE	9	Total 9	O 9	0	0
63	CF	6	Total 6	O 6	0	0
63	CN	1	Total 1	O 1	0	0
63	CO	1	Total 1	O 1	0	0
63	CP	11	Total 11	O 11	0	0
63	CQ	2	Total 2	O 2	0	0
63	CT	3	Total 3	O 3	0	0
63	CU	2	Total 2	O 2	0	0
63	CV	1	Total 1	O 1	0	0
63	CW	1	Total 1	O 1	0	0
63	CX	1	Total 1	O 1	0	0
63	CY	2	Total 2	O 2	0	0
63	C0	4	Total 4	O 4	0	0
63	C3	2	Total 2	O 2	0	0

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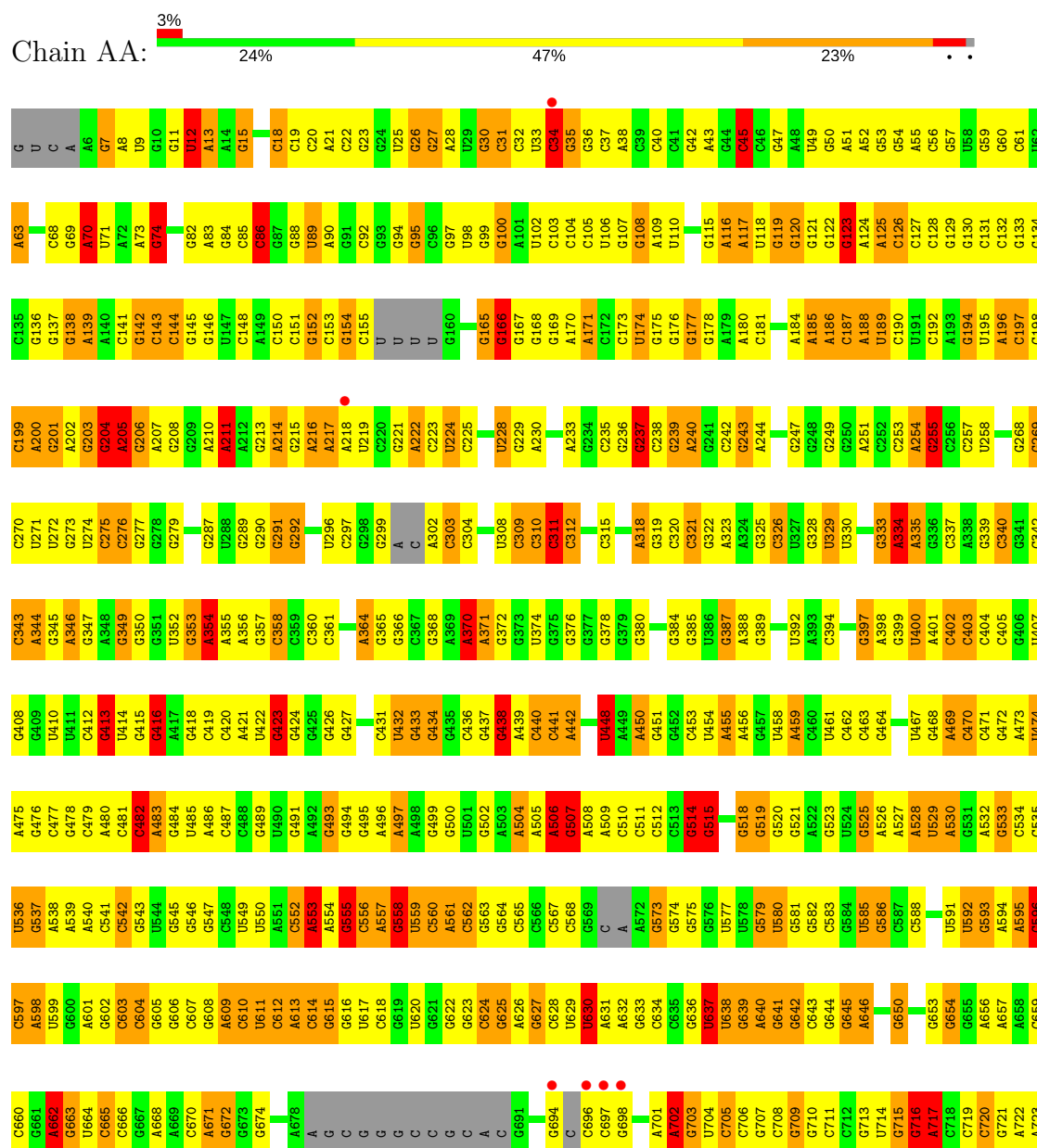
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C5	1	Total 1	O 1	0	0
63	C7	2	Total 2	O 2	0	0
63	C8	4	Total 4	O 4	0	0
63	DA	157	Total 157	O 157	0	0
63	DD	1	Total 1	O 1	0	0
63	DE	2	Total 2	O 2	0	0
63	DH	1	Total 1	O 1	0	0
63	DJ	1	Total 1	O 1	0	0
63	DK	2	Total 2	O 2	0	0
63	DL	1	Total 1	O 1	0	0
63	DT	1	Total 1	O 1	0	0

3 Residue-property plots

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

• Molecule 1: 23S Ribosomal RNA

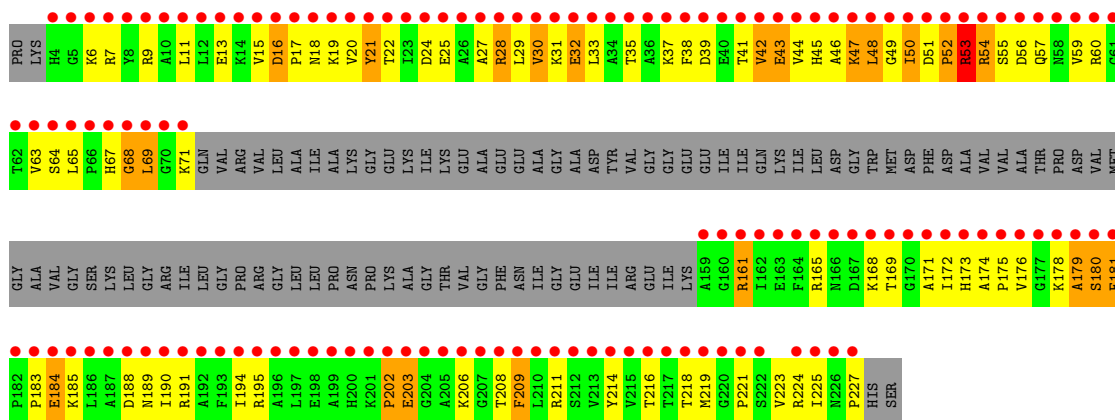


U1626	A1557	G1487	C1421	U1353	G1286	A1234	A1174	G1109	G1048	U988	U915	C853	A793	A724
A1626	G1558	G1487	C1422	C1360	C1287	G1235	A1175	C1110	G1049	G989	G916	U854	A793	C725
G1628	C1559	G1490	G1423	C1361	A1298	G1236	U1176	U1111	C1050	G990	A990	G855	U794	C726
C1629	C1560	A1491	A1424	A1299	G1237	G1237	U1177	U1112	C1051	G991	A919	G856	G795	G727
A1630	C1561	A1425	A1425	C1364	G1238	U1178	U1179	G1113	C1052	U857	G920	U858	G788	G728
C1631	G1562	G1426	G1426	C1365	A1239	G1239	U1180	G1114	C1053	G992	G921	C859	A798	G730
A1632	G1563	A1496	A1430	C1366	G1302	G1240	C1180	A1115	C1054	C994	G922	C860	A799	C730
A1633	C1564	G1497	A1431	C1367	C1303	C1241	G1181	A1116	A1055	U861	G927	C800	A799	G731
G1634	C1565	G1498	G1431	A1368	G1304	G1242	G1182	A1117	A1056	C960	G927	C801	C800	G732
C1635	C1566	C1432	C1432	G1369	G1305	U1243	G1183	C1118	G1057	C962	C932	C802	C803	C734
G1636	G1567	U1501	G1306	G1370	U1244	U1244	G1184	A1119	U1098	C963	C933	C804	U804	U735
U1637	U1502	G1435	C1307	G1371	C1245	C1245	C1185	U1166	U1060	C964	C934	C805	U805	A736
C1638	U1503	U1436	A1308	U1372	C1246	C1247	U1187	A1123	G1061	C967	C935	C806	G806	G737
G1639	A1504	U1437	U1309	C1373	G1248	G1248	A1188	A1124	G1062	U869	C936	C807	G807	C738
G1640	C1505	A1438	G1374	C1373	A1310	G1249	A1189	U1124	G1063	U870	C937	C808	A808	U741
A1643	U1506	A1439	A1311	G1375	G1312	U1250	C1125	U1125	U1003	U871	C938	C809	U809	G742
C1644	A1507	U1440	U1312	C1376	U1313	G1251	C1190	U1127	G1064	A871	C939	C810	G810	G743
C1645	A1508	U1441	U1314	G1377	A1314	C1252	C1191	U1128	U1065	C872	C940	C811	A811	C744
C1646	G1513	U1443	A1315	C1378	C1193	G1253	C1192	U1129	A1067	U873	C942	C812	C812	C745
A1647	C1444	C1444	C1316	C1379	A1194	G1259	G1197	G1135	U1072	U874	C943	C813	C813	C746
C1650	C1445	C1445	A1317	G1382	A1255	A1255	C1196	A1130	U1068	U875	C944	C814	U814	A746
C1651	C1449	C1449	A1321	G1383	U1256	G1257	C1197	A1131	U1069	U876	C945	C815	G815	G747
G1652	C1450	C1450	A1322	G1384	G1258	G1258	G1198	G1132	U1070	U877	C946	C816	G816	G748
C1653	C1451	C1451	A1323	U1385	A1259	G1260	C1199	G1133	G1071	U878	C947	C817	G817	G749
A1654	C1452	C1452	G1324	U1386	G1261	G1261	C1200	G1134	A1073	C879	C948	C818	G818	U750
C1655	C1453	C1453	A1324	C1387	G1262	G1262	A1201	C1138	U1074	U880	C949	C819	U820	G751
A1656	C1454	C1454	G1325	G1388	C1263	G1263	A1202	U1151	C1084	C881	C950	C820	A821	A752
C1657	C1455	C1455	G1326	G1389	C1264	G1264	G1203	A1141	G1076	A882	C951	C821	G821	A753
G1658	G1456	G1456	G1327	C1391	A1265	A1265	G1204	U1142	U1078	C883	C952	C822	G823	G760
C1659	C1457	C1457	U1328	G1392	U1266	U1266	U1205	U1143	U1079	C884	C953	C823	A824	U761
U1660	A1458	G1459	U1329	C1393	C1266	G1266	G1206	U1144	G1080	C885	C954	C824	G825	U762
C1663	U1459	G1460	A1330	G1394	C1267	G1267	U1207	G1145	U1081	U886	C955	C825	U826	A763
A1664	C1461	U1461	G1331	A1395	G1268	G1268	G1208	G1146	C1021	C987	C960	C826	U827	G764
G1665	C1462	U1462	U1334	C1396	G1269	G1269	G1209	A1149	G1023	A828	C963	C827	A828	A765
C1666	C1463	C1463	C1337	U1397	G1270	G1270	G1210	G1150	G1083	C891	C964	C828	A829	C766
U1667	G1464	G1464	A1338	U1398	G1271	G1271	U1211	U1151	G1085	C892	C965	C829	A830	A769
G1668	A1465	A1465	U1339	A1399	A1272	A1272	C1212	G1152	C1086	C893	C966	C830	A831	G770
C1669	U1466	U1466	G1401	C1400	G1273	G1273	U1213	U1153	G1087	U894	C967	C831	G832	U771
G1670	G1467	G1467	C1340	G1402	G1274	G1274	G1214	U1154	C1088	C895	C968	C832	U833	G772
C1671	C1470	C1470	U1341	U1403	G1275	G1275	G1215	C1155	G1090	A896	C969	C833	U834	G773
G1672	G1471	G1471	G1342	U1404	G1276	G1276	G1216	U1156	A1091	C897	C970	C834	A835	A774
G1673	G1472	G1472	C1343	A1405	C1277	C1277	G1217	A1157	A1092	U898	C971	C835	A836	G775
U1674	A1473	A1473	C1344	A1406	G1278	G1278	G1218	G1158	G1093	C899	C972	C836	C837	G776
G1675	G1474	G1474	G1345	C1407	G1282	G1282	A1219	U1159	A1094	C900	C973	C837	G838	C777
C1676	C1475	C1475	U1346	C1408	A1283	A1283	U1220	G1160	C1095	C901	G974	C838	G839	C778
G1677	G1476	G1476	A1347	C1409	G1284	G1284	G1221	G1161	A1096	C902	U975	C839	A840	G779
A1678	C1477	C1477	A1348	G1410	G1285	G1285	A1222	C1162	G1097	C903	G976	C840	G841	C780
G1679	U1477	U1477	C1349	A1411	U1286	U1286	C1223	G1163	C1098	C904	C977	C841	G842	G781
A1680	C1478	C1478	G1350	C1412	A1287	A1287	C1224	C1164	C1099	U905	A978	C842	C843	A781
C1681	U1479	U1479	C1351	A1413	U1288	U1288	C1225	G1165	A1100	C906	C979	C843	C844	A782
G1682	A1480	A1480	C1352	G1414	G1289	G1289	A1227	C1166	G1101	C907	C980	C844	G845	C783
A1683	C1481	C1481	A1353	G1415	G1290	G1290	G1228	G1167	G1102	C908	C981	C845	G846	C784
C1684	U1482	U1482	C1354	C1416	G1291	G1291	A1291	G1168	A1042	C909	U982	C846	A847	G785
U1685	C1483	C1483	G1355	G1417	A1292	A1292	G1229	C1169	G1104	C910	C982	C847	G848	G786
U1686	U1484	U1484	C1356	G1418	G1293	G1293	C1230	G1170	G1105	C911	C983	C848	A849	U787
C1687	A1485	A1485	G1357	U1419	A1294	A1294	G1231	U1171	U1066	C912	C984	C849	U850	G788
G1688	C1486	C1486	C1358	U1420	U1295	U1295	G1232	A1172	A1046	C913	C985	C850	A851	G789
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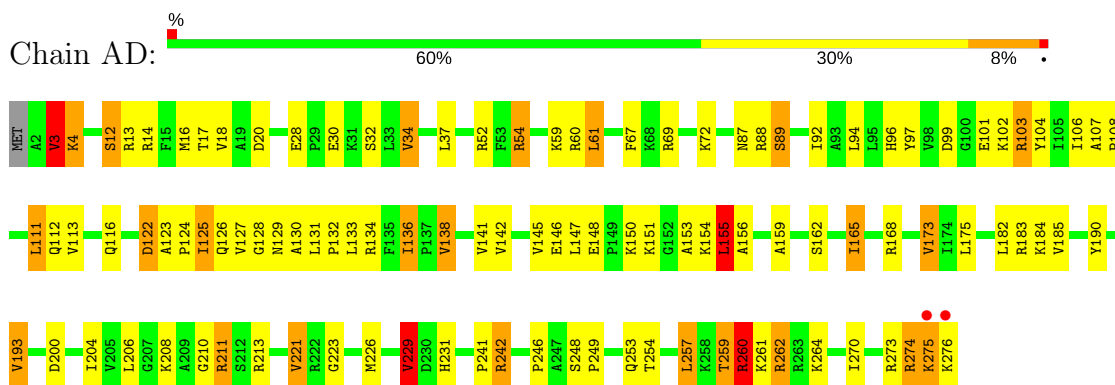
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G2600	C1691	G1754	U1825	G1996	G1967	G2034	U2097	C2160	A2220	G2262	A2348	G2412	C2476	G2540	G2600
A2601	G1692	G1755	U1826	G1997	G1971	A2035	U2098	C2161	A2221	G2263	G2349	G2413	C2477	G2541	A2601
G2602	C1693	G1756	U1827	G1998	G1972	A2036	U2099	C2162	A2222	G2264	G2350	G2414	C2478	G2542	G2602
C2603	G1694	U1765	U1828	G1999	U1973	A2037	C2100	C2163	C2223	A2285	G2351	G2415	C2479	A2543	C2603
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G2606	U1768	U1769	C1832	C1908	U1978	G2040	C2103	U2166	G2226	G2268	G2354	U2420	G2482	G2546	G2606
U2607	G1769	G1769	U1832	C1919	U1978	A2041	A2104	C2167	G2227	G2289	U2355	G2421	G2483	G2547	G2607
U2608	G1770	G1770	A1834	A1911	U1979	A2042	C2105	C2168	G2228	A2290	U2356	G2422	G2484	G2548	U2608
G2609	A1701	G1771	A1834	A1912	C1980	C2043	C2106	C2169	A2229	G2291	A2358	A2423	G2609	U2549	G2609
A2610	A1702	G1772	U1835	G1913	G1981	U2044	C2107	G2170	U2230	G2292	U2359	A2424	A2488	C2550	A2610
G2611	A1703	G1773	U1836	G1913	G1981	G2045	U2108	G2171	U2231	C2293	U2360	G2425	A2489	C2551	G2611
A2612	C1704	G1774	C1837	C1917	C1984	G2046	G2112	U2172	G2234	G2294	G2361	G2426	C2489	C2552	A2612
C2613	U1705	G1775	G1838	G1918	U1985	C2047	G2113	G2173	G2235	C2295	G2362	G2427	C2490	G2553	C2613
A2614	U1706	G1776	G1839	G1919	U1986	C2048	U2114	G2174	G2236	C2296	G2363	C2429	G2491	A2554	A2614
G2615	C1707	G1777	A1841	U1920	G1986	U2049	U2114	G2175	G2237	C2297	G2364	A2430	G2492	G2555	G2615
U2616	G1708	G1778	G1842	U1921	C1987	U2050	G2115	G2176	G2238	A2298	G2365	U2431	G2493	G2556	U2616
G2617	C1709	G1779	U1843	U1922	C1988	G2051	G2116	G2177	C2239	A2299	C2366	G2432	G2494	G2557	G2617
U2618	C1710	G1780	G1844	A1923	C1990	A2052	G2119	G2178	A2300	A2300	C2367	G2433	G2495	G2558	U2618
G2619	A1711	A1711	G1845	C1924	A1991	A2053	C2120	G2179	G2301	G2301	U2368	A2434	G2496	U2559	G2619
U2620	G1712	A1712	U1846	G1925	A1992	G2054	U2120	A2180	G2241	G2302	G2370	U2435	G2497	G2560	U2620
C2621	G1713	G1713	G1847	G1926	A1993	A2055	U2121	G2181	C2242	G2303	C2371	U2436	G2498	G2561	C2621
U2622	G1714	G1714	U1848	G1927	A1994	U2056	G2122	G2182	G2243	G2304	A2372	A2437	G2499	G2562	U2622
G2623	A1715	G1715	G1849	G1928	A1995	G2057	G2123	C2183	C2244	C2305	A2373	A2438	G2500	G2563	G2623
U2624	A1716	G1716	U1850	G1929	C1996	C2058	U2124	G2184	U2245	C2306	G2374	C2439	G2501	U2564	U2624
G2625	C1717	G1717	U1851	C1930	A1999	G2059	U2125	G2185	G2246	G2307	G2375	G2440	G2502	G2565	U2625
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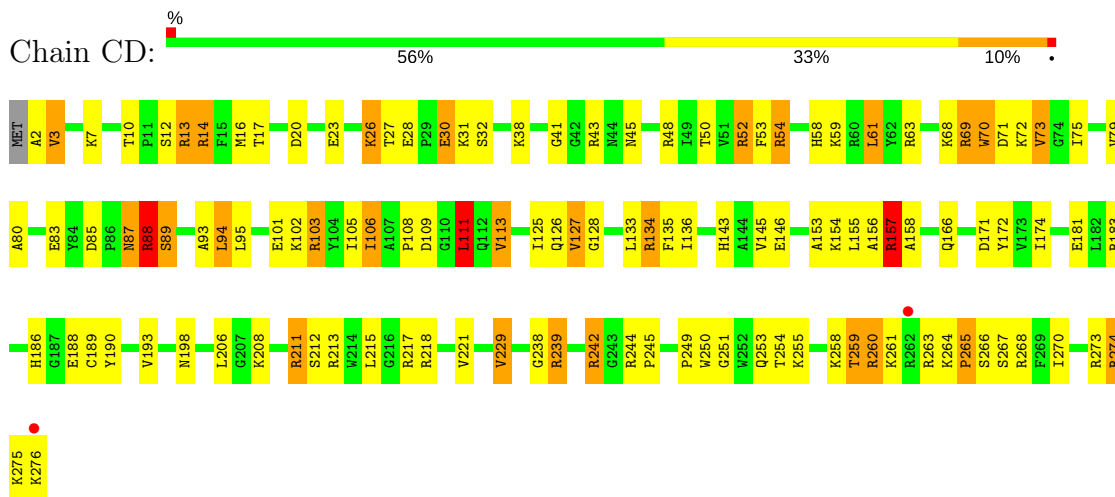
WORLDWIDE
PDB
PROTEIN DATA BANK



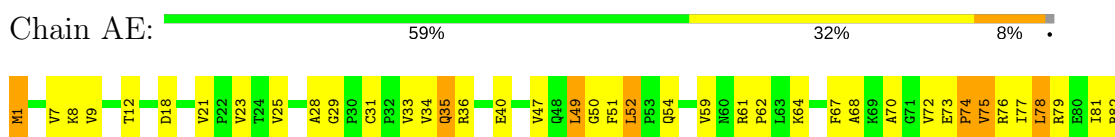
- Molecule 4: 50S ribosomal protein L2

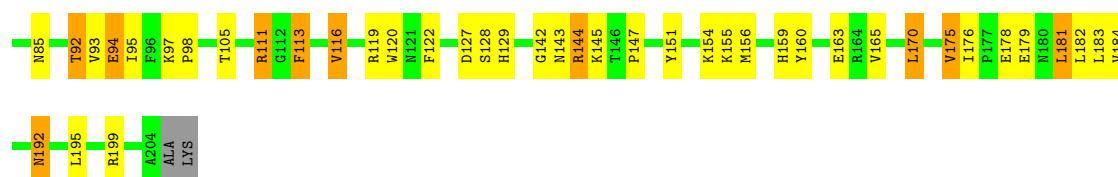


- Molecule 4: 50S ribosomal protein L2



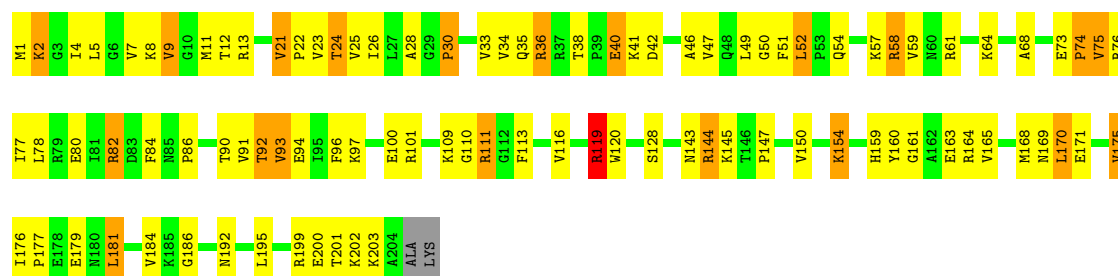
- Molecule 5: 50S ribosomal protein L3





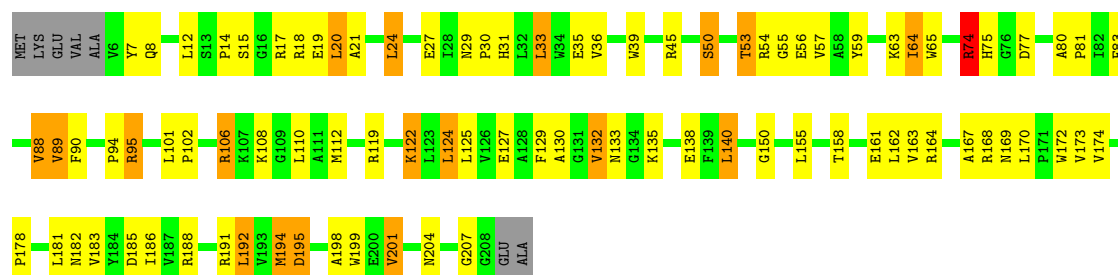
• Molecule 5: 50S ribosomal protein L3

Chain CE: 52% 36% 10%



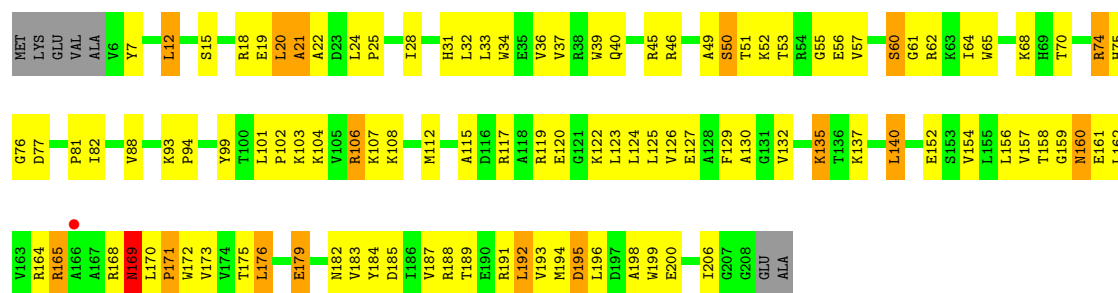
• Molecule 6: 50S ribosomal protein L4

Chain AF: 54% 33% 9%



• Molecule 6: 50S ribosomal protein L4

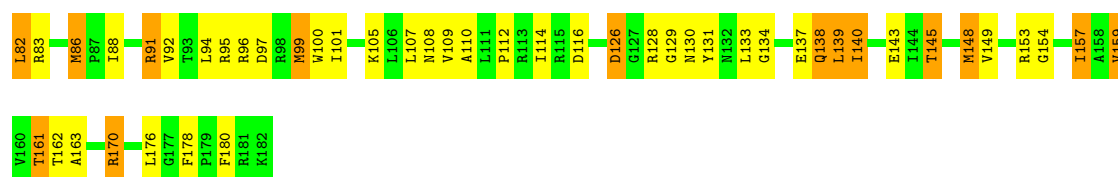
Chain CF: 46% 43% 8%



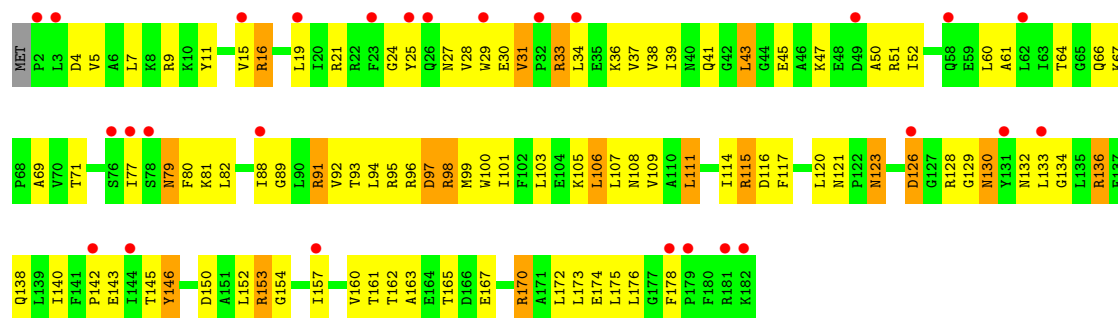
• Molecule 7: 50S ribosomal protein L5

Chain AG: 53% 34% 12%

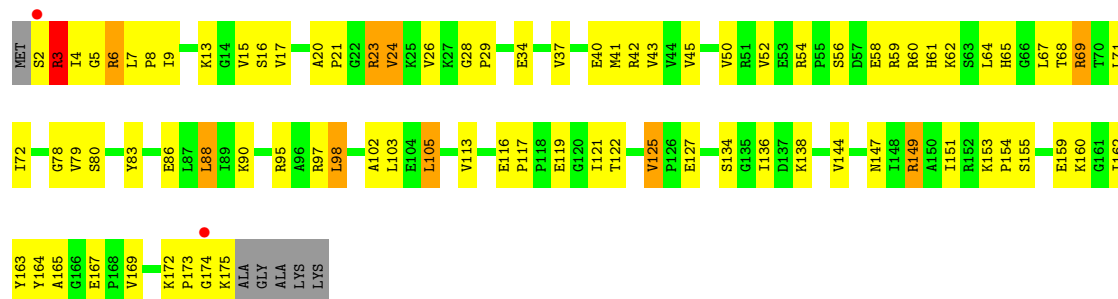




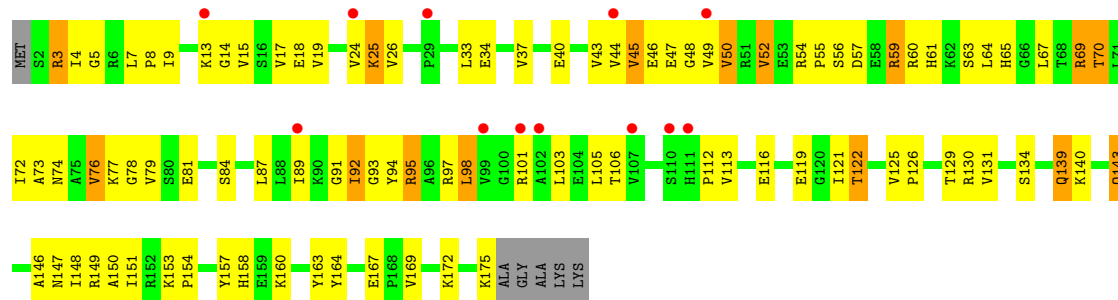
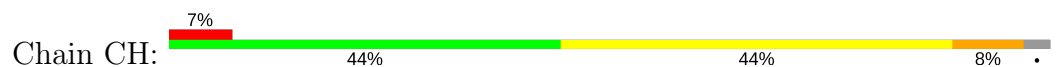
• Molecule 7: 50S ribosomal protein L5



• Molecule 8: 50S ribosomal protein L6

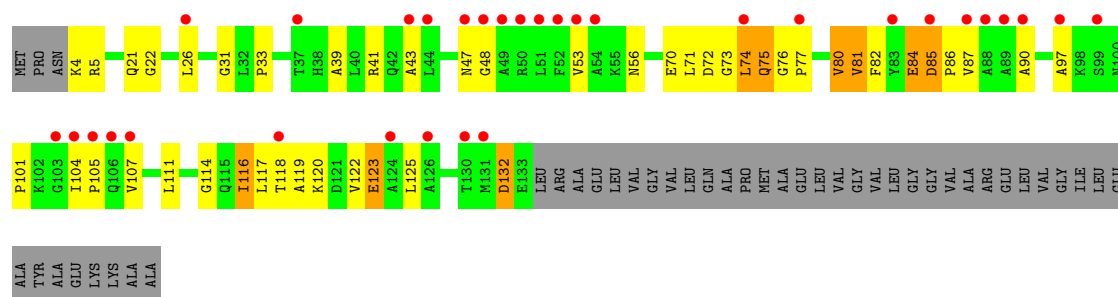


• Molecule 8: 50S ribosomal protein L6

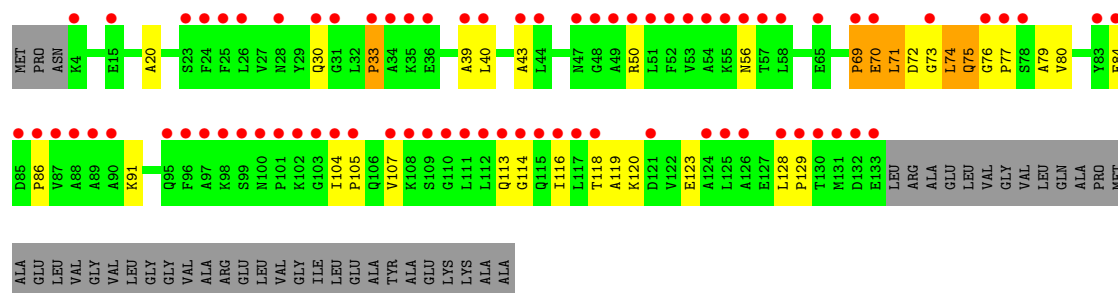


• Molecule 9: 50S ribosomal protein L10

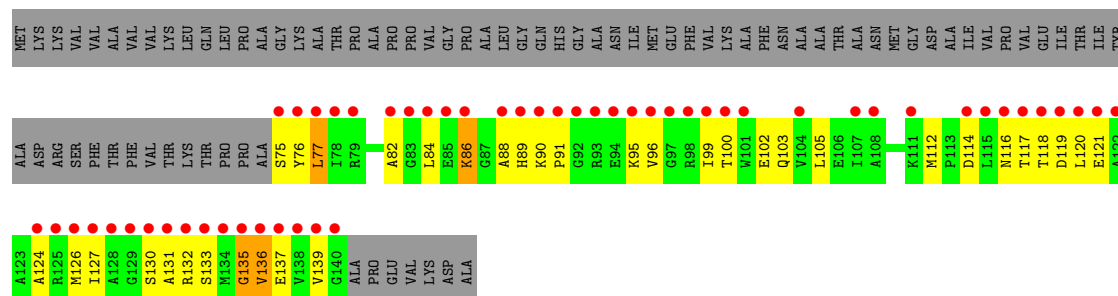
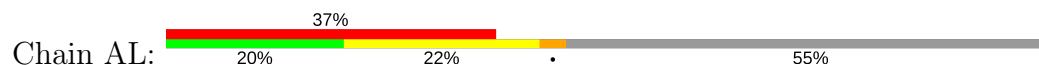




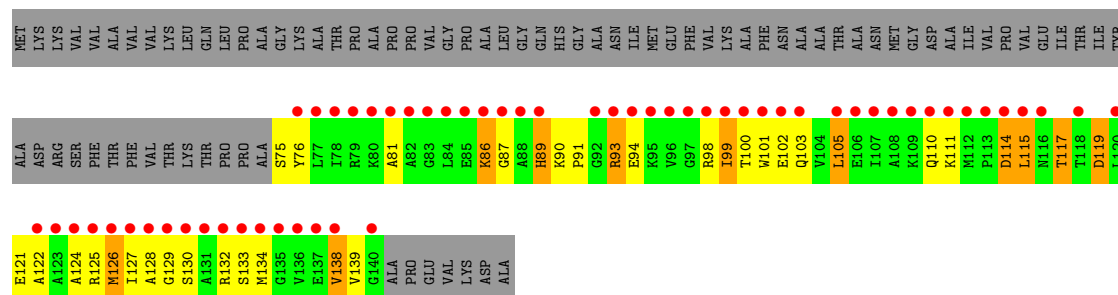
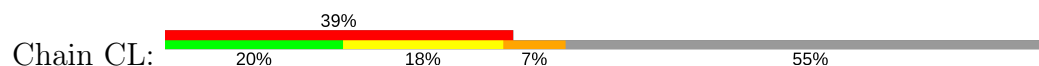
• Molecule 9: 50S ribosomal protein L10



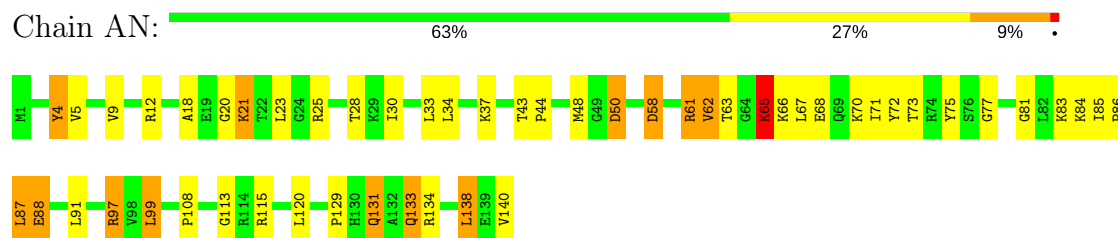
• Molecule 10: 50S ribosomal protein L11



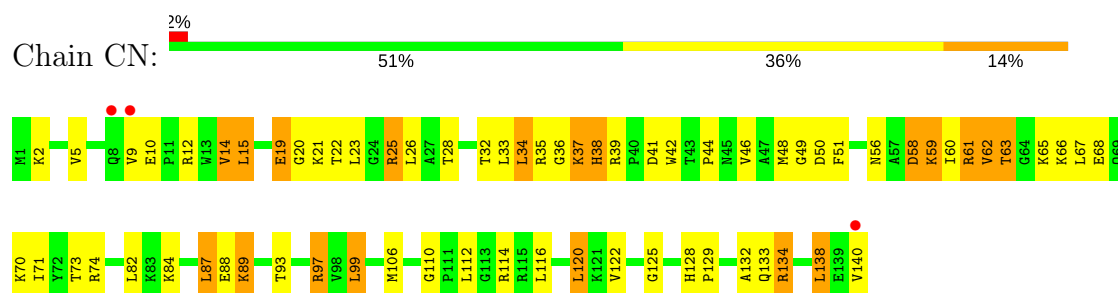
• Molecule 10: 50S ribosomal protein L11



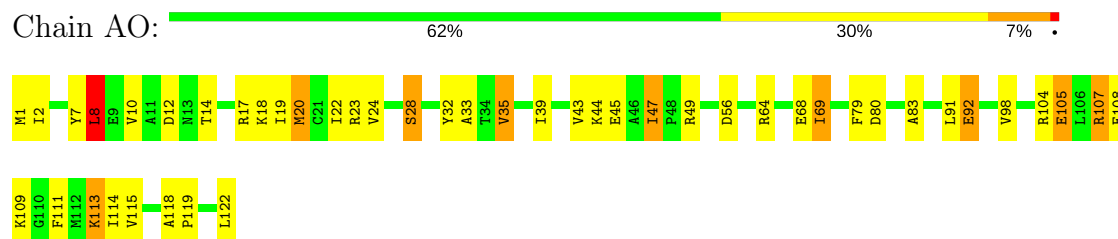
• Molecule 11: 50S ribosomal protein L13



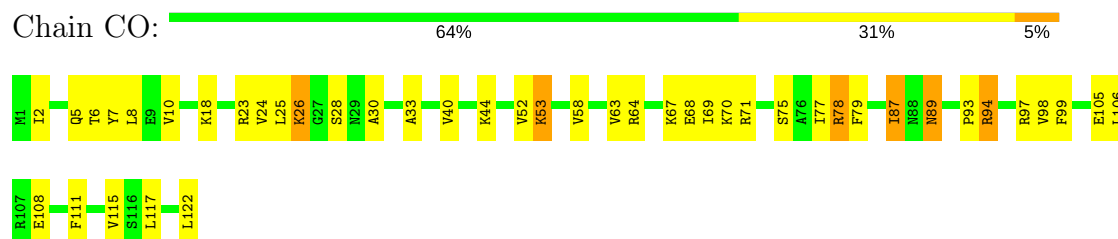
- Molecule 11: 50S ribosomal protein L13



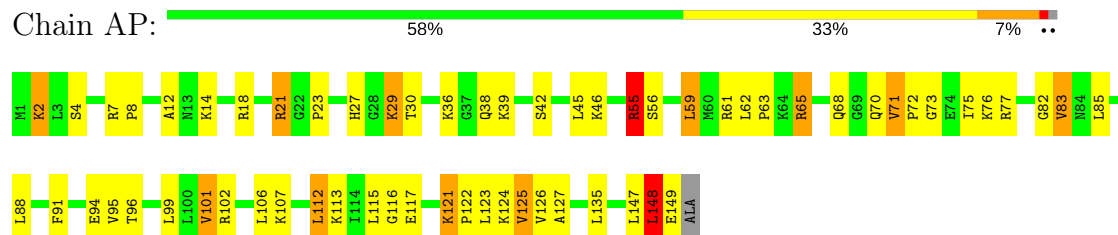
- Molecule 12: 50S ribosomal protein L14



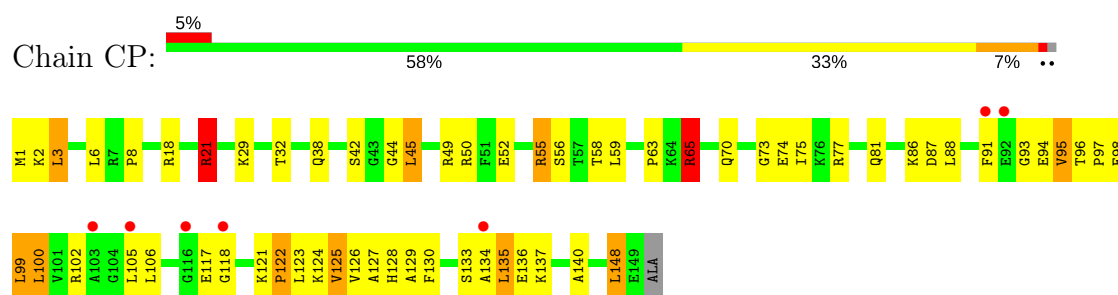
- Molecule 12: 50S ribosomal protein L14



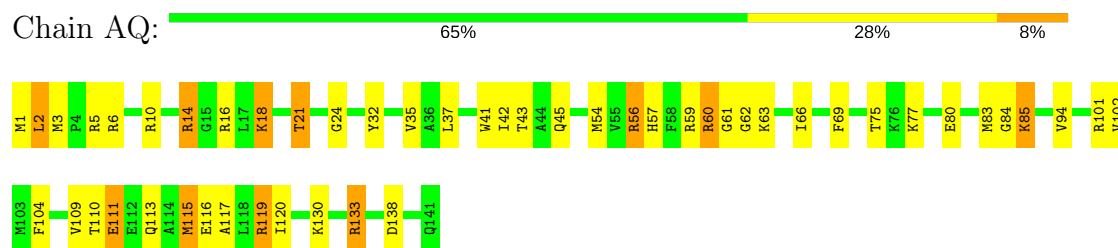
- Molecule 13: 50S ribosomal protein L15



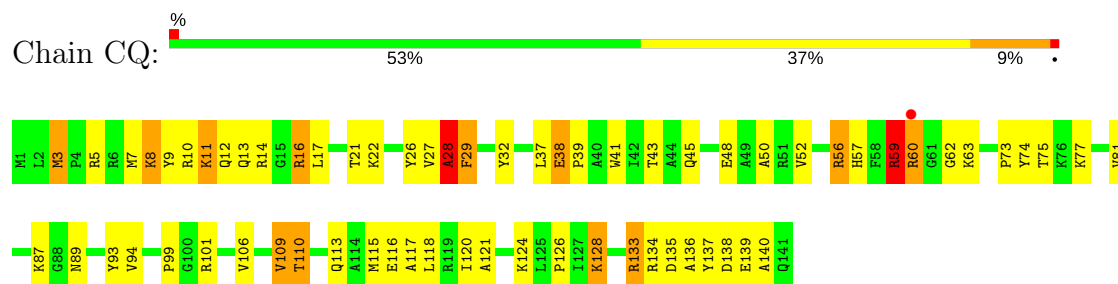
- Molecule 13: 50S ribosomal protein L15



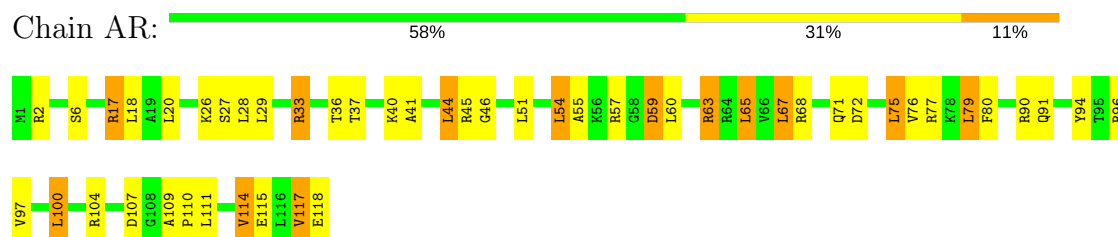
- Molecule 14: 50S ribosomal protein L16



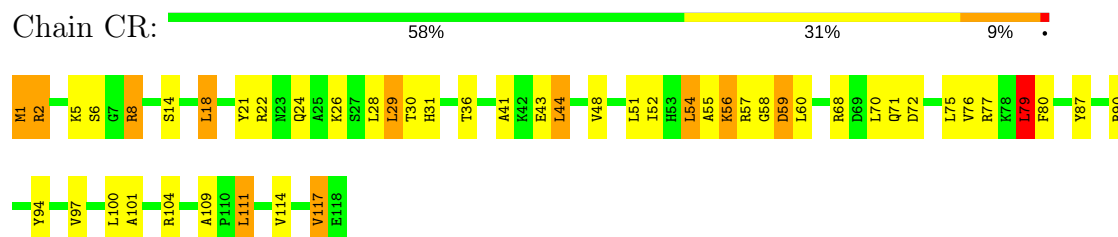
- Molecule 14: 50S ribosomal protein L16



- Molecule 15: 50S ribosomal protein L17

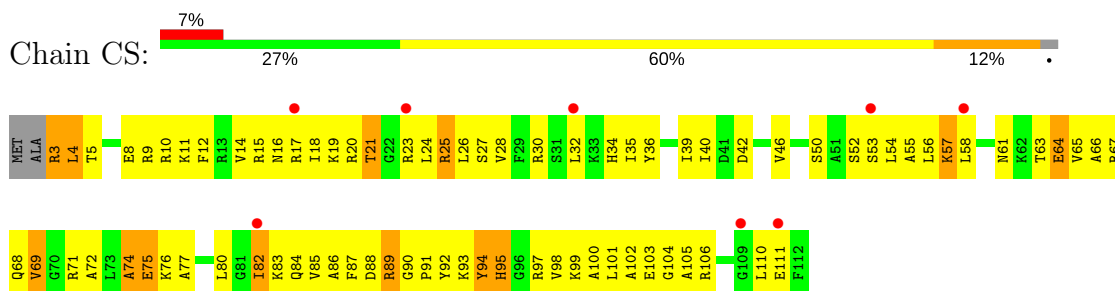


- Molecule 15: 50S ribosomal protein L17

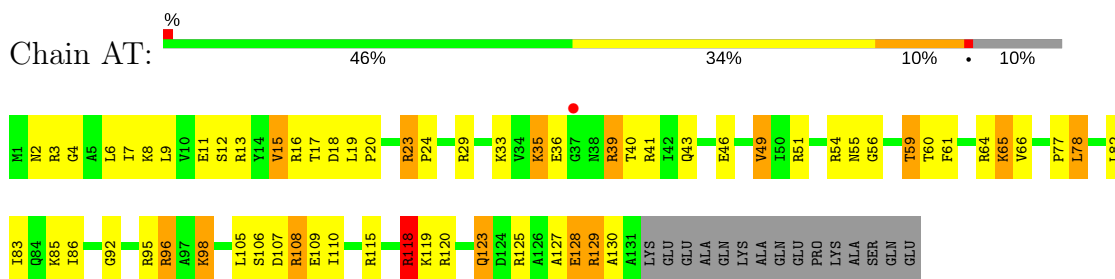


- Molecule 16: 50S ribosomal protein L18

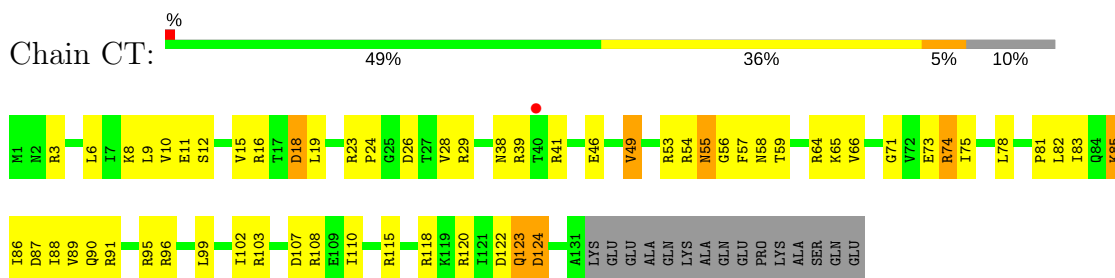
- Molecule 16: 50S ribosomal protein L18



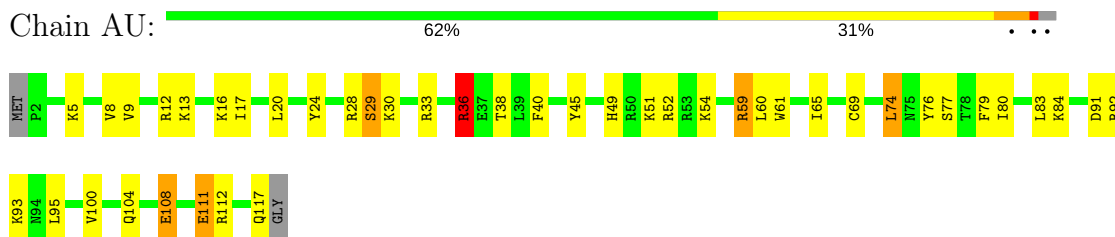
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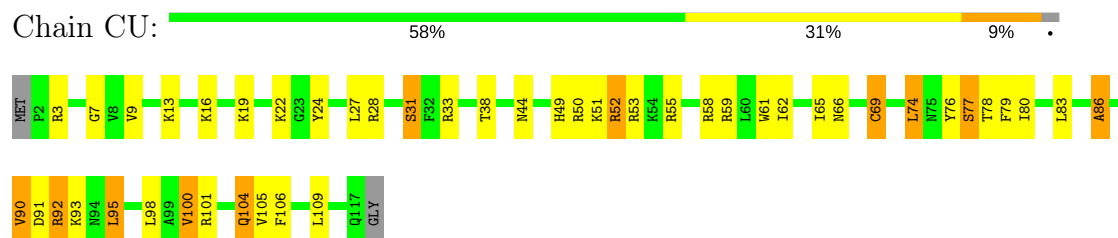
- Molecule 17: 50S ribosomal protein L19



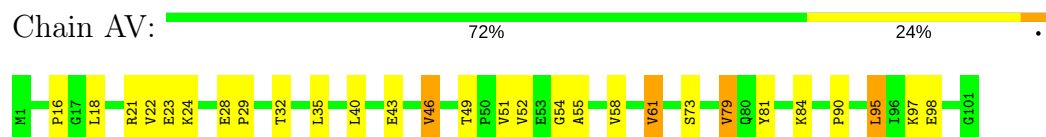
- Molecule 18: 50S ribosomal protein L20



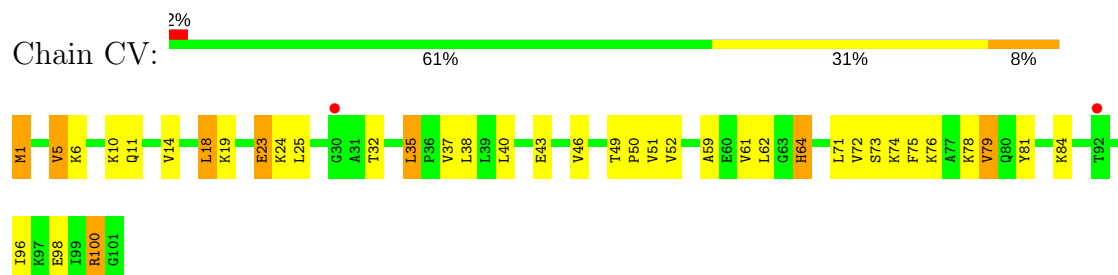
- Molecule 18: 50S ribosomal protein L20



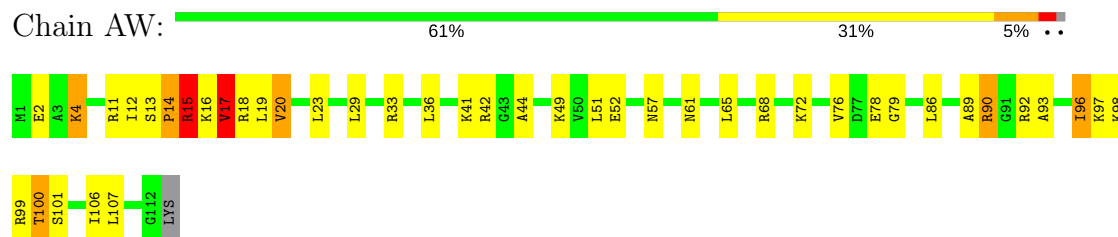
- Molecule 19: 50S ribosomal protein L21



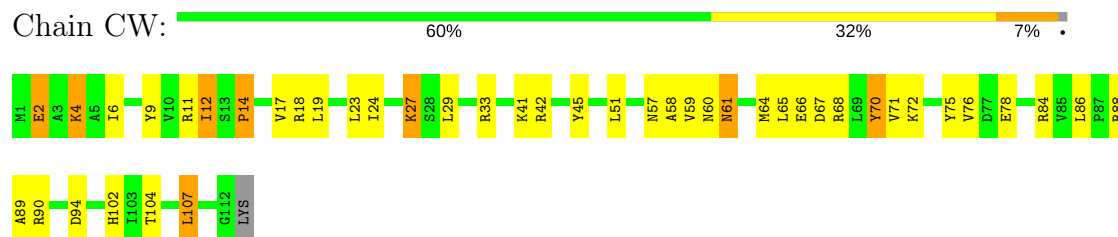
- Molecule 19: 50S ribosomal protein L21



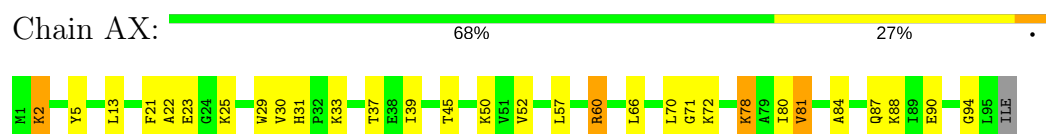
- Molecule 20: 50S ribosomal protein L22



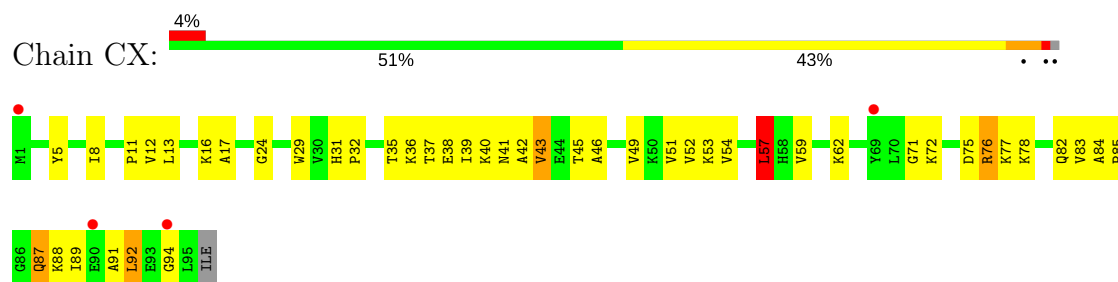
- Molecule 20: 50S ribosomal protein L22



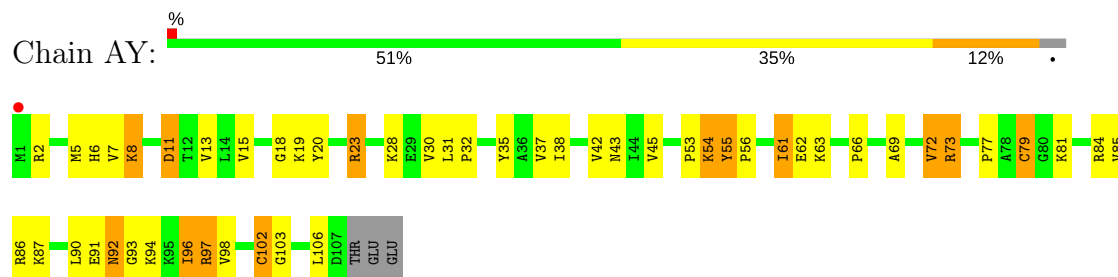
- Molecule 21: 50S ribosomal protein L23



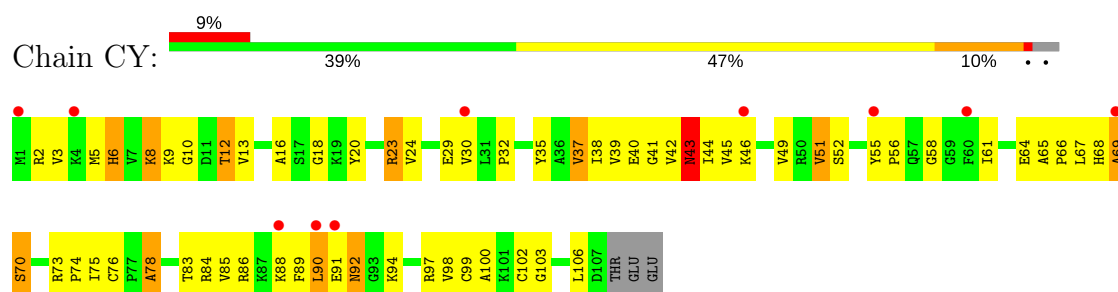
- Molecule 21: 50S ribosomal protein L23



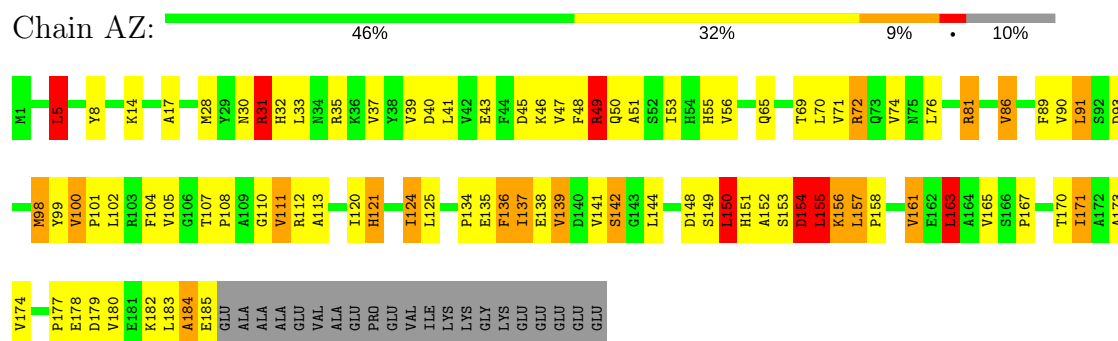
- Molecule 22: 50S ribosomal protein L24



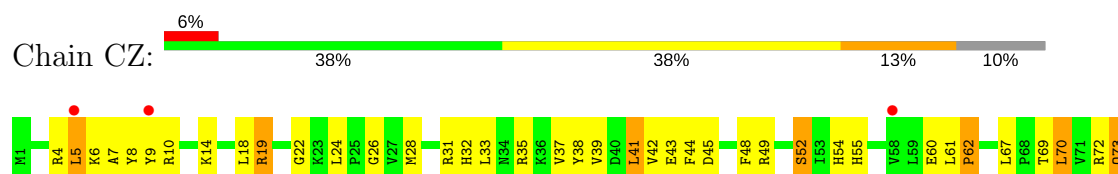
- Molecule 22: 50S ribosomal protein L24

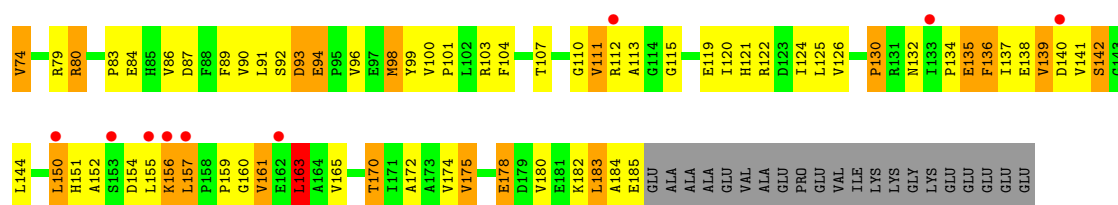


- Molecule 23: 50S ribosomal protein L25



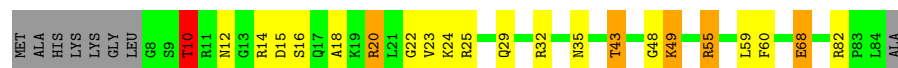
- Molecule 23: 50S ribosomal protein L25





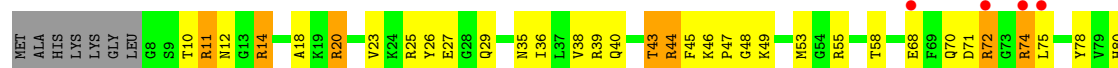
• Molecule 24: 50S ribosomal protein L27

Chain A0: 65% 19% 6% 9%



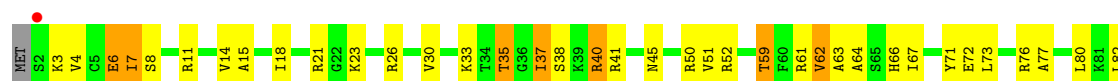
• Molecule 24: 50S ribosomal protein L27

Chain C0: 5% 48% 33% 9% 9%



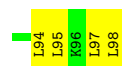
• Molecule 25: 50S ribosomal protein L28

Chain A1: % 55% 37% 7%



• Molecule 25: 50S ribosomal protein L28

Chain C1: % 57% 34% 8%

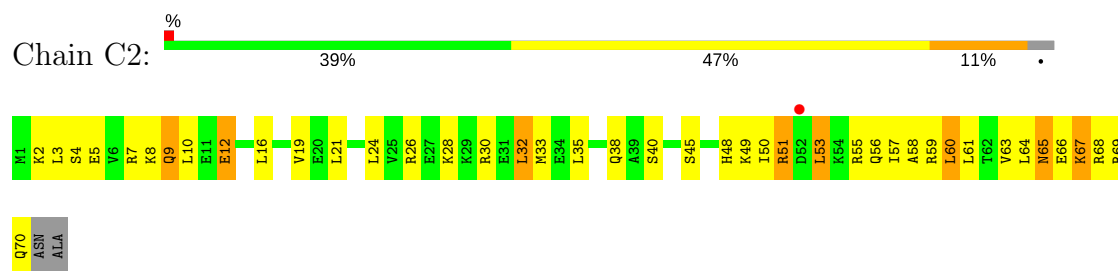


• Molecule 26: 50S ribosomal protein L29

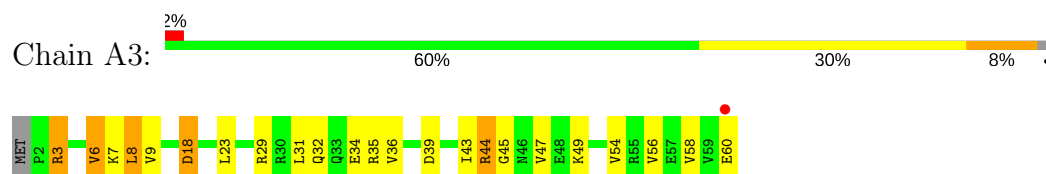
Chain A2: % 64% 26% 7%



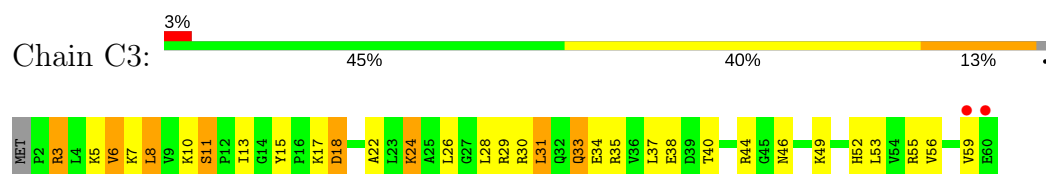
- Molecule 26: 50S ribosomal protein L29



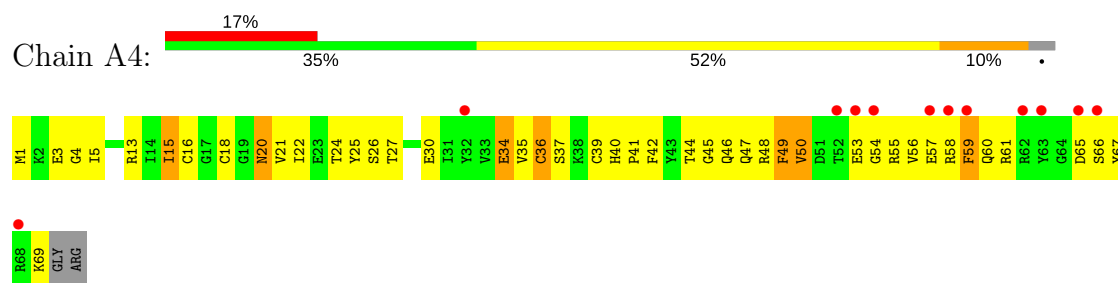
- Molecule 27: 50S ribosomal protein L30



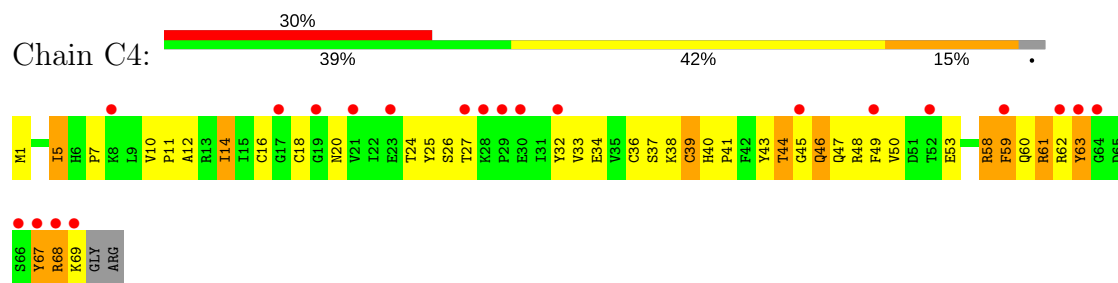
- Molecule 27: 50S ribosomal protein L30



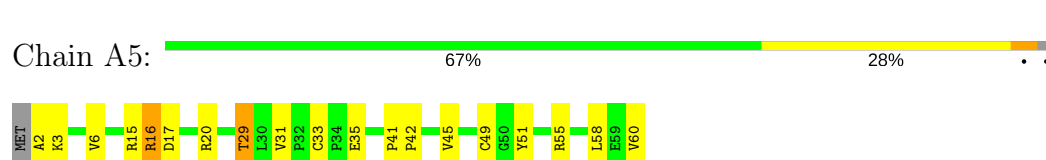
- Molecule 28: 50S ribosomal protein L31



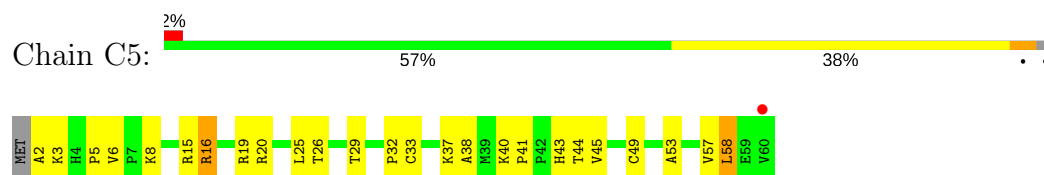
- Molecule 28: 50S ribosomal protein L31



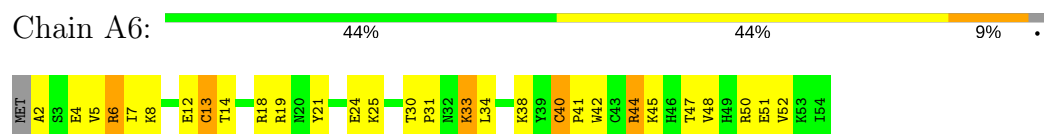
- Molecule 29: 50S ribosomal protein L32



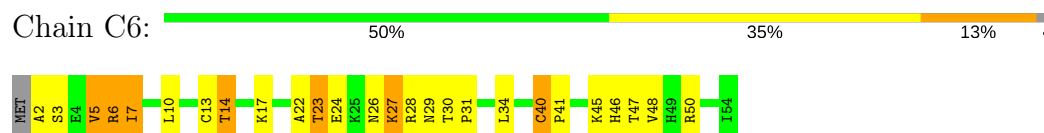
• Molecule 29: 50S ribosomal protein L32



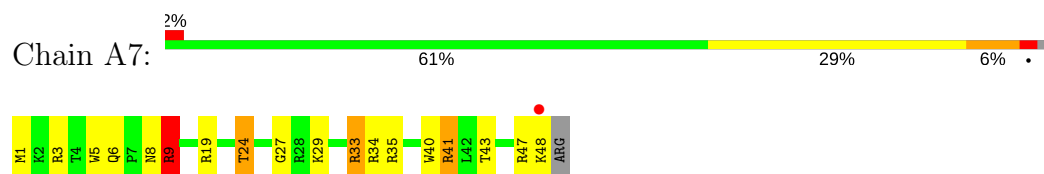
• Molecule 30: 50S ribosomal protein L33



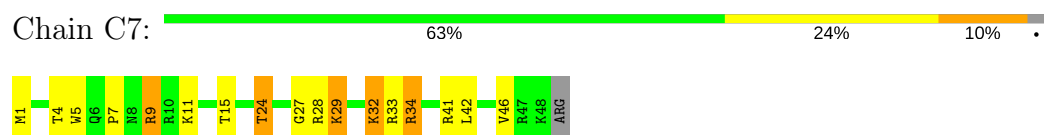
• Molecule 30: 50S ribosomal protein L33



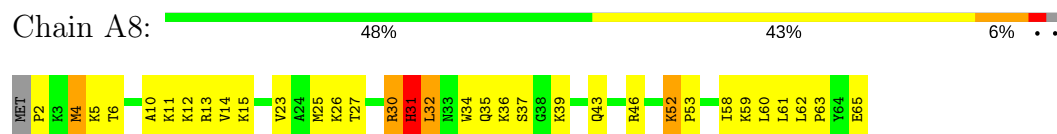
• Molecule 31: 50S ribosomal protein L34



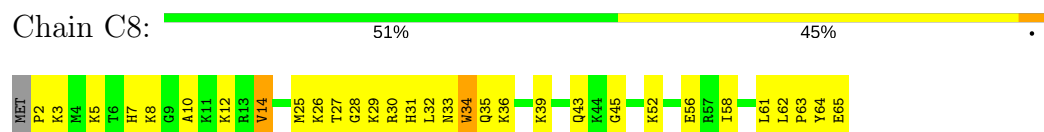
• Molecule 31: 50S ribosomal protein L34



• Molecule 32: 50S ribosomal protein L35



• Molecule 32: 50S ribosomal protein L35



• Molecule 33: 50S ribosomal protein L36

Chain A9: 



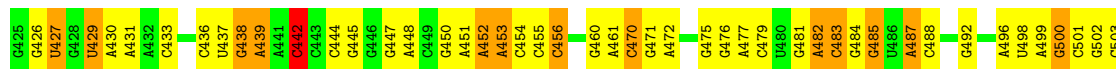
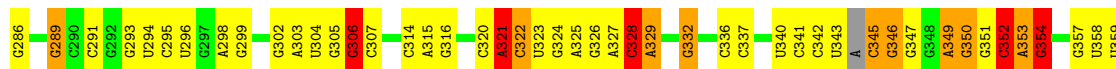
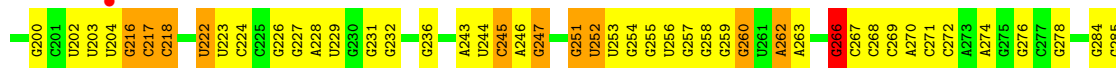
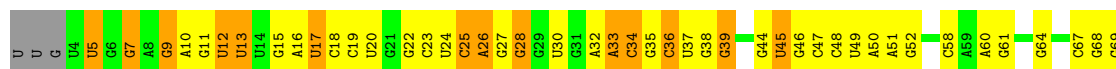
- Molecule 33: 50S ribosomal protein L36

Chain C9: 

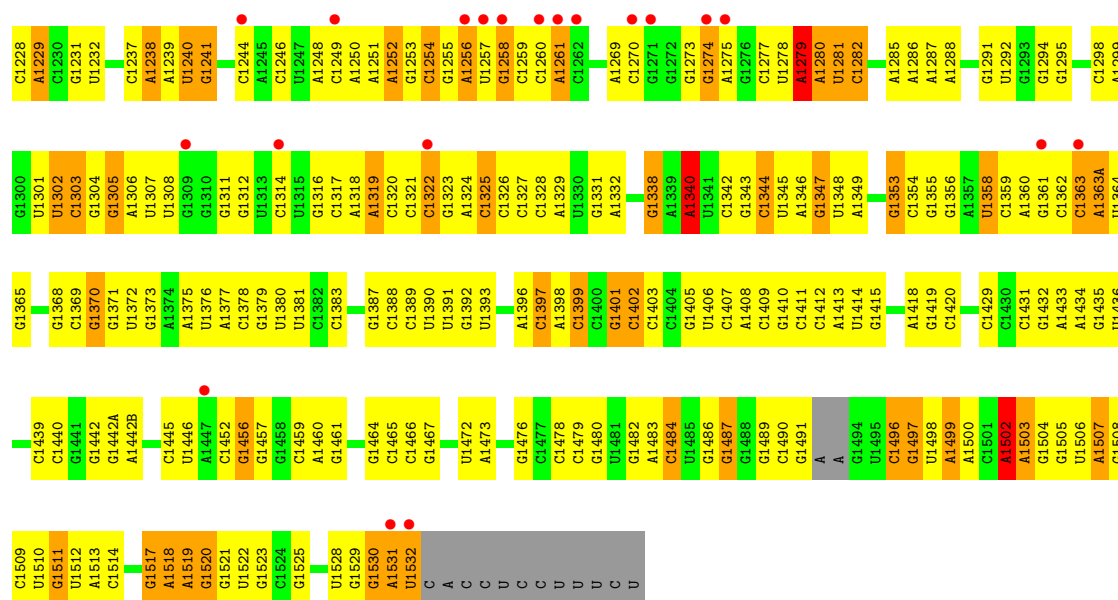


- Molecule 34: 16S Ribosomal RNA

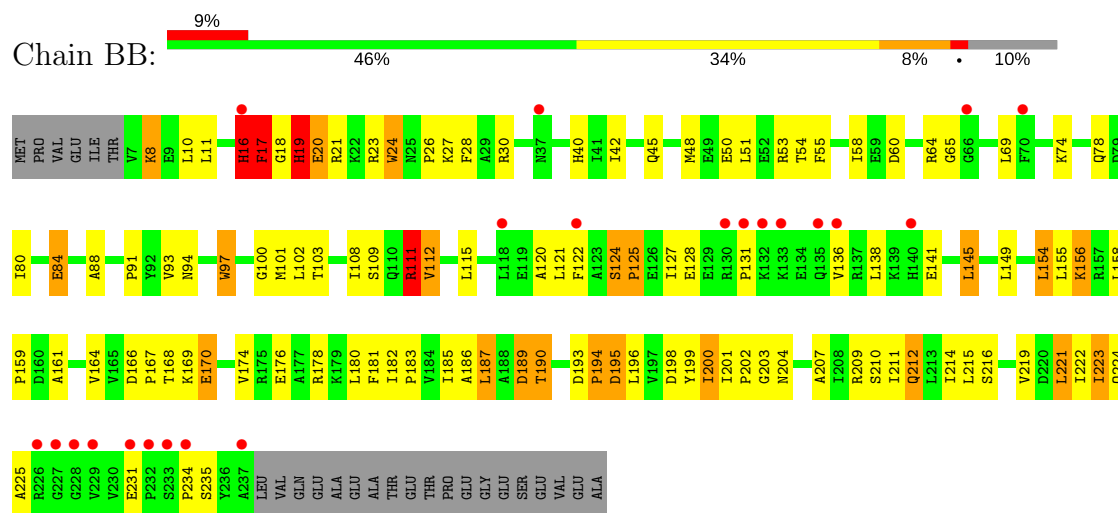
Chain BA: 



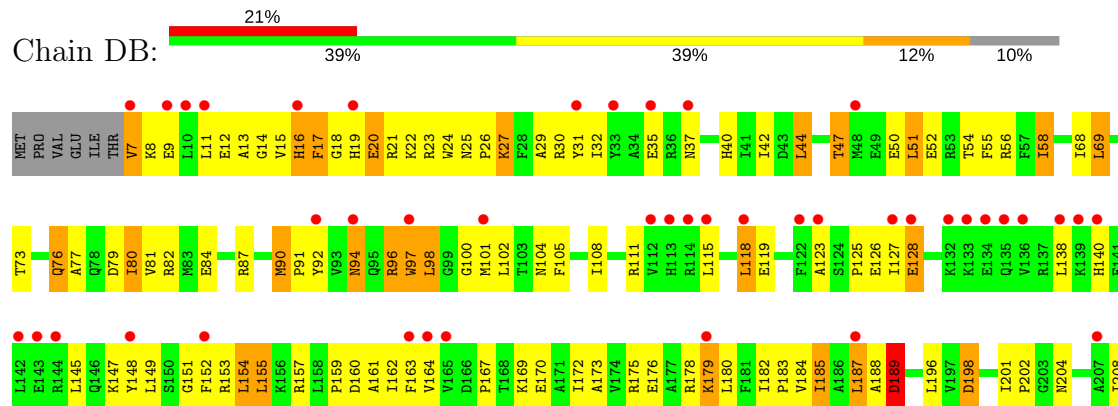


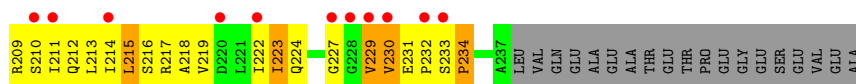


• Molecule 35: 30S ribosomal protein S2

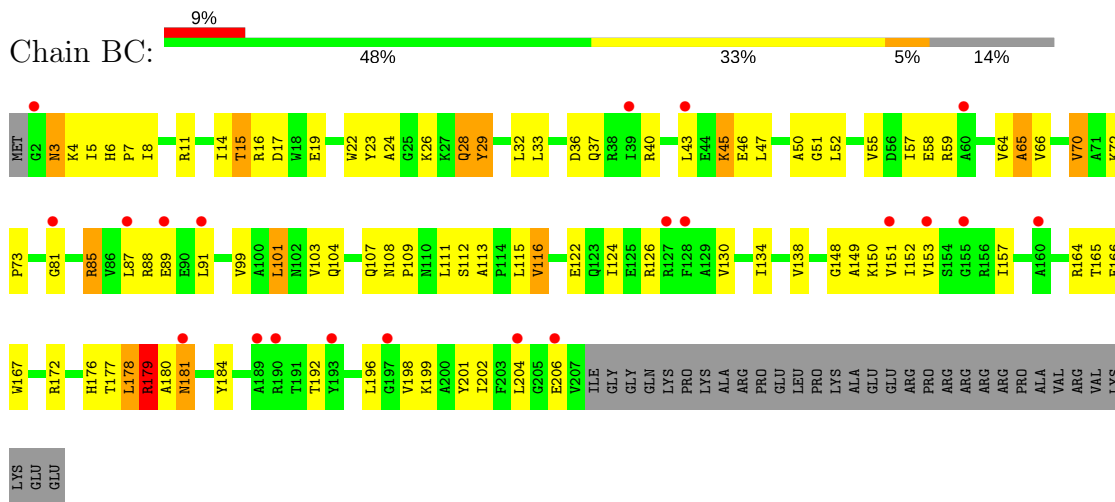


• Molecule 35: 30S ribosomal protein S2

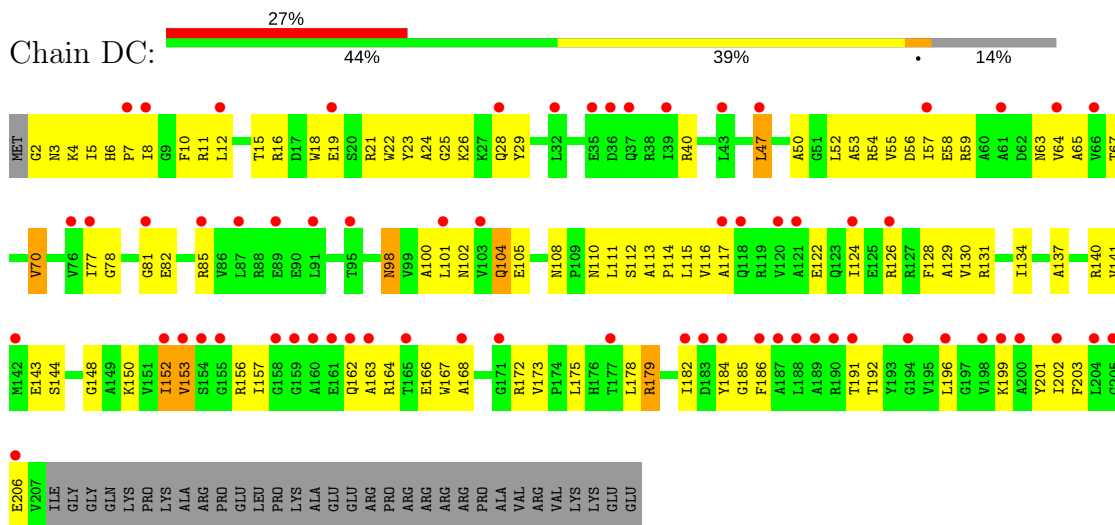




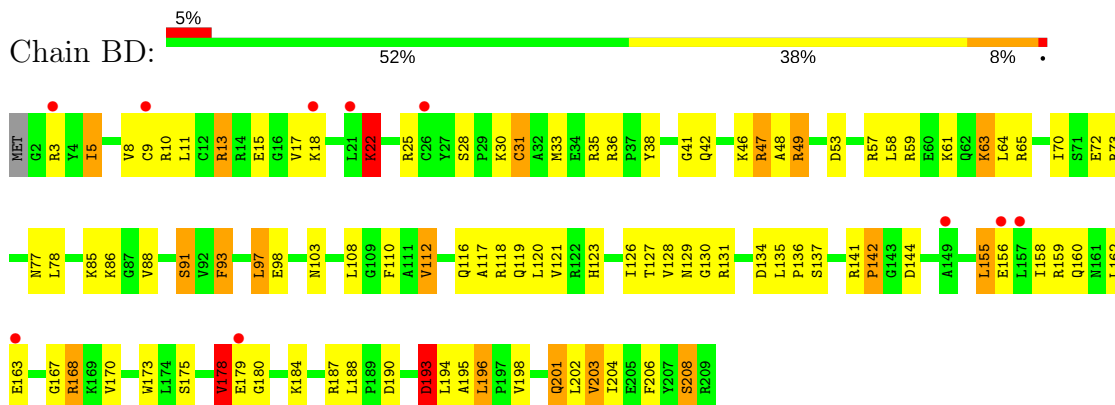
• Molecule 36: 30S ribosomal protein S3



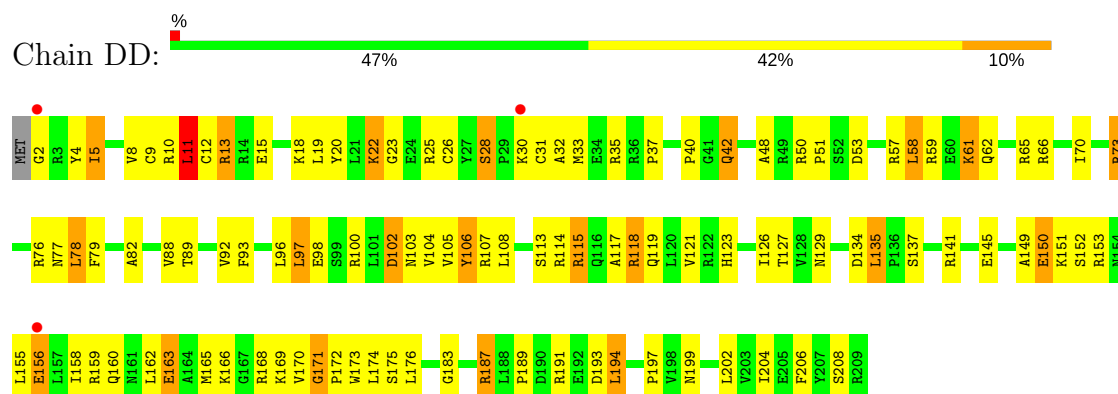
• Molecule 36: 30S ribosomal protein S3



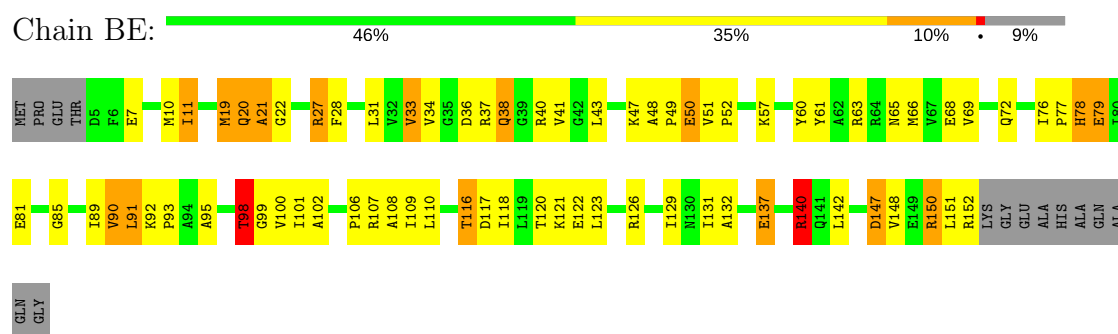
• Molecule 37: 30S ribosomal protein S4



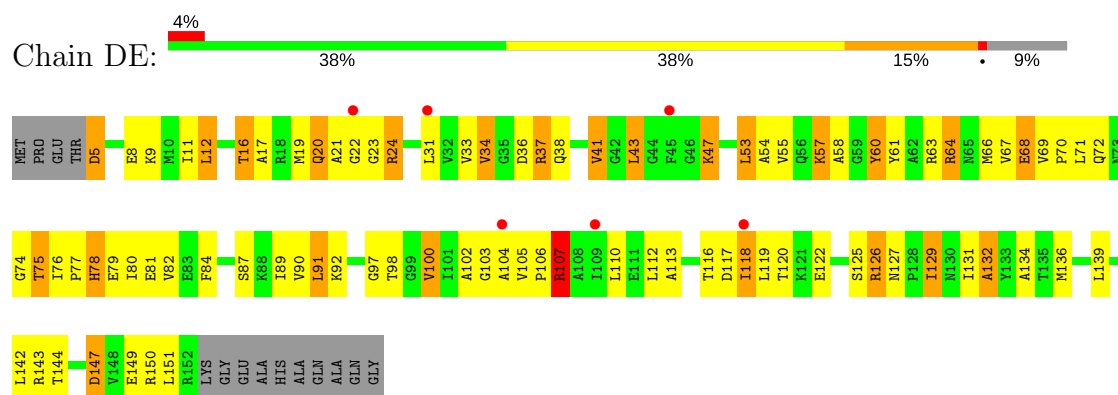
- Molecule 37: 30S ribosomal protein S4



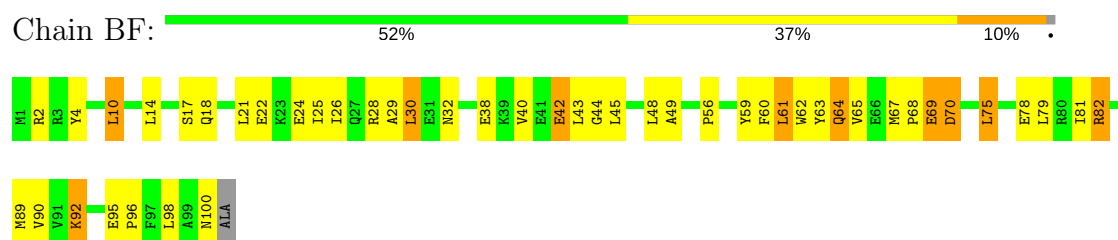
- Molecule 38: 30S ribosomal protein S5



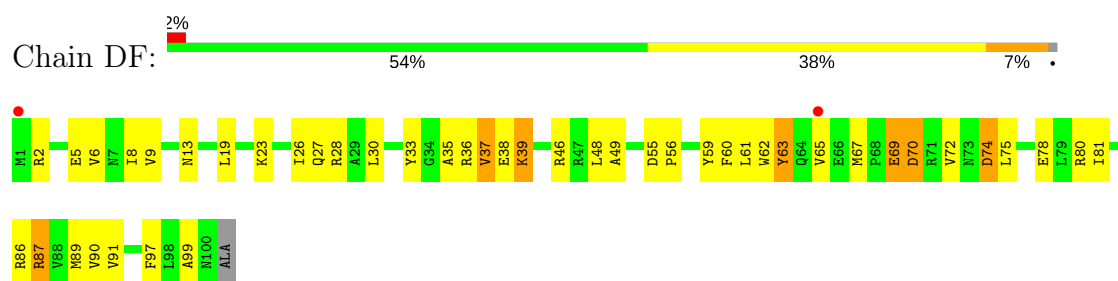
- Molecule 38: 30S ribosomal protein S5



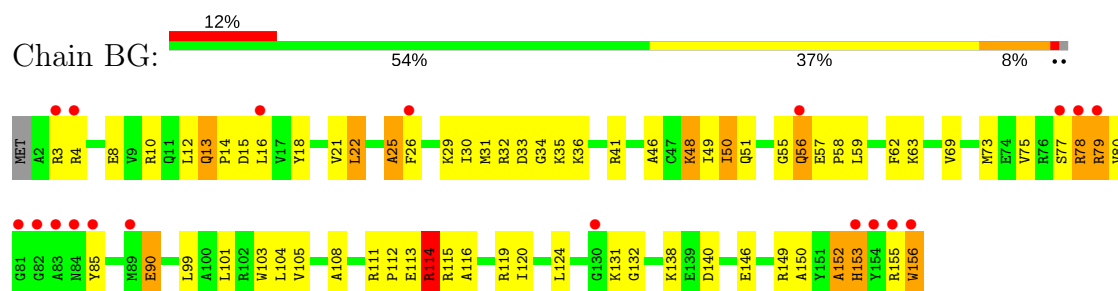
- Molecule 39: 30S ribosomal protein S6



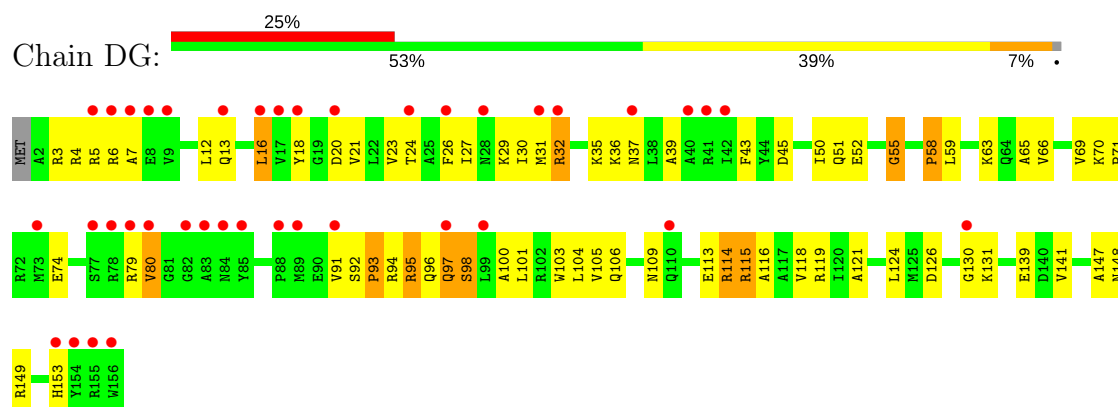
- Molecule 39: 30S ribosomal protein S6



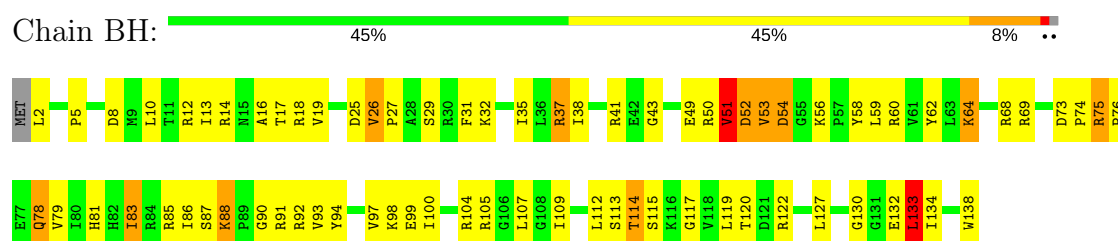
- Molecule 40: 30S ribosomal protein S7



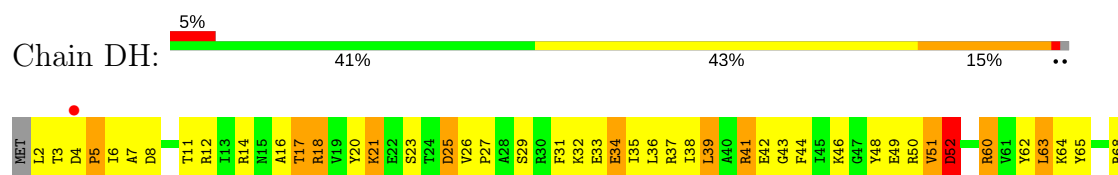
- Molecule 40: 30S ribosomal protein S7

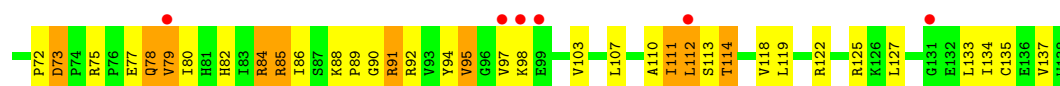


- Molecule 41: 30S ribosomal protein S8



- Molecule 41: 30S ribosomal protein S8

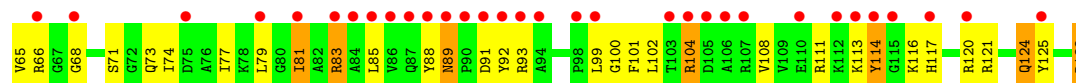
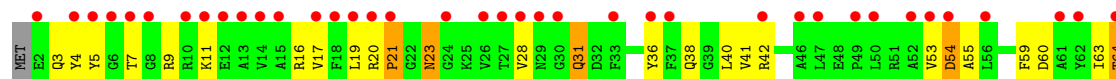




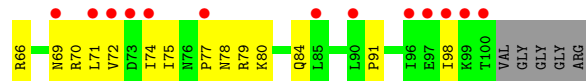
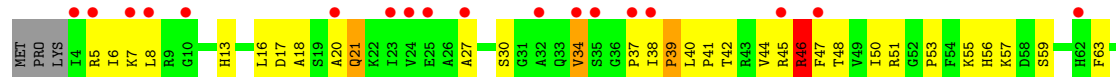
• Molecule 42: 30S ribosomal protein S9



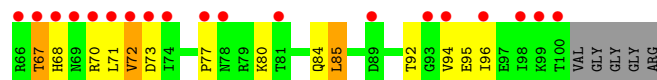
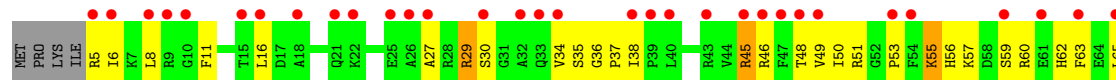
• Molecule 42: 30S ribosomal protein S9



• Molecule 43: 30S ribosomal protein S10

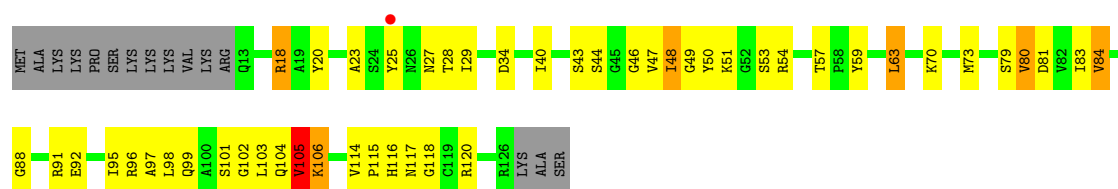


• Molecule 43: 30S ribosomal protein S10

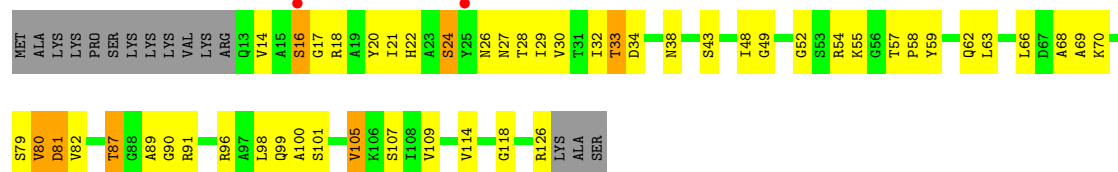


• Molecule 44: 30S ribosomal protein S11

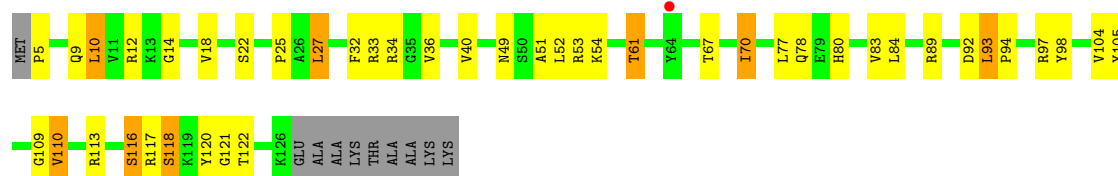




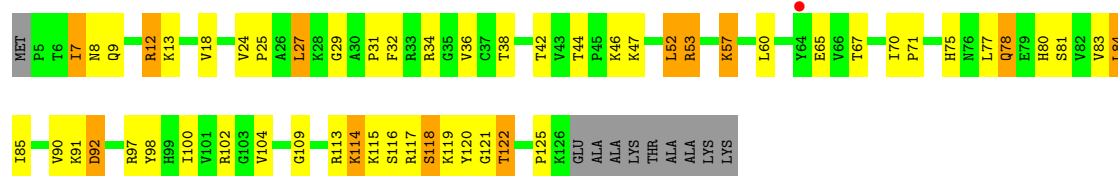
• Molecule 44: 30S ribosomal protein S11



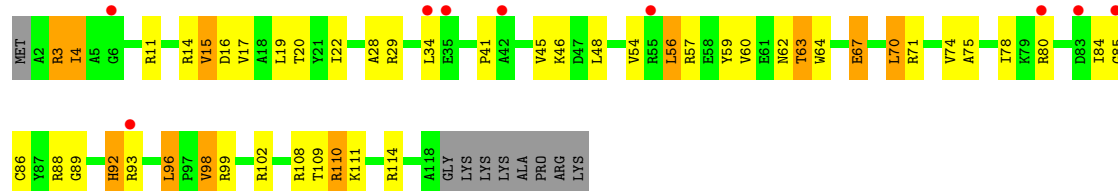
• Molecule 45: 30S ribosomal protein S12



• Molecule 45: 30S ribosomal protein S12

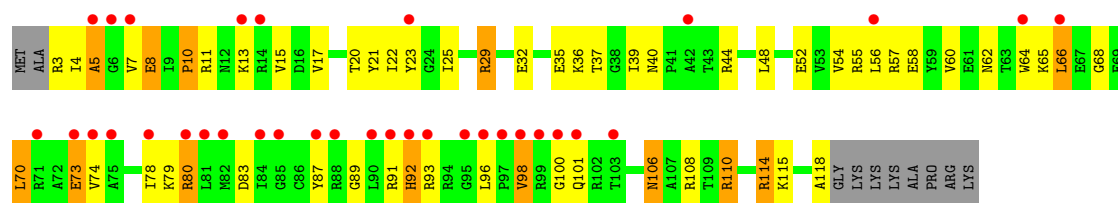


• Molecule 46: 30S ribosomal protein S13



• Molecule 46: 30S ribosomal protein S13

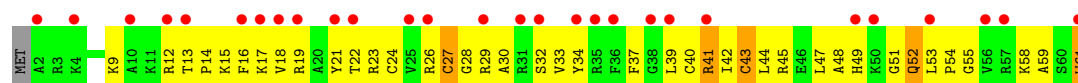




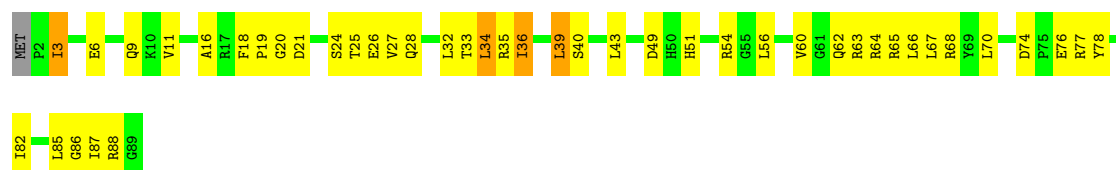
- Molecule 47: 30S ribosomal protein S14 type Z



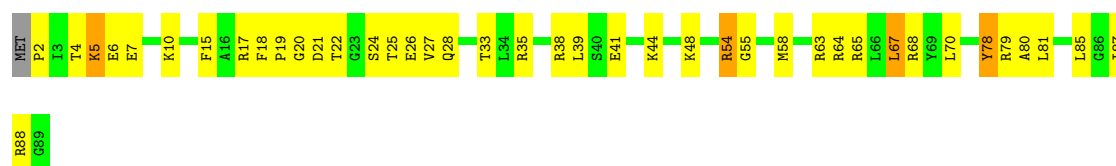
- Molecule 47: 30S ribosomal protein S14 type Z



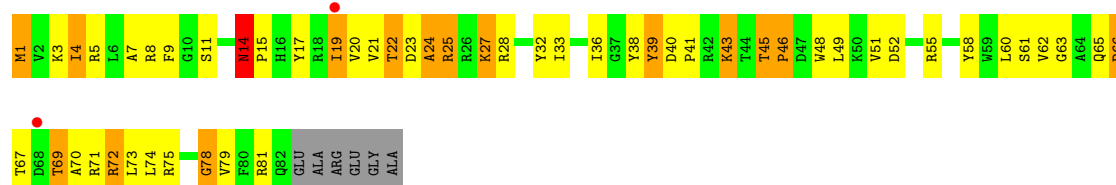
- Molecule 48: 30S ribosomal protein S15



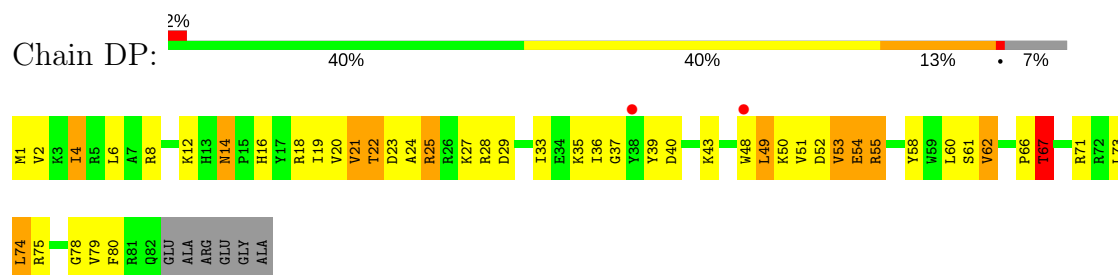
- Molecule 48: 30S ribosomal protein S15



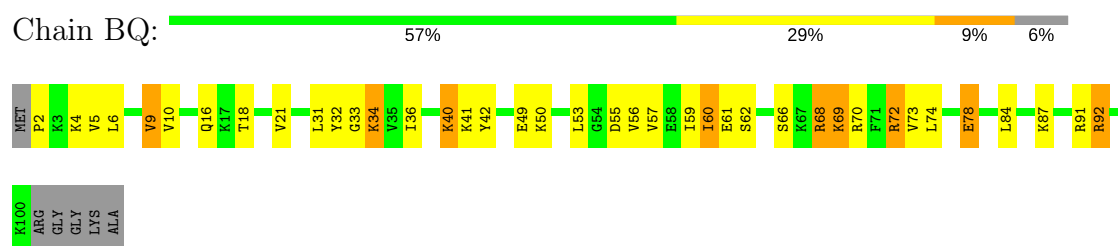
- Molecule 49: 30S ribosomal protein S16



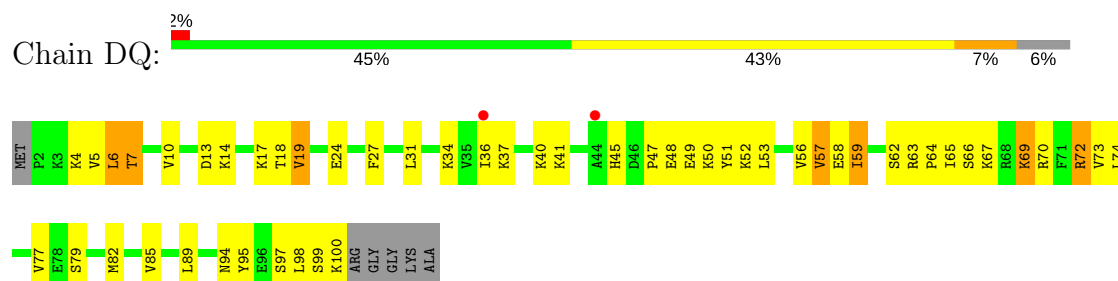
- Molecule 49: 30S ribosomal protein S16



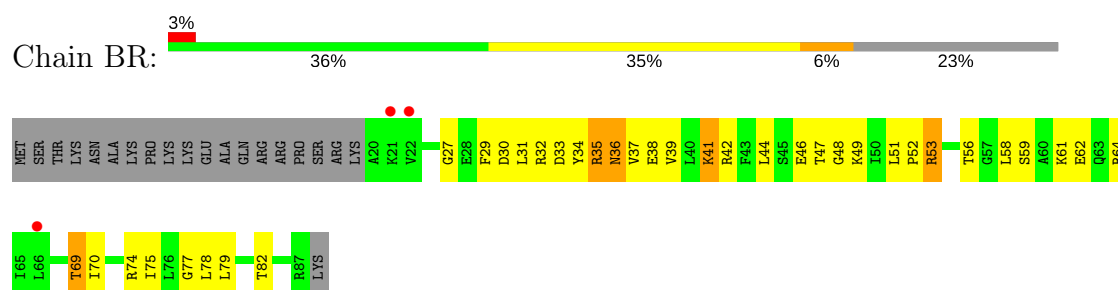
- Molecule 50: 30S ribosomal protein S17



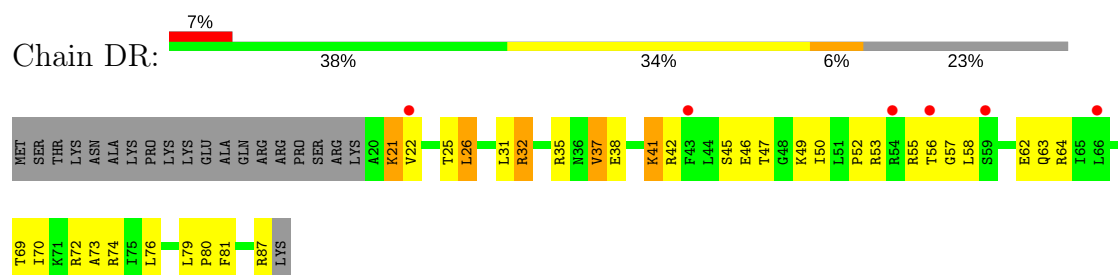
- Molecule 50: 30S ribosomal protein S17



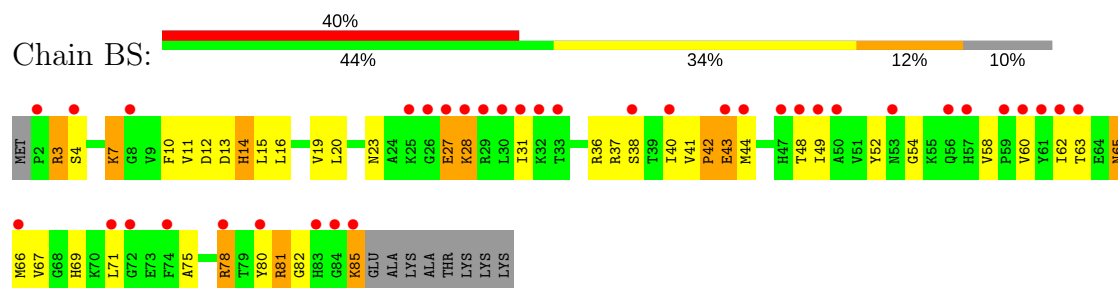
- Molecule 51: 30S ribosomal protein S18



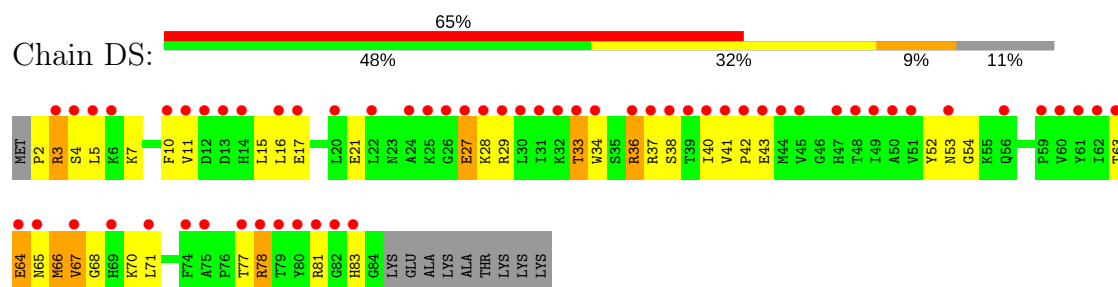
- Molecule 51: 30S ribosomal protein S18



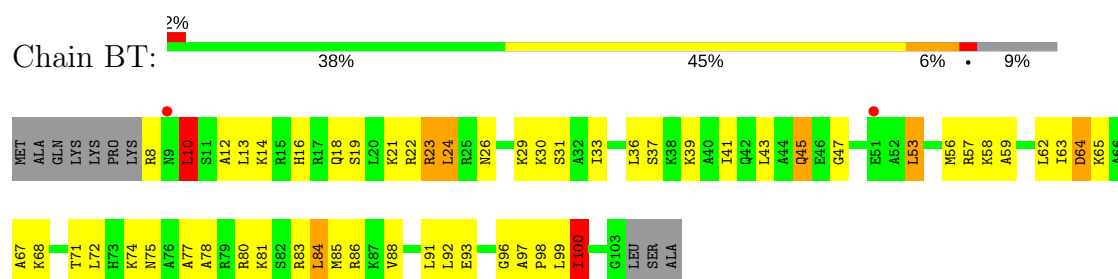
- Molecule 52: 30S ribosomal protein S19



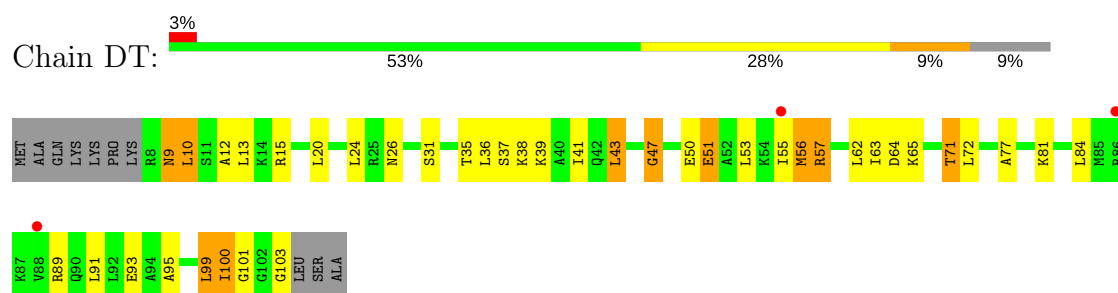
- Molecule 52: 30S ribosomal protein S19



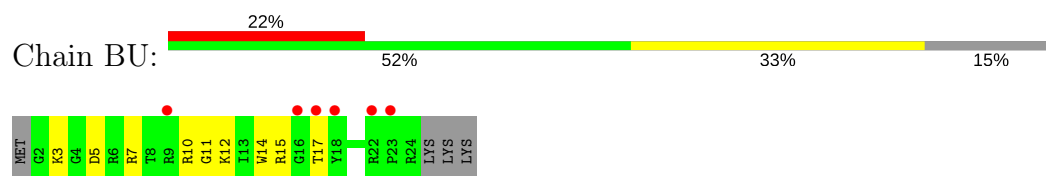
- Molecule 53: 30S ribosomal protein S20



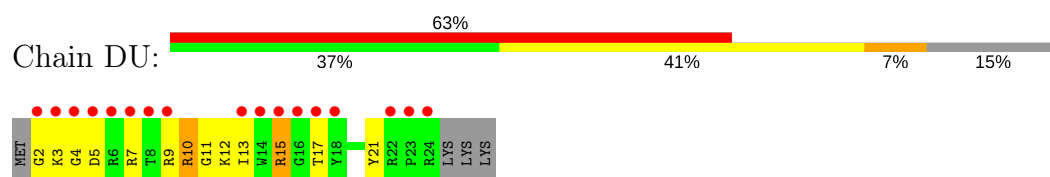
- Molecule 53: 30S ribosomal protein S20



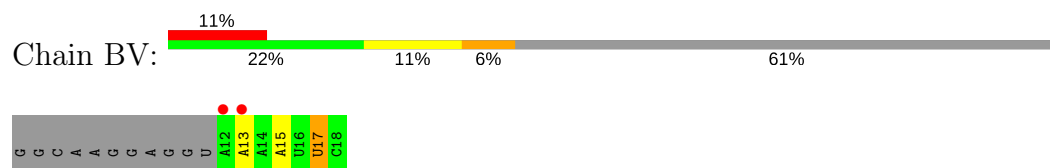
- Molecule 54: 30S ribosomal protein Thx



- Molecule 54: 30S ribosomal protein Thx



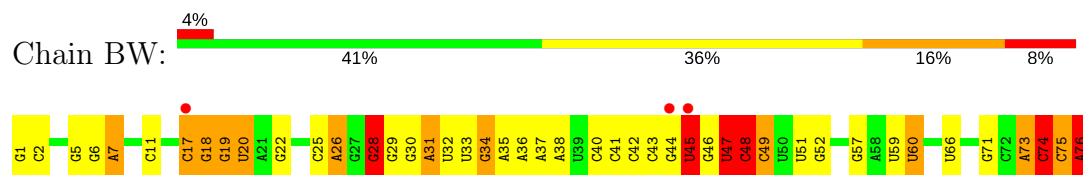
- Molecule 55: mRNA



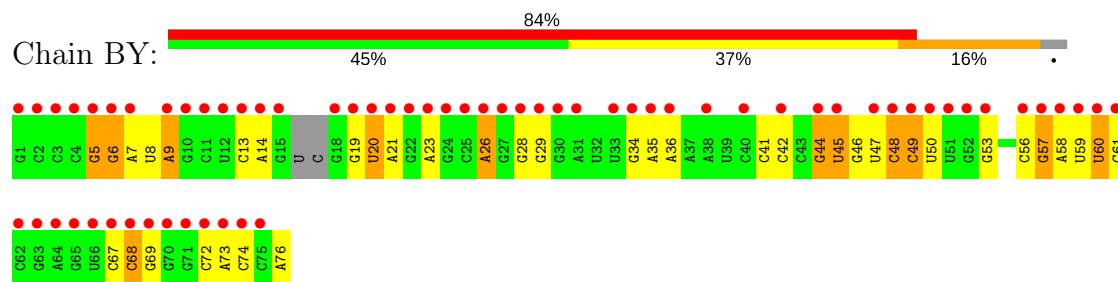
- Molecule 55: mRNA



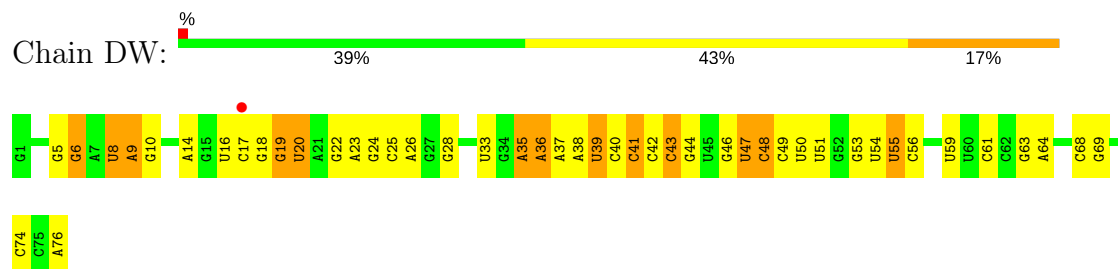
- Molecule 56: P-site tRNA



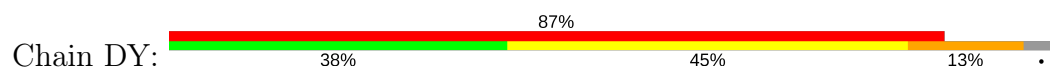
- Molecule 56: P-site tRNA

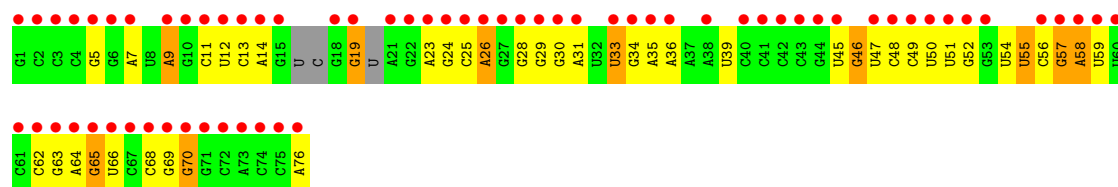


- Molecule 56: P-site tRNA



- Molecule 56: P-site tRNA

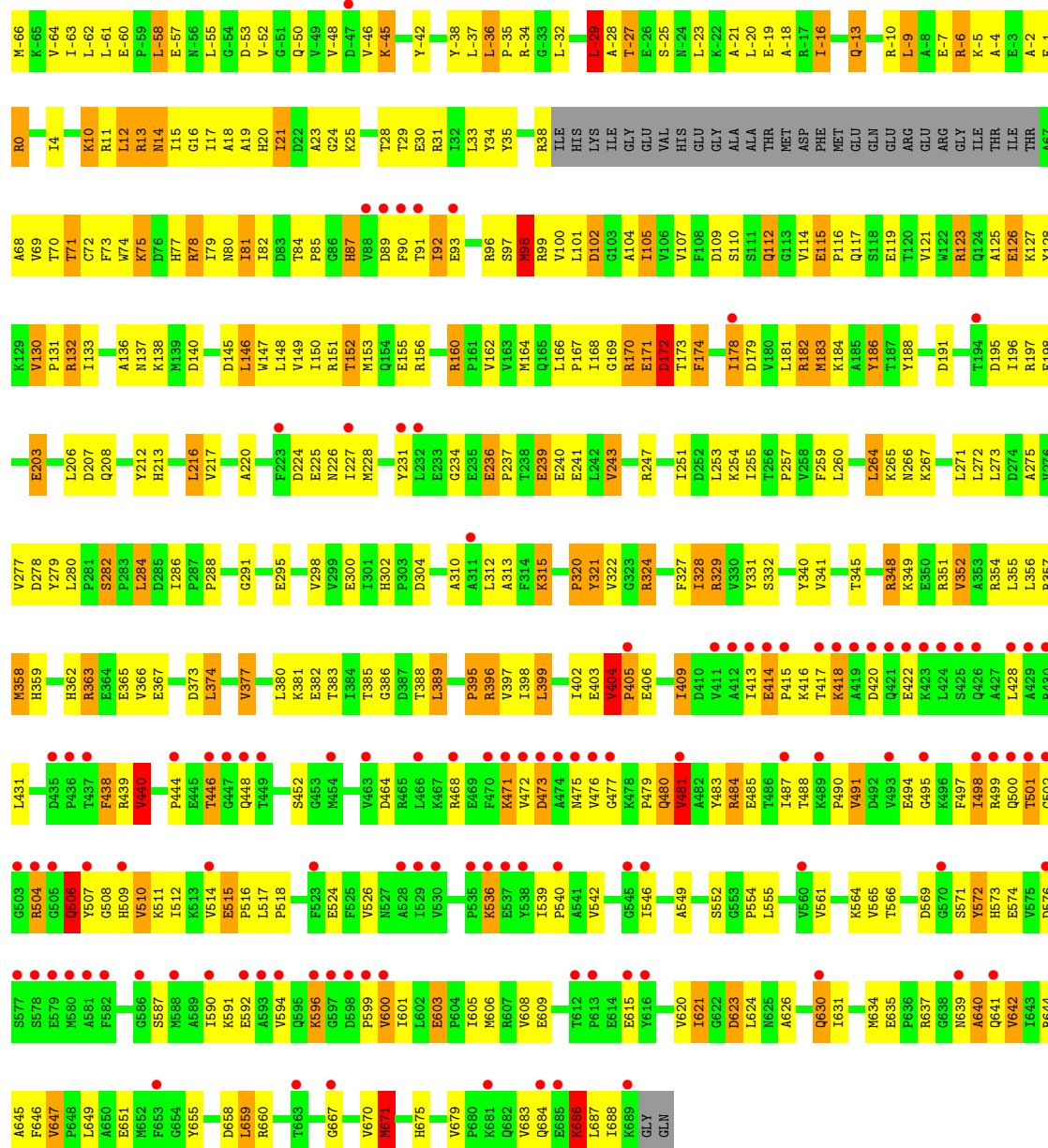




● Molecule 57: 50S ribosomal protein L9,Elongation factor G



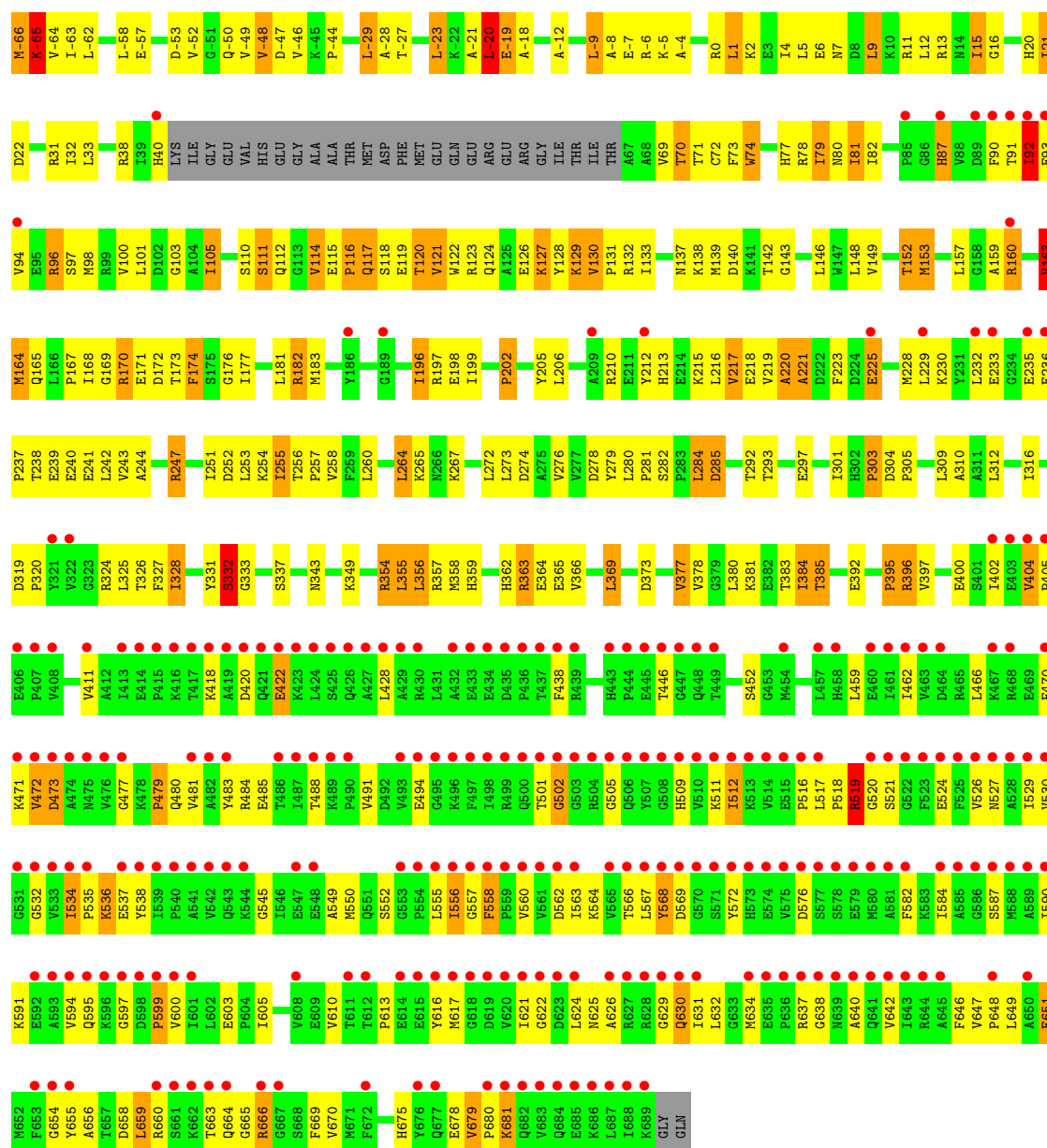
Chain BZ:



● Molecule 57: 50S ribosomal protein L9,Elongation factor G



Chain DZ:



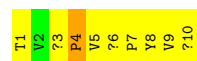
● Molecule 58: Dityromycin

Chain BX: 10% 60% 30%



● Molecule 58: Dityromycin

Chain DX: 10% 80% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.80-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 0.215 , 0.267	Depositor DCC
R_{free} test set	67916 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, ZN, MIA, 7MG, SF4, 2QZ, MG, 2QY, MVA, 004, 4SU, 2R3, 2R1, 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	1.41	444/69281 (0.6%)	2.07	3848/108144 (3.6%)
1	CA	1.00	75/69179 (0.1%)	1.66	1653/107984 (1.5%)
2	AB	1.17	7/2878 (0.2%)	1.92	120/4490 (2.7%)
2	CB	0.66	0/2878	1.33	24/4490 (0.5%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.94	2/2186 (0.1%)	1.04	5/2944 (0.2%)
4	CD	0.74	0/2192	0.95	6/2951 (0.2%)
5	AE	0.93	0/1592	1.08	2/2149 (0.1%)
5	CE	0.72	0/1592	0.91	1/2149 (0.0%)
6	AF	0.91	2/1619 (0.1%)	1.01	4/2193 (0.2%)
6	CF	0.63	0/1615	0.83	1/2188 (0.0%)
7	AG	0.60	0/1450	0.83	2/1959 (0.1%)
7	CG	0.36	0/1449	0.62	0/1958
8	AH	0.84	0/1356	0.96	1/1834 (0.1%)
8	CH	0.49	0/1356	0.67	0/1834
9	AK	0.34	0/640	0.67	0/889
9	CK	0.28	0/640	0.61	0/889
10	AL	0.31	0/503	0.54	0/673
10	CL	0.34	0/503	0.60	0/673
11	AN	0.95	0/1144	1.01	3/1543 (0.2%)
11	CN	0.61	0/1144	0.81	0/1543
12	AO	0.91	1/943 (0.1%)	1.02	3/1269 (0.2%)
12	CO	0.77	0/943	0.87	0/1269
13	AP	0.85	0/1156	1.03	4/1537 (0.3%)
13	CP	0.57	0/1152	0.87	2/1533 (0.1%)
14	AQ	0.91	0/1143	0.97	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.82	1/1527 (0.1%)
15	AR	0.90	0/982	1.07	4/1312 (0.3%)
15	CR	0.65	0/982	0.88	1/1312 (0.1%)
16	AS	0.76	0/887	0.95	1/1180 (0.1%)
16	CS	0.49	0/880	0.74	0/1172

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.89	0/1105	1.02	3/1477 (0.2%)
17	CT	0.65	0/1097	0.89	1/1468 (0.1%)
18	AU	1.11	3/977 (0.3%)	1.05	1/1301 (0.1%)
18	CU	0.69	1/977 (0.1%)	0.79	0/1301
19	AV	0.98	0/782	1.08	2/1049 (0.2%)
19	CV	0.58	0/782	0.79	0/1049
20	AW	1.10	2/897 (0.2%)	1.09	7/1205 (0.6%)
20	CW	0.80	0/897	0.92	0/1205
21	AX	0.96	0/764	0.99	0/1025
21	CX	0.67	0/764	0.83	1/1025 (0.1%)
22	AY	0.88	0/819	0.97	0/1095
22	CY	0.56	0/819	0.72	0/1095
23	AZ	0.72	1/1483 (0.1%)	0.93	4/2017 (0.2%)
23	CZ	0.45	0/1483	0.73	0/2017
24	A0	0.87	0/616	1.05	1/821 (0.1%)
24	C0	0.60	0/616	0.76	0/821
25	A1	0.87	0/762	0.92	0/1014
25	C1	0.67	0/762	0.89	1/1014 (0.1%)
26	A2	0.79	0/590	0.93	1/781 (0.1%)
26	C2	0.59	0/590	0.73	0/781
27	A3	1.01	0/474	1.06	0/635
27	C3	0.57	0/469	0.81	0/630
28	A4	0.50	0/571	0.72	0/768
28	C4	0.35	0/545	0.59	0/737
29	A5	0.99	0/469	1.05	0/635
29	C5	0.76	1/469 (0.2%)	0.86	0/635
30	A6	0.95	0/460	1.03	1/613 (0.2%)
30	C6	0.71	0/456	0.81	1/608 (0.2%)
31	A7	0.99	0/426	1.11	3/561 (0.5%)
31	C7	0.77	0/426	0.99	1/561 (0.2%)
32	A8	0.95	0/525	0.94	0/691
32	C8	0.63	0/525	0.82	0/691
33	A9	0.98	0/310	1.05	0/407
33	C9	0.64	0/310	0.80	0/407
34	BA	0.77	3/35976 (0.0%)	1.42	439/56145 (0.8%)
34	DA	0.68	1/36119 (0.0%)	1.30	238/56370 (0.4%)
35	BB	0.45	0/1881	0.69	1/2542 (0.0%)
35	DB	0.38	0/1860	0.66	0/2518
36	BC	0.40	0/1576	0.61	0/2130
36	DC	0.35	0/1568	0.55	0/2122
37	BD	0.49	0/1689	0.71	0/2267
37	DD	0.51	0/1708	0.73	1/2289 (0.0%)
38	BE	0.60	0/1145	0.79	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.51	0/1149	0.77	0/1548
39	BF	0.50	0/825	0.77	0/1118
39	DF	0.51	0/833	0.72	0/1128
40	BG	0.43	0/1250	0.60	0/1679
40	DG	0.35	0/1254	0.58	0/1683
41	BH	0.55	0/1108	0.76	0/1494
41	DH	0.45	0/1108	0.75	1/1494 (0.1%)
42	BI	0.44	0/1005	0.64	0/1350
42	DI	0.34	0/997	0.56	0/1343
43	BJ	0.39	0/722	0.71	2/982 (0.2%)
43	DJ	0.34	0/727	0.59	0/988
44	BK	0.56	0/848	0.72	0/1149
44	DK	0.48	0/848	0.63	0/1149
45	BL	0.65	0/946	0.79	0/1274
45	DL	0.64	0/946	0.84	1/1274 (0.1%)
46	BM	0.42	0/933	0.67	0/1253
46	DM	0.30	0/917	0.52	0/1234
47	BN	0.45	0/501	0.67	0/664
47	DN	0.33	0/501	0.60	0/664
48	BO	0.57	0/739	0.74	0/985
48	DO	0.50	0/739	0.70	0/985
49	BP	0.55	0/697	0.81	1/939 (0.1%)
49	DP	0.49	0/693	0.72	0/935
50	BQ	0.58	0/836	0.78	0/1117
50	DQ	0.51	0/836	0.72	0/1117
51	BR	0.55	0/560	0.83	0/746
51	DR	0.48	0/560	0.70	0/746
52	BS	0.34	0/676	0.59	0/911
52	DS	0.31	0/661	0.66	0/893
53	BT	0.50	0/730	0.81	0/965
53	DT	0.46	0/733	0.72	0/969
54	BU	0.42	0/203	0.69	0/266
54	DU	0.38	0/203	0.59	0/266
55	BV	0.64	0/165	1.06	0/254
55	DV	0.54	0/137	1.11	0/211
56	BW	0.86	0/1650	1.64	45/2569 (1.8%)
56	BY	0.42	0/1602	0.95	1/2493 (0.0%)
56	DW	0.65	0/1650	1.29	7/2569 (0.3%)
56	DY	0.35	0/1579	0.86	0/2455
57	BZ	0.49	0/5763	0.72	1/7804 (0.0%)
57	DZ	0.45	0/5784	0.69	1/7835 (0.0%)
58	BX	0.67	0/20	0.66	0/23
58	DX	0.70	0/20	1.43	0/23

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.95	543/329767 (0.2%)	1.50	6455/491645 (1.3%)

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
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

The worst 5 of 543 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	N9-C4	-15.28	1.28	1.37
1	AA	354	A	N9-C4	-13.92	1.29	1.37
1	AA	2299	A	N9-C4	-13.50	1.29	1.37
1	AA	1188	A	N9-C4	-13.32	1.29	1.37
1	AA	990	A	N9-C4	-11.81	1.30	1.37

The worst 5 of 6455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	553	A	N1-C6-N6	26.84	134.71	118.60
1	AA	990	A	N1-C2-N3	21.55	140.07	129.30
1	AA	990	A	C6-C5-N7	-21.18	117.48	132.30
1	AA	354	A	C2-N3-C4	-21.03	100.09	110.60
1	AA	553	A	C6-C5-N7	-20.90	117.67	132.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	74	PRO	Peptide
6	AF	194	MET	Peptide
19	AV	54	GLY	Peptide

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Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	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	31172	850	0
1	CA	61771	0	31146	1166	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	153	3
3	CC	1063	0	1090	186	15
4	AD	2136	0	2218	84	0
4	CD	2142	0	2229	85	0
5	AE	1559	0	1618	58	0
5	CE	1559	0	1618	76	0
6	AF	1584	0	1625	62	0
6	CF	1580	0	1619	75	0
7	AG	1425	0	1443	64	0
7	CG	1424	0	1434	82	0
8	AH	1330	0	1407	53	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	15	0
9	CK	641	0	309	9	0
10	AL	498	0	521	20	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	31	0
11	CN	1117	0	1184	38	0
12	AO	933	0	996	30	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	57	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	32	0
15	CR	968	0	1033	37	0
16	AS	877	0	938	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	CS	870	0	923	67	0
17	AT	1091	0	1151	48	0
17	CT	1083	0	1136	42	0
18	AU	959	0	1019	29	0
18	CU	959	0	1018	40	0
19	AV	771	0	830	11	0
19	CV	771	0	830	24	0
20	AW	886	0	940	23	0
20	CW	886	0	940	40	0
21	AX	750	0	814	24	0
21	CX	750	0	814	28	0
22	AY	806	0	881	37	0
22	CY	806	0	882	45	0
23	AZ	1451	0	1457	61	0
23	CZ	1451	0	1457	72	0
24	A0	608	0	622	20	0
24	C0	608	0	622	27	0
25	A1	755	0	826	29	0
25	C1	755	0	826	23	0
26	A2	588	0	643	16	0
26	C2	588	0	643	28	0
27	A3	469	0	518	12	0
27	C3	464	0	514	25	0
28	A4	558	0	545	31	0
28	C4	532	0	507	28	0
29	A5	455	0	465	15	0
29	C5	455	0	465	16	0
30	A6	453	0	473	17	0
30	C6	449	0	469	20	0
31	A7	418	0	467	16	0
31	C7	418	0	467	12	0
32	A8	517	0	582	25	0
32	C8	517	0	582	24	0
33	A9	307	0	335	11	0
33	C9	307	0	335	13	0
34	BA	32141	0	16224	681	0
34	DA	32268	0	16287	742	0
35	BB	1846	0	1867	78	0
35	DB	1825	0	1828	101	0
36	BC	1552	0	1546	65	0
36	DC	1544	0	1524	63	0
37	BD	1659	0	1679	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	DD	1678	0	1719	86	0
38	BE	1129	0	1185	51	0
38	DE	1133	0	1191	69	0
39	BF	812	0	804	29	0
39	DF	820	0	814	37	0
40	BG	1231	0	1238	45	0
40	DG	1235	0	1249	52	0
41	BH	1088	0	1126	53	0
41	DH	1088	0	1126	74	0
42	BI	986	0	995	52	0
42	DI	978	0	966	56	0
43	BJ	709	0	650	32	0
43	DJ	714	0	672	32	0
44	BK	833	0	836	34	0
44	DK	833	0	836	26	0
45	BL	930	0	980	39	0
45	DL	930	0	980	45	0
46	BM	923	0	970	37	0
46	DM	907	0	934	39	0
47	BN	492	0	529	30	0
47	DN	492	0	531	46	0
48	BO	728	0	760	29	0
48	DO	728	0	760	29	0
49	BP	681	0	697	50	0
49	DP	677	0	686	36	0
50	BQ	823	0	891	32	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	24	0
51	DR	555	0	618	30	0
52	BS	661	0	675	36	0
52	DS	646	0	644	34	0
53	BT	728	0	798	36	0
53	DT	731	0	807	27	0
54	BU	199	0	208	7	0
54	DU	199	0	208	9	0
55	BV	148	0	76	3	0
55	DV	123	0	66	1	0
56	BW	1631	0	839	25	0
56	BY	1581	0	805	24	0
56	DW	1631	0	839	33	0
56	DY	1561	0	796	34	0
57	BZ	5663	0	5747	265	15

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DZ	5682	0	5766	236	3
58	BX	93	0	85	14	0
58	DX	93	0	85	15	0
59	A0	5	0	0	0	0
59	A2	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	2	0	0	0	0
59	A7	1	0	0	0	0
59	A8	1	0	0	0	0
59	A9	1	0	0	0	0
59	AA	832	0	0	0	0
59	AB	23	0	0	0	0
59	AD	10	0	0	0	0
59	AE	5	0	0	0	0
59	AF	6	0	0	0	0
59	AG	2	0	0	0	0
59	AH	1	0	0	0	0
59	AN	3	0	0	0	0
59	AO	1	0	0	0	0
59	AP	3	0	0	0	0
59	AQ	4	0	0	0	0
59	AR	1	0	0	0	0
59	AU	5	0	0	0	0
59	AV	2	0	0	0	0
59	AW	3	0	0	0	0
59	AX	1	0	0	0	0
59	AY	1	0	0	0	0
59	AZ	1	0	0	0	0
59	BA	215	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
59	BK	1	0	0	0	0
59	BL	2	0	0	0	0
59	BM	1	0	0	0	0
59	BN	2	0	0	0	0
59	BS	1	0	0	0	0
59	BT	1	0	0	0	0
59	BW	3	0	0	0	0
59	BZ	1	0	0	0	0
59	C0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	C1	1	0	0	0	0
59	C3	1	0	0	0	0
59	C5	1	0	0	0	0
59	C7	1	0	0	0	0
59	C8	1	0	0	0	0
59	CA	664	0	0	0	0
59	CB	13	0	0	0	0
59	CD	4	0	0	0	0
59	CE	5	0	0	0	0
59	CF	4	0	0	0	0
59	CG	1	0	0	0	0
59	CN	1	0	0	0	0
59	CO	1	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	4	0	0	0	0
59	CR	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	2	0	0	0	0
59	CW	1	0	0	0	0
59	CX	1	0	0	0	0
59	DA	171	0	0	0	0
59	DD	1	0	0	0	0
59	DE	2	0	0	0	0
59	DF	1	0	0	0	0
59	DJ	1	0	0	0	0
59	DK	1	0	0	0	0
59	DT	1	0	0	0	0
59	DW	3	0	0	0	0
59	DZ	2	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	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	DD	8	0	0	2	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	7	0
63	A0	6	0	0	0	0
63	A1	2	0	0	0	0
63	A3	2	0	0	0	0
63	A5	3	0	0	0	0
63	A6	1	0	0	0	0
63	A7	2	0	0	1	0
63	A8	10	0	0	1	0
63	A9	1	0	0	0	0
63	AA	1413	0	0	66	0
63	AB	38	0	0	3	0
63	AD	10	0	0	2	0
63	AE	17	0	0	4	0
63	AF	11	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	1	0	0	0	0
63	AO	3	0	0	0	0
63	AP	16	0	0	1	0
63	AQ	4	0	0	1	0
63	AR	2	0	0	0	0
63	AS	1	0	0	1	0
63	AT	1	0	0	0	0
63	AU	4	0	0	0	0
63	AV	1	0	0	0	0
63	AW	1	0	0	0	0
63	AX	3	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	213	0	0	19	0
63	BD	1	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BP	1	0	0	0	0
63	BV	1	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	2	0	0	0	0
63	C0	4	0	0	0	0
63	C3	2	0	0	0	0
63	C5	1	0	0	0	0
63	C7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C8	4	0	0	0	0
63	CA	983	0	0	79	0
63	CB	9	0	0	1	0
63	CD	15	0	0	1	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CN	1	0	0	0	0
63	CO	1	0	0	0	0
63	CP	11	0	0	2	0
63	CQ	2	0	0	1	0
63	CT	3	0	0	0	0
63	CU	2	0	0	0	0
63	CV	1	0	0	1	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	2	0	0	1	0
63	DA	157	0	0	13	0
63	DD	1	0	0	0	0
63	DE	2	0	0	2	0
63	DH	1	0	0	0	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DT	1	0	0	0	0
All	All	310038	0	209219	7358	18

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 15.

The worst 5 of 7358 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:1891:G:H5''	3:AC:206:LYS:CG	1.32	1.59
1:AA:1891:G:C5'	3:AC:206:LYS:HD2	1.36	1.52
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.36	1.51
1:CA:2132:U:C4	3:CC:6:LYS:HE3	1.51	1.41
1:AA:1891:G:C5'	3:AC:206:LYS:CD	2.01	1.37

The worst 5 of 18 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)
57:BZ:502:GLY:N	3:CC:9:ARG:CD[2_655]	1.69	0.51
57:BZ:573:HIS:CE1	3:CC:13:GLU:OE1[2_655]	1.71	0.49
57:BZ:504:ARG:NH1	3:CC:9:ARG:NH2[2_655]	1.79	0.41
57:BZ:573:HIS:NE2	3:CC:13:GLU:OE1[2_655]	1.79	0.41
57:BZ:502:GLY:N	3:CC:9:ARG:CG[2_655]	1.79	0.41

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%)	249 (91%)	19 (7%)	5 (2%)	10	32
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	2	8
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	18	50
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	12	37
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	32	67
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	4	14
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	4	15
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	3	12
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	11	34
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	1	4
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	1	4
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	3	8
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	25	59
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	8	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	6	22
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	13	39
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	9	28
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	25	59
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	13	39
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	6	21
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	4	13
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	3	9
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	11	36
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	11	36
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	6	21
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	18	50
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	5	17
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	8	26
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	2	6
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	5	18
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	2	8
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	4
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	1	2
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	14	41
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	5	16
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	12	37
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	4	14
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	1
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	1
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	10	32
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	9	28
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	8	26
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	11	36
32	C8	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	11	36
33	A9	35/37 (95%)	35 (100%)	0	0	100	100
33	C9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	BB	229/256 (90%)	182 (80%)	33 (14%)	14 (6%)	2	4
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	2
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	2	6
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	5	18
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	2	5
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	3	12
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	2	6
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	2	8
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	5	16
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	5	16
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	4	15
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	8	26
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	2	7
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	2	6
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	5	16
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	3
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	5	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	10	32
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	4	13
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	22	55
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	4	15
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	4	14
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	2
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	7
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	4	15
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	4	14
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	3	8
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	2	7
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	5	16
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	5	17
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	2	8
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	4	13
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	3	10
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	1	4
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	1	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	3
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	2
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	3	9

5 of 586 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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	103 (93%)	8 (7%)	17	43
3	CC	111/180 (62%)	103 (93%)	8 (7%)	17	43
4	AD	215/218 (99%)	173 (80%)	42 (20%)	1	4
4	CD	216/218 (99%)	178 (82%)	38 (18%)	2	6
5	AE	164/166 (99%)	138 (84%)	26 (16%)	3	9
5	CE	164/166 (99%)	137 (84%)	27 (16%)	2	8
6	AF	160/166 (96%)	132 (82%)	28 (18%)	2	6
6	CF	159/166 (96%)	126 (79%)	33 (21%)	1	4
7	AG	143/156 (92%)	115 (80%)	28 (20%)	1	4
7	CG	142/156 (91%)	114 (80%)	28 (20%)	1	4
8	AH	144/148 (97%)	120 (83%)	24 (17%)	2	7
8	CH	144/148 (97%)	118 (82%)	26 (18%)	2	6
10	AL	50/111 (45%)	39 (78%)	11 (22%)	1	3
10	CL	50/111 (45%)	35 (70%)	15 (30%)	0	1
11	AN	118/119 (99%)	93 (79%)	25 (21%)	1	3
11	CN	118/119 (99%)	85 (72%)	33 (28%)	0	1
12	AO	100/100 (100%)	87 (87%)	13 (13%)	5	14
12	CO	100/100 (100%)	86 (86%)	14 (14%)	4	12
13	AP	116/116 (100%)	97 (84%)	19 (16%)	2	8
13	CP	115/116 (99%)	95 (83%)	20 (17%)	2	7
14	AQ	111/111 (100%)	94 (85%)	17 (15%)	3	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	CQ	111/111 (100%)	83 (75%)	28 (25%)	0	2
15	AR	101/101 (100%)	80 (79%)	21 (21%)	1	4
15	CR	101/101 (100%)	87 (86%)	14 (14%)	4	12
16	AS	87/88 (99%)	71 (82%)	16 (18%)	2	5
16	CS	85/88 (97%)	68 (80%)	17 (20%)	1	4
17	AT	115/127 (91%)	96 (84%)	19 (16%)	2	8
17	CT	113/127 (89%)	98 (87%)	15 (13%)	4	13
18	AU	93/94 (99%)	77 (83%)	16 (17%)	2	7
18	CU	93/94 (99%)	81 (87%)	12 (13%)	5	15
19	AV	80/82 (98%)	67 (84%)	13 (16%)	3	8
19	CV	80/82 (98%)	65 (81%)	15 (19%)	2	5
20	AW	90/92 (98%)	76 (84%)	14 (16%)	3	9
20	CW	90/92 (98%)	75 (83%)	15 (17%)	2	7
21	AX	77/78 (99%)	67 (87%)	10 (13%)	5	14
21	CX	77/78 (99%)	66 (86%)	11 (14%)	4	11
22	AY	85/91 (93%)	66 (78%)	19 (22%)	1	3
22	CY	85/91 (93%)	66 (78%)	19 (22%)	1	3
23	AZ	156/179 (87%)	120 (77%)	36 (23%)	1	2
23	CZ	156/179 (87%)	125 (80%)	31 (20%)	1	4
24	A0	61/67 (91%)	55 (90%)	6 (10%)	9	27
24	C0	61/67 (91%)	50 (82%)	11 (18%)	2	6
25	A1	80/83 (96%)	66 (82%)	14 (18%)	2	6
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2	6
26	A2	65/67 (97%)	56 (86%)	9 (14%)	4	12
26	C2	65/67 (97%)	51 (78%)	14 (22%)	1	3
27	A3	51/52 (98%)	41 (80%)	10 (20%)	1	4
27	C3	50/52 (96%)	38 (76%)	12 (24%)	1	2
28	A4	60/63 (95%)	52 (87%)	8 (13%)	4	13
28	C4	53/63 (84%)	39 (74%)	14 (26%)	0	1
29	A5	50/52 (96%)	43 (86%)	7 (14%)	4	12
29	C5	50/52 (96%)	42 (84%)	8 (16%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0	1
30	C6	50/52 (96%)	43 (86%)	7 (14%)	4	12
31	A7	41/42 (98%)	35 (85%)	6 (15%)	3	11
31	C7	41/42 (98%)	35 (85%)	6 (15%)	3	11
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1	4
32	C8	54/55 (98%)	48 (89%)	6 (11%)	7	21
33	A9	34/34 (100%)	30 (88%)	4 (12%)	6	18
33	C9	34/34 (100%)	30 (88%)	4 (12%)	6	18
35	BB	192/220 (87%)	157 (82%)	35 (18%)	2	6
35	DB	187/220 (85%)	148 (79%)	39 (21%)	1	4
36	BC	143/188 (76%)	127 (89%)	16 (11%)	7	21
36	DC	141/188 (75%)	113 (80%)	28 (20%)	1	4
37	BD	170/181 (94%)	136 (80%)	34 (20%)	1	4
37	DD	174/181 (96%)	143 (82%)	31 (18%)	2	6
38	BE	113/123 (92%)	86 (76%)	27 (24%)	1	2
38	DE	114/123 (93%)	82 (72%)	32 (28%)	0	1
39	BF	84/90 (93%)	70 (83%)	14 (17%)	2	7
39	DF	86/90 (96%)	74 (86%)	12 (14%)	4	12
40	BG	119/127 (94%)	99 (83%)	20 (17%)	2	7
40	DG	120/127 (94%)	104 (87%)	16 (13%)	4	13
41	BH	114/119 (96%)	90 (79%)	24 (21%)	1	3
41	DH	114/119 (96%)	86 (75%)	28 (25%)	1	2
42	BI	91/99 (92%)	78 (86%)	13 (14%)	4	11
42	DI	89/99 (90%)	73 (82%)	16 (18%)	2	6
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	6	17
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	3	9
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1	3
44	DK	83/99 (84%)	64 (77%)	19 (23%)	1	3
45	BL	97/109 (89%)	83 (86%)	14 (14%)	4	11
45	DL	97/109 (89%)	74 (76%)	23 (24%)	1	2
46	BM	91/101 (90%)	80 (88%)	11 (12%)	6	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	75 (85%)	13 (15%)	3	10
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	3
47	DN	49/50 (98%)	42 (86%)	7 (14%)	4	11
48	BO	78/80 (98%)	70 (90%)	8 (10%)	8	24
48	DO	78/80 (98%)	66 (85%)	12 (15%)	3	9
49	BP	69/74 (93%)	54 (78%)	15 (22%)	1	3
49	DP	68/74 (92%)	51 (75%)	17 (25%)	1	2
50	BQ	94/97 (97%)	82 (87%)	12 (13%)	5	15
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	3	10
51	BR	59/77 (77%)	49 (83%)	10 (17%)	2	7
51	DR	59/77 (77%)	52 (88%)	7 (12%)	6	18
52	BS	70/80 (88%)	59 (84%)	11 (16%)	3	9
52	DS	67/80 (84%)	55 (82%)	12 (18%)	2	6
53	BT	70/82 (85%)	53 (76%)	17 (24%)	1	2
53	DT	71/82 (87%)	59 (83%)	12 (17%)	2	7
54	BU	18/22 (82%)	17 (94%)	1 (6%)	25	57
54	DU	18/22 (82%)	16 (89%)	2 (11%)	7	21
57	BZ	604/636 (95%)	477 (79%)	127 (21%)	1	4
57	DZ	607/636 (95%)	509 (84%)	98 (16%)	3	8
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8760 (82%)	1904 (18%)	2	6

5 of 1904 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	186	TYR
7	CG	136	ARG
50	DQ	6	LEU
57	BZ	354	ARG
4	CD	113	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 172 such sidechains are listed below:

Mol	Chain	Res	Type
57	BZ	573	HIS
13	CP	38	GLN
48	DO	28	GLN
3	CC	67	HIS
6	CF	203	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2864/2915 (98%)	526 (18%)	0
1	CA	2860/2915 (98%)	611 (21%)	0
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	0
34	DA	1498/1521 (98%)	350 (23%)	0
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	16 (21%)	0
56	BY	71/76 (93%)	23 (32%)	0
56	DW	74/76 (97%)	23 (31%)	0
56	DY	69/76 (90%)	21 (30%)	0
All	All	9250/9454 (97%)	1946 (21%)	0

5 of 1946 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	U
1	AA	13	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

There are no RNA pucker outliers to report.

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

42 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	56	16,21,22	1.47	2 (12%)	20,30,33	3.85	8 (40%)
56	MIA	BW	37	56	23,31,32	1.78	4 (17%)	25,44,47	1.83	6 (24%)
56	PSU	BW	39	56	16,21,22	1.48	2 (12%)	20,30,33	3.43	6 (30%)
56	7MG	BW	46	56	20,26,27	1.42	2 (10%)	22,39,42	2.92	5 (22%)
56	5MU	BW	54	56	14,22,23	0.78	0	16,32,35	2.81	3 (18%)
56	PSU	BW	55	56	16,21,22	1.23	1 (6%)	20,30,33	3.71	6 (30%)
56	4SU	BW	8	56	14,21,22	1.19	1 (7%)	15,30,33	1.50	2 (13%)
58	2QZ	BX	1	58	7,8,9	0.81	0	4,10,12	5.73	3 (75%)
58	2QY	BX	10	58	13,13,14	2.39	2 (15%)	12,16,18	2.15	4 (33%)
58	004	BX	3	58	8,10,11	1.23	1 (12%)	11,12,14	2.35	4 (36%)
58	MVA	BX	5	58	7,7,8	1.28	1 (14%)	7,8,10	1.55	2 (28%)
58	2R1	BX	6	58	10,10,11	1.95	3 (30%)	7,13,15	4.01	2 (28%)
58	2R3	BX	8	58	14,14,15	0.85	0	16,18,20	2.08	7 (43%)
58	MVA	BX	9	58	7,7,8	1.14	1 (14%)	7,8,10	1.84	2 (28%)
56	PSU	BY	32	56	16,21,22	1.10	1 (6%)	20,30,33	3.52	6 (30%)
56	MIA	BY	37	56	18,24,32	1.28	2 (11%)	17,35,47	1.91	3 (17%)
56	PSU	BY	39	56	16,21,22	1.18	1 (6%)	20,30,33	3.66	6 (30%)
56	7MG	BY	46	56	20,26,27	1.66	2 (10%)	22,39,42	2.80	6 (27%)
56	5MU	BY	54	56	14,22,23	0.76	0	16,32,35	2.32	2 (12%)
56	PSU	BY	55	56	16,21,22	1.27	1 (6%)	20,30,33	3.57	6 (30%)
56	4SU	BY	8	56	14,21,22	1.20	1 (7%)	15,30,33	1.68	3 (20%)
56	PSU	DW	32	56	16,21,22	0.91	0	20,30,33	3.59	7 (35%)
56	MIA	DW	37	56	23,31,32	1.65	4 (17%)	25,44,47	1.53	5 (20%)
56	PSU	DW	39	56	16,21,22	1.23	2 (12%)	20,30,33	4.17	8 (40%)
56	7MG	DW	46	56	20,26,27	1.51	2 (10%)	22,39,42	2.79	6 (27%)
56	5MU	DW	54	56	14,22,23	0.72	0	16,32,35	2.29	3 (18%)
56	PSU	DW	55	56	16,21,22	1.27	1 (6%)	20,30,33	3.71	8 (40%)
56	4SU	DW	8	56	14,21,22	1.34	1 (7%)	15,30,33	1.41	2 (13%)
58	2QZ	DX	1	58	7,8,9	1.23	1 (14%)	4,10,12	5.55	2 (50%)
58	2QY	DX	10	58	13,13,14	2.47	2 (15%)	12,16,18	2.79	4 (33%)
58	004	DX	3	58	8,10,11	0.79	0	11,12,14	1.52	2 (18%)
58	MVA	DX	5	58	7,7,8	1.28	1 (14%)	7,8,10	1.44	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	2R1	DX	6	58	10,10,11	1.59	2 (20%)	7,13,15	2.61	4 (57%)
58	2R3	DX	8	58	14,14,15	0.60	0	16,18,20	1.76	5 (31%)
58	MVA	DX	9	58	7,7,8	1.58	2 (28%)	7,8,10	1.93	3 (42%)
56	PSU	DY	32	56	16,21,22	1.13	1 (6%)	20,30,33	3.57	6 (30%)
56	MIA	DY	37	56	18,24,32	1.18	2 (11%)	17,35,47	1.84	2 (11%)
56	PSU	DY	39	56	16,21,22	1.34	3 (18%)	20,30,33	3.77	6 (30%)
56	7MG	DY	46	56	20,26,27	1.65	3 (15%)	22,39,42	2.98	7 (31%)
56	5MU	DY	54	56	14,22,23	0.76	0	16,32,35	2.32	3 (18%)
56	PSU	DY	55	56	16,21,22	1.36	2 (12%)	20,30,33	3.53	6 (30%)
56	4SU	DY	8	56	14,21,22	1.27	1 (7%)	15,30,33	1.53	2 (13%)

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	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	4SU	BW	8	56	-	0/3/25/26	0/2/2/2
58	2QZ	BX	1	58	-	0/6/10/12	0/0/0/0
58	2QY	BX	10	58	-	0/3/8/10	0/1/1/1
58	004	BX	3	58	-	0/4/6/8	0/1/1/1
58	MVA	BX	5	58	-	0/5/8/10	0/0/0/0
58	2R1	BX	6	58	-	0/1/14/16	0/0/1/1
58	2R3	BX	8	58	-	0/10/12/14	0/1/1/1
58	MVA	BX	9	58	-	0/5/8/10	0/0/0/0
56	PSU	BY	32	56	-	0/7/25/26	0/2/2/2
56	MIA	BY	37	56	-	0/3/25/34	0/3/3/3
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	7MG	BY	46	56	-	0/7/37/38	0/3/3/3
56	5MU	BY	54	56	-	0/3/25/26	0/2/2/2
56	PSU	BY	55	56	-	0/7/25/26	0/2/2/2
56	4SU	BY	8	56	-	0/3/25/26	0/2/2/2
56	PSU	DW	32	56	-	1/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4SU	DW	8	56	-	0/3/25/26	0/2/2/2
58	2QZ	DX	1	58	-	0/6/10/12	0/0/0/0
58	2QY	DX	10	58	-	0/3/8/10	0/1/1/1
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
58	MVA	DX	5	58	-	0/5/8/10	0/0/0/0
58	2R1	DX	6	58	-	0/1/14/16	0/0/1/1
58	2R3	DX	8	58	-	0/10/12/14	0/1/1/1
58	MVA	DX	9	58	-	0/5/8/10	0/0/0/0
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	MIA	DY	37	56	-	0/3/25/34	0/3/3/3
56	PSU	DY	39	56	-	0/7/25/26	0/2/2/2
56	7MG	DY	46	56	-	0/7/37/38	0/3/3/3
56	5MU	DY	54	56	-	0/3/25/26	0/2/2/2
56	PSU	DY	55	56	-	0/7/25/26	0/2/2/2
56	4SU	DY	8	56	-	0/3/25/26	0/2/2/2

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-6.97	1.69	1.75
56	DW	37	MIA	C2-S10	-5.54	1.71	1.75
56	BW	39	PSU	C5-C1'	-4.77	1.48	1.52
56	BW	32	PSU	C5-C1'	-4.44	1.48	1.52
56	DW	8	4SU	C4-S4	-4.08	1.59	1.67

The worst 5 of 184 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	32	PSU	N1-C2-N3	-11.61	120.05	128.40
56	BW	55	PSU	N1-C2-N3	-9.96	121.23	128.40
56	DY	32	PSU	N1-C2-N3	-9.92	121.26	128.40
56	DW	39	PSU	N1-C2-N3	-9.78	121.36	128.40
56	BY	39	PSU	N1-C2-N3	-9.75	121.38	128.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	DW	32	PSU	O4'-C1'-C5-C4

There are no ring outliers.

23 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	32	PSU	1	0
56	BW	37	MIA	2	0
58	BX	10	2QY	1	0
58	BX	3	004	4	0
58	BX	5	MVA	2	0
58	BX	6	2R1	5	0
58	BX	8	2R3	2	0
58	BX	9	MVA	2	0
56	BY	8	4SU	1	0
56	DW	37	MIA	2	0
56	DW	39	PSU	6	0
56	DW	54	5MU	1	0
56	DW	55	PSU	1	0
56	DW	8	4SU	1	0
58	DX	1	2QZ	2	0
58	DX	10	2QY	9	0
58	DX	3	004	1	0
58	DX	5	MVA	2	0
58	DX	6	2R1	2	0
58	DX	8	2R3	2	0
58	DX	9	MVA	4	0
56	DY	46	7MG	2	0
56	DY	55	PSU	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2056 ligands modelled in this entry, 2052 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	$\# Z > 2$
61	SF4	BD	501	-	0,12,12	0.00	-	0,24,24	0.00	-
62	GDP	BZ	702	59	25,30,30	1.22	2 (8%)	26,47,47	2.19	9 (34%)
61	SF4	DD	501	37	0,12,12	0.00	-	0,24,24	0.00	-
62	GDP	DZ	703	59	25,30,30	1.20	2 (8%)	26,47,47	2.07	5 (19%)

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
61	SF4	BD	501	-	-	0/0/48/48	0/6/5/5
62	GDP	BZ	702	59	-	0/12/32/32	0/3/3/3
61	SF4	DD	501	37	-	0/0/48/48	0/6/5/5
62	GDP	DZ	703	59	-	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)
62	DZ	703	GDP	C5-C4	3.24	1.47	1.40
62	BZ	702	GDP	C5-C4	3.38	1.48	1.40
62	DZ	703	GDP	C6-C5	3.47	1.48	1.41
62	BZ	702	GDP	C6-C5	3.63	1.48	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	702	GDP	C5-C6-N1	-5.42	115.77	123.48
62	DZ	703	GDP	C5-C6-N1	-4.75	116.72	123.48
62	DZ	703	GDP	C6-C5-C4	-4.29	116.58	120.84
62	DZ	703	GDP	N3-C2-N1	-3.14	122.87	127.46
62	BZ	702	GDP	C6-C5-C4	-3.10	117.76	120.84

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
61	BD	501	SF4	1	0
62	BZ	702	GDP	5	0
61	DD	501	SF4	2	0
62	DZ	703	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2872/2915 (98%)	-0.06	94 (3%) 47 36	13, 31, 166, 313	0
1	CA	2868/2915 (98%)	0.06	121 (4%) 37 26	24, 55, 177, 331	0
2	AB	120/121 (99%)	-0.41	0 100 100	24, 47, 66, 112	0
2	CB	120/121 (99%)	0.01	1 (0%) 86 81	56, 104, 146, 178	0
3	AC	137/228 (60%)	5.84	122 (89%) 0 0	89, 187, 231, 259	0
3	CC	137/228 (60%)	8.37	136 (99%) 0 0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.46	2 (0%) 87 83	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.37	2 (0%) 87 83	13, 44, 77, 134	0
5	AE	204/206 (99%)	-0.47	0 100 100	7, 31, 60, 100	0
5	CE	204/206 (99%)	-0.31	0 100 100	16, 51, 87, 143	0
6	AF	203/210 (96%)	-0.41	0 100 100	6, 32, 76, 141	0
6	CF	203/210 (96%)	-0.19	1 (0%) 90 88	20, 66, 123, 158	0
7	AG	181/182 (99%)	-0.28	2 (1%) 80 74	34, 67, 114, 180	0
7	CG	181/182 (99%)	0.81	27 (14%) 3 1	75, 125, 183, 211	0
8	AH	174/180 (96%)	-0.46	2 (1%) 80 74	21, 46, 74, 199	0
8	CH	174/180 (96%)	0.66	12 (6%) 18 10	52, 92, 139, 174	0
9	AK	130/173 (75%)	1.27	32 (24%) 1 0	65, 131, 198, 223	0
9	CK	130/173 (75%)	2.85	77 (59%) 0 0	85, 163, 212, 233	0
10	AL	66/147 (44%)	4.22	54 (81%) 0 0	112, 182, 229, 247	0
10	CL	66/147 (44%)	5.46	58 (87%) 0 0	105, 183, 232, 263	0
11	AN	140/140 (100%)	-0.58	0 100 100	11, 28, 57, 97	0
11	CN	140/140 (100%)	-0.12	3 (2%) 64 54	35, 59, 92, 143	0
12	AO	122/122 (100%)	-0.43	0 100 100	16, 35, 66, 93	0
12	CO	122/122 (100%)	-0.32	0 100 100	30, 49, 80, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.35	0 100 100	8, 38, 78, 128	0
13	CP	149/150 (99%)	0.27	7 (4%) 32 22	26, 75, 123, 155	0
14	AQ	141/141 (100%)	-0.48	0 100 100	9, 32, 54, 99	0
14	CQ	141/141 (100%)	-0.27	1 (0%) 87 83	19, 63, 95, 146	0
15	AR	118/118 (100%)	-0.48	0 100 100	14, 27, 52, 76	0
15	CR	118/118 (100%)	-0.32	0 100 100	26, 49, 75, 106	0
16	AS	110/112 (98%)	-0.28	0 100 100	24, 47, 76, 86	0
16	CS	110/112 (98%)	0.66	8 (7%) 16 8	61, 96, 140, 166	0
17	AT	131/146 (89%)	-0.30	1 (0%) 86 81	20, 40, 95, 219	0
17	CT	131/146 (89%)	-0.22	1 (0%) 86 81	36, 56, 104, 152	0
18	AU	116/118 (98%)	-0.51	0 100 100	7, 22, 39, 87	0
18	CU	116/118 (98%)	-0.18	0 100 100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-0.60	0 100 100	11, 27, 58, 77	0
19	CV	101/101 (100%)	-0.07	2 (1%) 65 56	29, 69, 102, 162	0
20	AW	112/113 (99%)	-0.46	0 100 100	10, 24, 49, 145	0
20	CW	112/113 (99%)	-0.21	0 100 100	26, 45, 76, 159	0
21	AX	95/96 (98%)	-0.48	0 100 100	12, 33, 64, 108	0
21	CX	95/96 (98%)	0.15	4 (4%) 37 26	37, 63, 100, 173	0
22	AY	107/110 (97%)	-0.39	1 (0%) 84 79	18, 43, 88, 120	0
22	CY	107/110 (97%)	0.57	10 (9%) 9 5	48, 81, 124, 171	0
23	AZ	185/206 (89%)	-0.44	0 100 100	28, 56, 94, 136	0
23	CZ	185/206 (89%)	0.38	12 (6%) 20 12	52, 98, 145, 175	0
24	A0	77/85 (90%)	-0.42	0 100 100	10, 31, 54, 82	0
24	C0	77/85 (90%)	0.28	4 (5%) 28 19	27, 69, 104, 127	0
25	A1	97/98 (98%)	-0.31	1 (1%) 82 77	15, 39, 80, 98	0
25	C1	97/98 (98%)	-0.16	1 (1%) 82 77	31, 56, 95, 144	0
26	A2	70/72 (97%)	-0.39	1 (1%) 75 69	15, 43, 65, 135	0
26	C2	70/72 (97%)	-0.03	1 (1%) 75 69	47, 79, 110, 151	0
27	A3	59/60 (98%)	-0.40	1 (1%) 70 63	11, 26, 53, 112	0
27	C3	59/60 (98%)	0.39	2 (3%) 46 34	31, 63, 103, 162	0
28	A4	69/71 (97%)	0.72	12 (17%) 2 1	47, 102, 188, 221	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.33	21 (30%) 0 0	88, 158, 196, 229	0
29	A5	59/60 (98%)	-0.51	0 100 100	11, 23, 50, 68	0
29	C5	59/60 (98%)	-0.26	1 (1%) 70 63	16, 47, 82, 121	0
30	A6	53/54 (98%)	-0.44	0 100 100	17, 36, 62, 77	0
30	C6	53/54 (98%)	-0.11	0 100 100	41, 63, 86, 104	0
31	A7	48/49 (97%)	-0.34	1 (2%) 64 54	11, 21, 54, 100	0
31	C7	48/49 (97%)	-0.23	0 100 100	23, 36, 96, 120	0
32	A8	64/65 (98%)	-0.43	0 100 100	14, 26, 39, 63	0
32	C8	64/65 (98%)	-0.20	0 100 100	27, 53, 71, 94	0
33	A9	37/37 (100%)	-0.29	0 100 100	20, 33, 64, 67	0
33	C9	37/37 (100%)	0.05	0 100 100	44, 62, 90, 101	0
34	BA	1495/1521 (98%)	0.14	49 (3%) 47 36	24, 82, 180, 330	0
34	DA	1501/1521 (98%)	0.33	93 (6%) 21 13	40, 94, 207, 307	0
35	BB	231/256 (90%)	0.51	22 (9%) 9 5	53, 104, 167, 195	0
35	DB	231/256 (90%)	1.21	54 (23%) 1 1	67, 135, 197, 228	0
36	BC	206/239 (86%)	0.73	21 (10%) 7 4	74, 114, 169, 187	0
36	DC	206/239 (86%)	1.71	65 (31%) 0 0	88, 151, 198, 221	0
37	BD	208/209 (99%)	0.27	10 (4%) 31 21	54, 91, 141, 182	0
37	DD	208/209 (99%)	0.12	3 (1%) 75 69	53, 88, 134, 199	0
38	BE	148/162 (91%)	-0.09	0 100 100	37, 72, 110, 150	0
38	DE	148/162 (91%)	0.35	6 (4%) 38 27	43, 90, 131, 177	0
39	BF	100/101 (99%)	-0.12	0 100 100	43, 81, 124, 145	0
39	DF	100/101 (99%)	0.02	2 (2%) 65 56	49, 90, 133, 146	0
40	BG	155/156 (99%)	0.62	19 (12%) 5 2	66, 100, 155, 194	0
40	DG	155/156 (99%)	1.52	39 (25%) 1 0	81, 131, 178, 214	0
41	BH	137/138 (99%)	0.11	0 100 100	45, 73, 105, 121	0
41	DH	137/138 (99%)	0.35	7 (5%) 29 19	52, 92, 126, 160	0
42	BI	127/128 (99%)	1.37	31 (24%) 1 1	59, 115, 169, 192	0
42	DI	127/128 (99%)	2.47	70 (55%) 0 0	79, 154, 192, 248	0
43	BJ	97/105 (92%)	1.59	31 (31%) 0 0	75, 123, 173, 194	0
43	DJ	96/105 (91%)	2.40	51 (53%) 0 0	77, 160, 201, 221	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	-0.28	1 (0%) 84 79	30, 73, 117, 125	0
44	DK	114/129 (88%)	0.23	2 (1%) 69 60	61, 93, 139, 170	0
45	BL	122/132 (92%)	-0.21	1 (0%) 86 81	27, 61, 88, 110	0
45	DL	122/132 (92%)	0.04	1 (0%) 86 81	41, 70, 101, 142	0
46	BM	117/126 (92%)	0.53	9 (7%) 14 8	62, 108, 154, 187	0
46	DM	116/126 (92%)	1.45	34 (29%) 1 0	64, 156, 202, 235	0
47	BN	60/61 (98%)	0.80	5 (8%) 12 6	60, 110, 153, 173	0
47	DN	60/61 (98%)	1.96	28 (46%) 0 0	95, 142, 192, 210	0
48	BO	88/89 (98%)	-0.18	0 100 100	36, 69, 107, 139	0
48	DO	88/89 (98%)	0.09	0 100 100	50, 83, 115, 140	0
49	BP	82/88 (93%)	0.19	2 (2%) 59 49	46, 81, 126, 151	0
49	DP	82/88 (93%)	0.30	2 (2%) 59 49	50, 76, 108, 121	0
50	BQ	99/105 (94%)	-0.10	0 100 100	46, 72, 103, 119	0
50	DQ	99/105 (94%)	0.22	2 (2%) 65 56	47, 80, 116, 148	0
51	BR	68/88 (77%)	0.25	3 (4%) 35 25	45, 71, 115, 136	0
51	DR	68/88 (77%)	0.52	6 (8%) 11 5	58, 90, 129, 147	0
52	BS	84/93 (90%)	2.00	37 (44%) 0 0	68, 127, 168, 222	0
52	DS	83/93 (89%)	3.09	60 (72%) 0 0	98, 164, 213, 222	0
53	BT	96/106 (90%)	0.31	2 (2%) 64 54	49, 84, 117, 160	0
53	DT	96/106 (90%)	0.15	3 (3%) 49 38	48, 81, 126, 145	0
54	BU	23/27 (85%)	1.33	6 (26%) 1 0	60, 100, 114, 154	0
54	DU	23/27 (85%)	2.80	17 (73%) 0 0	78, 134, 159, 181	0
55	BV	7/18 (38%)	1.21	2 (28%) 1 0	61, 69, 175, 190	0
55	DV	6/18 (33%)	1.83	3 (50%) 0 0	89, 95, 181, 204	0
56	BW	69/76 (90%)	0.28	3 (4%) 36 26	38, 69, 118, 210	0
56	BY	67/76 (88%)	4.16	64 (95%) 0 0	76, 232, 280, 304	0
56	DW	69/76 (90%)	0.57	1 (1%) 75 69	48, 108, 151, 254	0
56	DY	66/76 (86%)	6.45	66 (100%) 0 0	145, 283, 315, 338	0
57	BZ	728/758 (96%)	0.71	113 (15%) 2 1	38, 97, 190, 248	0
57	DZ	730/758 (96%)	1.48	243 (33%) 0 0	27, 113, 212, 264	0
58	BX	3/10 (30%)	-0.19	0 100 100	83, 83, 83, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
58	DX	3/10 (30%)	0.19	0 100 100	81, 81, 81, 81	0
All	All	22705/23918 (94%)	0.37	2128 (9%) 9 5	6, 70, 189, 338	0

The worst 5 of 2128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CC	166	ASN	26.5
3	CC	167	ASP	25.1
3	CC	179	ALA	24.5
3	AC	171	ALA	21.6
3	CC	175	PRO	19.6

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	2QZ	BX	1	9/10	0.93	0.25	-	82,82,82,82	0
56	7MG	DY	46	24/25	0.52	0.41	-	266,266,266,266	0
58	MVA	DX	9	8/9	0.94	0.24	-	81,81,81,81	0
56	MIA	DY	37	22/30	0.46	0.85	-	271,271,271,271	0
56	PSU	BY	39	20/21	0.68	0.54	-	197,197,197,197	0
58	004	BX	3	10/11	0.90	0.12	-	82,82,82,82	0
56	MIA	BW	37	29/30	0.94	0.22	-	79,79,79,79	0
56	5MU	BY	54	21/22	0.47	0.58	-	246,246,246,246	0
56	7MG	BW	46	24/25	0.89	0.19	-	76,76,76,76	3
58	004	DX	3	10/11	0.83	0.20	-	81,81,81,81	0
58	2QZ	DX	1	9/10	0.94	0.24	-	81,81,81,81	0
58	2R1	DX	6	10/11	0.83	0.15	-	81,81,81,81	0
56	PSU	BW	39	20/21	0.96	0.14	-	65,65,65,65	0
56	PSU	DY	39	20/21	0.18	1.03	-	291,291,291,291	0
56	PSU	DW	39	20/21	0.86	0.28	-	112,112,112,112	1
56	5MU	DY	54	21/22	0.38	0.84	-	303,303,303,303	0
56	PSU	DY	32	20/21	0.14	1.12	-	275,275,275,275	0
56	PSU	BW	55	20/21	0.91	0.17	-	79,79,79,79	0
58	2R3	DX	8	14/15	0.96	0.13	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	7MG	DW	46	24/25	0.87	0.23	-	124,124,124,124	0
58	2QY	DX	10	13/14	0.92	0.17	-	81,81,81,81	0
56	5MU	DW	54	21/22	0.89	0.20	-	95,95,95,95	1
56	4SU	DW	8	20/21	0.91	0.14	-	103,103,103,103	0
56	4SU	BW	8	20/21	0.96	0.14	-	60,60,60,60	1
56	MIA	DW	37	29/30	0.91	0.23	-	109,109,109,109	0
56	PSU	BY	32	20/21	0.47	0.55	-	226,226,226,226	0
56	PSU	BW	32	20/21	0.94	0.20	-	73,73,73,73	1
56	PSU	DW	55	20/21	0.88	0.19	-	92,92,92,92	0
56	7MG	BY	46	24/25	0.49	0.34	-	276,276,276,276	0
58	MVA	BX	5	8/9	0.87	0.15	-	82,82,82,82	0
56	PSU	BY	55	20/21	0.27	0.51	-	243,243,243,243	0
58	2R3	BX	8	14/15	0.92	0.14	-	82,82,82,82	0
56	5MU	BW	54	21/22	0.92	0.18	-	80,80,80,80	0
56	4SU	BY	8	20/21	0.52	0.34	-	239,239,239,239	0
56	PSU	DY	55	20/21	0.28	0.66	-	252,252,252,252	0
58	MVA	DX	5	8/9	0.95	0.37	-	81,81,81,81	0
56	4SU	DY	8	20/21	0.40	0.43	-	277,277,277,277	0
58	2QY	BX	10	13/14	0.90	0.19	-	82,82,82,82	0
58	2R1	BX	6	10/11	0.89	0.16	-	82,82,82,82	1
58	MVA	BX	9	8/9	0.90	0.31	-	82,82,82,82	0
56	PSU	DW	32	20/21	0.82	0.31	-	126,126,126,126	0
56	MIA	BY	37	22/30	0.72	0.42	-	186,186,186,186	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3018	1/1	0.82	1.43	122.96	67,67,67,67	0
59	MG	AA	3039	1/1	0.94	0.52	108.43	34,34,34,34	1
59	MG	AA	3710	1/1	0.96	0.51	69.24	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3087	1/1	0.86	0.81	58.96	68,68,68,68	0
59	MG	AA	3136	1/1	0.96	0.65	57.81	63,63,63,63	0
59	MG	AA	3216	1/1	0.97	0.60	56.87	38,38,38,38	0
59	MG	AA	3706	1/1	0.95	0.54	56.54	41,41,41,41	1
59	MG	CA	3499	1/1	0.72	0.50	56.42	62,62,62,62	0
59	MG	AA	3137	1/1	0.95	0.64	47.47	53,53,53,53	0
59	MG	AA	3772	1/1	0.91	0.61	46.36	61,61,61,61	1
59	MG	CA	3442	1/1	0.92	0.59	45.39	74,74,74,74	0
59	MG	AA	3179	1/1	0.91	0.50	40.29	45,45,45,45	1
59	MG	AH	201	1/1	0.95	0.85	38.31	64,64,64,64	0
59	MG	CA	3502	1/1	0.75	0.66	38.04	90,90,90,90	0
59	MG	CA	3025	1/1	0.98	0.39	37.76	59,59,59,59	0
59	MG	AA	3235	1/1	0.88	0.45	36.78	93,93,93,93	0
59	MG	CA	3146	1/1	0.63	0.95	35.38	82,82,82,82	0
59	MG	CA	3157	1/1	0.93	0.55	35.31	81,81,81,81	0
59	MG	AA	3101	1/1	0.93	0.64	34.75	68,68,68,68	0
59	MG	AA	3147	1/1	0.97	0.52	34.38	40,40,40,40	1
59	MG	C7	101	1/1	0.83	0.43	33.54	56,56,56,56	0
59	MG	AA	3214	1/1	0.97	0.81	32.29	58,58,58,58	1
59	MG	AA	3712	1/1	0.76	0.69	30.90	70,70,70,70	0
59	MG	AA	3174	1/1	0.94	0.45	29.35	59,59,59,59	0
59	MG	AA	3820	1/1	0.80	0.43	29.07	85,85,85,85	0
59	MG	AU	202	1/1	0.96	0.45	28.83	82,82,82,82	0
59	MG	AA	3775	1/1	0.93	0.59	28.34	25,25,25,25	1
59	MG	AA	3824	1/1	0.95	0.58	28.10	72,72,72,72	0
59	MG	CA	3168	1/1	0.92	0.42	27.05	58,58,58,58	0
59	MG	AA	3140	1/1	0.72	0.58	26.77	62,62,62,62	0
59	MG	CA	3218	1/1	0.96	0.36	26.64	40,40,40,40	0
59	MG	AD	301	1/1	0.90	0.72	26.59	58,58,58,58	0
59	MG	C5	101	1/1	0.95	0.49	26.14	66,66,66,66	0
59	MG	AA	3131	1/1	0.96	0.26	25.85	63,63,63,63	0
59	MG	CA	3140	1/1	0.86	0.38	25.79	63,63,63,63	0
59	MG	CA	3503	1/1	0.88	0.35	25.76	52,52,52,52	0
59	MG	CA	3221	1/1	0.91	0.58	25.75	65,65,65,65	0
59	MG	CA	3162	1/1	0.96	0.39	25.59	31,31,31,31	0
59	MG	AA	3110	1/1	0.92	0.48	25.04	52,52,52,52	0
59	MG	AA	3217	1/1	0.94	0.44	24.35	29,29,29,29	1
59	MG	AA	3060	1/1	0.97	0.32	24.26	20,20,20,20	0
59	MG	CA	3041	1/1	0.75	0.41	24.22	61,61,61,61	0
59	MG	BA	1665	1/1	0.77	0.45	23.17	73,73,73,73	0
59	MG	CA	3113	1/1	0.89	0.39	22.97	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3133	1/1	0.92	0.33	22.64	50,50,50,50	0
59	MG	AA	3608	1/1	0.90	0.36	22.59	60,60,60,60	0
59	MG	AA	3171	1/1	0.88	0.27	22.27	54,54,54,54	0
59	MG	AA	3158	1/1	0.86	0.88	22.16	68,68,68,68	0
59	MG	CA	3033	1/1	0.90	0.40	21.75	55,55,55,55	0
59	MG	CA	3058	1/1	0.82	0.34	21.61	67,67,67,67	0
59	MG	AD	305	1/1	0.69	0.63	21.60	86,86,86,86	0
59	MG	CA	3658	1/1	0.93	0.39	21.11	64,64,64,64	0
59	MG	AA	3176	1/1	0.95	0.32	20.49	70,70,70,70	0
59	MG	CA	3544	1/1	0.86	0.32	20.39	60,60,60,60	0
59	MG	AA	3257	1/1	0.94	0.32	20.02	54,54,54,54	0
59	MG	AA	3113	1/1	0.96	0.32	19.91	45,45,45,45	0
59	MG	AA	3199	1/1	0.90	0.34	19.75	41,41,41,41	0
59	MG	CA	3028	1/1	0.96	0.64	19.58	51,51,51,51	0
59	MG	AA	3044	1/1	0.95	0.37	19.48	52,52,52,52	0
59	MG	AA	3823	1/1	0.93	0.48	19.36	39,39,39,39	0
59	MG	AE	305	1/1	0.88	0.35	18.99	48,48,48,48	0
59	MG	CA	3225	1/1	0.83	0.34	18.89	64,64,64,64	0
59	MG	AA	3038	1/1	0.93	0.44	18.75	29,29,29,29	1
59	MG	DA	1671	1/1	0.96	0.36	18.28	56,56,56,56	0
59	MG	CA	3618	1/1	0.99	0.30	18.11	40,40,40,40	0
59	MG	BA	1628	1/1	0.80	0.30	17.55	87,87,87,87	0
59	MG	AA	3255	1/1	0.94	0.22	17.54	38,38,38,38	0
59	MG	CA	3291	1/1	0.86	0.41	17.41	48,48,48,48	0
59	MG	CA	3182	1/1	0.94	0.31	17.24	38,38,38,38	0
59	MG	BA	1714	1/1	0.75	0.28	16.96	74,74,74,74	0
59	MG	CA	3226	1/1	0.85	0.33	16.82	52,52,52,52	0
59	MG	AU	204	1/1	0.97	0.38	16.81	25,25,25,25	0
59	MG	AA	3261	1/1	0.93	0.31	16.79	25,25,25,25	0
59	MG	CA	3432	1/1	0.84	0.27	16.79	32,32,32,32	0
59	MG	DA	1769	1/1	0.76	0.44	16.54	74,74,74,74	0
59	MG	CA	3166	1/1	0.94	0.31	16.48	27,27,27,27	0
59	MG	CA	3420	1/1	0.74	0.33	16.42	69,69,69,69	0
59	MG	CA	3440	1/1	0.95	0.31	16.04	49,49,49,49	0
59	MG	AA	3109	1/1	0.81	0.34	15.73	56,56,56,56	0
59	MG	AA	3184	1/1	0.92	0.25	15.58	75,75,75,75	0
59	MG	AA	3315	1/1	0.82	0.22	15.56	65,65,65,65	0
59	MG	CA	3441	1/1	0.94	0.23	15.35	56,56,56,56	0
59	MG	AA	3826	1/1	0.91	0.29	15.34	46,46,46,46	0
59	MG	AA	3209	1/1	0.89	0.31	15.05	62,62,62,62	0
59	MG	AA	3213	1/1	0.86	0.65	14.81	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3603	1/1	0.84	0.35	14.78	49,49,49,49	0
59	MG	AA	3307	1/1	0.96	0.33	14.67	61,61,61,61	0
59	MG	AA	3403	1/1	0.96	0.34	14.63	42,42,42,42	0
59	MG	CF	301	1/1	0.85	0.47	14.60	61,61,61,61	0
59	MG	DA	1745	1/1	0.99	0.38	14.56	50,50,50,50	0
59	MG	CA	3428	1/1	0.89	0.26	14.41	58,58,58,58	0
59	MG	BA	1663	1/1	0.87	0.23	14.35	43,43,43,43	0
59	MG	DA	1601	1/1	0.91	0.41	14.33	74,74,74,74	0
59	MG	CA	3455	1/1	0.95	0.28	14.11	49,49,49,49	0
59	MG	AA	3043	1/1	0.91	0.30	13.94	45,45,45,45	0
59	MG	CA	3642	1/1	0.93	0.52	13.84	52,52,52,52	0
59	MG	AA	3818	1/1	0.84	0.31	13.83	61,61,61,61	0
59	MG	AA	3144	1/1	0.97	0.36	13.79	50,50,50,50	0
59	MG	CA	3159	1/1	0.84	0.59	13.76	69,69,69,69	0
59	MG	CA	3230	1/1	0.97	0.33	13.73	49,49,49,49	0
59	MG	CA	3163	1/1	0.97	0.30	13.54	30,30,30,30	0
59	MG	CA	3210	1/1	0.85	0.34	13.39	62,62,62,62	0
59	MG	AA	3186	1/1	0.92	0.29	13.29	48,48,48,48	0
59	MG	AA	3280	1/1	0.91	0.29	13.16	53,53,53,53	0
59	MG	AA	3822	1/1	0.90	0.32	13.15	47,47,47,47	0
59	MG	CA	3035	1/1	0.88	0.28	13.13	69,69,69,69	0
59	MG	AA	3828	1/1	0.94	0.38	13.05	38,38,38,38	0
59	MG	AA	3286	1/1	0.93	0.45	12.87	40,40,40,40	0
59	MG	CA	3333	1/1	0.82	0.36	12.83	68,68,68,68	0
59	MG	CA	3619	1/1	0.92	0.38	12.78	40,40,40,40	0
59	MG	CA	3348	1/1	0.77	0.28	12.68	44,44,44,44	0
59	MG	DA	1652	1/1	0.88	0.84	12.61	80,80,80,80	0
59	MG	CA	3160	1/1	0.96	0.39	12.45	57,57,57,57	0
59	MG	AD	304	1/1	0.95	0.34	12.44	41,41,41,41	0
59	MG	CA	3655	1/1	0.93	0.41	12.29	52,52,52,52	0
59	MG	AA	3809	1/1	0.83	0.29	12.25	57,57,57,57	0
59	MG	AA	3301	1/1	0.96	0.30	12.18	39,39,39,39	0
59	MG	BA	1740	1/1	0.98	0.31	12.16	50,50,50,50	0
59	MG	CA	3068	1/1	0.81	0.43	11.96	66,66,66,66	0
59	MG	AA	3825	1/1	0.89	0.39	11.90	63,63,63,63	0
59	MG	CV	201	1/1	0.77	0.81	11.83	117,117,117,117	0
59	MG	CA	3054	1/1	0.96	0.25	11.79	36,36,36,36	0
59	MG	AA	3102	1/1	0.92	0.23	11.35	47,47,47,47	0
59	MG	AA	3012	1/1	0.80	0.35	11.30	49,49,49,49	0
59	MG	CA	3375	1/1	0.95	0.33	11.28	68,68,68,68	0
59	MG	AA	3034	1/1	0.89	0.31	11.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3421	1/1	0.98	0.21	11.23	28,28,28,28	0
59	MG	AA	3740	1/1	0.85	0.29	11.05	61,61,61,61	0
59	MG	AX	3001	1/1	0.79	0.31	11.04	52,52,52,52	0
59	MG	AA	3023	1/1	0.98	0.62	11.00	53,53,53,53	0
59	MG	BA	1672	1/1	0.93	0.30	10.93	65,65,65,65	0
59	MG	CA	3207	1/1	0.92	0.28	10.91	75,75,75,75	0
59	MG	CA	3213	1/1	0.95	0.27	10.83	51,51,51,51	0
59	MG	CA	3036	1/1	0.91	0.28	10.51	32,32,32,32	0
59	MG	CA	3657	1/1	0.97	0.39	10.40	41,41,41,41	0
59	MG	AA	3050	1/1	0.94	0.27	10.36	28,28,28,28	0
59	MG	CA	3322	1/1	0.99	0.26	10.31	40,40,40,40	0
59	MG	CA	3409	1/1	0.91	0.28	10.26	42,42,42,42	0
59	MG	CA	3532	1/1	0.92	0.23	10.25	49,49,49,49	0
59	MG	BA	1691	1/1	0.59	0.44	10.20	86,86,86,86	0
59	MG	AA	3177	1/1	0.86	0.28	10.15	59,59,59,59	0
59	MG	AA	3036	1/1	0.95	0.24	9.99	25,25,25,25	0
59	MG	AA	3667	1/1	0.93	0.29	9.93	41,41,41,41	0
59	MG	AA	3033	1/1	0.92	0.27	9.89	55,55,55,55	0
59	MG	CA	3326	1/1	0.96	0.24	9.70	28,28,28,28	0
59	MG	AA	3423	1/1	0.96	0.20	9.64	16,16,16,16	0
59	MG	CA	3358	1/1	0.98	0.30	9.55	36,36,36,36	0
59	MG	AP	201	1/1	0.96	0.32	9.44	21,21,21,21	1
59	MG	DA	1634	1/1	0.68	0.29	9.36	66,66,66,66	0
59	MG	AA	3803	1/1	0.89	0.32	9.24	45,45,45,45	0
59	MG	CA	3090	1/1	0.88	0.28	9.20	77,77,77,77	0
59	MG	CU	201	1/1	0.95	0.48	9.17	74,74,74,74	0
59	MG	AA	3161	1/1	0.92	0.23	9.13	43,43,43,43	0
59	MG	CA	3650	1/1	0.98	0.25	9.11	14,14,14,14	0
59	MG	BA	1758	1/1	0.72	0.36	9.03	76,76,76,76	0
59	MG	AA	3606	1/1	0.94	0.24	9.02	34,34,34,34	0
59	MG	AA	3253	1/1	0.86	0.34	8.78	64,64,64,64	0
59	MG	AA	3228	1/1	0.96	0.30	8.66	32,32,32,32	0
59	MG	AA	3398	1/1	0.97	0.22	8.60	31,31,31,31	0
59	MG	DA	1650	1/1	0.93	0.28	8.58	50,50,50,50	0
59	MG	CA	3212	1/1	0.92	0.24	8.52	84,84,84,84	0
59	MG	BA	1630	1/1	0.87	0.29	8.50	61,61,61,61	0
59	MG	AF	304	1/1	0.96	0.29	8.25	36,36,36,36	0
59	MG	AA	3827	1/1	0.80	0.38	8.18	38,38,38,38	0
59	MG	AA	3172	1/1	0.93	0.22	8.17	47,47,47,47	0
59	MG	CA	3500	1/1	0.89	0.23	8.09	75,75,75,75	0
59	MG	AA	3215	1/1	0.85	0.33	8.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3452	1/1	0.94	0.20	8.08	36,36,36,36	0
59	MG	AA	3653	1/1	0.81	0.22	8.07	60,60,60,60	0
59	MG	CA	3415	1/1	0.98	0.26	8.03	34,34,34,34	0
59	MG	AA	3832	1/1	0.93	0.42	7.94	55,55,55,55	0
59	MG	CA	3635	1/1	0.94	0.23	7.93	48,48,48,48	0
59	MG	AA	3771	1/1	0.91	0.24	7.92	60,60,60,60	0
59	MG	AA	3224	1/1	0.91	0.24	7.90	56,56,56,56	0
59	MG	AA	3130	1/1	0.98	0.23	7.83	34,34,34,34	0
59	MG	AA	3117	1/1	0.95	0.24	7.72	25,25,25,25	1
59	MG	AA	3547	1/1	0.96	0.26	7.69	60,60,60,60	0
59	MG	AA	3128	1/1	0.81	0.47	7.60	89,89,89,89	0
59	MG	CA	3108	1/1	0.65	0.27	7.59	78,78,78,78	0
59	MG	AA	3244	1/1	0.92	0.25	7.57	52,52,52,52	0
59	MG	CA	3463	1/1	0.92	0.23	7.57	56,56,56,56	0
59	MG	AW	3003	1/1	0.95	0.25	7.42	28,28,28,28	0
59	MG	BA	1787	1/1	0.93	0.27	7.23	55,55,55,55	0
59	MG	BA	1780	1/1	0.93	0.36	7.23	60,60,60,60	0
59	MG	CA	3457	1/1	0.82	0.26	7.18	43,43,43,43	0
59	MG	CA	3217	1/1	0.97	0.26	7.15	62,62,62,62	0
59	MG	AD	310	1/1	0.94	0.39	7.15	78,78,78,78	0
59	MG	BA	1687	1/1	0.87	0.22	7.12	52,52,52,52	0
59	MG	AA	3814	1/1	0.74	0.59	7.12	72,72,72,72	0
59	MG	CA	3427	1/1	0.98	0.19	7.11	37,37,37,37	0
59	MG	AA	3534	1/1	0.97	0.19	7.10	14,14,14,14	0
59	MG	CE	303	1/1	0.92	0.40	7.04	51,51,51,51	0
59	MG	CA	3039	1/1	0.98	0.28	7.00	37,37,37,37	0
59	MG	DA	1640	1/1	0.94	0.31	6.97	77,77,77,77	0
59	MG	AA	3082	1/1	0.98	0.27	6.93	60,60,60,60	0
59	MG	DA	1622	1/1	0.77	0.36	6.88	60,60,60,60	0
59	MG	AA	3081	1/1	0.94	0.21	6.81	56,56,56,56	0
59	MG	CA	3314	1/1	0.91	0.29	6.80	57,57,57,57	0
59	MG	AA	3625	1/1	0.75	0.20	6.63	51,51,51,51	0
59	MG	CA	3486	1/1	0.73	0.24	6.61	81,81,81,81	0
59	MG	AA	3120	1/1	0.90	0.24	6.49	33,33,33,33	0
59	MG	CE	301	1/1	0.88	0.32	6.44	53,53,53,53	0
59	MG	AA	3042	1/1	0.96	0.23	6.38	32,32,32,32	0
59	MG	CA	3410	1/1	0.93	0.22	6.38	25,25,25,25	0
59	MG	AA	3045	1/1	0.92	0.32	6.37	55,55,55,55	0
59	MG	CA	3309	1/1	0.97	0.24	6.37	22,22,22,22	0
59	MG	AA	3799	1/1	0.99	0.33	6.36	42,42,42,42	0
59	MG	AA	3569	1/1	0.98	0.22	6.27	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AQ	202	1/1	0.93	0.25	6.14	35,35,35,35	0
59	MG	AA	3519	1/1	0.97	0.23	6.11	27,27,27,27	0
59	MG	CA	3243	1/1	0.92	0.27	6.10	58,58,58,58	0
59	MG	AB	3003	1/1	0.80	0.23	6.04	60,60,60,60	0
59	MG	CA	3105	1/1	0.97	0.25	6.01	39,39,39,39	0
59	MG	AA	3532	1/1	0.96	0.20	6.00	20,20,20,20	0
59	MG	AV	201	1/1	0.99	0.26	5.95	42,42,42,42	0
59	MG	AA	3690	1/1	0.96	0.20	5.88	50,50,50,50	0
59	MG	BA	1684	1/1	0.96	0.27	5.83	61,61,61,61	0
59	MG	AA	3543	1/1	0.97	0.22	5.75	32,32,32,32	0
59	MG	AA	3254	1/1	0.94	0.25	5.73	52,52,52,52	0
59	MG	CA	3458	1/1	0.90	0.22	5.65	54,54,54,54	0
59	MG	BA	1612	1/1	0.74	0.25	5.63	92,92,92,92	0
59	MG	BA	1679	1/1	0.85	0.31	5.53	59,59,59,59	0
59	MG	AD	307	1/1	0.84	0.24	5.44	56,56,56,56	0
59	MG	AA	3830	1/1	0.97	0.27	5.41	47,47,47,47	0
59	MG	CA	3229	1/1	0.85	0.19	5.37	53,53,53,53	0
59	MG	BA	1656	1/1	0.90	0.32	5.29	75,75,75,75	0
59	MG	CA	3137	1/1	0.91	0.23	5.27	69,69,69,69	0
59	MG	AA	3721	1/1	0.97	0.20	5.22	40,40,40,40	0
59	MG	AA	3360	1/1	0.97	0.23	5.22	22,22,22,22	0
59	MG	AD	309	1/1	0.94	0.25	5.21	37,37,37,37	0
59	MG	AA	3563	1/1	0.97	0.21	5.18	34,34,34,34	0
59	MG	CA	3100	1/1	0.49	0.25	5.16	81,81,81,81	0
59	MG	CA	3227	1/1	0.99	0.22	5.07	41,41,41,41	0
59	MG	CA	3492	1/1	0.88	0.24	5.02	59,59,59,59	0
59	MG	AA	3152	1/1	0.98	0.24	5.01	10,10,10,10	0
59	MG	AA	3134	1/1	0.92	0.23	5.00	62,62,62,62	0
59	MG	BA	1725	1/1	0.97	0.24	4.99	54,54,54,54	0
59	MG	CA	3332	1/1	0.97	0.24	4.87	29,29,29,29	0
59	MG	BA	1735	1/1	0.97	0.21	4.87	41,41,41,41	0
59	MG	AA	3691	1/1	0.97	0.23	4.84	62,62,62,62	0
59	MG	AU	205	1/1	0.95	0.26	4.83	45,45,45,45	0
59	MG	AA	3404	1/1	0.96	0.20	4.69	27,27,27,27	0
59	MG	AA	3466	1/1	0.90	0.20	4.62	76,76,76,76	0
59	MG	CW	201	1/1	0.95	0.36	4.58	46,46,46,46	0
59	MG	CA	3252	1/1	0.94	0.19	4.54	62,62,62,62	0
59	MG	CA	3589	1/1	0.92	0.23	4.48	71,71,71,71	0
59	MG	AA	3510	1/1	0.95	0.24	4.46	17,17,17,17	0
59	MG	CA	3169	1/1	0.98	0.21	4.43	34,34,34,34	0
59	MG	AA	3593	1/1	0.96	0.22	4.42	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AD	308	1/1	0.93	0.42	4.41	46,46,46,46	0
59	MG	CA	3372	1/1	0.99	0.18	4.38	35,35,35,35	0
59	MG	CA	3201	1/1	0.93	0.23	4.35	45,45,45,45	0
59	MG	CA	3636	1/1	0.91	0.19	4.31	64,64,64,64	0
59	MG	DA	1665	1/1	0.84	0.20	4.29	63,63,63,63	0
59	MG	AA	3392	1/1	0.95	0.24	4.24	17,17,17,17	0
59	MG	AA	3813	1/1	0.96	0.19	4.20	29,29,29,29	1
59	MG	CA	3330	1/1	0.96	0.21	4.19	36,36,36,36	0
59	MG	AA	3344	1/1	0.85	0.23	4.18	22,22,22,22	0
59	MG	BA	1607	1/1	0.89	0.27	4.18	64,64,64,64	0
59	MG	BA	1723	1/1	0.82	0.24	4.16	70,70,70,70	0
59	MG	CA	3413	1/1	0.82	0.22	4.11	39,39,39,39	0
59	MG	CA	3103	1/1	0.97	0.19	3.97	53,53,53,53	0
59	MG	AA	3226	1/1	0.90	0.22	3.95	46,46,46,46	0
59	MG	AA	3384	1/1	0.95	0.21	3.89	22,22,22,22	0
59	MG	AA	3829	1/1	0.95	0.24	3.88	47,47,47,47	0
59	MG	BA	1676	1/1	0.92	0.19	3.85	61,61,61,61	0
59	MG	CA	3026	1/1	0.92	0.22	3.84	32,32,32,32	1
59	MG	BA	1615	1/1	0.96	0.28	3.83	62,62,62,62	0
59	MG	CA	3383	1/1	0.98	0.20	3.79	30,30,30,30	0
59	MG	DA	1609	1/1	0.86	0.30	3.74	89,89,89,89	0
59	MG	AA	3515	1/1	0.97	0.22	3.74	12,12,12,12	0
59	MG	CA	3557	1/1	0.80	0.22	3.71	76,76,76,76	0
59	MG	CB	3007	1/1	0.89	0.22	3.67	52,52,52,52	0
59	MG	AA	3193	1/1	0.95	0.20	3.59	40,40,40,40	0
59	MG	AA	3511	1/1	0.96	0.20	3.56	14,14,14,14	0
59	MG	AA	3250	1/1	0.98	0.18	3.56	123,123,123,123	0
59	MG	AA	3188	1/1	0.95	0.18	3.56	31,31,31,31	0
59	MG	AA	3182	1/1	0.98	0.22	3.50	46,46,46,46	0
59	MG	BA	1788	1/1	0.77	0.19	3.48	79,79,79,79	0
59	MG	AA	3241	1/1	0.65	0.21	3.47	65,65,65,65	0
59	MG	A0	101	1/1	0.83	0.20	3.46	69,69,69,69	0
59	MG	CA	3010	1/1	0.96	0.19	3.46	43,43,43,43	0
59	MG	AA	3317	1/1	0.97	0.16	3.44	24,24,24,24	0
59	MG	CA	3353	1/1	0.98	0.22	3.40	45,45,45,45	0
59	MG	AA	3794	1/1	0.95	0.43	3.38	60,60,60,60	0
59	MG	CA	3285	1/1	0.94	0.19	3.24	63,63,63,63	0
59	MG	CA	3361	1/1	0.98	0.20	3.20	43,43,43,43	0
59	MG	AF	301	1/1	0.91	0.21	3.19	35,35,35,35	1
59	MG	AA	3565	1/1	0.97	0.21	3.14	44,44,44,44	0
59	MG	AA	3718	1/1	0.92	0.21	3.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3335	1/1	0.98	0.24	3.13	15,15,15,15	0
59	MG	DA	1642	1/1	0.67	0.20	3.12	62,62,62,62	0
59	MG	CA	3552	1/1	0.95	0.18	3.12	30,30,30,30	0
59	MG	C3	3001	1/1	0.92	0.39	3.11	72,72,72,72	0
59	MG	AA	3708	1/1	0.81	0.29	3.08	61,61,61,61	0
59	MG	AA	3795	1/1	0.89	0.25	3.07	22,22,22,22	0
59	MG	AB	3020	1/1	0.86	0.18	3.02	62,62,62,62	0
59	MG	CQ	202	1/1	0.64	0.29	2.97	74,74,74,74	0
59	MG	CA	3526	1/1	0.93	0.21	2.93	58,58,58,58	0
59	MG	AA	3576	1/1	0.90	0.18	2.93	52,52,52,52	0
59	MG	AA	3443	1/1	0.94	0.19	2.93	33,33,33,33	0
59	MG	AA	3806	1/1	0.95	0.19	2.92	42,42,42,42	0
59	MG	CA	3277	1/1	0.96	0.18	2.90	55,55,55,55	0
59	MG	AA	3393	1/1	0.95	0.20	2.80	23,23,23,23	0
59	MG	AA	3391	1/1	0.91	0.20	2.78	19,19,19,19	0
59	MG	AA	3561	1/1	0.98	0.20	2.78	21,21,21,21	0
59	MG	AA	3702	1/1	0.99	0.20	2.69	14,14,14,14	0
59	MG	CA	3661	1/1	0.94	0.23	2.69	27,27,27,27	0
59	MG	AA	3529	1/1	0.96	0.20	2.69	30,30,30,30	0
59	MG	AA	3793	1/1	0.98	0.22	2.67	7,7,7,7	0
59	MG	CA	3002	1/1	0.97	0.23	2.67	28,28,28,28	0
59	MG	AA	3429	1/1	0.93	0.19	2.53	31,31,31,31	0
59	MG	BA	1757	1/1	0.93	0.22	2.50	43,43,43,43	0
59	MG	CA	3318	1/1	0.95	0.21	2.44	24,24,24,24	0
59	MG	AA	3053	1/1	0.99	0.18	2.43	19,19,19,19	0
59	MG	BA	1616	1/1	0.54	0.27	2.43	122,122,122,122	0
59	MG	BA	1641	1/1	0.89	0.20	2.32	54,54,54,54	0
59	MG	CA	3346	1/1	0.95	0.19	2.31	30,30,30,30	0
59	MG	AA	3509	1/1	0.95	0.16	2.29	40,40,40,40	0
59	MG	AA	3294	1/1	0.98	0.17	2.28	37,37,37,37	0
59	MG	BA	1627	1/1	0.95	0.23	2.27	51,51,51,51	0
59	MG	AA	3659	1/1	0.88	0.18	2.26	73,73,73,73	0
59	MG	DT	3001	1/1	0.64	0.42	2.26	60,60,60,60	0
59	MG	CA	3660	1/1	0.93	0.19	2.26	60,60,60,60	0
59	MG	BA	1631	1/1	0.72	0.17	2.25	71,71,71,71	0
59	MG	AA	3413	1/1	0.94	0.19	2.23	25,25,25,25	0
59	MG	AA	3730	1/1	0.97	0.17	2.22	75,75,75,75	0
59	MG	DA	1655	1/1	0.63	0.24	2.16	83,83,83,83	0
59	MG	DA	1683	1/1	0.87	0.32	2.11	58,58,58,58	0
59	MG	CA	3045	1/1	0.98	0.17	2.10	60,60,60,60	0
59	MG	AA	3766	1/1	0.94	0.17	2.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	AA	3688	1/1	0.96	0.15	2.10	25,25,25,25	0
59	MG	AA	3682	1/1	0.97	0.17	2.09	31,31,31,31	0
59	MG	AA	3047	1/1	0.88	0.18	2.08	29,29,29,29	0
59	MG	CA	3653	1/1	0.97	0.20	2.06	32,32,32,32	0
59	MG	AA	3362	1/1	0.98	0.16	1.99	46,46,46,46	0
59	MG	CA	3569	1/1	0.88	0.19	1.99	41,41,41,41	0
59	MG	CV	202	1/1	0.98	0.21	1.97	38,38,38,38	0
59	MG	DA	1641	1/1	0.87	0.25	1.94	74,74,74,74	0
59	MG	AU	203	1/1	0.97	0.21	1.92	31,31,31,31	0
59	MG	CA	3013	1/1	0.81	0.23	1.90	42,42,42,42	0
59	MG	DA	1661	1/1	0.92	0.18	1.89	66,66,66,66	0
59	MG	AA	3568	1/1	0.96	0.18	1.84	15,15,15,15	0
59	MG	CA	3448	1/1	0.91	0.21	1.83	37,37,37,37	0
59	MG	CA	3627	1/1	0.97	0.19	1.82	60,60,60,60	0
59	MG	AA	3745	1/1	0.99	0.18	1.78	68,68,68,68	0
59	MG	AA	3407	1/1	0.98	0.20	1.77	10,10,10,10	0
59	MG	CA	3615	1/1	0.89	0.20	1.75	28,28,28,28	0
59	MG	CA	3572	1/1	0.78	0.16	1.71	70,70,70,70	0
59	MG	AA	3020	1/1	0.98	0.18	1.69	11,11,11,11	0
59	MG	AA	3313	1/1	0.90	0.16	1.65	39,39,39,39	0
59	MG	BA	1680	1/1	0.95	0.18	1.64	40,40,40,40	0
59	MG	AA	3049	1/1	0.97	0.17	1.64	35,35,35,35	0
59	MG	CD	304	1/1	0.94	0.29	1.62	28,28,28,28	0
59	MG	AA	3328	1/1	0.99	0.16	1.54	42,42,42,42	0
59	MG	CA	3264	1/1	0.88	0.19	1.53	60,60,60,60	0
59	MG	AA	3319	1/1	0.92	0.19	1.51	58,58,58,58	0
59	MG	AA	3276	1/1	0.94	0.24	1.49	67,67,67,67	0
59	MG	BA	1726	1/1	0.94	0.19	1.47	46,46,46,46	0
59	MG	BA	1705	1/1	0.90	0.23	1.47	53,53,53,53	0
59	MG	AA	3743	1/1	0.93	0.16	1.45	67,67,67,67	0
59	MG	C1	101	1/1	0.94	0.18	1.42	57,57,57,57	0
59	MG	AU	201	1/1	0.97	0.19	1.39	25,25,25,25	0
59	MG	CA	3232	1/1	0.95	0.17	1.34	54,54,54,54	0
59	MG	BA	1742	1/1	0.94	0.18	1.33	48,48,48,48	0
59	MG	AA	3821	1/1	0.97	0.19	1.31	38,38,38,38	0
59	MG	BA	1671	1/1	0.89	0.21	1.30	101,101,101,101	0
59	MG	AA	3623	1/1	0.97	0.17	1.29	28,28,28,28	0
59	MG	CQ	201	1/1	0.88	0.23	1.28	72,72,72,72	0
59	MG	DA	1696	1/1	0.96	0.17	1.28	53,53,53,53	0
59	MG	AA	3738	1/1	0.93	0.19	1.27	24,24,24,24	0
59	MG	AA	3815	1/1	0.97	0.17	1.25	30,30,30,30	0
59	MG	BA	1815	1/1	0.85	0.22	1.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3421	1/1	0.94	0.20	1.22	57,57,57,57	0
59	MG	AA	3035	1/1	0.86	0.15	1.21	48,48,48,48	0
59	MG	BA	1730	1/1	0.89	0.18	1.20	53,53,53,53	0
59	MG	AA	3831	1/1	0.98	0.20	1.09	37,37,37,37	0
59	MG	DA	1697	1/1	0.98	0.17	1.09	48,48,48,48	0
59	MG	CA	3523	1/1	0.98	0.14	1.08	37,37,37,37	0
59	MG	CA	3324	1/1	0.96	0.17	1.06	26,26,26,26	0
59	MG	AA	3537	1/1	0.96	0.17	1.05	20,20,20,20	0
59	MG	CA	3268	1/1	0.95	0.17	1.04	52,52,52,52	0
59	MG	AA	3222	1/1	0.97	0.17	1.04	4,4,4,4	0
59	MG	AA	3627	1/1	0.81	0.15	0.97	76,76,76,76	0
59	MG	AF	303	1/1	0.98	0.20	0.95	19,19,19,19	0
59	MG	AA	3489	1/1	0.97	0.18	0.91	15,15,15,15	0
59	MG	AA	3318	1/1	0.96	0.16	0.86	23,23,23,23	0
59	MG	CA	3417	1/1	0.89	0.21	0.84	56,56,56,56	0
59	MG	CA	3614	1/1	0.93	0.24	0.83	62,62,62,62	0
59	MG	CA	3598	1/1	0.83	0.15	0.82	65,65,65,65	0
59	MG	AA	3546	1/1	0.96	0.14	0.79	60,60,60,60	0
59	MG	AB	3016	1/1	0.97	0.14	0.79	34,34,34,34	0
59	MG	AA	3528	1/1	0.98	0.16	0.71	19,19,19,19	0
59	MG	AA	3676	1/1	0.90	0.15	0.70	26,26,26,26	0
59	MG	BA	1702	1/1	0.97	0.19	0.70	46,46,46,46	0
59	MG	CA	3392	1/1	0.84	0.19	0.61	43,43,43,43	0
59	MG	AA	3058	1/1	0.93	0.15	0.57	22,22,22,22	0
59	MG	AA	3007	1/1	0.96	0.14	0.56	12,12,12,12	0
59	MG	AA	3521	1/1	0.95	0.18	0.55	19,19,19,19	0
59	MG	DA	1717	1/1	0.59	0.28	0.52	95,95,95,95	0
59	MG	BA	1625	1/1	0.85	0.16	0.47	86,86,86,86	0
59	MG	CA	3279	1/1	0.77	0.17	0.39	26,26,26,26	0
59	MG	CA	3360	1/1	0.96	0.17	0.39	38,38,38,38	0
59	MG	AA	3205	1/1	0.91	0.15	0.39	42,42,42,42	0
59	MG	AA	3477	1/1	0.99	0.18	0.37	14,14,14,14	0
59	MG	BA	1655	1/1	0.80	0.15	0.35	59,59,59,59	0
59	MG	DA	1689	1/1	0.89	0.17	0.34	56,56,56,56	0
59	MG	DA	1614	1/1	0.82	0.18	0.30	65,65,65,65	0
59	MG	CA	3132	1/1	0.94	0.16	0.28	48,48,48,48	0
59	MG	CA	3070	1/1	0.83	0.16	0.26	60,60,60,60	0
59	MG	BA	1760	1/1	0.92	0.17	0.26	53,53,53,53	0
59	MG	CA	3464	1/1	0.96	0.18	0.26	36,36,36,36	0
59	MG	BA	1649	1/1	0.91	0.16	0.25	35,35,35,35	0
59	MG	AA	3674	1/1	0.95	0.14	0.23	30,30,30,30	0
59	MG	AA	3396	1/1	0.96	0.17	0.22	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3601	1/1	0.95	0.13	0.19	57,57,57,57	0
59	MG	CA	3296	1/1	0.84	0.15	0.18	79,79,79,79	0
59	MG	AA	3052	1/1	0.95	0.16	0.17	11,11,11,11	0
59	MG	AA	3518	1/1	0.94	0.17	0.17	14,14,14,14	0
59	MG	BB	3001	1/1	0.78	0.16	0.16	91,91,91,91	0
59	MG	AA	3245	1/1	0.94	0.17	0.14	11,11,11,11	0
59	MG	CA	3282	1/1	0.99	0.18	0.13	36,36,36,36	0
59	MG	DA	1669	1/1	0.82	0.20	0.12	65,65,65,65	0
59	MG	AD	303	1/1	0.86	0.15	0.07	50,50,50,50	0
59	MG	AA	3739	1/1	0.72	0.17	0.06	38,38,38,38	0
59	MG	CA	3266	1/1	0.99	0.15	0.05	36,36,36,36	0
59	MG	CA	3310	1/1	0.89	0.17	0.00	47,47,47,47	0
59	MG	AA	3463	1/1	0.98	0.16	-0.02	15,15,15,15	0
59	MG	CA	3170	1/1	0.94	0.15	-0.05	32,32,32,32	0
59	MG	AA	3753	1/1	0.98	0.15	-0.06	30,30,30,30	0
59	MG	AA	3800	1/1	0.92	0.16	-0.06	35,35,35,35	0
59	MG	AA	3460	1/1	0.97	0.14	-0.08	27,27,27,27	0
59	MG	DA	1672	1/1	0.91	0.23	-0.13	77,77,77,77	0
59	MG	DA	1747	1/1	0.95	0.14	-0.15	48,48,48,48	0
59	MG	CA	3397	1/1	0.95	0.15	-0.15	57,57,57,57	0
59	MG	AD	302	1/1	0.90	0.15	-0.16	17,17,17,17	0
59	MG	CA	3274	1/1	0.91	0.15	-0.21	52,52,52,52	0
59	MG	AA	3390	1/1	0.97	0.16	-0.21	23,23,23,23	0
59	MG	CA	3419	1/1	0.89	0.15	-0.22	59,59,59,59	0
59	MG	AA	3585	1/1	0.98	0.16	-0.24	35,35,35,35	0
60	ZN	A5	501	1/1	0.99	0.13	-0.30	30,30,30,30	0
59	MG	AA	3587	1/1	0.98	0.14	-0.32	28,28,28,28	0
59	MG	CA	3357	1/1	0.94	0.12	-0.32	66,66,66,66	0
59	MG	CA	3269	1/1	0.94	0.14	-0.35	81,81,81,81	0
59	MG	AA	3522	1/1	0.95	0.16	-0.35	30,30,30,30	0
60	ZN	A6	102	1/1	0.99	0.12	-0.39	40,40,40,40	0
62	GDP	DZ	703	28/28	0.96	0.14	-0.39	66,66,66,66	1
59	MG	AA	3004	1/1	0.94	0.15	-0.39	21,21,21,21	0
59	MG	CA	3320	1/1	0.96	0.16	-0.40	36,36,36,36	0
59	MG	AA	3438	1/1	0.99	0.15	-0.41	17,17,17,17	0
59	MG	CA	3315	1/1	0.97	0.13	-0.46	47,47,47,47	0
59	MG	AA	3436	1/1	0.98	0.17	-0.49	12,12,12,12	0
59	MG	CA	3189	1/1	0.87	0.14	-0.51	50,50,50,50	0
59	MG	CF	303	1/1	0.93	0.14	-0.57	51,51,51,51	0
59	MG	AA	3303	1/1	0.99	0.15	-0.59	24,24,24,24	0
59	MG	AA	3523	1/1	0.98	0.16	-0.61	13,13,13,13	0
59	MG	CO	5001	1/1	0.96	0.17	-0.62	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3399	1/1	0.96	0.15	-0.62	16,16,16,16	0
59	MG	CA	3177	1/1	0.93	0.15	-0.64	29,29,29,29	0
59	MG	DA	1680	1/1	0.93	0.17	-0.66	56,56,56,56	0
59	MG	DA	1700	1/1	0.93	0.16	-0.66	61,61,61,61	0
59	MG	BA	1696	1/1	0.84	0.16	-0.66	98,98,98,98	0
59	MG	DE	201	1/1	0.92	0.16	-0.68	84,84,84,84	0
59	MG	AA	3744	1/1	0.88	0.15	-0.69	34,34,34,34	0
60	ZN	A9	501	1/1	1.00	0.12	-0.69	42,42,42,42	0
59	MG	AD	306	1/1	0.90	0.14	-0.71	65,65,65,65	0
62	GDP	BZ	702	28/28	0.97	0.12	-0.71	57,57,57,57	0
59	MG	CA	3370	1/1	0.94	0.14	-0.73	41,41,41,41	0
59	MG	DA	1625	1/1	0.92	0.15	-0.73	50,50,50,50	0
59	MG	CA	3433	1/1	0.99	0.12	-0.75	82,82,82,82	0
59	MG	CA	3012	1/1	0.95	0.15	-0.76	65,65,65,65	0
59	MG	CA	3664	1/1	0.94	0.14	-0.77	48,48,48,48	0
59	MG	CA	3339	1/1	0.97	0.14	-0.78	24,24,24,24	0
59	MG	DA	1723	1/1	0.94	0.13	-0.78	53,53,53,53	0
59	MG	DA	1771	1/1	0.83	0.12	-0.81	60,60,60,60	0
60	ZN	C4	501	1/1	0.92	0.11	-0.82	194,194,194,194	0
59	MG	CA	3104	1/1	0.94	0.15	-0.84	80,80,80,80	0
59	MG	CA	3311	1/1	0.99	0.13	-0.89	50,50,50,50	0
59	MG	CA	3317	1/1	0.87	0.14	-0.92	49,49,49,49	0
60	ZN	AY	501	1/1	0.99	0.10	-0.94	61,61,61,61	0
59	MG	AA	3512	1/1	0.99	0.15	-0.94	38,38,38,38	0
59	MG	AA	3411	1/1	0.98	0.14	-0.95	12,12,12,12	0
59	MG	CA	3223	1/1	0.89	0.15	-0.99	59,59,59,59	0
59	MG	CA	3085	1/1	0.99	0.16	-1.00	25,25,25,25	0
59	MG	AA	3445	1/1	0.88	0.13	-1.00	23,23,23,23	0
59	MG	AA	3490	1/1	0.94	0.16	-1.02	27,27,27,27	0
60	ZN	C9	501	1/1	0.98	0.09	-1.03	75,75,75,75	0
59	MG	AA	3001	1/1	0.94	0.14	-1.04	25,25,25,25	0
59	MG	DA	1703	1/1	0.90	0.21	-1.05	89,89,89,89	0
59	MG	BA	1750	1/1	0.84	0.21	-1.05	55,55,55,55	0
59	MG	AA	3112	1/1	0.95	0.14	-1.07	61,61,61,61	0
59	MG	AA	3305	1/1	0.96	0.16	-1.10	25,25,25,25	0
59	MG	AA	3551	1/1	0.85	0.12	-1.11	39,39,39,39	0
60	ZN	C5	102	1/1	0.97	0.10	-1.13	66,66,66,66	0
59	MG	BA	1748	1/1	0.92	0.14	-1.14	63,63,63,63	0
59	MG	BA	1686	1/1	0.98	0.15	-1.17	36,36,36,36	0
59	MG	CA	3299	1/1	0.96	0.14	-1.17	64,64,64,64	0
59	MG	AA	3539	1/1	0.97	0.14	-1.18	34,34,34,34	0
59	MG	CA	3300	1/1	0.96	0.12	-1.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CF	304	1/1	0.97	0.13	-1.23	65,65,65,65	0
59	MG	CA	3004	1/1	0.96	0.14	-1.28	49,49,49,49	0
59	MG	AA	3386	1/1	0.96	0.12	-1.29	45,45,45,45	0
59	MG	AA	3452	1/1	0.98	0.14	-1.31	14,14,14,14	0
59	MG	AA	3600	1/1	0.98	0.15	-1.35	25,25,25,25	0
59	MG	CA	3562	1/1	0.95	0.14	-1.35	29,29,29,29	0
59	MG	BA	1603	1/1	0.83	0.11	-1.37	61,61,61,61	0
59	MG	AA	3727	1/1	0.97	0.14	-1.43	23,23,23,23	0
59	MG	BE	3001	1/1	0.93	0.11	-1.46	78,78,78,78	0
59	MG	AA	3575	1/1	0.85	0.14	-1.46	35,35,35,35	0
60	ZN	DN	501	1/1	0.96	0.08	-1.46	117,117,117,117	0
59	MG	AA	3282	1/1	0.90	0.12	-1.49	33,33,33,33	0
59	MG	AA	3762	1/1	0.95	0.14	-1.49	23,23,23,23	0
59	MG	CA	3048	1/1	0.94	0.10	-1.50	47,47,47,47	0
59	MG	CA	3337	1/1	0.95	0.14	-1.50	20,20,20,20	0
61	SF4	BD	501	8/8	0.98	0.10	-1.51	78,78,78,78	0
60	ZN	C6	501	1/1	0.97	0.10	-1.51	66,66,66,66	0
59	MG	BA	1766	1/1	0.96	0.14	-1.52	62,62,62,62	0
59	MG	CA	3321	1/1	0.95	0.13	-1.54	28,28,28,28	0
59	MG	CA	3462	1/1	0.92	0.11	-1.55	63,63,63,63	0
60	ZN	BN	501	1/1	0.93	0.10	-1.56	132,132,132,132	0
59	MG	CA	3663	1/1	0.89	0.11	-1.59	64,64,64,64	0
59	MG	CA	3490	1/1	0.79	0.13	-1.60	50,50,50,50	0
60	ZN	CY	501	1/1	0.97	0.06	-1.62	101,101,101,101	0
59	MG	CA	3453	1/1	0.90	0.16	-1.64	35,35,35,35	0
59	MG	BN	503	1/1	0.91	0.14	-1.66	62,62,62,62	0
59	MG	DA	1711	1/1	0.96	0.12	-1.70	60,60,60,60	0
59	MG	BA	1700	1/1	0.86	0.14	-1.70	52,52,52,52	0
59	MG	DA	1648	1/1	0.99	0.12	-1.71	40,40,40,40	0
59	MG	AA	3779	1/1	0.97	0.12	-1.73	22,22,22,22	0
59	MG	AA	3624	1/1	0.91	0.12	-1.75	42,42,42,42	0
59	MG	AA	3397	1/1	0.97	0.13	-1.77	13,13,13,13	0
59	MG	BA	1754	1/1	0.92	0.13	-1.79	49,49,49,49	0
59	MG	BK	201	1/1	0.93	0.10	-1.81	44,44,44,44	0
59	MG	AA	3401	1/1	0.99	0.14	-1.82	21,21,21,21	0
59	MG	DE	202	1/1	0.85	0.08	-1.85	100,100,100,100	0
59	MG	AA	3416	1/1	0.98	0.14	-1.86	14,14,14,14	0
59	MG	BA	1613	1/1	0.85	0.12	-1.86	76,76,76,76	0
59	MG	CA	3192	1/1	0.91	0.11	-1.88	45,45,45,45	0
59	MG	AB	3014	1/1	0.98	0.11	-1.93	56,56,56,56	0
59	MG	BA	1795	1/1	0.94	0.10	-1.98	59,59,59,59	0
59	MG	CA	3178	1/1	0.93	0.12	-2.03	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CX	5001	1/1	0.90	0.13	-2.05	65,65,65,65	0
59	MG	AA	3236	1/1	0.94	0.14	-2.05	57,57,57,57	0
59	MG	BA	1746	1/1	0.91	0.12	-2.05	33,33,33,33	0
59	MG	CA	3498	1/1	0.97	0.12	-2.07	49,49,49,49	0
60	ZN	A4	501	1/1	0.94	0.07	-2.07	117,117,117,117	0
59	MG	DA	1768	1/1	0.94	0.07	-2.08	59,59,59,59	0
59	MG	AG	201	1/1	0.97	0.07	-2.15	38,38,38,38	0
59	MG	CA	3079	1/1	0.91	0.10	-2.17	41,41,41,41	0
59	MG	CA	3009	1/1	0.95	0.10	-2.18	27,27,27,27	0
59	MG	BA	1617	1/1	0.93	0.12	-2.19	118,118,118,118	0
59	MG	CG	3001	1/1	0.96	0.10	-2.23	65,65,65,65	0
61	SF4	DD	501	8/8	0.98	0.11	-2.27	82,82,82,82	1
59	MG	AA	3190	1/1	0.94	0.13	-2.29	24,24,24,24	0
59	MG	AA	3502	1/1	0.95	0.13	-2.32	29,29,29,29	1
59	MG	AA	3725	1/1	0.96	0.15	-2.33	13,13,13,13	0
59	MG	CA	3594	1/1	0.91	0.11	-2.36	73,73,73,73	0
59	MG	BA	1611	1/1	0.92	0.13	-2.42	31,31,31,31	0
59	MG	CA	3123	1/1	0.96	0.09	-2.43	29,29,29,29	0
59	MG	AA	3084	1/1	0.96	0.10	-2.43	23,23,23,23	0
59	MG	CB	3004	1/1	0.93	0.13	-2.46	55,55,55,55	0
59	MG	CA	3214	1/1	0.98	0.11	-2.47	22,22,22,22	0
59	MG	AA	3578	1/1	0.97	0.13	-2.49	28,28,28,28	0
59	MG	CA	3017	1/1	0.97	0.14	-2.58	30,30,30,30	0
59	MG	CA	3592	1/1	0.98	0.13	-2.60	64,64,64,64	0
59	MG	CE	305	1/1	0.95	0.04	-2.68	58,58,58,58	0
59	MG	AA	3497	1/1	0.97	0.13	-2.71	44,44,44,44	0
59	MG	CA	3561	1/1	0.94	0.14	-2.71	41,41,41,41	1
59	MG	CA	3283	1/1	0.94	0.12	-2.72	31,31,31,31	0
59	MG	BM	201	1/1	0.96	0.04	-2.76	62,62,62,62	0
59	MG	AA	3099	1/1	0.95	0.10	-2.77	53,53,53,53	0
59	MG	AG	202	1/1	0.95	0.06	-2.81	54,54,54,54	0
59	MG	CA	3528	1/1	0.82	0.10	-2.82	38,38,38,38	0
59	MG	CA	3425	1/1	0.97	0.12	-2.88	50,50,50,50	0
59	MG	AA	3673	1/1	0.93	0.11	-2.99	38,38,38,38	0
59	MG	DA	1621	1/1	0.89	0.09	-3.00	42,42,42,42	0
59	MG	AA	3382	1/1	0.96	0.12	-3.06	37,37,37,37	0
59	MG	AA	3021	1/1	0.95	0.13	-3.09	33,33,33,33	0
59	MG	CA	3064	1/1	0.97	0.09	-3.10	48,48,48,48	0
59	MG	CA	3211	1/1	0.97	0.09	-3.11	29,29,29,29	0
59	MG	DA	1722	1/1	0.80	0.13	-3.11	77,77,77,77	0
59	MG	AA	3218	1/1	0.94	0.09	-3.13	67,67,67,67	0
59	MG	CA	3275	1/1	0.93	0.10	-3.20	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3069	1/1	0.91	0.09	-3.29	28,28,28,28	0
59	MG	CA	3489	1/1	0.94	0.10	-3.36	39,39,39,39	0
59	MG	CA	3019	1/1	0.97	0.11	-3.37	22,22,22,22	0
59	MG	BT	3001	1/1	0.96	0.12	-3.52	46,46,46,46	0
59	MG	CA	3617	1/1	0.96	0.13	-3.55	41,41,41,41	0
59	MG	AA	3320	1/1	0.97	0.13	-3.57	37,37,37,37	0
59	MG	DA	1685	1/1	0.95	0.10	-3.59	46,46,46,46	0
59	MG	AA	3777	1/1	0.98	0.12	-3.61	41,41,41,41	0
59	MG	AA	3757	1/1	0.95	0.07	-3.62	14,14,14,14	0
59	MG	AA	3203	1/1	0.92	0.07	-3.63	59,59,59,59	0
59	MG	AB	3007	1/1	0.96	0.07	-3.70	39,39,39,39	0
59	MG	CA	3262	1/1	0.96	0.12	-3.71	11,11,11,11	0
59	MG	BA	1681	1/1	0.96	0.09	-3.74	53,53,53,53	0
59	MG	DA	1657	1/1	0.96	0.10	-3.84	23,23,23,23	0
59	MG	CA	3018	1/1	0.94	0.08	-3.86	41,41,41,41	0
59	MG	AA	3037	1/1	0.98	0.11	-3.95	4,4,4,4	0
59	MG	AA	3017	1/1	0.90	0.10	-4.04	61,61,61,61	0
59	MG	AA	3022	1/1	0.95	0.12	-4.04	5,5,5,5	0
59	MG	AA	3406	1/1	0.97	0.09	-4.10	20,20,20,20	0
59	MG	CA	3438	1/1	0.98	0.14	-4.14	24,24,24,24	0
59	MG	CA	3652	1/1	0.97	0.13	-4.17	23,23,23,23	0
59	MG	CA	3595	1/1	0.90	0.10	-4.23	70,70,70,70	0
59	MG	BA	1621	1/1	0.93	0.11	-4.37	51,51,51,51	0
59	MG	BA	1794	1/1	0.91	0.07	-4.52	38,38,38,38	0
59	MG	CA	3364	1/1	0.97	0.10	-4.58	22,22,22,22	0
59	MG	CA	3027	1/1	0.97	0.06	-4.61	31,31,31,31	0
59	MG	AA	3326	1/1	0.97	0.09	-4.61	36,36,36,36	1
59	MG	CA	3056	1/1	0.93	0.09	-4.62	63,63,63,63	0
59	MG	AA	3380	1/1	0.99	0.12	-4.64	18,18,18,18	0
59	MG	AA	3009	1/1	0.91	0.09	-4.68	22,22,22,22	0
59	MG	AA	3345	1/1	0.99	0.13	-4.81	6,6,6,6	0
59	MG	CA	3604	1/1	0.91	0.09	-4.93	62,62,62,62	0
59	MG	AA	3621	1/1	0.96	0.07	-4.95	17,17,17,17	0
59	MG	AA	3350	1/1	0.96	0.08	-5.03	36,36,36,36	0
59	MG	AA	3262	1/1	0.96	0.14	-5.05	15,15,15,15	0
59	MG	AA	3506	1/1	0.96	0.10	-5.15	48,48,48,48	0
59	MG	CA	3306	1/1	0.98	0.08	-5.38	24,24,24,24	0
59	MG	BA	1743	1/1	0.97	0.06	-5.39	41,41,41,41	0
59	MG	DA	1628	1/1	0.96	0.09	-5.48	39,39,39,39	0
59	MG	CA	3468	1/1	0.97	0.06	-5.52	53,53,53,53	0
59	MG	CA	3292	1/1	0.99	0.09	-5.56	12,12,12,12	0
59	MG	BA	1813	1/1	0.90	0.07	-5.85	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3342	1/1	0.98	0.11	-5.87	33,33,33,33	0
59	MG	CA	3138	1/1	0.97	0.04	-6.18	86,86,86,86	0
59	MG	AA	3011	1/1	0.99	0.08	-6.27	16,16,16,16	0
59	MG	AA	3654	1/1	0.91	0.06	-6.33	67,67,67,67	0
59	MG	AA	3473	1/1	0.97	0.07	-6.38	53,53,53,53	0
59	MG	AA	3620	1/1	0.94	0.11	-6.52	22,22,22,22	0
59	MG	AA	3377	1/1	0.98	0.06	-6.77	20,20,20,20	0
59	MG	AA	3560	1/1	0.95	0.13	-7.08	29,29,29,29	0
59	MG	DA	1750	1/1	0.95	0.08	-7.11	67,67,67,67	0
59	MG	AA	3388	1/1	0.96	0.08	-7.23	28,28,28,28	0
59	MG	AA	3072	1/1	0.98	0.08	-7.84	19,19,19,19	0
59	MG	AA	3338	1/1	0.98	0.08	-9.18	28,28,28,28	0
59	MG	CA	3491	1/1	0.96	0.06	-9.99	44,44,44,44	0
59	MG	CA	3581	1/1	0.85	0.11	-9.99	38,38,38,38	0
59	MG	AA	3770	1/1	0.97	0.12	-10.01	43,43,43,43	0
59	MG	AA	3387	1/1	0.94	0.08	-10.15	29,29,29,29	0
59	MG	AA	3589	1/1	0.93	0.08	-10.88	55,55,55,55	0
59	MG	CA	3644	1/1	0.83	0.20	-	66,66,66,66	0
59	MG	AB	3018	1/1	0.94	0.22	-	69,69,69,69	0
59	MG	AA	3488	1/1	0.98	0.19	-	36,36,36,36	0
59	MG	AA	3494	1/1	0.95	0.09	-	34,34,34,34	0
59	MG	AA	3373	1/1	0.91	0.17	-	48,48,48,48	0
59	MG	AA	3311	1/1	0.98	0.14	-	2,2,2,2	0
59	MG	BA	1812	1/1	0.48	0.20	-	79,79,79,79	0
59	MG	AA	3048	1/1	0.95	0.16	-	28,28,28,28	0
59	MG	AB	3022	1/1	0.95	0.12	-	61,61,61,61	0
59	MG	CA	3343	1/1	0.91	0.12	-	32,32,32,32	0
59	MG	AA	3437	1/1	0.98	0.18	-	17,17,17,17	0
59	MG	CA	3259	1/1	0.92	0.26	-	80,80,80,80	0
59	MG	BA	1652	1/1	0.86	0.12	-	59,59,59,59	0
59	MG	CA	3549	1/1	0.92	0.16	-	70,70,70,70	0
59	MG	AA	3157	1/1	0.87	0.48	-	91,91,91,91	0
59	MG	CA	3504	1/1	0.94	0.13	-	79,79,79,79	0
59	MG	AA	3453	1/1	0.97	0.23	-	39,39,39,39	0
59	MG	BA	1668	1/1	0.80	0.16	-	69,69,69,69	0
59	MG	BA	1620	1/1	0.91	0.17	-	52,52,52,52	0
59	MG	AA	3479	1/1	0.84	0.23	-	55,55,55,55	0
59	MG	CA	3304	1/1	0.70	0.12	-	67,67,67,67	0
59	MG	AA	3776	1/1	0.83	0.12	-	69,69,69,69	0
59	MG	AA	3722	1/1	0.91	0.12	-	37,37,37,37	0
59	MG	CA	3155	1/1	0.31	0.23	-	112,112,112,112	0
59	MG	AA	3714	1/1	0.84	0.24	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3006	1/1	0.95	0.34	-	52,52,52,52	0
59	MG	DA	1737	1/1	0.87	0.20	-	69,69,69,69	0
59	MG	AA	3234	1/1	0.93	0.29	-	36,36,36,36	0
59	MG	AA	3003	1/1	0.98	0.06	-	8,8,8,8	0
59	MG	AN	3003	1/1	0.88	0.07	-	55,55,55,55	0
59	MG	BA	1803	1/1	0.86	0.12	-	64,64,64,64	0
59	MG	AA	3626	1/1	0.84	0.18	-	35,35,35,35	0
59	MG	AA	3432	1/1	0.98	0.23	-	42,42,42,42	0
59	MG	AA	3426	1/1	0.96	0.17	-	20,20,20,20	0
59	MG	CA	3021	1/1	0.90	0.44	-	69,69,69,69	0
59	MG	BA	1677	1/1	0.98	0.17	-	28,28,28,28	0
59	MG	AB	3012	1/1	0.98	0.15	-	23,23,23,23	1
59	MG	AA	3125	1/1	0.97	0.16	-	22,22,22,22	1
59	MG	AA	3267	1/1	0.90	0.34	-	53,53,53,53	0
59	MG	CA	3319	1/1	0.86	0.14	-	65,65,65,65	0
59	MG	CA	3273	1/1	0.84	0.35	-	58,58,58,58	0
59	MG	AA	3325	1/1	0.95	0.16	-	70,70,70,70	0
59	MG	CA	3362	1/1	0.96	0.12	-	43,43,43,43	0
59	MG	CA	3553	1/1	0.74	0.19	-	90,90,90,90	0
59	MG	DA	1673	1/1	0.98	0.13	-	82,82,82,82	0
59	MG	BA	1777	1/1	0.97	0.28	-	71,71,71,71	0
59	MG	AA	3656	1/1	0.83	0.23	-	80,80,80,80	0
59	MG	DA	1617	1/1	0.89	0.17	-	64,64,64,64	0
59	MG	AB	3006	1/1	0.84	0.19	-	57,57,57,57	0
59	MG	AA	3769	1/1	0.72	0.17	-	63,63,63,63	0
59	MG	DA	1603	1/1	0.84	0.10	-	72,72,72,72	0
59	MG	DA	1733	1/1	0.57	0.34	-	92,92,92,92	0
59	MG	AA	3486	1/1	0.91	0.21	-	67,67,67,67	0
59	MG	AA	3449	1/1	0.91	0.23	-	50,50,50,50	0
59	MG	AA	3817	1/1	0.81	0.18	-	75,75,75,75	0
59	MG	CA	3508	1/1	0.92	0.18	-	52,52,52,52	0
59	MG	AA	3619	1/1	0.88	0.12	-	47,47,47,47	0
59	MG	AA	3232	1/1	0.91	0.25	-	58,58,58,58	0
59	MG	AA	3418	1/1	0.89	0.13	-	74,74,74,74	0
59	MG	AA	3630	1/1	0.91	0.34	-	72,72,72,72	0
59	MG	AA	3571	1/1	0.73	0.34	-	94,94,94,94	0
59	MG	AA	3183	1/1	0.90	0.35	-	58,58,58,58	0
59	MG	AA	3289	1/1	0.94	0.43	-	53,53,53,53	0
59	MG	CA	3600	1/1	0.79	0.51	-	86,86,86,86	0
59	MG	AA	3671	1/1	0.95	0.23	-	19,19,19,19	0
59	MG	AA	3264	1/1	0.87	0.41	-	51,51,51,51	0
59	MG	DA	1721	1/1	0.96	0.09	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3626	1/1	0.89	0.18	-	61,61,61,61	0
59	MG	CA	3174	1/1	0.91	0.52	-	50,50,50,50	0
59	MG	CA	3637	1/1	0.96	0.47	-	61,61,61,61	0
59	MG	CA	3539	1/1	0.90	0.18	-	90,90,90,90	0
59	MG	CA	3450	1/1	0.90	0.11	-	54,54,54,54	0
59	MG	AA	3163	1/1	0.93	0.24	-	72,72,72,72	0
59	MG	DA	1715	1/1	0.78	0.28	-	79,79,79,79	0
59	MG	AA	3655	1/1	0.89	0.33	-	55,55,55,55	0
59	MG	AA	3367	1/1	0.94	0.17	-	60,60,60,60	0
59	MG	AA	3415	1/1	0.99	0.23	-	62,62,62,62	0
59	MG	CA	3515	1/1	0.92	0.20	-	54,54,54,54	0
59	MG	CA	3303	1/1	0.95	0.35	-	43,43,43,43	0
59	MG	BA	1669	1/1	0.86	0.37	-	66,66,66,66	0
59	MG	CA	3096	1/1	0.32	0.24	-	125,125,125,125	0
59	MG	CA	3101	1/1	0.58	1.11	-	84,84,84,84	0
59	MG	CA	3265	1/1	0.95	0.29	-	61,61,61,61	0
59	MG	BL	202	1/1	0.96	0.17	-	54,54,54,54	0
59	MG	CA	3449	1/1	0.97	0.07	-	55,55,55,55	0
59	MG	DA	1649	1/1	0.96	0.33	-	69,69,69,69	0
59	MG	AA	3359	1/1	0.94	0.18	-	31,31,31,31	0
59	MG	CA	3081	1/1	0.84	0.31	-	63,63,63,63	0
59	MG	DA	1687	1/1	0.95	0.42	-	56,56,56,56	0
59	MG	CA	3647	1/1	0.85	0.15	-	85,85,85,85	0
59	MG	BA	1805	1/1	0.92	0.25	-	71,71,71,71	0
59	MG	DA	1666	1/1	0.89	0.19	-	53,53,53,53	0
59	MG	CA	3172	1/1	0.83	0.34	-	81,81,81,81	0
59	MG	BW	501	1/1	0.94	0.22	-	47,47,47,47	0
59	MG	AA	3514	1/1	0.93	0.18	-	42,42,42,42	0
59	MG	CA	3276	1/1	0.85	0.18	-	44,44,44,44	0
59	MG	AA	3602	1/1	0.90	0.15	-	51,51,51,51	0
59	MG	AA	3402	1/1	0.99	0.13	-	27,27,27,27	0
59	MG	AA	3553	1/1	0.98	0.05	-	43,43,43,43	0
59	MG	CA	3161	1/1	0.93	0.25	-	57,57,57,57	0
59	MG	CA	3380	1/1	0.99	0.21	-	59,59,59,59	0
59	MG	CA	3190	1/1	0.94	0.23	-	66,66,66,66	0
59	MG	AA	3713	1/1	0.96	0.22	-	27,27,27,27	0
59	MG	CA	3278	1/1	0.91	0.12	-	58,58,58,58	0
59	MG	CA	3194	1/1	0.77	0.23	-	52,52,52,52	0
59	MG	AA	3223	1/1	0.97	0.11	-	15,15,15,15	0
59	MG	DA	1761	1/1	0.85	0.30	-	72,72,72,72	0
59	MG	CA	3037	1/1	0.79	0.72	-	57,57,57,57	0
59	MG	BA	1782	1/1	0.93	0.19	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	DA	1718	1/1	0.67	0.32	-	101,101,101,101	0
59	MG	CA	3554	1/1	0.97	0.09	-	66,66,66,66	0
59	MG	BA	1632	1/1	0.96	0.08	-	48,48,48,48	0
59	MG	AA	3749	1/1	0.92	0.17	-	73,73,73,73	0
59	MG	AA	3164	1/1	0.87	0.63	-	71,71,71,71	0
59	MG	CA	3077	1/1	0.80	0.23	-	42,42,42,42	0
59	MG	CA	3571	1/1	0.97	0.27	-	45,45,45,45	0
59	MG	BA	1690	1/1	0.82	0.40	-	71,71,71,71	0
59	MG	CA	3608	1/1	0.84	0.32	-	50,50,50,50	1
59	MG	AA	3166	1/1	0.91	0.41	-	40,40,40,40	0
59	MG	A0	105	1/1	0.90	0.08	-	30,30,30,30	0
59	MG	CA	3573	1/1	0.89	0.12	-	65,65,65,65	0
59	MG	DA	1744	1/1	0.93	0.22	-	66,66,66,66	0
59	MG	AA	3249	1/1	0.85	0.17	-	59,59,59,59	0
59	MG	DA	1616	1/1	0.90	0.23	-	51,51,51,51	0
59	MG	CA	3368	1/1	0.92	0.16	-	44,44,44,44	0
59	MG	AE	304	1/1	0.86	0.19	-	52,52,52,52	0
59	MG	CA	3312	1/1	0.92	0.18	-	38,38,38,38	0
59	MG	AA	3496	1/1	0.97	0.36	-	31,31,31,31	0
59	MG	CA	3006	1/1	0.97	0.08	-	22,22,22,22	0
59	MG	AF	302	1/1	0.88	0.11	-	41,41,41,41	0
59	MG	AA	3409	1/1	0.84	0.08	-	60,60,60,60	0
59	MG	DA	1678	1/1	0.92	0.28	-	66,66,66,66	0
59	MG	DW	503	1/1	0.91	0.22	-	85,85,85,85	0
59	MG	CA	3247	1/1	0.92	0.28	-	39,39,39,39	0
59	MG	CA	3095	1/1	0.86	0.32	-	58,58,58,58	0
59	MG	DA	1647	1/1	0.94	0.15	-	51,51,51,51	0
59	MG	AA	3032	1/1	0.96	0.33	-	59,59,59,59	0
59	MG	AA	3819	1/1	0.94	0.51	-	57,57,57,57	0
59	MG	DA	1726	1/1	0.92	0.29	-	60,60,60,60	0
59	MG	CA	3386	1/1	0.97	0.20	-	50,50,50,50	0
59	MG	CA	3565	1/1	0.47	0.19	-	95,95,95,95	0
59	MG	AA	3444	1/1	0.87	0.24	-	66,66,66,66	0
59	MG	CA	3446	1/1	0.98	0.18	-	33,33,33,33	0
59	MG	CA	3209	1/1	0.98	0.13	-	73,73,73,73	0
59	MG	AA	3485	1/1	0.89	0.11	-	48,48,48,48	0
59	MG	AA	3090	1/1	0.91	0.38	-	53,53,53,53	0
59	MG	CA	3154	1/1	0.70	0.20	-	64,64,64,64	0
59	MG	CA	3514	1/1	0.79	0.42	-	64,64,64,64	0
59	MG	CA	3509	1/1	0.89	0.11	-	83,83,83,83	0
59	MG	CA	3524	1/1	0.91	0.24	-	52,52,52,52	0
59	MG	AA	3729	1/1	0.98	0.20	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3640	1/1	0.98	0.28	-	43,43,43,43	0
59	MG	AA	3185	1/1	0.96	0.16	-	76,76,76,76	0
59	MG	CA	3089	1/1	0.76	0.48	-	87,87,87,87	0
59	MG	CA	3122	1/1	0.81	0.70	-	58,58,58,58	0
59	MG	AA	3187	1/1	0.95	0.29	-	56,56,56,56	0
59	MG	AA	3059	1/1	0.96	0.36	-	40,40,40,40	0
59	MG	AA	3277	1/1	0.71	0.69	-	99,99,99,99	0
59	MG	AA	3304	1/1	0.93	0.15	-	47,47,47,47	0
59	MG	AA	3225	1/1	0.78	0.15	-	73,73,73,73	0
59	MG	BA	1761	1/1	0.97	0.16	-	62,62,62,62	0
59	MG	BA	1727	1/1	0.85	0.09	-	77,77,77,77	0
59	MG	BA	1604	1/1	0.75	0.19	-	63,63,63,63	0
59	MG	DA	1719	1/1	0.95	0.38	-	61,61,61,61	0
59	MG	AA	3456	1/1	0.93	0.14	-	56,56,56,56	0
59	MG	DA	1607	1/1	0.93	0.10	-	86,86,86,86	0
59	MG	CA	3106	1/1	0.96	0.13	-	66,66,66,66	0
59	MG	AA	3156	1/1	0.88	0.43	-	49,49,49,49	0
59	MG	AB	3023	1/1	0.96	0.35	-	54,54,54,54	0
59	MG	CA	3125	1/1	0.82	0.32	-	78,78,78,78	0
59	MG	AA	3469	1/1	0.96	0.12	-	32,32,32,32	0
59	MG	AA	3169	1/1	0.84	0.34	-	35,35,35,35	0
59	MG	DA	1730	1/1	0.90	0.25	-	71,71,71,71	0
59	MG	CA	3451	1/1	0.95	0.21	-	62,62,62,62	0
59	MG	CA	3328	1/1	0.88	0.20	-	35,35,35,35	0
59	MG	AA	3704	1/1	0.94	0.19	-	49,49,49,49	0
59	MG	BA	1747	1/1	0.97	0.19	-	65,65,65,65	0
59	MG	AA	3306	1/1	0.96	0.25	-	52,52,52,52	0
59	MG	DA	1638	1/1	0.88	0.29	-	80,80,80,80	0
59	MG	BA	1745	1/1	0.94	0.20	-	46,46,46,46	0
59	MG	DA	1667	1/1	0.90	0.06	-	66,66,66,66	0
59	MG	CA	3564	1/1	0.97	0.13	-	80,80,80,80	0
59	MG	CA	3127	1/1	0.55	0.41	-	94,94,94,94	0
59	MG	C0	101	1/1	0.96	0.17	-	59,59,59,59	0
59	MG	AA	3540	1/1	0.99	0.09	-	36,36,36,36	0
59	MG	CA	3253	1/1	0.94	0.17	-	70,70,70,70	0
59	MG	AA	3334	1/1	0.97	0.14	-	63,63,63,63	0
59	MG	CA	3599	1/1	0.84	0.08	-	70,70,70,70	0
59	MG	AA	3097	1/1	0.98	0.20	-	22,22,22,22	0
59	MG	A0	102	1/1	0.83	0.09	-	56,56,56,56	0
59	MG	AA	3029	1/1	0.96	0.24	-	28,28,28,28	0
59	MG	AA	3055	1/1	0.89	0.28	-	65,65,65,65	0
59	MG	AA	3389	1/1	0.96	0.15	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3420	1/1	0.95	0.15	-	25,25,25,25	1
59	MG	CA	3298	1/1	0.90	0.36	-	57,57,57,57	0
59	MG	BA	1642	1/1	0.90	0.15	-	60,60,60,60	0
59	MG	CA	3043	1/1	0.92	0.41	-	61,61,61,61	0
59	MG	A0	103	1/1	0.85	0.10	-	70,70,70,70	0
59	MG	CR	201	1/1	0.90	0.26	-	34,34,34,34	0
59	MG	AA	3556	1/1	0.81	0.32	-	66,66,66,66	0
59	MG	CA	3239	1/1	0.91	0.17	-	69,69,69,69	0
59	MG	CA	3550	1/1	0.78	0.09	-	62,62,62,62	1
59	MG	AA	3191	1/1	0.90	0.11	-	16,16,16,16	0
59	MG	DD	502	1/1	0.96	0.48	-	50,50,50,50	0
59	MG	CA	3376	1/1	0.86	0.10	-	78,78,78,78	0
59	MG	DA	1759	1/1	0.93	0.17	-	53,53,53,53	0
59	MG	CA	3352	1/1	0.85	0.18	-	79,79,79,79	0
59	MG	AA	3584	1/1	0.89	0.13	-	17,17,17,17	0
59	MG	AA	3146	1/1	0.99	0.08	-	29,29,29,29	0
59	MG	BA	1786	1/1	0.58	0.22	-	82,82,82,82	0
59	MG	CA	3529	1/1	0.92	0.07	-	68,68,68,68	0
59	MG	CA	3281	1/1	0.95	0.23	-	21,21,21,21	0
59	MG	AA	3741	1/1	0.99	0.10	-	21,21,21,21	0
59	MG	BA	1749	1/1	0.95	0.31	-	61,61,61,61	0
59	MG	AA	3505	1/1	0.98	0.15	-	30,30,30,30	0
59	MG	AR	201	1/1	0.88	0.16	-	28,28,28,28	0
59	MG	CA	3416	1/1	0.95	0.14	-	44,44,44,44	0
59	MG	AA	3201	1/1	0.96	0.09	-	53,53,53,53	0
59	MG	CA	3060	1/1	0.82	0.39	-	72,72,72,72	0
59	MG	DA	1639	1/1	0.55	0.55	-	69,69,69,69	0
59	MG	CA	3469	1/1	0.95	0.22	-	61,61,61,61	0
59	MG	DA	1714	1/1	0.96	0.15	-	68,68,68,68	0
59	MG	AA	3030	1/1	0.94	0.29	-	24,24,24,24	1
59	MG	CA	3086	1/1	0.90	0.26	-	85,85,85,85	0
59	MG	BA	1739	1/1	0.90	0.19	-	62,62,62,62	0
59	MG	CA	3228	1/1	0.98	0.36	-	59,59,59,59	0
59	MG	AA	3369	1/1	0.97	0.12	-	47,47,47,47	0
59	MG	CA	3069	1/1	0.85	0.72	-	81,81,81,81	0
59	MG	AA	3475	1/1	0.99	0.25	-	45,45,45,45	0
59	MG	AA	3327	1/1	0.86	0.17	-	31,31,31,31	0
59	MG	AA	3129	1/1	0.96	0.18	-	34,34,34,34	1
59	MG	A9	502	1/1	0.95	0.25	-	41,41,41,41	0
59	MG	CA	3355	1/1	0.96	0.14	-	35,35,35,35	0
59	MG	CA	3116	1/1	0.87	0.32	-	52,52,52,52	0
59	MG	AA	3684	1/1	0.95	0.25	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BZ	701	1/1	0.96	0.19	-	49,49,49,49	0
59	MG	CA	3206	1/1	0.98	0.41	-	44,44,44,44	0
59	MG	AA	3080	1/1	0.92	0.50	-	61,61,61,61	0
59	MG	AA	3493	1/1	0.95	0.10	-	77,77,77,77	0
59	MG	AA	3143	1/1	0.89	0.23	-	48,48,48,48	0
59	MG	AA	3566	1/1	0.96	0.05	-	56,56,56,56	0
59	MG	AA	3337	1/1	0.94	0.16	-	75,75,75,75	0
59	MG	CA	3525	1/1	0.98	0.28	-	23,23,23,23	0
59	MG	CA	3046	1/1	0.89	0.29	-	68,68,68,68	0
59	MG	AA	3526	1/1	0.99	0.20	-	19,19,19,19	0
59	MG	AA	3535	1/1	0.97	0.13	-	48,48,48,48	0
59	MG	CA	3459	1/1	0.98	0.09	-	28,28,28,28	0
59	MG	CA	3235	1/1	0.86	0.28	-	78,78,78,78	0
59	MG	AA	3342	1/1	0.97	0.23	-	51,51,51,51	0
59	MG	DA	1676	1/1	0.97	0.15	-	74,74,74,74	0
59	MG	AA	3204	1/1	0.93	0.34	-	54,54,54,54	0
59	MG	AA	3057	1/1	0.85	0.18	-	46,46,46,46	0
59	MG	CB	3013	1/1	0.62	0.17	-	100,100,100,100	0
59	MG	AA	3647	1/1	0.96	0.11	-	43,43,43,43	0
59	MG	CA	3187	1/1	0.91	0.22	-	37,37,37,37	0
59	MG	BA	1653	1/1	0.96	0.10	-	56,56,56,56	0
59	MG	AA	3508	1/1	0.95	0.18	-	43,43,43,43	0
59	MG	BA	1635	1/1	0.82	0.51	-	65,65,65,65	0
59	MG	DA	1646	1/1	0.88	0.12	-	57,57,57,57	0
59	MG	AA	3812	1/1	0.95	0.17	-	41,41,41,41	0
59	MG	CA	3476	1/1	0.93	0.17	-	38,38,38,38	0
59	MG	AA	3442	1/1	0.97	0.14	-	23,23,23,23	0
59	MG	CA	3444	1/1	0.91	0.10	-	67,67,67,67	0
59	MG	DA	1734	1/1	0.95	0.14	-	65,65,65,65	0
59	MG	AA	3095	1/1	0.85	0.32	-	75,75,75,75	0
59	MG	AA	3065	1/1	0.87	0.58	-	62,62,62,62	0
59	MG	CA	3256	1/1	0.86	0.29	-	65,65,65,65	0
59	MG	CA	3075	1/1	0.62	0.65	-	90,90,90,90	0
59	MG	AA	3083	1/1	0.85	0.38	-	61,61,61,61	0
59	MG	AA	3024	1/1	0.93	0.13	-	48,48,48,48	0
59	MG	CA	3308	1/1	0.98	0.10	-	39,39,39,39	0
59	MG	CA	3566	1/1	0.83	0.35	-	30,30,30,30	1
59	MG	CA	3488	1/1	0.85	0.15	-	88,88,88,88	0
59	MG	AP	202	1/1	0.88	0.18	-	44,44,44,44	0
59	MG	AA	3077	1/1	0.92	0.27	-	43,43,43,43	0
59	MG	DA	1713	1/1	0.92	0.17	-	49,49,49,49	0
59	MG	AA	3675	1/1	0.81	0.14	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1618	1/1	0.92	0.31	-	52,52,52,52	0
59	MG	AA	3781	1/1	0.91	0.20	-	72,72,72,72	0
59	MG	AA	3558	1/1	0.82	0.08	-	48,48,48,48	0
59	MG	CA	3531	1/1	0.95	0.09	-	47,47,47,47	0
59	MG	CA	3145	1/1	0.82	0.44	-	76,76,76,76	0
59	MG	DA	1637	1/1	0.92	0.39	-	68,68,68,68	0
59	MG	AA	3093	1/1	0.84	1.05	-	92,92,92,92	0
59	MG	BA	1755	1/1	0.38	0.14	-	86,86,86,86	0
59	MG	AA	3104	1/1	0.95	0.32	-	54,54,54,54	0
59	MG	DA	1702	1/1	0.89	0.13	-	63,63,63,63	0
59	MG	AA	3439	1/1	0.98	0.28	-	37,37,37,37	0
59	MG	AA	3010	1/1	0.84	0.44	-	46,46,46,46	0
59	MG	DA	1681	1/1	0.87	0.37	-	70,70,70,70	0
59	MG	AA	3597	1/1	0.98	0.11	-	33,33,33,33	0
59	MG	CA	3051	1/1	0.93	0.74	-	57,57,57,57	0
59	MG	AA	3103	1/1	0.99	0.03	-	5,5,5,5	0
59	MG	AA	3379	1/1	0.97	0.26	-	23,23,23,23	0
59	MG	AA	3538	1/1	0.96	0.15	-	15,15,15,15	0
59	MG	CA	3020	1/1	0.90	0.18	-	47,47,47,47	0
59	MG	CA	3062	1/1	0.96	0.30	-	38,38,38,38	0
59	MG	BA	1629	1/1	0.92	0.28	-	61,61,61,61	0
59	MG	AB	3008	1/1	0.82	0.38	-	52,52,52,52	0
59	MG	AA	3284	1/1	0.91	0.58	-	60,60,60,60	0
59	MG	AA	3689	1/1	0.95	0.09	-	35,35,35,35	0
59	MG	AA	3628	1/1	0.94	0.23	-	70,70,70,70	0
59	MG	CA	3065	1/1	0.87	0.54	-	56,56,56,56	0
59	MG	CA	3391	1/1	0.92	0.07	-	51,51,51,51	0
59	MG	AA	3634	1/1	0.85	0.19	-	76,76,76,76	0
59	MG	DA	1710	1/1	0.94	0.25	-	104,104,104,104	0
59	MG	CA	3040	1/1	0.61	0.47	-	79,79,79,79	0
59	MG	CA	3245	1/1	0.92	0.41	-	62,62,62,62	0
59	MG	DA	1635	1/1	0.90	0.28	-	75,75,75,75	0
59	MG	AE	303	1/1	0.98	0.21	-	19,19,19,19	0
59	MG	AA	3068	1/1	0.87	0.56	-	73,73,73,73	0
59	MG	BA	1614	1/1	0.78	0.14	-	72,72,72,72	0
59	MG	CA	3632	1/1	0.89	0.18	-	74,74,74,74	0
59	MG	AA	3221	1/1	0.95	0.15	-	30,30,30,30	0
59	MG	AA	3603	1/1	0.86	0.62	-	76,76,76,76	0
59	MG	AA	3041	1/1	0.85	0.26	-	37,37,37,37	0
59	MG	CA	3611	1/1	0.96	0.15	-	59,59,59,59	0
59	MG	AQ	204	1/1	0.94	0.23	-	86,86,86,86	0
59	MG	AA	3347	1/1	0.89	0.13	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3242	1/1	0.64	0.30	-	85,85,85,85	0
59	MG	BA	1638	1/1	0.66	0.21	-	66,66,66,66	0
59	MG	BA	1801	1/1	0.94	0.09	-	65,65,65,65	0
59	MG	AA	3159	1/1	0.97	0.27	-	55,55,55,55	0
59	MG	CA	3517	1/1	0.76	0.16	-	62,62,62,62	0
59	MG	CA	3257	1/1	0.89	0.16	-	35,35,35,35	0
59	MG	CA	3429	1/1	0.94	0.26	-	59,59,59,59	0
59	MG	AA	3735	1/1	0.99	0.13	-	25,25,25,25	0
59	MG	AA	3308	1/1	0.90	0.22	-	18,18,18,18	0
59	MG	BA	1688	1/1	0.99	0.43	-	61,61,61,61	0
59	MG	AA	3066	1/1	0.78	0.14	-	51,51,51,51	0
59	MG	CE	302	1/1	0.97	0.13	-	64,64,64,64	0
59	MG	BA	1695	1/1	0.86	0.08	-	83,83,83,83	0
59	MG	AA	3495	1/1	0.94	0.15	-	35,35,35,35	0
59	MG	BA	1640	1/1	0.98	0.44	-	52,52,52,52	0
59	MG	CA	3605	1/1	0.80	0.21	-	70,70,70,70	0
59	MG	BA	1768	1/1	0.89	0.10	-	64,64,64,64	0
59	MG	AA	3541	1/1	0.66	0.12	-	74,74,74,74	0
59	MG	AA	3170	1/1	0.94	0.19	-	54,54,54,54	0
59	MG	BA	1648	1/1	0.82	0.11	-	74,74,74,74	0
59	MG	CA	3584	1/1	0.96	0.15	-	32,32,32,32	0
59	MG	AA	3240	1/1	0.65	0.16	-	69,69,69,69	0
59	MG	AA	3737	1/1	0.95	0.16	-	54,54,54,54	0
59	MG	AA	3312	1/1	0.96	0.10	-	23,23,23,23	0
59	MG	AA	3353	1/1	0.96	0.22	-	39,39,39,39	0
59	MG	CA	3066	1/1	0.90	0.16	-	69,69,69,69	0
59	MG	AA	3381	1/1	0.98	0.16	-	16,16,16,16	0
59	MG	AA	3070	1/1	0.82	0.40	-	81,81,81,81	0
59	MG	CD	301	1/1	0.96	0.44	-	43,43,43,43	0
59	MG	AA	3663	1/1	0.98	0.19	-	11,11,11,11	0
59	MG	CA	3396	1/1	0.92	0.23	-	39,39,39,39	0
59	MG	CA	3129	1/1	0.89	0.59	-	64,64,64,64	0
59	MG	AY	502	1/1	0.91	0.28	-	60,60,60,60	0
59	MG	AA	3732	1/1	0.78	0.28	-	70,70,70,70	0
59	MG	AA	3370	1/1	0.94	0.15	-	47,47,47,47	0
59	MG	CA	3345	1/1	0.92	0.17	-	46,46,46,46	0
59	MG	CA	3024	1/1	0.95	0.29	-	100,100,100,100	0
59	MG	AA	3168	1/1	0.89	0.31	-	47,47,47,47	0
59	MG	CA	3388	1/1	0.78	0.14	-	90,90,90,90	0
59	MG	CA	3403	1/1	0.92	0.07	-	70,70,70,70	0
59	MG	BA	1662	1/1	0.86	0.72	-	70,70,70,70	0
59	MG	BA	1751	1/1	0.97	0.12	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3480	1/1	0.95	0.21	-	50,50,50,50	0
59	MG	CA	3171	1/1	0.90	0.37	-	56,56,56,56	0
59	MG	CA	3609	1/1	0.92	0.16	-	52,52,52,52	0
59	MG	AA	3139	1/1	0.89	0.33	-	60,60,60,60	0
59	MG	AA	3607	1/1	0.90	0.14	-	60,60,60,60	1
59	MG	CA	3121	1/1	0.95	0.12	-	49,49,49,49	0
59	MG	CA	3082	1/1	0.75	0.76	-	76,76,76,76	0
59	MG	DA	1688	1/1	0.93	0.25	-	51,51,51,51	0
59	MG	AA	3783	1/1	0.90	0.48	-	53,53,53,53	1
59	MG	DA	1752	1/1	0.95	0.16	-	52,52,52,52	0
59	MG	DA	1630	1/1	0.96	0.71	-	62,62,62,62	0
59	MG	AA	3582	1/1	0.69	0.59	-	76,76,76,76	0
59	MG	CA	3143	1/1	0.92	0.56	-	41,41,41,41	0
59	MG	CA	3623	1/1	0.91	0.15	-	64,64,64,64	0
59	MG	AA	3804	1/1	0.95	0.18	-	50,50,50,50	0
59	MG	BA	1810	1/1	0.81	0.13	-	82,82,82,82	0
59	MG	AA	3348	1/1	0.95	0.06	-	53,53,53,53	0
59	MG	BA	1799	1/1	0.95	0.13	-	64,64,64,64	0
59	MG	AA	3687	1/1	0.94	0.29	-	52,52,52,52	0
59	MG	BA	1722	1/1	0.98	0.29	-	51,51,51,51	0
59	MG	AA	3281	1/1	0.79	0.29	-	75,75,75,75	0
59	MG	BA	1643	1/1	0.69	0.34	-	66,66,66,66	0
59	MG	AA	3400	1/1	0.95	0.17	-	13,13,13,13	0
59	MG	CA	3585	1/1	0.92	0.16	-	36,36,36,36	1
59	MG	AA	3333	1/1	0.95	0.20	-	11,11,11,11	0
59	MG	AA	3167	1/1	0.79	0.19	-	45,45,45,45	0
59	MG	BA	1682	1/1	0.84	0.82	-	70,70,70,70	0
59	MG	BA	1753	1/1	0.91	0.12	-	48,48,48,48	0
59	MG	BA	1689	1/1	0.82	0.51	-	71,71,71,71	0
59	MG	CA	3072	1/1	0.80	0.38	-	66,66,66,66	0
59	MG	CA	3156	1/1	0.93	0.38	-	52,52,52,52	0
59	MG	CA	3613	1/1	0.98	0.22	-	57,57,57,57	0
59	MG	BA	1651	1/1	0.94	0.33	-	55,55,55,55	0
59	MG	BA	1601	1/1	0.72	0.35	-	95,95,95,95	0
59	MG	DA	1679	1/1	0.88	0.12	-	70,70,70,70	0
59	MG	CA	3001	1/1	0.83	0.25	-	64,64,64,64	0
59	MG	DA	1763	1/1	0.95	0.30	-	76,76,76,76	0
59	MG	AA	3554	1/1	0.97	0.19	-	40,40,40,40	0
59	MG	AA	3707	1/1	0.92	0.09	-	59,59,59,59	0
59	MG	CA	3578	1/1	0.94	0.09	-	38,38,38,38	0
59	MG	AA	3220	1/1	0.98	0.15	-	62,62,62,62	0
59	MG	BA	1658	1/1	0.87	0.61	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3122	1/1	0.53	0.69	-	99,99,99,99	0
59	MG	CA	3536	1/1	0.73	0.26	-	84,84,84,84	0
59	MG	BA	1778	1/1	0.80	0.16	-	54,54,54,54	0
59	MG	AA	3601	1/1	0.82	0.11	-	61,61,61,61	0
59	MG	AA	3567	1/1	0.96	0.11	-	26,26,26,26	0
59	MG	CA	3538	1/1	0.70	0.15	-	72,72,72,72	0
59	MG	AA	3750	1/1	0.96	0.33	-	51,51,51,51	0
59	MG	CA	3180	1/1	0.79	0.36	-	62,62,62,62	0
59	MG	AW	3002	1/1	0.81	0.25	-	47,47,47,47	0
59	MG	AA	3087	1/1	0.82	0.48	-	55,55,55,55	0
59	MG	CA	3582	1/1	0.90	0.08	-	99,99,99,99	0
59	MG	BA	1775	1/1	0.57	0.34	-	90,90,90,90	0
59	MG	AA	3728	1/1	0.96	0.26	-	29,29,29,29	0
59	MG	AA	3650	1/1	0.97	0.11	-	49,49,49,49	0
59	MG	AA	3219	1/1	0.80	0.21	-	61,61,61,61	0
59	MG	AA	3116	1/1	0.96	0.63	-	35,35,35,35	0
59	MG	AA	3263	1/1	0.96	0.42	-	24,24,24,24	1
59	MG	CA	3185	1/1	0.95	0.29	-	48,48,48,48	0
59	MG	CA	3286	1/1	0.96	0.20	-	58,58,58,58	0
59	MG	BA	1664	1/1	0.94	0.14	-	56,56,56,56	0
59	MG	BD	502	1/1	0.86	0.53	-	64,64,64,64	0
59	MG	CA	3336	1/1	0.88	0.09	-	64,64,64,64	0
59	MG	DA	1748	1/1	0.92	0.18	-	70,70,70,70	0
59	MG	AA	3472	1/1	0.90	0.23	-	42,42,42,42	0
59	MG	CA	3400	1/1	0.98	0.13	-	57,57,57,57	0
59	MG	AA	3572	1/1	0.94	0.20	-	17,17,17,17	0
59	MG	CA	3602	1/1	0.75	0.10	-	84,84,84,84	0
59	MG	BA	1678	1/1	0.96	0.21	-	54,54,54,54	0
59	MG	AA	3581	1/1	0.96	0.17	-	52,52,52,52	0
59	MG	AA	3645	1/1	0.92	0.21	-	58,58,58,58	0
59	MG	CA	3493	1/1	0.94	0.53	-	65,65,65,65	0
59	MG	AA	3268	1/1	0.92	0.07	-	66,66,66,66	0
59	MG	CA	3495	1/1	0.88	0.21	-	70,70,70,70	0
59	MG	CP	201	1/1	0.65	0.17	-	62,62,62,62	1
59	MG	AA	3356	1/1	0.93	0.15	-	80,80,80,80	0
59	MG	AA	3637	1/1	0.95	0.33	-	17,17,17,17	1
59	MG	AA	3322	1/1	0.96	0.20	-	61,61,61,61	0
59	MG	AA	3724	1/1	0.88	0.23	-	47,47,47,47	0
59	MG	CA	3607	1/1	0.94	0.09	-	64,64,64,64	0
59	MG	CA	3533	1/1	0.94	0.18	-	45,45,45,45	0
59	MG	AA	3108	1/1	0.40	0.65	-	101,101,101,101	0
59	MG	CA	3511	1/1	0.87	0.20	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1718	1/1	0.92	0.09	-	63,63,63,63	0
59	MG	AN	3001	1/1	0.92	0.32	-	58,58,58,58	0
59	MG	DA	1620	1/1	0.91	0.21	-	57,57,57,57	0
59	MG	AA	3153	1/1	0.87	0.32	-	59,59,59,59	0
59	MG	AA	3784	1/1	0.94	0.21	-	59,59,59,59	0
59	MG	BA	1784	1/1	0.86	0.27	-	68,68,68,68	0
59	MG	AA	3015	1/1	0.88	0.35	-	57,57,57,57	0
59	MG	AA	3726	1/1	0.99	0.16	-	12,12,12,12	0
59	MG	AA	3693	1/1	0.82	0.14	-	69,69,69,69	0
59	MG	AA	3550	1/1	0.96	0.20	-	38,38,38,38	0
59	MG	CA	3622	1/1	0.94	0.17	-	50,50,50,50	0
59	MG	AA	3808	1/1	0.84	0.40	-	72,72,72,72	0
59	MG	AA	3148	1/1	0.94	0.45	-	29,29,29,29	1
59	MG	AA	3270	1/1	0.91	0.55	-	55,55,55,55	0
59	MG	AB	3015	1/1	0.97	0.14	-	28,28,28,28	0
59	MG	DA	1739	1/1	0.88	0.12	-	73,73,73,73	0
59	MG	CA	3363	1/1	0.84	0.16	-	88,88,88,88	0
59	MG	BA	1716	1/1	0.74	0.24	-	86,86,86,86	0
59	MG	CA	3435	1/1	0.98	0.11	-	55,55,55,55	0
59	MG	AA	3716	1/1	0.92	0.24	-	66,66,66,66	0
59	MG	CA	3408	1/1	0.85	0.11	-	58,58,58,58	0
59	MG	A2	3001	1/1	0.87	0.25	-	53,53,53,53	0
59	MG	DA	1662	1/1	0.86	0.23	-	75,75,75,75	0
59	MG	AA	3499	1/1	0.89	0.14	-	48,48,48,48	0
59	MG	CA	3341	1/1	0.86	0.34	-	73,73,73,73	0
59	MG	AA	3026	1/1	0.84	0.23	-	47,47,47,47	0
59	MG	CA	3034	1/1	0.80	0.29	-	77,77,77,77	0
59	MG	AA	3040	1/1	0.42	0.17	-	113,113,113,113	0
59	MG	CA	3219	1/1	0.97	0.25	-	42,42,42,42	0
59	MG	AA	3468	1/1	0.96	0.06	-	55,55,55,55	0
59	MG	CA	3290	1/1	0.96	0.33	-	34,34,34,34	0
59	MG	CA	3014	1/1	0.85	0.24	-	50,50,50,50	0
59	MG	AA	3788	1/1	0.88	0.28	-	61,61,61,61	0
59	MG	BA	1703	1/1	0.88	0.30	-	51,51,51,51	0
59	MG	AA	3247	1/1	0.96	0.16	-	55,55,55,55	0
59	MG	AA	3756	1/1	0.89	0.14	-	49,49,49,49	0
59	MG	AA	3162	1/1	0.89	0.26	-	67,67,67,67	0
59	MG	AA	3615	1/1	0.94	0.26	-	43,43,43,43	0
59	MG	CA	3377	1/1	0.83	0.10	-	52,52,52,52	0
59	MG	AA	3181	1/1	0.79	0.33	-	79,79,79,79	0
59	MG	DA	1660	1/1	0.87	0.14	-	80,80,80,80	0
59	MG	AA	3451	1/1	0.94	0.07	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3341	1/1	0.96	0.19	-	25,25,25,25	0
59	MG	CA	3649	1/1	0.89	0.26	-	51,51,51,51	0
59	MG	AB	3017	1/1	0.59	0.17	-	59,59,59,59	0
59	MG	CA	3316	1/1	0.94	0.17	-	43,43,43,43	0
59	MG	AA	3786	1/1	0.84	0.17	-	53,53,53,53	0
59	MG	AA	3258	1/1	0.82	0.44	-	68,68,68,68	0
59	MG	CA	3575	1/1	0.82	0.20	-	71,71,71,71	0
59	MG	BL	201	1/1	0.66	0.37	-	84,84,84,84	0
59	MG	AA	3778	1/1	0.98	0.14	-	43,43,43,43	0
59	MG	CA	3347	1/1	0.96	0.15	-	45,45,45,45	0
59	MG	DA	1631	1/1	0.76	0.09	-	74,74,74,74	0
59	MG	AA	3365	1/1	0.94	0.39	-	77,77,77,77	0
59	MG	DA	1684	1/1	0.90	0.18	-	69,69,69,69	0
59	MG	DA	1725	1/1	0.95	0.17	-	58,58,58,58	0
59	MG	AA	3173	1/1	0.94	0.28	-	46,46,46,46	0
59	MG	AA	3430	1/1	0.97	0.16	-	39,39,39,39	0
59	MG	CA	3411	1/1	0.87	0.24	-	57,57,57,57	0
59	MG	AA	3298	1/1	0.97	0.15	-	58,58,58,58	0
59	MG	DA	1770	1/1	0.84	0.15	-	63,63,63,63	0
59	MG	CA	3202	1/1	0.81	0.71	-	73,73,73,73	0
59	MG	BA	1719	1/1	0.84	0.15	-	62,62,62,62	0
59	MG	CA	3631	1/1	0.81	0.11	-	65,65,65,65	0
59	MG	AA	3025	1/1	0.87	0.43	-	68,68,68,68	0
59	MG	AA	3470	1/1	0.98	0.08	-	39,39,39,39	0
59	MG	AA	3336	1/1	0.96	0.14	-	51,51,51,51	0
59	MG	AA	3734	1/1	0.98	0.24	-	26,26,26,26	0
59	MG	CA	3551	1/1	0.87	0.07	-	63,63,63,63	0
59	MG	AA	3455	1/1	0.94	0.20	-	32,32,32,32	1
59	MG	BA	1699	1/1	0.91	0.19	-	72,72,72,72	0
59	MG	CA	3088	1/1	0.85	0.31	-	67,67,67,67	0
59	MG	CA	3148	1/1	0.91	0.34	-	62,62,62,62	0
59	MG	DA	1707	1/1	0.95	0.07	-	61,61,61,61	0
59	MG	CA	3305	1/1	0.95	0.27	-	48,48,48,48	0
59	MG	AA	3231	1/1	0.93	0.21	-	64,64,64,64	0
59	MG	CA	3356	1/1	0.95	0.19	-	44,44,44,44	0
59	MG	CA	3196	1/1	0.94	0.66	-	68,68,68,68	0
59	MG	CA	3633	1/1	0.84	0.27	-	68,68,68,68	0
59	MG	AA	3114	1/1	0.96	0.21	-	26,26,26,26	0
59	MG	CA	3593	1/1	0.89	0.60	-	61,61,61,61	0
59	MG	CA	3546	1/1	0.56	0.15	-	88,88,88,88	0
59	MG	DA	1751	1/1	0.92	0.16	-	64,64,64,64	0
59	MG	AA	3046	1/1	0.93	0.33	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3697	1/1	0.95	0.23	-	40,40,40,40	0
59	MG	AA	3586	1/1	0.80	0.35	-	74,74,74,74	0
59	MG	CA	3475	1/1	0.97	0.25	-	50,50,50,50	0
59	MG	AA	3056	1/1	0.84	1.05	-	96,96,96,96	0
59	MG	BA	1650	1/1	0.92	0.14	-	55,55,55,55	0
59	MG	DA	1645	1/1	0.96	0.10	-	58,58,58,58	0
59	MG	AA	3061	1/1	0.84	0.57	-	59,59,59,59	0
59	MG	BA	1708	1/1	0.91	0.22	-	64,64,64,64	0
59	MG	BA	1773	1/1	0.97	0.13	-	40,40,40,40	0
59	MG	AB	3019	1/1	0.97	0.12	-	70,70,70,70	0
59	MG	CA	3393	1/1	0.94	0.07	-	68,68,68,68	0
59	MG	AA	3761	1/1	0.80	0.38	-	92,92,92,92	0
59	MG	CA	3580	1/1	0.91	0.23	-	76,76,76,76	0
59	MG	AA	3525	1/1	0.97	0.18	-	35,35,35,35	0
59	MG	AA	3210	1/1	0.96	0.31	-	59,59,59,59	1
59	MG	CA	3260	1/1	0.87	0.15	-	35,35,35,35	0
59	MG	BA	1637	1/1	0.91	0.46	-	72,72,72,72	0
59	MG	AA	3595	1/1	0.98	0.15	-	42,42,42,42	0
59	MG	AA	3135	1/1	0.91	0.56	-	55,55,55,55	0
59	MG	BA	1770	1/1	0.96	0.12	-	54,54,54,54	0
59	MG	AA	3516	1/1	0.91	0.23	-	65,65,65,65	0
59	MG	AA	3564	1/1	0.96	0.20	-	44,44,44,44	0
59	MG	CA	3654	1/1	0.66	0.40	-	90,90,90,90	0
59	MG	AA	3196	1/1	0.88	0.19	-	55,55,55,55	0
59	MG	CA	3092	1/1	0.78	0.77	-	79,79,79,79	0
59	MG	CA	3042	1/1	0.91	0.31	-	65,65,65,65	0
59	MG	DA	1623	1/1	0.65	0.24	-	72,72,72,72	0
59	MG	CA	3246	1/1	0.87	0.50	-	57,57,57,57	0
59	MG	AA	3618	1/1	0.90	0.15	-	72,72,72,72	0
59	MG	AQ	201	1/1	0.97	0.44	-	48,48,48,48	0
59	MG	AP	203	1/1	0.84	0.18	-	59,59,59,59	0
59	MG	CA	3102	1/1	0.96	0.50	-	62,62,62,62	0
59	MG	CA	3130	1/1	0.85	0.16	-	55,55,55,55	0
59	MG	AA	3802	1/1	0.95	0.15	-	86,86,86,86	0
59	MG	AA	3478	1/1	0.95	0.24	-	33,33,33,33	0
59	MG	AA	3605	1/1	0.96	0.32	-	45,45,45,45	0
59	MG	CA	3430	1/1	0.93	0.36	-	41,41,41,41	0
59	MG	DA	1758	1/1	0.93	0.17	-	75,75,75,75	0
59	MG	AA	3580	1/1	0.94	0.22	-	54,54,54,54	0
59	MG	DA	1675	1/1	0.91	0.41	-	70,70,70,70	0
59	MG	AA	3797	1/1	0.92	0.17	-	52,52,52,52	0
59	MG	AA	3132	1/1	0.95	0.21	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CQ	203	1/1	0.88	0.34	-	54,54,54,54	0
59	MG	CA	3496	1/1	0.88	0.13	-	56,56,56,56	0
59	MG	CA	3165	1/1	0.86	0.25	-	57,57,57,57	0
59	MG	AA	3755	1/1	0.97	0.64	-	78,78,78,78	0
59	MG	AA	3662	1/1	0.94	0.07	-	60,60,60,60	0
59	MG	AA	3358	1/1	0.91	0.12	-	45,45,45,45	0
59	MG	AA	3248	1/1	0.99	0.14	-	22,22,22,22	0
59	MG	CA	3567	1/1	0.98	0.22	-	26,26,26,26	0
59	MG	CA	3244	1/1	0.54	0.30	-	89,89,89,89	0
59	MG	AA	3664	1/1	0.88	0.20	-	62,62,62,62	0
59	MG	AA	3078	1/1	0.91	0.32	-	70,70,70,70	0
59	MG	CA	3295	1/1	0.96	0.26	-	66,66,66,66	0
59	MG	CA	3080	1/1	0.58	0.23	-	75,75,75,75	0
59	MG	BW	503	1/1	0.88	0.20	-	60,60,60,60	0
59	MG	CD	303	1/1	0.92	0.08	-	70,70,70,70	0
59	MG	CA	3656	1/1	0.86	0.57	-	63,63,63,63	0
59	MG	AA	3433	1/1	0.98	0.14	-	37,37,37,37	0
59	MG	CA	3335	1/1	0.96	0.20	-	66,66,66,66	0
59	MG	CA	3011	1/1	0.97	0.38	-	63,63,63,63	0
59	MG	AA	3435	1/1	0.96	0.17	-	52,52,52,52	0
59	MG	BA	1798	1/1	0.96	0.41	-	73,73,73,73	0
59	MG	CA	3135	1/1	0.73	0.31	-	59,59,59,59	0
59	MG	AA	3119	1/1	0.96	0.31	-	47,47,47,47	0
59	MG	AA	3385	1/1	0.89	0.21	-	49,49,49,49	0
59	MG	BA	1608	1/1	0.90	0.52	-	57,57,57,57	0
59	MG	AA	3609	1/1	0.93	0.11	-	58,58,58,58	0
59	MG	BA	1622	1/1	0.88	0.51	-	65,65,65,65	0
59	MG	DA	1656	1/1	0.83	0.13	-	63,63,63,63	0
59	MG	AA	3229	1/1	0.87	0.36	-	67,67,67,67	0
59	MG	AA	3256	1/1	0.90	0.34	-	49,49,49,49	0
59	MG	CA	3350	1/1	0.74	0.09	-	82,82,82,82	0
59	MG	BA	1752	1/1	0.97	0.27	-	59,59,59,59	0
59	MG	BA	1729	1/1	0.84	0.16	-	53,53,53,53	0
59	MG	CA	3591	1/1	0.79	0.11	-	60,60,60,60	0
59	MG	CA	3050	1/1	0.82	0.45	-	75,75,75,75	0
59	MG	CA	3186	1/1	0.59	0.61	-	77,77,77,77	0
59	MG	AA	3154	1/1	0.98	0.18	-	57,57,57,57	0
59	MG	AA	3194	1/1	0.88	0.25	-	82,82,82,82	0
59	MG	BS	101	1/1	0.80	0.16	-	79,79,79,79	0
59	MG	CA	3271	1/1	0.91	0.18	-	48,48,48,48	0
59	MG	CA	3548	1/1	0.70	0.10	-	90,90,90,90	0
59	MG	CA	3251	1/1	0.85	0.18	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3610	1/1	0.94	0.22	-	59,59,59,59	0
59	MG	CA	3541	1/1	0.78	0.28	-	63,63,63,63	0
59	MG	AA	3807	1/1	0.50	0.31	-	77,77,77,77	0
59	MG	AA	3719	1/1	0.94	0.10	-	59,59,59,59	0
59	MG	AA	3668	1/1	0.96	0.17	-	54,54,54,54	0
59	MG	AA	3285	1/1	0.88	0.30	-	51,51,51,51	0
59	MG	CA	3149	1/1	0.59	0.17	-	100,100,100,100	0
59	MG	DA	1720	1/1	0.96	0.10	-	60,60,60,60	0
59	MG	CA	3354	1/1	0.95	0.25	-	49,49,49,49	0
59	MG	DA	1709	1/1	0.94	0.16	-	70,70,70,70	0
59	MG	A5	502	1/1	0.94	0.16	-	51,51,51,51	0
59	MG	CA	3456	1/1	0.85	0.09	-	54,54,54,54	0
59	MG	CB	3002	1/1	0.90	0.10	-	63,63,63,63	0
59	MG	AA	3790	1/1	0.95	0.47	-	57,57,57,57	0
59	MG	DA	1746	1/1	0.66	0.10	-	81,81,81,81	0
59	MG	CA	3422	1/1	0.97	0.24	-	43,43,43,43	0
59	MG	CA	3109	1/1	0.97	0.22	-	35,35,35,35	0
59	MG	AA	3202	1/1	0.86	0.11	-	61,61,61,61	0
59	MG	BA	1806	1/1	0.90	0.33	-	55,55,55,55	0
59	MG	BA	1657	1/1	0.47	0.25	-	78,78,78,78	0
59	MG	BA	1710	1/1	0.93	0.25	-	81,81,81,81	0
59	MG	AA	3346	1/1	0.99	0.14	-	59,59,59,59	0
59	MG	AA	3665	1/1	0.97	0.30	-	40,40,40,40	0
59	MG	BA	1624	1/1	0.84	0.18	-	58,58,58,58	0
59	MG	AA	3063	1/1	0.93	0.26	-	54,54,54,54	0
59	MG	CA	3395	1/1	0.86	0.42	-	50,50,50,50	0
59	MG	AA	3692	1/1	0.96	0.15	-	36,36,36,36	1
59	MG	AA	3686	1/1	0.95	0.20	-	61,61,61,61	0
59	MG	AA	3703	1/1	0.96	0.23	-	56,56,56,56	0
59	MG	CA	3176	1/1	0.83	0.41	-	60,60,60,60	0
59	MG	DA	1740	1/1	0.96	0.57	-	68,68,68,68	0
59	MG	DA	1695	1/1	0.94	0.17	-	63,63,63,63	0
59	MG	CA	3142	1/1	0.94	0.44	-	61,61,61,61	0
59	MG	CA	3639	1/1	0.95	0.59	-	61,61,61,61	0
59	MG	CA	3329	1/1	0.98	0.14	-	21,21,21,21	0
59	MG	CA	3470	1/1	0.94	0.19	-	74,74,74,74	0
59	MG	CA	3520	1/1	0.92	0.16	-	73,73,73,73	0
59	MG	AA	3699	1/1	0.88	0.27	-	71,71,71,71	0
59	MG	AZ	301	1/1	0.93	0.14	-	55,55,55,55	0
59	MG	DA	1619	1/1	0.95	0.59	-	59,59,59,59	0
59	MG	AA	3500	1/1	0.96	0.12	-	59,59,59,59	0
59	MG	AA	3309	1/1	0.97	0.25	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3295	1/1	0.89	0.14	-	57,57,57,57	0
59	MG	BA	1683	1/1	0.87	0.21	-	71,71,71,71	0
59	MG	AA	3354	1/1	0.99	0.12	-	27,27,27,27	0
59	MG	AA	3796	1/1	0.88	0.50	-	78,78,78,78	0
59	MG	BA	1724	1/1	0.91	0.19	-	67,67,67,67	0
59	MG	CA	3586	1/1	0.90	0.17	-	93,93,93,93	0
59	MG	CA	3057	1/1	0.88	0.29	-	60,60,60,60	0
59	MG	AA	3395	1/1	0.97	0.17	-	54,54,54,54	0
59	MG	AA	3791	1/1	0.96	0.17	-	51,51,51,51	0
59	MG	AA	3748	1/1	0.93	0.20	-	45,45,45,45	0
59	MG	BA	1781	1/1	0.94	0.14	-	63,63,63,63	0
59	MG	AA	3573	1/1	0.94	0.16	-	12,12,12,12	0
59	MG	CB	3009	1/1	0.97	0.18	-	67,67,67,67	0
59	MG	CD	302	1/1	0.83	0.53	-	56,56,56,56	0
59	MG	AA	3091	1/1	0.98	0.76	-	47,47,47,47	1
59	MG	CA	3078	1/1	0.81	0.48	-	57,57,57,57	0
59	MG	CA	3338	1/1	0.96	0.14	-	64,64,64,64	0
59	MG	CA	3016	1/1	0.86	0.25	-	52,52,52,52	0
59	MG	CA	3512	1/1	0.90	0.15	-	53,53,53,53	0
59	MG	CA	3394	1/1	0.96	0.12	-	69,69,69,69	0
59	MG	AA	3197	1/1	0.87	0.19	-	45,45,45,45	0
59	MG	CA	3507	1/1	0.85	0.27	-	83,83,83,83	0
59	MG	BA	1733	1/1	0.91	0.20	-	78,78,78,78	0
59	MG	CA	3414	1/1	0.93	0.19	-	34,34,34,34	1
59	MG	DA	1658	1/1	0.90	0.33	-	51,51,51,51	0
59	MG	AA	3331	1/1	0.86	0.16	-	15,15,15,15	0
59	MG	AB	3005	1/1	0.97	0.20	-	44,44,44,44	0
59	MG	DZ	702	1/1	0.96	0.22	-	57,57,57,57	0
59	MG	BA	1673	1/1	0.60	0.20	-	80,80,80,80	0
59	MG	AA	3491	1/1	0.96	0.09	-	46,46,46,46	0
59	MG	CA	3374	1/1	0.91	0.30	-	60,60,60,60	0
59	MG	CA	3128	1/1	0.92	0.39	-	50,50,50,50	0
59	MG	A7	101	1/1	0.82	0.16	-	55,55,55,55	0
59	MG	BA	1661	1/1	0.89	0.32	-	63,63,63,63	0
59	MG	AA	3677	1/1	0.87	0.10	-	69,69,69,69	0
59	MG	AA	3089	1/1	0.94	0.28	-	49,49,49,49	0
59	MG	CA	3073	1/1	0.93	0.26	-	49,49,49,49	0
59	MG	DA	1705	1/1	0.91	0.10	-	68,68,68,68	0
59	MG	CA	3471	1/1	0.96	0.19	-	33,33,33,33	0
59	MG	CA	3098	1/1	0.87	0.14	-	70,70,70,70	0
59	MG	AA	3717	1/1	0.70	0.56	-	68,68,68,68	0
59	MG	BA	1644	1/1	0.79	0.19	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3410	1/1	0.99	0.14	-	57,57,57,57	0
59	MG	DF	3001	1/1	0.90	0.20	-	54,54,54,54	0
59	MG	DA	1694	1/1	0.91	0.34	-	106,106,106,106	0
59	MG	CA	3402	1/1	0.93	0.09	-	66,66,66,66	0
59	MG	CA	3188	1/1	0.94	0.81	-	94,94,94,94	0
59	MG	AA	3251	1/1	0.94	0.35	-	56,56,56,56	0
59	MG	DA	1729	1/1	0.85	0.17	-	49,49,49,49	0
59	MG	DA	1728	1/1	0.92	0.08	-	71,71,71,71	0
59	MG	AA	3273	1/1	0.79	0.76	-	90,90,90,90	0
59	MG	AA	3383	1/1	0.96	0.16	-	20,20,20,20	0
59	MG	AA	3126	1/1	0.87	0.37	-	79,79,79,79	0
59	MG	AA	3484	1/1	0.98	0.11	-	53,53,53,53	0
59	MG	CA	3443	1/1	0.98	0.18	-	28,28,28,28	0
59	MG	AW	3001	1/1	0.89	0.29	-	54,54,54,54	0
59	MG	DA	1674	1/1	0.77	0.28	-	77,77,77,77	0
59	MG	CA	3003	1/1	0.94	0.30	-	62,62,62,62	0
59	MG	CA	3134	1/1	0.90	0.66	-	71,71,71,71	0
59	MG	AA	3638	1/1	0.91	0.35	-	71,71,71,71	0
59	MG	AA	3681	1/1	0.97	0.13	-	42,42,42,42	0
59	MG	CA	3587	1/1	0.67	0.33	-	70,70,70,70	0
59	MG	CA	3477	1/1	0.90	0.14	-	69,69,69,69	0
59	MG	AA	3524	1/1	0.97	0.19	-	41,41,41,41	0
59	MG	AA	3088	1/1	0.89	0.42	-	39,39,39,39	0
59	MG	BA	1785	1/1	0.97	0.17	-	62,62,62,62	0
59	MG	CB	3011	1/1	0.88	0.23	-	56,56,56,56	0
59	MG	DA	1701	1/1	0.91	0.24	-	68,68,68,68	0
59	MG	DA	1760	1/1	0.95	0.14	-	61,61,61,61	0
59	MG	BA	1666	1/1	0.92	0.37	-	61,61,61,61	0
59	MG	AA	3329	1/1	0.96	0.08	-	40,40,40,40	1
59	MG	AA	3591	1/1	0.90	0.26	-	52,52,52,52	0
59	MG	AA	3507	1/1	0.96	0.15	-	50,50,50,50	0
59	MG	AA	3394	1/1	0.92	0.16	-	39,39,39,39	0
59	MG	AA	3293	1/1	0.88	0.15	-	27,27,27,27	0
59	MG	AA	3557	1/1	0.89	0.19	-	37,37,37,37	0
59	MG	AA	3098	1/1	0.97	0.27	-	51,51,51,51	0
59	MG	DA	1677	1/1	0.91	0.42	-	78,78,78,78	0
59	MG	DA	1738	1/1	0.29	0.48	-	95,95,95,95	0
59	MG	BA	1802	1/1	0.70	0.24	-	76,76,76,76	0
59	MG	AA	3206	1/1	0.81	0.53	-	106,106,106,106	0
59	MG	CA	3379	1/1	0.85	0.23	-	83,83,83,83	0
59	MG	AA	3661	1/1	0.93	0.24	-	41,41,41,41	1
59	MG	AA	3574	1/1	0.95	0.17	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3678	1/1	0.92	0.15	-	77,77,77,77	0
59	MG	AA	3138	1/1	0.90	0.12	-	38,38,38,38	0
59	MG	AA	3212	1/1	0.45	0.82	-	81,81,81,81	0
59	MG	AA	3211	1/1	0.91	0.27	-	56,56,56,56	0
59	MG	DA	1698	1/1	0.94	0.33	-	97,97,97,97	0
59	MG	CA	3074	1/1	0.96	0.33	-	49,49,49,49	0
59	MG	CA	3307	1/1	0.80	0.31	-	60,60,60,60	0
59	MG	AA	3700	1/1	0.90	0.22	-	70,70,70,70	0
59	MG	CA	3577	1/1	0.85	0.16	-	51,51,51,51	1
59	MG	CA	3465	1/1	0.90	0.30	-	70,70,70,70	0
59	MG	BA	1772	1/1	0.84	0.12	-	66,66,66,66	0
59	MG	AA	3751	1/1	0.86	0.34	-	61,61,61,61	0
59	MG	AA	3450	1/1	0.83	0.10	-	58,58,58,58	0
59	MG	DA	1691	1/1	0.92	0.18	-	63,63,63,63	0
59	MG	AA	3290	1/1	0.95	0.13	-	64,64,64,64	0
59	MG	AA	3227	1/1	0.81	0.18	-	22,22,22,22	0
59	MG	AA	3096	1/1	0.93	0.20	-	59,59,59,59	0
59	MG	CA	3494	1/1	0.78	0.24	-	97,97,97,97	0
59	MG	DA	1654	1/1	0.71	0.35	-	63,63,63,63	0
59	MG	DA	1732	1/1	0.84	0.15	-	85,85,85,85	0
59	MG	DA	1767	1/1	0.89	0.13	-	74,74,74,74	0
59	MG	BA	1685	1/1	0.85	0.14	-	50,50,50,50	0
59	MG	AA	3243	1/1	0.98	0.23	-	43,43,43,43	0
59	MG	CA	3111	1/1	0.85	0.24	-	79,79,79,79	0
59	MG	AA	3149	1/1	0.82	0.33	-	51,51,51,51	0
59	MG	BA	1734	1/1	0.93	0.13	-	61,61,61,61	0
59	MG	BA	1674	1/1	0.95	0.57	-	48,48,48,48	0
59	MG	DA	1613	1/1	0.92	0.24	-	48,48,48,48	0
59	MG	DA	1765	1/1	0.96	0.13	-	64,64,64,64	0
59	MG	AA	3679	1/1	0.90	0.08	-	36,36,36,36	0
59	MG	AA	3680	1/1	0.70	0.33	-	79,79,79,79	0
59	MG	A8	5001	1/1	0.94	0.27	-	30,30,30,30	0
59	MG	AA	3644	1/1	0.78	0.33	-	56,56,56,56	0
59	MG	BA	1654	1/1	0.67	0.23	-	76,76,76,76	0
59	MG	CA	3340	1/1	0.86	0.17	-	66,66,66,66	0
59	MG	AO	5001	1/1	0.95	0.09	-	34,34,34,34	0
59	MG	CA	3173	1/1	0.87	0.36	-	61,61,61,61	0
59	MG	AA	3559	1/1	0.97	0.23	-	46,46,46,46	0
59	MG	AA	3545	1/1	0.98	0.19	-	43,43,43,43	0
59	MG	AA	3366	1/1	0.97	0.23	-	35,35,35,35	1
59	MG	CA	3625	1/1	0.89	0.27	-	64,64,64,64	0
59	MG	AA	3759	1/1	0.94	0.10	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3160	1/1	0.95	0.15	-	30,30,30,30	0
59	MG	AA	3492	1/1	0.89	0.18	-	26,26,26,26	0
59	MG	CA	3327	1/1	0.96	0.16	-	38,38,38,38	0
59	MG	CA	3431	1/1	0.92	0.20	-	75,75,75,75	0
59	MG	BA	1796	1/1	0.89	0.26	-	57,57,57,57	0
59	MG	AA	3810	1/1	0.90	0.27	-	67,67,67,67	0
59	MG	CA	3053	1/1	0.97	0.45	-	32,32,32,32	0
59	MG	BA	1738	1/1	0.91	0.08	-	66,66,66,66	0
59	MG	CA	3153	1/1	0.84	0.23	-	73,73,73,73	0
59	MG	BA	1790	1/1	0.60	0.15	-	96,96,96,96	0
59	MG	BA	1606	1/1	0.96	0.28	-	126,126,126,126	0
59	MG	AA	3092	1/1	0.96	0.17	-	39,39,39,39	0
59	MG	BA	1646	1/1	0.85	0.95	-	66,66,66,66	0
59	MG	CA	3485	1/1	0.56	0.30	-	85,85,85,85	0
59	MG	CA	3418	1/1	0.96	0.29	-	34,34,34,34	0
59	MG	CA	3579	1/1	0.70	0.22	-	65,65,65,65	0
59	MG	CA	3289	1/1	0.80	0.28	-	65,65,65,65	0
59	MG	CA	3114	1/1	0.88	0.19	-	66,66,66,66	0
59	MG	CA	3501	1/1	0.70	0.45	-	74,74,74,74	0
59	MG	CA	3424	1/1	0.97	0.19	-	66,66,66,66	0
59	MG	DA	1636	1/1	0.86	0.50	-	62,62,62,62	0
59	MG	BA	1797	1/1	0.90	0.17	-	59,59,59,59	0
59	MG	AA	3296	1/1	0.72	0.25	-	67,67,67,67	0
59	MG	AA	3617	1/1	0.53	0.15	-	77,77,77,77	0
59	MG	AA	3787	1/1	0.90	0.20	-	82,82,82,82	0
59	MG	BA	1779	1/1	0.89	0.19	-	85,85,85,85	0
59	MG	DA	1643	1/1	0.85	0.25	-	79,79,79,79	0
59	MG	AB	3002	1/1	0.93	0.17	-	52,52,52,52	0
59	MG	AA	3419	1/1	0.97	0.17	-	20,20,20,20	0
59	MG	CA	3629	1/1	0.84	0.08	-	55,55,55,55	0
59	MG	CA	3193	1/1	0.83	0.44	-	89,89,89,89	0
59	MG	CB	3012	1/1	0.87	0.26	-	62,62,62,62	0
59	MG	CB	3010	1/1	0.96	0.13	-	51,51,51,51	0
59	MG	AA	3340	1/1	0.96	0.22	-	3,3,3,3	0
59	MG	CA	3119	1/1	0.97	0.54	-	55,55,55,55	0
59	MG	AA	3431	1/1	0.95	0.15	-	25,25,25,25	0
59	MG	AA	3533	1/1	0.95	0.17	-	22,22,22,22	0
59	MG	DA	1624	1/1	0.84	0.12	-	82,82,82,82	0
59	MG	AA	3646	1/1	0.93	0.22	-	53,53,53,53	0
59	MG	AA	3635	1/1	0.89	0.31	-	49,49,49,49	0
59	MG	DA	1754	1/1	0.48	0.40	-	120,120,120,120	0
59	MG	AA	3271	1/1	0.95	0.33	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1741	1/1	0.62	0.19	-	88,88,88,88	0
59	MG	CA	3152	1/1	0.72	0.35	-	64,64,64,64	0
59	MG	CA	3234	1/1	0.91	0.35	-	50,50,50,50	0
59	MG	BA	1791	1/1	0.85	0.17	-	72,72,72,72	0
59	MG	CA	3023	1/1	0.84	0.42	-	68,68,68,68	0
59	MG	DA	1606	1/1	0.91	0.30	-	85,85,85,85	0
59	MG	AA	3260	1/1	0.95	0.17	-	21,21,21,21	0
59	MG	AA	3639	1/1	0.97	0.13	-	18,18,18,18	0
59	MG	CA	3648	1/1	0.98	0.35	-	52,52,52,52	0
59	MG	DA	1659	1/1	0.68	0.29	-	78,78,78,78	0
59	MG	BA	1639	1/1	0.93	0.46	-	61,61,61,61	0
59	MG	BA	1715	1/1	0.96	0.11	-	60,60,60,60	0
59	MG	CA	3482	1/1	0.97	0.17	-	61,61,61,61	0
59	MG	AA	3754	1/1	0.58	0.25	-	64,64,64,64	0
59	MG	CA	3099	1/1	0.96	0.24	-	58,58,58,58	0
59	MG	BA	1707	1/1	0.76	0.11	-	72,72,72,72	0
59	MG	AA	3801	1/1	0.99	0.15	-	27,27,27,27	0
59	MG	DA	1611	1/1	0.72	0.39	-	89,89,89,89	0
59	MG	CA	3183	1/1	0.94	0.21	-	49,49,49,49	0
59	MG	CA	3044	1/1	0.78	0.21	-	89,89,89,89	0
59	MG	CA	3249	1/1	0.90	0.15	-	61,61,61,61	0
59	MG	AA	3076	1/1	0.99	0.13	-	0,0,0,0	0
59	MG	AA	3660	1/1	0.82	0.22	-	61,61,61,61	0
59	MG	CA	3167	1/1	0.93	0.08	-	50,50,50,50	0
59	MG	AA	3720	1/1	0.96	0.16	-	55,55,55,55	0
59	MG	CA	3117	1/1	0.70	0.28	-	67,67,67,67	0
59	MG	BA	1728	1/1	0.90	0.19	-	47,47,47,47	0
59	MG	CA	3497	1/1	0.97	0.09	-	45,45,45,45	0
59	MG	AA	3115	1/1	0.92	0.34	-	44,44,44,44	0
59	MG	AA	3596	1/1	0.83	0.31	-	65,65,65,65	0
59	MG	CA	3179	1/1	0.98	0.32	-	60,60,60,60	0
59	MG	CA	3560	1/1	0.85	0.22	-	79,79,79,79	0
59	MG	CA	3030	1/1	0.80	0.51	-	59,59,59,59	0
59	MG	AA	3310	1/1	0.91	0.15	-	56,56,56,56	0
59	MG	DA	1693	1/1	0.96	0.14	-	67,67,67,67	0
59	MG	AA	3760	1/1	0.98	0.37	-	55,55,55,55	0
59	MG	DA	1653	1/1	0.98	0.30	-	55,55,55,55	0
59	MG	AA	3178	1/1	0.93	0.36	-	48,48,48,48	0
59	MG	AA	3287	1/1	0.92	0.39	-	43,43,43,43	0
59	MG	AA	3316	1/1	0.98	0.23	-	36,36,36,36	0
59	MG	DA	1663	1/1	0.88	0.42	-	91,91,91,91	0
59	MG	CA	3454	1/1	0.85	0.16	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3505	1/1	0.74	0.09	-	67,67,67,67	0
59	MG	AA	3583	1/1	0.83	0.14	-	63,63,63,63	0
59	MG	AA	3685	1/1	0.95	0.19	-	72,72,72,72	0
59	MG	AA	3375	1/1	0.96	0.29	-	48,48,48,48	0
59	MG	AA	3542	1/1	0.85	0.23	-	58,58,58,58	0
59	MG	BA	1610	1/1	0.85	0.08	-	78,78,78,78	0
59	MG	AA	3085	1/1	0.92	0.20	-	46,46,46,46	0
59	MG	AA	3641	1/1	0.92	0.28	-	51,51,51,51	0
59	MG	AA	3071	1/1	0.94	0.60	-	40,40,40,40	0
59	MG	CA	3545	1/1	0.87	0.46	-	86,86,86,86	0
59	MG	AA	3611	1/1	0.85	0.18	-	47,47,47,47	0
59	MG	DA	1629	1/1	0.93	0.42	-	59,59,59,59	0
59	MG	CA	3643	1/1	0.94	0.17	-	79,79,79,79	0
59	MG	AA	3323	1/1	0.77	0.21	-	64,64,64,64	0
59	MG	AA	3517	1/1	0.97	0.07	-	23,23,23,23	0
59	MG	AA	3180	1/1	0.85	0.26	-	69,69,69,69	0
59	MG	AA	3266	1/1	0.49	0.78	-	90,90,90,90	0
59	MG	AA	3612	1/1	0.91	0.14	-	68,68,68,68	0
59	MG	CA	3597	1/1	0.91	0.21	-	58,58,58,58	0
59	MG	CA	3110	1/1	0.91	0.26	-	56,56,56,56	0
59	MG	AA	3758	1/1	0.96	0.28	-	43,43,43,43	1
59	MG	CA	3404	1/1	0.97	0.16	-	65,65,65,65	0
59	MG	AA	3363	1/1	0.74	0.20	-	82,82,82,82	0
59	MG	AA	3457	1/1	0.98	0.13	-	30,30,30,30	0
59	MG	AA	3330	1/1	0.95	0.07	-	66,66,66,66	0
59	MG	BA	1675	1/1	0.92	0.07	-	100,100,100,100	0
59	MG	BA	1706	1/1	0.90	0.20	-	63,63,63,63	0
59	MG	AA	3723	1/1	0.88	0.09	-	49,49,49,49	0
59	MG	CA	3293	1/1	0.93	0.16	-	60,60,60,60	0
59	MG	CA	3472	1/1	0.90	0.47	-	62,62,62,62	0
59	MG	DA	1644	1/1	0.84	0.35	-	94,94,94,94	0
59	MG	AA	3405	1/1	0.99	0.27	-	44,44,44,44	0
59	MG	CA	3423	1/1	0.99	0.23	-	46,46,46,46	0
59	MG	AA	3111	1/1	0.97	0.24	-	24,24,24,24	0
59	MG	AA	3482	1/1	0.99	0.12	-	41,41,41,41	0
59	MG	AA	3378	1/1	0.94	0.17	-	56,56,56,56	0
59	MG	BA	1807	1/1	0.91	0.12	-	61,61,61,61	0
59	MG	AA	3711	1/1	0.94	0.36	-	43,43,43,43	1
59	MG	CA	3384	1/1	0.98	0.12	-	55,55,55,55	0
59	MG	CA	3521	1/1	0.84	0.22	-	74,74,74,74	0
59	MG	AB	3013	1/1	0.95	0.15	-	53,53,53,53	0
59	MG	AA	3005	1/1	0.88	0.16	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3107	1/1	0.96	0.13	-	49,49,49,49	0
59	MG	CA	3646	1/1	0.37	0.17	-	91,91,91,91	0
59	MG	CA	3107	1/1	0.95	0.26	-	77,77,77,77	0
59	MG	AA	3434	1/1	0.98	0.06	-	17,17,17,17	0
59	MG	CA	3248	1/1	0.94	0.42	-	53,53,53,53	0
59	MG	AA	3531	1/1	0.96	0.13	-	24,24,24,24	0
59	MG	DA	1632	1/1	0.82	0.29	-	57,57,57,57	0
59	MG	AA	3643	1/1	0.81	0.24	-	84,84,84,84	0
59	MG	CA	3284	1/1	0.83	0.17	-	75,75,75,75	0
59	MG	CA	3049	1/1	0.98	0.36	-	46,46,46,46	0
59	MG	CA	3351	1/1	0.97	0.14	-	46,46,46,46	0
59	MG	CA	3063	1/1	0.94	0.10	-	34,34,34,34	0
59	MG	BA	1693	1/1	0.81	0.48	-	76,76,76,76	0
59	MG	AA	3314	1/1	0.93	0.26	-	57,57,57,57	0
59	MG	CA	3147	1/1	0.95	0.29	-	55,55,55,55	0
59	MG	BA	1694	1/1	0.85	0.24	-	83,83,83,83	0
59	MG	CA	3297	1/1	0.97	0.34	-	36,36,36,36	0
59	MG	DA	1716	1/1	0.96	0.10	-	57,57,57,57	0
59	MG	CA	3032	1/1	0.91	0.56	-	100,100,100,100	0
59	MG	CA	3120	1/1	0.84	0.21	-	42,42,42,42	0
59	MG	CA	3301	1/1	0.92	0.20	-	60,60,60,60	0
59	MG	AA	3016	1/1	0.65	0.45	-	64,64,64,64	0
59	MG	BA	1712	1/1	0.87	0.40	-	57,57,57,57	0
59	MG	CA	3474	1/1	0.88	0.22	-	59,59,59,59	0
59	MG	BA	1811	1/1	0.79	0.20	-	77,77,77,77	0
59	MG	AE	301	1/1	0.76	0.57	-	69,69,69,69	0
59	MG	CA	3583	1/1	0.80	0.17	-	80,80,80,80	0
59	MG	AA	3376	1/1	0.93	0.21	-	35,35,35,35	0
59	MG	DW	501	1/1	0.98	0.17	-	44,44,44,44	0
59	MG	DA	1741	1/1	0.92	0.35	-	67,67,67,67	0
59	MG	DA	1757	1/1	0.26	1.13	-	111,111,111,111	0
59	MG	AN	3002	1/1	0.96	0.45	-	69,69,69,69	0
59	MG	AA	3562	1/1	0.97	0.09	-	56,56,56,56	0
59	MG	DA	1743	1/1	0.94	0.13	-	59,59,59,59	0
59	MG	CA	3175	1/1	0.97	0.19	-	31,31,31,31	0
59	MG	BA	1769	1/1	0.97	0.10	-	58,58,58,58	0
59	MG	CA	3240	1/1	0.78	0.48	-	71,71,71,71	0
59	MG	CA	3479	1/1	0.99	0.17	-	50,50,50,50	0
59	MG	BA	1645	1/1	0.89	0.18	-	74,74,74,74	0
59	MG	CA	3624	1/1	0.65	0.16	-	118,118,118,118	0
59	MG	CA	3250	1/1	0.90	0.14	-	38,38,38,38	0
59	MG	CA	3237	1/1	0.69	0.49	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3288	1/1	0.85	0.16	-	49,49,49,49	0
59	MG	CA	3136	1/1	0.97	0.10	-	63,63,63,63	0
59	MG	AA	3105	1/1	0.90	0.15	-	52,52,52,52	0
59	MG	BA	1647	1/1	0.92	0.51	-	57,57,57,57	0
59	MG	AA	3141	1/1	0.92	0.09	-	68,68,68,68	0
59	MG	AA	3054	1/1	0.97	0.17	-	21,21,21,21	0
59	MG	BA	1764	1/1	0.60	0.09	-	71,71,71,71	0
59	MG	AA	3792	1/1	0.84	0.13	-	48,48,48,48	0
59	MG	AA	3374	1/1	0.94	0.31	-	49,49,49,49	0
59	MG	AA	3368	1/1	0.98	0.24	-	49,49,49,49	0
59	MG	CA	3662	1/1	0.96	0.32	-	33,33,33,33	0
59	MG	DA	1610	1/1	0.82	0.71	-	71,71,71,71	0
59	MG	CA	3238	1/1	0.92	0.24	-	69,69,69,69	0
59	MG	AA	3487	1/1	0.92	0.03	-	49,49,49,49	0
59	MG	CA	3197	1/1	0.97	0.40	-	45,45,45,45	0
59	MG	AA	3349	1/1	0.96	0.17	-	47,47,47,47	0
59	MG	BA	1771	1/1	0.95	0.21	-	65,65,65,65	0
59	MG	AA	3474	1/1	0.94	0.15	-	18,18,18,18	1
59	MG	AA	3014	1/1	0.91	0.12	-	31,31,31,31	0
59	MG	DA	1612	1/1	0.94	0.13	-	57,57,57,57	0
59	MG	AA	3275	1/1	0.85	0.34	-	89,89,89,89	0
59	MG	BA	1737	1/1	0.87	0.20	-	79,79,79,79	0
59	MG	AA	3614	1/1	0.84	0.28	-	50,50,50,50	1
59	MG	AA	3669	1/1	0.93	0.18	-	81,81,81,81	0
59	MG	AA	3683	1/1	0.90	0.27	-	62,62,62,62	0
59	MG	BA	1756	1/1	0.84	0.07	-	85,85,85,85	0
59	MG	AA	3736	1/1	0.86	0.30	-	59,59,59,59	0
59	MG	DA	1704	1/1	0.81	0.18	-	49,49,49,49	0
59	MG	CA	3263	1/1	0.95	0.14	-	64,64,64,64	0
59	MG	CA	3150	1/1	0.78	0.19	-	57,57,57,57	0
59	MG	CA	3436	1/1	0.93	0.11	-	64,64,64,64	0
59	MG	AA	3124	1/1	0.93	0.73	-	62,62,62,62	0
59	MG	DA	1753	1/1	0.90	0.29	-	79,79,79,79	0
59	MG	BA	1623	1/1	0.92	0.62	-	67,67,67,67	0
59	MG	DA	1651	1/1	0.98	0.11	-	63,63,63,63	0
59	MG	CA	3645	1/1	0.95	0.11	-	69,69,69,69	0
59	MG	AA	3696	1/1	0.92	0.17	-	66,66,66,66	0
59	MG	AA	3175	1/1	0.88	0.56	-	63,63,63,63	0
59	MG	AA	3252	1/1	0.90	0.21	-	44,44,44,44	0
59	MG	AA	3715	1/1	0.90	0.54	-	33,33,33,33	1
59	MG	AA	3027	1/1	0.89	0.51	-	75,75,75,75	0
59	MG	CA	3588	1/1	0.93	0.12	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3471	1/1	0.96	0.08	-	56,56,56,56	0
59	MG	CA	3094	1/1	0.93	0.21	-	59,59,59,59	0
59	MG	CA	3061	1/1	0.69	0.35	-	68,68,68,68	0
59	MG	CA	3371	1/1	0.89	0.18	-	52,52,52,52	0
59	MG	BA	1721	1/1	0.75	0.20	-	66,66,66,66	0
59	MG	AA	3288	1/1	0.91	0.27	-	39,39,39,39	0
59	MG	BA	1767	1/1	0.44	0.42	-	96,96,96,96	0
59	MG	BA	1619	1/1	0.80	0.21	-	59,59,59,59	0
59	MG	BA	1713	1/1	0.80	0.58	-	68,68,68,68	0
59	MG	BA	1626	1/1	0.95	0.12	-	41,41,41,41	0
59	MG	DA	1708	1/1	0.87	0.25	-	77,77,77,77	0
59	MG	CA	3236	1/1	0.77	0.68	-	81,81,81,81	0
59	MG	DA	1735	1/1	0.88	0.12	-	73,73,73,73	0
59	MG	AA	3302	1/1	0.98	0.06	-	51,51,51,51	0
59	MG	BA	1670	1/1	0.75	0.23	-	69,69,69,69	0
59	MG	CA	3272	1/1	0.97	0.32	-	49,49,49,49	0
59	MG	CA	3369	1/1	0.98	0.14	-	48,48,48,48	0
59	MG	CA	3242	1/1	0.70	0.39	-	82,82,82,82	0
59	MG	CA	3621	1/1	0.94	0.21	-	61,61,61,61	0
59	MG	AA	3462	1/1	0.96	0.09	-	54,54,54,54	0
59	MG	CA	3367	1/1	0.83	0.21	-	63,63,63,63	0
59	MG	AA	3440	1/1	0.88	0.24	-	63,63,63,63	0
59	MG	AA	3672	1/1	0.94	0.15	-	48,48,48,48	0
59	MG	AA	3192	1/1	0.98	0.23	-	30,30,30,30	0
59	MG	CN	5001	1/1	0.93	0.16	-	65,65,65,65	0
59	MG	CB	3005	1/1	0.93	0.38	-	63,63,63,63	0
59	MG	BA	1709	1/1	0.87	0.29	-	50,50,50,50	0
59	MG	AA	3701	1/1	0.91	0.15	-	81,81,81,81	0
59	MG	BA	1609	1/1	0.87	0.13	-	62,62,62,62	0
59	MG	AA	3577	1/1	0.93	0.08	-	42,42,42,42	0
59	MG	CA	3651	1/1	0.93	0.53	-	76,76,76,76	0
59	MG	BA	1809	1/1	0.95	0.23	-	61,61,61,61	0
59	MG	AA	3816	1/1	0.80	0.70	-	66,66,66,66	0
59	MG	AA	3142	1/1	0.88	0.26	-	64,64,64,64	0
59	MG	AA	3300	1/1	0.83	0.16	-	22,22,22,22	0
59	MG	AA	3062	1/1	0.93	0.17	-	47,47,47,47	0
59	MG	AA	3364	1/1	0.99	0.18	-	23,23,23,23	0
59	MG	AA	3123	1/1	0.90	0.34	-	54,54,54,54	0
59	MG	AA	3019	1/1	0.83	0.29	-	70,70,70,70	0
59	MG	BA	1762	1/1	0.97	0.06	-	74,74,74,74	0
59	MG	CA	3390	1/1	0.76	0.23	-	80,80,80,80	0
59	MG	AA	3165	1/1	0.98	0.16	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3705	1/1	0.86	0.57	-	53,53,53,53	1
59	MG	CA	3031	1/1	0.90	0.48	-	68,68,68,68	0
59	MG	AA	3805	1/1	0.96	0.21	-	58,58,58,58	0
59	MG	AQ	203	1/1	0.91	0.29	-	32,32,32,32	0
59	MG	AB	3021	1/1	0.87	0.26	-	65,65,65,65	0
59	MG	AA	3013	1/1	0.95	0.18	-	28,28,28,28	0
59	MG	AA	3357	1/1	0.89	0.16	-	55,55,55,55	0
59	MG	CA	3302	1/1	0.98	0.28	-	37,37,37,37	0
59	MG	CA	3412	1/1	0.93	0.18	-	59,59,59,59	0
59	MG	AA	3579	1/1	0.91	0.18	-	54,54,54,54	0
59	MG	CA	3401	1/1	0.98	0.22	-	28,28,28,28	0
59	MG	CA	3224	1/1	0.88	0.53	-	59,59,59,59	0
59	MG	CA	3052	1/1	0.93	0.18	-	44,44,44,44	0
59	MG	CA	3568	1/1	0.94	0.10	-	39,39,39,39	0
59	MG	AA	3100	1/1	0.97	0.24	-	29,29,29,29	0
59	MG	CA	3184	1/1	0.85	0.33	-	77,77,77,77	0
59	MG	CA	3516	1/1	0.86	0.35	-	79,79,79,79	0
59	MG	AA	3481	1/1	0.86	0.13	-	78,78,78,78	0
59	MG	AA	3067	1/1	0.75	0.42	-	61,61,61,61	0
59	MG	CA	3270	1/1	0.89	0.28	-	76,76,76,76	0
59	MG	AA	3458	1/1	0.99	0.09	-	40,40,40,40	0
59	MG	CQ	204	1/1	0.75	0.33	-	74,74,74,74	0
59	MG	AA	3292	1/1	0.98	0.20	-	24,24,24,24	0
59	MG	AA	3321	1/1	0.99	0.10	-	61,61,61,61	0
59	MG	CA	3205	1/1	0.73	0.53	-	81,81,81,81	0
59	MG	CF	302	1/1	0.90	0.53	-	69,69,69,69	0
59	MG	AA	3636	1/1	0.88	0.34	-	86,86,86,86	0
59	MG	CA	3556	1/1	0.97	0.19	-	62,62,62,62	0
59	MG	AA	3649	1/1	0.85	0.33	-	62,62,62,62	0
59	MG	AA	3051	1/1	0.81	0.47	-	48,48,48,48	0
59	MG	AA	3189	1/1	0.92	0.20	-	62,62,62,62	0
59	MG	CA	3527	1/1	0.92	0.14	-	76,76,76,76	0
59	MG	CA	3220	1/1	0.97	0.07	-	59,59,59,59	0
59	MG	CA	3231	1/1	0.97	0.71	-	60,60,60,60	0
59	MG	AF	305	1/1	0.57	0.53	-	76,76,76,76	0
59	MG	CA	3382	1/1	0.98	0.22	-	38,38,38,38	0
59	MG	CA	3076	1/1	0.93	0.34	-	64,64,64,64	0
59	MG	AA	3230	1/1	0.89	0.28	-	69,69,69,69	0
59	MG	AA	3461	1/1	0.84	0.19	-	62,62,62,62	0
59	MG	AA	3570	1/1	0.96	0.15	-	14,14,14,14	0
59	MG	DA	1756	1/1	0.71	0.57	-	86,86,86,86	0
59	MG	AA	3631	1/1	0.98	0.18	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AB	3001	1/1	0.84	0.37	-	74,74,74,74	0
59	MG	DA	1764	1/1	0.96	0.08	-	71,71,71,71	0
59	MG	CA	3487	1/1	0.97	0.20	-	60,60,60,60	0
59	MG	BA	1633	1/1	0.83	0.25	-	63,63,63,63	0
59	MG	DA	1670	1/1	0.92	0.12	-	49,49,49,49	0
59	MG	CA	3570	1/1	0.99	0.12	-	36,36,36,36	0
59	MG	AB	3009	1/1	0.91	0.09	-	50,50,50,50	0
59	MG	CE	304	1/1	0.90	0.36	-	75,75,75,75	0
59	MG	DA	1731	1/1	0.96	0.09	-	49,49,49,49	0
59	MG	AE	302	1/1	0.70	0.24	-	57,57,57,57	0
59	MG	AA	3598	1/1	0.97	0.24	-	51,51,51,51	0
59	MG	CA	3634	1/1	0.84	0.23	-	82,82,82,82	0
59	MG	AA	3361	1/1	0.94	0.16	-	53,53,53,53	0
59	MG	BA	1720	1/1	0.93	0.21	-	61,61,61,61	0
59	MG	AA	3731	1/1	0.93	0.14	-	51,51,51,51	0
59	MG	AA	3237	1/1	0.86	0.39	-	76,76,76,76	0
59	MG	DW	502	1/1	0.92	0.08	-	58,58,58,58	0
59	MG	AA	3552	1/1	0.97	0.18	-	63,63,63,63	0
59	MG	CA	3439	1/1	0.96	0.23	-	32,32,32,32	0
59	MG	AA	3207	1/1	0.94	0.20	-	60,60,60,60	0
59	MG	AA	3441	1/1	0.95	0.29	-	58,58,58,58	0
59	MG	DA	1605	1/1	0.83	0.33	-	105,105,105,105	0
59	MG	AA	3074	1/1	0.97	0.29	-	14,14,14,14	0
59	MG	AA	3094	1/1	0.96	0.24	-	80,80,80,80	0
59	MG	CA	3543	1/1	0.95	0.19	-	71,71,71,71	0
59	MG	CA	3097	1/1	0.77	0.29	-	66,66,66,66	0
59	MG	AA	3150	1/1	0.86	0.28	-	45,45,45,45	0
59	MG	DJ	5001	1/1	0.93	0.32	-	82,82,82,82	0
59	MG	CA	3398	1/1	0.89	0.16	-	67,67,67,67	0
59	MG	DZ	701	1/1	0.88	0.25	-	72,72,72,72	0
59	MG	CA	3481	1/1	0.86	0.21	-	64,64,64,64	0
59	MG	CA	3365	1/1	0.97	0.19	-	55,55,55,55	0
59	MG	CA	3015	1/1	0.99	0.28	-	51,51,51,51	0
59	MG	CA	3233	1/1	0.93	0.12	-	59,59,59,59	0
59	MG	AA	3480	1/1	0.84	0.31	-	88,88,88,88	0
59	MG	AA	3299	1/1	0.95	0.26	-	47,47,47,47	0
59	MG	CA	3067	1/1	0.91	0.19	-	63,63,63,63	0
59	MG	CA	3641	1/1	0.97	0.21	-	46,46,46,46	0
59	MG	DA	1668	1/1	0.93	0.38	-	65,65,65,65	0
59	MG	CA	3537	1/1	0.97	0.30	-	59,59,59,59	0
59	MG	CA	3467	1/1	0.89	0.63	-	77,77,77,77	0
59	MG	AA	3648	1/1	0.93	0.17	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	CA	3473	1/1	0.91	0.16	-	51,51,51,51	0
59	MG	CA	3055	1/1	0.78	0.12	-	77,77,77,77	0
59	MG	AA	3339	1/1	0.91	0.17	-	49,49,49,49	0
59	MG	AA	3640	1/1	0.82	0.21	-	68,68,68,68	0
59	MG	DA	1608	1/1	0.90	0.17	-	57,57,57,57	0
59	MG	AA	3520	1/1	0.95	0.14	-	17,17,17,17	0
59	MG	CA	3659	1/1	0.96	0.10	-	55,55,55,55	0
59	MG	AB	3011	1/1	0.97	0.16	-	29,29,29,29	0
59	MG	AA	3763	1/1	0.90	0.26	-	47,47,47,47	0
59	MG	CA	3091	1/1	0.85	0.28	-	69,69,69,69	0
59	MG	AA	3351	1/1	0.94	0.21	-	29,29,29,29	0
59	MG	AA	3476	1/1	0.92	0.17	-	28,28,28,28	0
59	MG	DA	1664	1/1	0.90	0.12	-	66,66,66,66	0
59	MG	AA	3447	1/1	0.92	0.34	-	56,56,56,56	0
59	MG	CA	3200	1/1	0.84	0.30	-	51,51,51,51	0
59	MG	BA	1783	1/1	0.95	0.18	-	57,57,57,57	0
59	MG	BA	1711	1/1	0.89	0.14	-	61,61,61,61	0
59	MG	CA	3638	1/1	0.90	0.34	-	76,76,76,76	0
59	MG	AA	3527	1/1	0.97	0.16	-	27,27,27,27	0
59	MG	CA	3519	1/1	0.96	0.22	-	48,48,48,48	0
59	MG	AA	3008	1/1	0.96	0.21	-	26,26,26,26	0
59	MG	AA	3633	1/1	0.91	0.16	-	48,48,48,48	0
59	MG	DA	1762	1/1	0.94	0.20	-	61,61,61,61	0
59	MG	BA	1776	1/1	0.64	0.21	-	97,97,97,97	0
59	MG	DA	1682	1/1	0.93	0.33	-	52,52,52,52	0
59	MG	AA	3555	1/1	0.94	0.15	-	45,45,45,45	0
59	MG	AA	3780	1/1	0.79	0.40	-	72,72,72,72	0
59	MG	DA	1699	1/1	0.91	0.19	-	74,74,74,74	0
59	MG	AA	3698	1/1	0.92	0.16	-	41,41,41,41	0
59	MG	BA	1789	1/1	0.94	0.15	-	72,72,72,72	0
59	MG	BA	1602	1/1	0.72	0.18	-	79,79,79,79	0
59	MG	CA	3084	1/1	0.77	0.41	-	56,56,56,56	0
59	MG	CA	3258	1/1	0.98	0.36	-	51,51,51,51	0
59	MG	CA	3483	1/1	0.94	0.32	-	64,64,64,64	0
59	MG	AA	3278	1/1	0.94	0.21	-	60,60,60,60	0
59	MG	AA	3454	1/1	0.93	0.24	-	61,61,61,61	0
59	MG	A0	104	1/1	0.89	0.36	-	51,51,51,51	0
59	MG	DA	1727	1/1	0.81	0.12	-	61,61,61,61	0
59	MG	BN	502	1/1	0.91	0.17	-	87,87,87,87	0
59	MG	DA	1618	1/1	0.84	0.63	-	91,91,91,91	0
59	MG	DA	1604	1/1	0.89	0.12	-	80,80,80,80	0
59	MG	CA	3007	1/1	0.78	0.40	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3534	1/1	0.88	0.11	-	73,73,73,73	0
59	MG	DA	1766	1/1	0.95	0.12	-	74,74,74,74	0
59	MG	CA	3029	1/1	0.93	0.09	-	56,56,56,56	0
59	MG	AA	3498	1/1	0.98	0.24	-	47,47,47,47	0
59	MG	AA	3742	1/1	0.96	0.12	-	68,68,68,68	0
59	MG	BA	1744	1/1	0.88	0.17	-	57,57,57,57	0
59	MG	CA	3334	1/1	0.97	0.21	-	47,47,47,47	0
59	MG	CA	3460	1/1	0.10	0.96	-	104,104,104,104	0
59	MG	CA	3294	1/1	0.72	0.09	-	72,72,72,72	0
59	MG	CA	3616	1/1	0.91	0.64	-	74,74,74,74	0
59	MG	CA	3484	1/1	0.93	0.26	-	78,78,78,78	0
59	MG	CA	3478	1/1	0.87	0.32	-	65,65,65,65	0
59	MG	CA	3437	1/1	0.97	0.18	-	64,64,64,64	0
59	MG	AA	3239	1/1	0.96	0.27	-	25,25,25,25	1
59	MG	CA	3434	1/1	0.93	0.16	-	32,32,32,32	0
59	MG	CA	3141	1/1	0.89	0.45	-	68,68,68,68	0
59	MG	AA	3785	1/1	0.95	0.16	-	61,61,61,61	0
59	MG	BA	1660	1/1	0.10	0.39	-	82,82,82,82	0
59	MG	AB	3010	1/1	0.92	0.10	-	62,62,62,62	0
59	MG	CA	3555	1/1	0.81	0.14	-	71,71,71,71	0
59	MG	CA	3373	1/1	0.85	0.30	-	58,58,58,58	0
59	MG	AA	3503	1/1	0.95	0.06	-	54,54,54,54	0
59	MG	CA	3191	1/1	0.88	0.21	-	46,46,46,46	0
59	MG	DA	1706	1/1	0.94	0.33	-	66,66,66,66	0
59	MG	BA	1808	1/1	0.96	0.16	-	54,54,54,54	0
59	MG	AA	3651	1/1	0.93	0.22	-	77,77,77,77	0
59	MG	BA	1793	1/1	0.93	0.09	-	65,65,65,65	0
59	MG	AA	3504	1/1	0.95	0.09	-	29,29,29,29	0
59	MG	CA	3426	1/1	0.90	0.20	-	38,38,38,38	0
59	MG	BA	1814	1/1	0.85	0.21	-	69,69,69,69	0
59	MG	CA	3606	1/1	0.94	0.48	-	73,73,73,73	0
59	MG	CA	3164	1/1	0.93	0.56	-	64,64,64,64	0
59	MG	CA	3126	1/1	0.91	0.31	-	62,62,62,62	0
59	MG	BA	1698	1/1	0.78	0.42	-	63,63,63,63	0
59	MG	DA	1602	1/1	0.94	0.10	-	45,45,45,45	0
59	MG	AA	3424	1/1	0.97	0.18	-	14,14,14,14	0
59	MG	CA	3255	1/1	0.96	0.24	-	28,28,28,28	0
59	MG	AA	3332	1/1	0.98	0.18	-	17,17,17,17	0
59	MG	AA	3594	1/1	0.94	0.24	-	56,56,56,56	0
59	MG	CA	3466	1/1	0.98	0.40	-	56,56,56,56	0
59	MG	CA	3610	1/1	0.91	0.13	-	69,69,69,69	0
59	MG	CA	3620	1/1	0.48	0.64	-	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3031	1/1	0.88	0.48	-	63,63,63,63	0
59	MG	AA	3414	1/1	0.88	0.17	-	37,37,37,37	0
59	MG	CA	3461	1/1	0.96	0.16	-	34,34,34,34	0
59	MG	BA	1659	1/1	0.86	0.33	-	67,67,67,67	0
59	MG	CA	3022	1/1	0.93	0.52	-	69,69,69,69	0
59	MG	AA	3588	1/1	0.95	0.15	-	47,47,47,47	0
59	MG	AA	3590	1/1	0.95	0.17	-	60,60,60,60	0
59	MG	AA	3658	1/1	0.95	0.21	-	42,42,42,42	0
59	MG	AA	3752	1/1	0.97	0.12	-	42,42,42,42	0
59	MG	AA	3106	1/1	0.91	0.17	-	33,33,33,33	0
59	MG	AA	3352	1/1	0.80	0.36	-	47,47,47,47	0
59	MG	CA	3574	1/1	0.96	0.15	-	37,37,37,37	0
59	MG	BA	1692	1/1	0.95	0.28	-	55,55,55,55	0
59	MG	DA	1749	1/1	0.85	0.33	-	77,77,77,77	0
59	MG	CB	3003	1/1	0.90	0.09	-	65,65,65,65	0
59	MG	DA	1755	1/1	0.93	0.51	-	88,88,88,88	0
59	MG	AA	3408	1/1	0.94	0.34	-	41,41,41,41	0
59	MG	AA	3028	1/1	0.90	0.28	-	39,39,39,39	0
59	MG	AA	3798	1/1	0.96	0.22	-	25,25,25,25	0
59	MG	CA	3576	1/1	0.92	0.11	-	71,71,71,71	0
59	MG	AA	3446	1/1	0.91	0.09	-	59,59,59,59	0
59	MG	AA	3269	1/1	0.55	0.33	-	63,63,63,63	0
59	MG	CA	3215	1/1	0.89	0.07	-	54,54,54,54	0
59	MG	DA	1692	1/1	0.87	0.16	-	53,53,53,53	0
59	MG	DK	5001	1/1	0.65	0.16	-	76,76,76,76	0
59	MG	AA	3657	1/1	0.86	0.17	-	63,63,63,63	0
59	MG	AA	3616	1/1	0.89	0.17	-	57,57,57,57	0
59	MG	BA	1774	1/1	0.91	0.27	-	50,50,50,50	0
59	MG	AA	3238	1/1	0.70	0.44	-	76,76,76,76	0
59	MG	AF	306	1/1	0.95	0.24	-	57,57,57,57	0
59	MG	AA	3002	1/1	0.78	0.21	-	57,57,57,57	0
59	MG	CA	3518	1/1	0.83	0.11	-	65,65,65,65	0
59	MG	AA	3151	1/1	0.99	0.23	-	62,62,62,62	0
59	MG	AA	3629	1/1	0.81	0.17	-	77,77,77,77	0
59	MG	CA	3261	1/1	0.99	0.15	-	47,47,47,47	0
59	MG	CA	3366	1/1	0.96	0.16	-	49,49,49,49	0
59	MG	CA	3199	1/1	0.91	0.22	-	55,55,55,55	0
59	MG	DA	1742	1/1	0.75	0.21	-	72,72,72,72	0
59	MG	BA	1804	1/1	0.97	0.10	-	45,45,45,45	0
59	MG	AA	3427	1/1	0.92	0.12	-	61,61,61,61	0
59	MG	AA	3483	1/1	0.92	0.21	-	46,46,46,46	0
59	MG	CA	3151	1/1	0.94	0.16	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3344	1/1	0.96	0.07	-	68,68,68,68	0
59	MG	AA	3279	1/1	0.94	0.23	-	34,34,34,34	0
59	MG	CA	3530	1/1	0.84	0.50	-	71,71,71,71	0
59	MG	AA	3272	1/1	0.96	0.16	-	55,55,55,55	0
59	MG	BA	1704	1/1	0.80	0.31	-	71,71,71,71	0
59	MG	AA	3666	1/1	0.97	0.14	-	41,41,41,41	0
59	MG	AA	3371	1/1	0.89	0.23	-	53,53,53,53	0
59	MG	AA	3622	1/1	0.83	0.22	-	60,60,60,60	0
59	MG	AA	3283	1/1	0.97	0.33	-	43,43,43,43	0
59	MG	AA	3246	1/1	0.91	0.13	-	52,52,52,52	0
59	MG	CA	3181	1/1	0.99	0.16	-	40,40,40,40	0
59	MG	AA	3652	1/1	0.95	0.14	-	53,53,53,53	0
59	MG	CA	3133	1/1	0.97	0.20	-	85,85,85,85	0
59	MG	CA	3124	1/1	0.85	0.26	-	65,65,65,65	0
59	MG	CA	3323	1/1	0.83	0.40	-	87,87,87,87	0
59	MG	AA	3064	1/1	0.95	0.13	-	32,32,32,32	0
59	MG	AA	3789	1/1	0.98	0.21	-	44,44,44,44	0
59	MG	CA	3325	1/1	0.72	0.13	-	38,38,38,38	0
59	MG	AA	3544	1/1	0.84	0.22	-	26,26,26,26	0
59	MG	AA	3075	1/1	0.97	0.29	-	49,49,49,49	0
59	MG	AA	3811	1/1	0.97	0.15	-	56,56,56,56	0
59	MG	CA	3385	1/1	0.89	0.37	-	61,61,61,61	0
59	MG	BA	1717	1/1	0.95	0.18	-	78,78,78,78	0
59	MG	AA	3670	1/1	0.96	0.08	-	54,54,54,54	0
59	MG	AA	3259	1/1	0.96	0.34	-	41,41,41,41	1
59	MG	AA	3536	1/1	0.74	0.24	-	66,66,66,66	0
59	MG	CA	3198	1/1	0.95	0.23	-	34,34,34,34	0
59	MG	CA	3144	1/1	0.95	0.23	-	40,40,40,40	0
59	MG	DA	1615	1/1	0.95	0.25	-	58,58,58,58	0
59	MG	DA	1690	1/1	0.93	0.19	-	73,73,73,73	0
59	MG	A6	103	1/1	0.92	0.36	-	72,72,72,72	0
59	MG	CA	3059	1/1	0.87	0.43	-	58,58,58,58	0
59	MG	CA	3115	1/1	0.86	0.41	-	67,67,67,67	0
59	MG	AA	3592	1/1	0.87	0.15	-	26,26,26,26	0
59	MG	CA	3331	1/1	0.98	0.26	-	52,52,52,52	0
59	MG	CA	3407	1/1	0.97	0.19	-	36,36,36,36	0
59	MG	A6	101	1/1	0.87	0.23	-	60,60,60,60	0
59	MG	AA	3747	1/1	0.48	0.34	-	85,85,85,85	0
59	MG	CA	3280	1/1	0.90	0.15	-	48,48,48,48	0
59	MG	CA	3612	1/1	0.86	0.36	-	83,83,83,83	0
59	MG	AA	3694	1/1	0.87	0.15	-	53,53,53,53	0
59	MG	BA	1765	1/1	0.98	0.23	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3200	1/1	0.95	0.22	-	30,30,30,30	0
59	MG	AA	3274	1/1	0.86	0.38	-	75,75,75,75	0
59	MG	AA	3198	1/1	0.93	0.15	-	63,63,63,63	0
59	MG	AA	3086	1/1	0.93	0.40	-	55,55,55,55	0
59	MG	AA	3632	1/1	0.95	0.20	-	54,54,54,54	0
59	MG	AA	3530	1/1	0.95	0.19	-	20,20,20,20	1
59	MG	AA	3513	1/1	0.95	0.10	-	41,41,41,41	0
59	MG	AA	3464	1/1	0.88	0.40	-	66,66,66,66	0
59	MG	AA	3599	1/1	0.96	0.16	-	59,59,59,59	0
59	MG	CA	3506	1/1	0.90	0.12	-	63,63,63,63	0
59	MG	AA	3297	1/1	0.99	0.23	-	27,27,27,27	0
59	MG	BA	1605	1/1	0.87	0.13	-	73,73,73,73	0
59	MG	CB	3006	1/1	0.96	0.06	-	71,71,71,71	0
59	MG	CA	3513	1/1	0.81	0.16	-	70,70,70,70	0
59	MG	BA	1792	1/1	0.84	0.19	-	80,80,80,80	0
59	MG	BA	1634	1/1	0.79	0.39	-	64,64,64,64	0
59	MG	DA	1686	1/1	0.87	0.19	-	56,56,56,56	0
59	MG	AA	3425	1/1	0.94	0.05	-	77,77,77,77	0
59	MG	CA	3203	1/1	0.84	0.19	-	73,73,73,73	0
59	MG	AA	3127	1/1	0.97	0.34	-	57,57,57,57	0
59	MG	AA	3501	1/1	0.95	0.06	-	49,49,49,49	0
59	MG	BW	502	1/1	0.90	0.10	-	59,59,59,59	0
59	MG	AA	3145	1/1	0.97	0.29	-	44,44,44,44	0
59	MG	AA	3448	1/1	0.94	0.12	-	62,62,62,62	0
59	MG	CA	3378	1/1	0.72	0.24	-	97,97,97,97	0
59	MG	AA	3549	1/1	0.94	0.05	-	66,66,66,66	0
59	MG	AA	3773	1/1	0.76	0.44	-	35,35,35,35	1
59	MG	BA	1697	1/1	0.72	1.08	-	99,99,99,99	0
59	MG	AA	3118	1/1	0.91	0.39	-	76,76,76,76	0
59	MG	DA	1712	1/1	0.99	0.33	-	53,53,53,53	0
59	MG	CA	3131	1/1	0.92	0.23	-	26,26,26,26	0
59	MG	BA	1800	1/1	0.92	0.46	-	77,77,77,77	0
59	MG	CA	3510	1/1	0.85	0.11	-	95,95,95,95	0
59	MG	AA	3372	1/1	0.98	0.23	-	37,37,37,37	0
59	MG	BA	1759	1/1	0.93	0.32	-	63,63,63,63	0
59	MG	CA	3630	1/1	0.78	0.10	-	65,65,65,65	0
59	MG	CA	3547	1/1	0.93	0.13	-	69,69,69,69	0
59	MG	CB	3001	1/1	0.89	0.28	-	72,72,72,72	0
59	MG	AA	3417	1/1	0.95	0.18	-	25,25,25,25	0
59	MG	CA	3208	1/1	0.80	0.63	-	74,74,74,74	0
59	MG	AA	3642	1/1	0.88	0.34	-	71,71,71,71	0
59	MG	AA	3195	1/1	0.65	0.37	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3467	1/1	0.84	0.31	-	49,49,49,49	0
59	MG	CA	3071	1/1	0.91	0.27	-	45,45,45,45	0
59	MG	CA	3112	1/1	0.72	0.38	-	69,69,69,69	0
59	MG	AA	3265	1/1	0.94	0.17	-	43,43,43,43	0
59	MG	CA	3445	1/1	0.95	0.20	-	22,22,22,22	0
59	MG	AA	3355	1/1	0.97	0.17	-	57,57,57,57	0
59	MG	AA	3733	1/1	0.93	0.15	-	49,49,49,49	0
59	MG	CA	3287	1/1	0.98	0.22	-	45,45,45,45	0
59	MG	CA	3349	1/1	0.95	0.20	-	23,23,23,23	0
59	MG	CA	3158	1/1	0.78	0.37	-	54,54,54,54	0
59	MG	CA	3535	1/1	0.88	0.21	-	77,77,77,77	0
59	MG	CA	3254	1/1	0.93	0.16	-	85,85,85,85	0
59	MG	CB	3008	1/1	0.72	0.20	-	66,66,66,66	0
59	MG	CA	3083	1/1	0.92	0.41	-	61,61,61,61	0
59	MG	AA	3121	1/1	0.96	0.16	-	53,53,53,53	0
59	MG	BA	1701	1/1	0.90	0.09	-	54,54,54,54	0
59	MG	AA	3412	1/1	0.98	0.20	-	39,39,39,39	0
59	MG	CA	3559	1/1	0.83	0.12	-	75,75,75,75	0
59	MG	CA	3590	1/1	0.94	0.10	-	59,59,59,59	0
59	MG	AA	3233	1/1	0.89	0.18	-	46,46,46,46	0
59	MG	AA	3746	1/1	0.92	0.17	-	73,73,73,73	0
59	MG	BF	3001	1/1	0.96	0.17	-	49,49,49,49	0
59	MG	AA	3613	1/1	0.97	0.17	-	48,48,48,48	0
59	MG	AA	3324	1/1	0.94	0.14	-	15,15,15,15	0
59	MG	AA	3465	1/1	0.98	0.20	-	42,42,42,42	0
59	MG	CA	3596	1/1	0.92	0.12	-	51,51,51,51	0
59	MG	CA	3628	1/1	0.89	0.18	-	54,54,54,54	0
59	MG	AA	3695	1/1	0.86	0.08	-	67,67,67,67	0
59	MG	CA	3204	1/1	0.87	0.19	-	54,54,54,54	0
59	MG	CA	3005	1/1	0.80	0.19	-	48,48,48,48	0
59	MG	AA	3767	1/1	0.75	0.35	-	67,67,67,67	0
59	MG	CA	3387	1/1	0.92	0.33	-	50,50,50,50	0
59	MG	AA	3428	1/1	0.97	0.19	-	18,18,18,18	0
59	MG	CA	3313	1/1	0.93	0.26	-	38,38,38,38	0
59	MG	AA	3765	1/1	0.98	0.38	-	60,60,60,60	0
59	MG	AA	3073	1/1	0.97	0.14	-	31,31,31,31	0
59	MG	CA	3038	1/1	0.81	0.51	-	97,97,97,97	0
59	MG	CA	3008	1/1	0.94	0.38	-	46,46,46,46	0
59	MG	AV	202	1/1	0.96	0.23	-	33,33,33,33	0
59	MG	CA	3399	1/1	0.94	0.07	-	57,57,57,57	0
59	MG	DA	1633	1/1	0.81	0.26	-	55,55,55,55	0
59	MG	CA	3267	1/1	0.98	0.13	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3195	1/1	0.98	0.31	-	47,47,47,47	0
59	MG	CA	3118	1/1	0.87	0.64	-	65,65,65,65	0
59	MG	AA	3422	1/1	0.97	0.18	-	23,23,23,23	0
59	MG	BA	1732	1/1	0.93	0.25	-	70,70,70,70	0
59	MG	AB	3004	1/1	0.72	0.32	-	69,69,69,69	0
59	MG	AA	3343	1/1	0.96	0.10	-	46,46,46,46	0
59	MG	CA	3389	1/1	0.78	0.34	-	59,59,59,59	0
59	MG	CA	3563	1/1	0.80	0.09	-	75,75,75,75	0
59	MG	CA	3406	1/1	0.82	0.13	-	77,77,77,77	0
59	MG	AA	3155	1/1	0.90	0.21	-	93,93,93,93	0
59	MG	CA	3447	1/1	0.97	0.25	-	73,73,73,73	0
59	MG	AA	3774	1/1	0.98	0.35	-	25,25,25,25	1
59	MG	DA	1627	1/1	0.89	0.08	-	77,77,77,77	0
59	MG	CA	3540	1/1	0.86	0.08	-	54,54,54,54	0
59	MG	CA	3381	1/1	0.96	0.14	-	50,50,50,50	0
59	MG	AA	3764	1/1	0.93	0.16	-	73,73,73,73	0
59	MG	BA	1667	1/1	0.92	0.25	-	74,74,74,74	0
59	MG	AA	3709	1/1	0.99	0.42	-	23,23,23,23	1
59	MG	AA	3782	1/1	0.89	0.20	-	44,44,44,44	0
59	MG	AA	3548	1/1	0.95	0.11	-	7,7,7,7	0
59	MG	CA	3047	1/1	0.96	0.16	-	84,84,84,84	0
59	MG	CA	3405	1/1	0.98	0.10	-	55,55,55,55	0
59	MG	C8	5001	1/1	0.97	0.34	-	37,37,37,37	0
59	MG	DA	1626	1/1	0.47	0.30	-	71,71,71,71	0
59	MG	AA	3208	1/1	0.84	0.42	-	54,54,54,54	0
59	MG	BA	1731	1/1	0.92	0.17	-	45,45,45,45	0
59	MG	CA	3216	1/1	0.75	0.46	-	79,79,79,79	0
59	MG	AA	3291	1/1	0.96	0.27	-	45,45,45,45	0
59	MG	CA	3558	1/1	0.92	0.09	-	64,64,64,64	0
59	MG	AA	3459	1/1	0.97	0.20	-	53,53,53,53	0
59	MG	CA	3139	1/1	0.32	0.70	-	126,126,126,126	0
59	MG	BA	1763	1/1	0.93	0.17	-	76,76,76,76	0
59	MG	BA	1736	1/1	0.91	0.17	-	67,67,67,67	0
59	MG	CA	3542	1/1	0.75	0.40	-	87,87,87,87	0
59	MG	DA	1724	1/1	0.74	0.41	-	70,70,70,70	0
59	MG	DA	1736	1/1	0.89	0.12	-	78,78,78,78	0
59	MG	CA	3359	1/1	0.94	0.08	-	33,33,33,33	0
59	MG	CA	3522	1/1	0.94	0.13	-	54,54,54,54	0
59	MG	CA	3241	1/1	0.89	0.17	-	72,72,72,72	0
59	MG	BA	1636	1/1	0.94	0.17	-	57,57,57,57	0
59	MG	AA	3604	1/1	0.86	0.43	-	81,81,81,81	0
59	MG	AA	3079	1/1	0.87	0.12	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3768	1/1	0.79	0.19	-	58,58,58,58	0
59	MG	CA	3222	1/1	0.92	0.34	-	57,57,57,57	0
59	MG	CA	3093	1/1	0.74	0.71	-	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.