



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:55 PM GMT

PDB ID : 4WQF
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with elongation factor G and fusidic acid in the post-translocational state
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-21
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

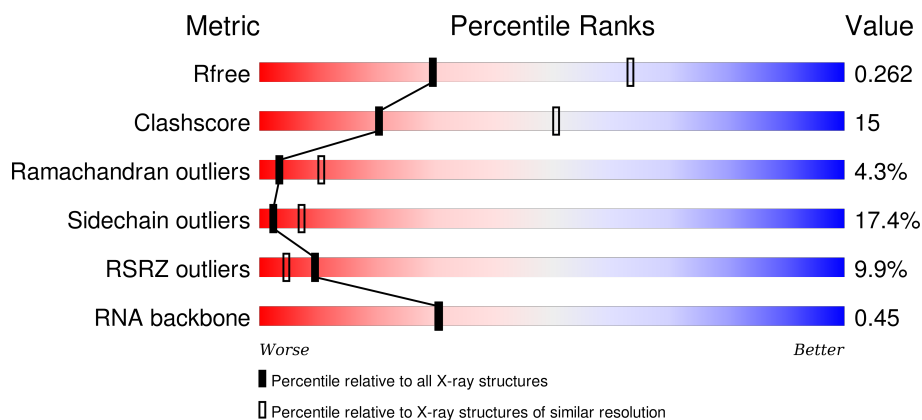
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>4%</div> <div>19%</div> <div>49%</div> <div>25%</div> <div>5%</div> </div>
1	CA	2915	<div> <div>4%</div> <div>32%</div> <div>44%</div> <div>19%</div> </div>
2	AB	121	<div> <div>25%</div> <div>46%</div> <div>24%</div> </div>
2	CB	121	<div> <div>%</div> <div>44%</div> <div>41%</div> <div>13%</div> </div>





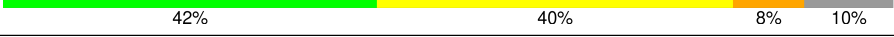



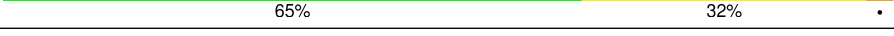

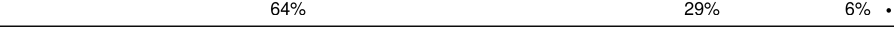
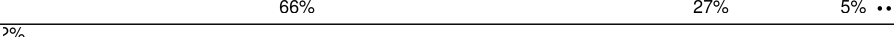

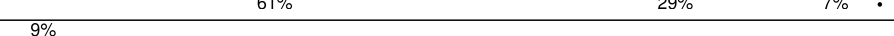


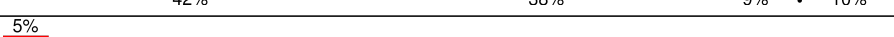

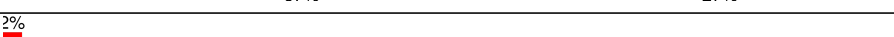






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Mol	Chain	Length	Quality of chain
3	AC	228	
3	CC	228	
4	AD	276	
4	CD	276	
5	AE	206	
5	CE	206	
6	AF	210	
6	CF	210	
7	AG	182	
7	CG	182	
8	AH	180	
8	CH	180	
9	AK	173	
9	CK	173	
10	AL	147	
10	CL	147	
11	AN	140	
11	CN	140	
12	AO	122	
12	CO	122	
13	AP	150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

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	MG	A7	103	-	-	-	X
58	MG	A8	5001	-	-	-	X
58	MG	AA	3012	-	-	-	X
58	MG	AA	3014	-	-	-	X
58	MG	AA	3018	-	-	-	X
58	MG	AA	3020	-	-	-	X
58	MG	AA	3023	-	-	-	X
58	MG	AA	3034	-	-	-	X
58	MG	AA	3035	-	-	-	X
58	MG	AA	3036	-	-	-	X
58	MG	AA	3037	-	-	-	X
58	MG	AA	3039	-	-	-	X
58	MG	AA	3040	-	-	-	X
58	MG	AA	3043	-	-	-	X
58	MG	AA	3044	-	-	-	X
58	MG	AA	3048	-	-	-	X
58	MG	AA	3051	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	3059	-	-	-	X
58	MG	AA	3061	-	-	-	X
58	MG	AA	3081	-	-	-	X
58	MG	AA	3082	-	-	-	X
58	MG	AA	3101	-	-	-	X
58	MG	AA	3102	-	-	-	X
58	MG	AA	3109	-	-	-	X
58	MG	AA	3110	-	-	-	X
58	MG	AA	3112	-	-	-	X
58	MG	AA	3113	-	-	-	X
58	MG	AA	3116	-	-	-	X
58	MG	AA	3117	-	-	-	X
58	MG	AA	3120	-	-	-	X
58	MG	AA	3128	-	-	-	X
58	MG	AA	3130	-	-	-	X
58	MG	AA	3132	-	-	-	X
58	MG	AA	3133	-	-	-	X
58	MG	AA	3134	-	-	-	X
58	MG	AA	3135	-	-	-	X
58	MG	AA	3138	-	-	-	X
58	MG	AA	3142	-	-	-	X
58	MG	AA	3150	-	-	-	X
58	MG	AA	3162	-	-	-	X
58	MG	AA	3168	-	-	-	X
58	MG	AA	3171	-	-	-	X
58	MG	AA	3173	-	-	-	X
58	MG	AA	3174	-	-	-	X
58	MG	AA	3179	-	-	-	X
58	MG	AA	3183	-	-	-	X
58	MG	AA	3184	-	-	-	X
58	MG	AA	3185	-	-	-	X
58	MG	AA	3187	-	-	-	X
58	MG	AA	3190	-	-	-	X
58	MG	AA	3196	-	-	-	X
58	MG	AA	3206	-	-	-	X
58	MG	AA	3210	-	-	-	X
58	MG	AA	3211	-	-	-	X
58	MG	AA	3212	-	-	-	X
58	MG	AA	3221	-	-	-	X
58	MG	AA	3223	-	-	-	X
58	MG	AA	3231	-	-	-	X
58	MG	AA	3240	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	3247	-	-	-	X
58	MG	AA	3249	-	-	-	X
58	MG	AA	3250	-	-	-	X
58	MG	AA	3253	-	-	-	X
58	MG	AA	3257	-	-	-	X
58	MG	AA	3267	-	-	-	X
58	MG	AA	3272	-	-	-	X
58	MG	AA	3282	-	-	-	X
58	MG	AA	3297	-	-	-	X
58	MG	AA	3301	-	-	-	X
58	MG	AA	3309	-	-	-	X
58	MG	AA	3311	-	-	-	X
58	MG	AA	3314	-	-	-	X
58	MG	AA	3316	-	-	-	X
58	MG	AA	3329	-	-	-	X
58	MG	AA	3331	-	-	-	X
58	MG	AA	3354	-	-	-	X
58	MG	AA	3357	-	-	-	X
58	MG	AA	3372	-	-	-	X
58	MG	AA	3381	-	-	-	X
58	MG	AA	3388	-	-	-	X
58	MG	AA	3395	-	-	-	X
58	MG	AA	3400	-	-	-	X
58	MG	AA	3410	-	-	-	X
58	MG	AA	3418	-	-	-	X
58	MG	AA	3420	-	-	-	X
58	MG	AA	3436	-	-	-	X
58	MG	AA	3439	-	-	-	X
58	MG	AA	3440	-	-	-	X
58	MG	AA	3442	-	-	-	X
58	MG	AA	3443	-	-	-	X
58	MG	AA	3453	-	-	-	X
58	MG	AA	3456	-	-	-	X
58	MG	AA	3462	-	-	-	X
58	MG	AA	3485	-	-	-	X
58	MG	AA	3488	-	-	-	X
58	MG	AA	3499	-	-	-	X
58	MG	AA	3506	-	-	-	X
58	MG	AA	3507	-	-	-	X
58	MG	AA	3508	-	-	-	X
58	MG	AA	3525	-	-	-	X
58	MG	AA	3551	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	3559	-	-	-	X
58	MG	AA	3564	-	-	-	X
58	MG	AA	3565	-	-	-	X
58	MG	AA	3581	-	-	-	X
58	MG	AA	3589	-	-	-	X
58	MG	AA	3596	-	-	-	X
58	MG	AA	3602	-	-	-	X
58	MG	AA	3604	-	-	-	X
58	MG	AA	3606	-	-	-	X
58	MG	AA	3617	-	-	-	X
58	MG	AA	3620	-	-	-	X
58	MG	AA	3621	-	-	-	X
58	MG	AA	3623	-	-	-	X
58	MG	AA	3663	-	-	-	X
58	MG	AA	3698	-	-	-	X
58	MG	AA	3702	-	-	-	X
58	MG	AA	3704	-	-	-	X
58	MG	AA	3706	-	-	-	X
58	MG	AA	3708	-	-	-	X
58	MG	AA	3711	-	-	-	X
58	MG	AA	3717	-	-	-	X
58	MG	AA	3726	-	-	-	X
58	MG	AA	3735	-	-	-	X
58	MG	AA	3736	-	-	-	X
58	MG	AA	3739	-	-	-	X
58	MG	AA	3741	-	-	-	X
58	MG	AA	3768	-	-	-	X
58	MG	AA	3770	-	-	-	X
58	MG	AA	3771	-	-	-	X
58	MG	AA	3773	-	-	-	X
58	MG	AA	3791	-	-	-	X
58	MG	AA	3793	-	-	-	X
58	MG	AA	3798	-	-	-	X
58	MG	AA	3805	-	-	-	X
58	MG	AA	3806	-	-	-	X
58	MG	AA	3811	-	-	-	X
58	MG	AA	3812	-	-	-	X
58	MG	AA	3815	-	-	-	X
58	MG	AA	3816	-	-	-	X
58	MG	AA	3817	-	-	-	X
58	MG	AA	3819	-	-	-	X
58	MG	AA	3820	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	AA	3822	-	-	-	X
58	MG	AA	3823	-	-	-	X
58	MG	AA	3824	-	-	-	X
58	MG	AA	3827	-	-	-	X
58	MG	AA	3828	-	-	-	X
58	MG	AA	3829	-	-	-	X
58	MG	AA	3830	-	-	-	X
58	MG	AA	3831	-	-	-	X
58	MG	AA	3832	-	-	-	X
58	MG	AA	3833	-	-	-	X
58	MG	AA	3835	-	-	-	X
58	MG	AB	3003	-	-	-	X
58	MG	AB	3008	-	-	-	X
58	MG	AB	3023	-	-	-	X
58	MG	AD	301	-	-	-	X
58	MG	AD	302	-	-	-	X
58	MG	AD	304	-	-	-	X
58	MG	AD	305	-	-	-	X
58	MG	AD	308	-	-	-	X
58	MG	AD	309	-	-	-	X
58	MG	AD	310	-	-	-	X
58	MG	AE	304	-	-	-	X
58	MG	AF	302	-	-	-	X
58	MG	AF	303	-	-	-	X
58	MG	AH	3001	-	-	-	X
58	MG	AH	3002	-	-	-	X
58	MG	AN	3001	-	-	-	X
58	MG	AQ	202	-	-	-	X
58	MG	AU	201	-	-	-	X
58	MG	AU	202	-	-	-	X
58	MG	AU	203	-	-	-	X
58	MG	AV	202	-	-	-	X
58	MG	AW	3003	-	-	-	X
58	MG	AX	101	-	-	-	X
58	MG	BA	1615	-	-	-	X
58	MG	BA	1616	-	-	-	X
58	MG	BA	1623	-	-	-	X
58	MG	BA	1626	-	-	-	X
58	MG	BA	1629	-	-	-	X
58	MG	BA	1630	-	-	-	X
58	MG	BA	1648	-	-	-	X
58	MG	BA	1657	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	BA	1664	-	-	-	X
58	MG	BA	1671	-	-	-	X
58	MG	BA	1678	-	-	-	X
58	MG	BA	1683	-	-	-	X
58	MG	BA	1686	-	-	-	X
58	MG	BA	1690	-	-	-	X
58	MG	BA	1693	-	-	-	X
58	MG	BA	1695	-	-	-	X
58	MG	BA	1711	-	-	-	X
58	MG	BA	1721	-	-	-	X
58	MG	BA	1723	-	-	-	X
58	MG	BA	1738	-	-	-	X
58	MG	BA	1740	-	-	-	X
58	MG	BA	1755	-	-	-	X
58	MG	BA	1756	-	-	-	X
58	MG	BA	1763	-	-	-	X
58	MG	BA	1783	-	-	-	X
58	MG	BA	1801	-	-	-	X
58	MG	BA	1811	-	-	-	X
58	MG	BT	3001	-	-	-	X
58	MG	C3	3001	-	-	-	X
58	MG	C7	101	-	-	-	X
58	MG	CA	3002	-	-	-	X
58	MG	CA	3011	-	-	-	X
58	MG	CA	3013	-	-	-	X
58	MG	CA	3014	-	-	-	X
58	MG	CA	3023	-	-	-	X
58	MG	CA	3027	-	-	-	X
58	MG	CA	3028	-	-	-	X
58	MG	CA	3030	-	-	-	X
58	MG	CA	3035	-	-	-	X
58	MG	CA	3037	-	-	-	X
58	MG	CA	3038	-	-	-	X
58	MG	CA	3041	-	-	-	X
58	MG	CA	3043	-	-	-	X
58	MG	CA	3073	-	-	-	X
58	MG	CA	3084	-	-	-	X
58	MG	CA	3086	-	-	-	X
58	MG	CA	3088	-	-	-	X
58	MG	CA	3091	-	-	-	X
58	MG	CA	3106	-	-	-	X
58	MG	CA	3109	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3110	-	-	-	X
58	MG	CA	3114	-	-	-	X
58	MG	CA	3119	-	-	-	X
58	MG	CA	3124	-	-	-	X
58	MG	CA	3127	-	-	-	X
58	MG	CA	3133	-	-	-	X
58	MG	CA	3137	-	-	-	X
58	MG	CA	3146	-	-	-	X
58	MG	CA	3159	-	-	-	X
58	MG	CA	3163	-	-	-	X
58	MG	CA	3166	-	-	-	X
58	MG	CA	3168	-	-	-	X
58	MG	CA	3169	-	-	-	X
58	MG	CA	3177	-	-	-	X
58	MG	CA	3178	-	-	-	X
58	MG	CA	3182	-	-	-	X
58	MG	CA	3185	-	-	-	X
58	MG	CA	3190	-	-	-	X
58	MG	CA	3201	-	-	-	X
58	MG	CA	3212	-	-	-	X
58	MG	CA	3213	-	-	-	X
58	MG	CA	3217	-	-	-	X
58	MG	CA	3218	-	-	-	X
58	MG	CA	3221	-	-	-	X
58	MG	CA	3223	-	-	-	X
58	MG	CA	3226	-	-	-	X
58	MG	CA	3229	-	-	-	X
58	MG	CA	3230	-	-	-	X
58	MG	CA	3251	-	-	-	X
58	MG	CA	3263	-	-	-	X
58	MG	CA	3266	-	-	-	X
58	MG	CA	3276	-	-	-	X
58	MG	CA	3281	-	-	-	X
58	MG	CA	3290	-	-	-	X
58	MG	CA	3302	-	-	-	X
58	MG	CA	3309	-	-	-	X
58	MG	CA	3313	-	-	-	X
58	MG	CA	3314	-	-	-	X
58	MG	CA	3322	-	-	-	X
58	MG	CA	3324	-	-	-	X
58	MG	CA	3326	-	-	-	X
58	MG	CA	3328	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3330	-	-	-	X
58	MG	CA	3340	-	-	-	X
58	MG	CA	3348	-	-	-	X
58	MG	CA	3353	-	-	-	X
58	MG	CA	3358	-	-	-	X
58	MG	CA	3361	-	-	-	X
58	MG	CA	3364	-	-	-	X
58	MG	CA	3375	-	-	-	X
58	MG	CA	3383	-	-	-	X
58	MG	CA	3392	-	-	-	X
58	MG	CA	3396	-	-	-	X
58	MG	CA	3409	-	-	-	X
58	MG	CA	3420	-	-	-	X
58	MG	CA	3428	-	-	-	X
58	MG	CA	3432	-	-	-	X
58	MG	CA	3441	-	-	-	X
58	MG	CA	3452	-	-	-	X
58	MG	CA	3455	-	-	-	X
58	MG	CA	3458	-	-	-	X
58	MG	CA	3463	-	-	-	X
58	MG	CA	3467	-	-	-	X
58	MG	CA	3476	-	-	-	X
58	MG	CA	3489	-	-	-	X
58	MG	CA	3490	-	-	-	X
58	MG	CA	3491	-	-	-	X
58	MG	CA	3498	-	-	-	X
58	MG	CA	3500	-	-	-	X
58	MG	CA	3530	-	-	-	X
58	MG	CA	3542	-	-	-	X
58	MG	CA	3555	-	-	-	X
58	MG	CA	3567	-	-	-	X
58	MG	CA	3588	-	-	-	X
58	MG	CA	3596	-	-	-	X
58	MG	CA	3597	-	-	-	X
58	MG	CA	3603	-	-	-	X
58	MG	CA	3607	-	-	-	X
58	MG	CA	3618	-	-	-	X
58	MG	CA	3619	-	-	-	X
58	MG	CA	3626	-	-	-	X
58	MG	CA	3650	-	-	-	X
58	MG	CA	3654	-	-	-	X
58	MG	CA	3660	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	CA	3661	-	-	-	X
58	MG	CD	303	-	-	-	X
58	MG	CE	301	-	-	-	X
58	MG	CE	303	-	-	-	X
58	MG	CF	301	-	-	-	X
58	MG	CF	303	-	-	-	X
58	MG	CQ	201	-	-	-	X
58	MG	CU	201	-	-	-	X
58	MG	CV	202	-	-	-	X
58	MG	DA	1606	-	-	-	X
58	MG	DA	1610	-	-	-	X
58	MG	DA	1618	-	-	-	X
58	MG	DA	1636	-	-	-	X
58	MG	DA	1638	-	-	-	X
58	MG	DA	1647	-	-	-	X
58	MG	DA	1649	-	-	-	X
58	MG	DA	1651	-	-	-	X
58	MG	DA	1658	-	-	-	X
58	MG	DA	1668	-	-	-	X
58	MG	DA	1669	-	-	-	X
58	MG	DA	1672	-	-	-	X
58	MG	DA	1680	-	-	-	X
58	MG	DA	1684	-	-	-	X
58	MG	DA	1689	-	-	-	X
58	MG	DA	1694	-	-	-	X
58	MG	DA	1697	-	-	-	X
58	MG	DA	1722	-	-	-	X
58	MG	DA	1743	-	-	-	X
58	MG	DA	1768	-	-	-	X
58	MG	DF	3001	-	-	-	X
58	MG	DT	3001	-	-	-	X
60	SF4	DD	501	-	-	X	-
62	GDP	DZ	704	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 310279 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	2852	Total	C	N	O	P	0	0	0
			61426	27339	11489	19747	2851			
1	CA	2848	Total	C	N	O	P	0	0	0
			61337	27299	11470	19721	2847			

- 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	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CL	139	Total	C	N	O	S	0	0	0
			1025	653	181	186	5			

- 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	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
24	C0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	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	S	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	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	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	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			
57	DZ	730	Total	C	N	O	S	0	0	0
			5690	3616	980	1075	19			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AP	2	Total 2 Mg 2	0	0
58	CR	1	Total 1 Mg 1	0	0
58	BA	211	Total 211 Mg 211	0	0
58	CA	664	Total 664 Mg 664	0	0
58	C8	1	Total 1 Mg 1	0	0
58	C5	1	Total 1 Mg 1	0	0
58	AB	23	Total 23 Mg 23	0	0
58	BL	2	Total 2 Mg 2	0	0
58	CV	2	Total 2 Mg 2	0	0
58	A6	1	Total 1 Mg 1	0	0
58	BE	1	Total 1 Mg 1	0	0
58	AW	4	Total 4 Mg 4	0	0
58	AN	3	Total 3 Mg 3	0	0
58	DZ	2	Total 2 Mg 2	0	0
58	AX	1	Total 1 Mg 1	0	0
58	CN	1	Total 1 Mg 1	0	0
58	A2	2	Total 2 Mg 2	0	0
58	CY	1	Total 1 Mg 1	0	0
58	DD	1	Total 1 Mg 1	0	0
58	BB	1	Total 1 Mg 1	0	0
58	BT	1	Total 1 Mg 1	0	0
58	AE	4	Total 4 Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BM	2	Total 2	Mg 2	0	0
58	CU	1	Total 1	Mg 1	0	0
58	BF	1	Total 1	Mg 1	0	0
58	AV	3	Total 3	Mg 3	0	0
58	DA	168	Total 168	Mg 168	0	0
58	CB	13	Total 13	Mg 13	0	0
58	AA	835	Total 835	Mg 835	0	0
58	CQ	5	Total 5	Mg 5	0	0
58	A5	1	Total 1	Mg 1	0	0
58	AR	1	Total 1	Mg 1	0	0
58	CG	1	Total 1	Mg 1	0	0
58	DK	1	Total 1	Mg 1	0	0
58	DF	1	Total 1	Mg 1	0	0
58	AD	10	Total 10	Mg 10	0	0
58	BN	1	Total 1	Mg 1	0	0
58	DJ	1	Total 1	Mg 1	0	0
58	C7	1	Total 1	Mg 1	0	0
58	C3	1	Total 1	Mg 1	0	0
58	AZ	2	Total 2	Mg 2	0	0
58	A4	1	Total 1	Mg 1	0	0
58	BK	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AU	3	Total 3	Mg 3	0	0
58	DW	3	Total 3	Mg 3	0	0
58	A9	1	Total 1	Mg 1	0	0
58	CF	5	Total 5	Mg 5	0	0
58	BV	1	Total 1	Mg 1	0	0
58	A0	3	Total 3	Mg 3	0	0
58	AG	2	Total 2	Mg 2	0	0
58	DE	2	Total 2	Mg 2	0	0
58	AQ	3	Total 3	Mg 3	0	0
58	CE	6	Total 6	Mg 6	0	0
58	AH	2	Total 2	Mg 2	0	0
58	BZ	2	Total 2	Mg 2	0	0
58	CO	2	Total 2	Mg 2	0	0
58	CP	3	Total 3	Mg 3	0	0
58	CW	1	Total 1	Mg 1	0	0
58	A7	3	Total 3	Mg 3	0	0
58	CD	3	Total 3	Mg 3	0	0
58	BD	1	Total 1	Mg 1	0	0
58	DT	1	Total 1	Mg 1	0	0
58	A8	2	Total 2	Mg 2	0	0
58	AO	1	Total 1	Mg 1	0	0

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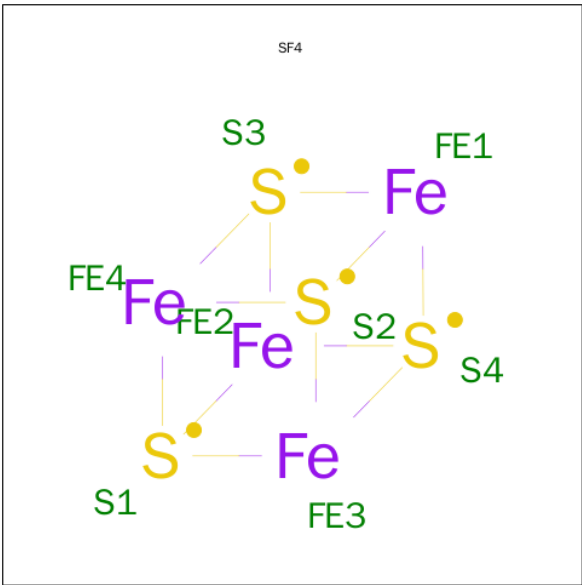
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BW	3	Total 3	Mg 3	0	0
58	AY	1	Total 1	Mg 1	0	0
58	AF	5	Total 5	Mg 5	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

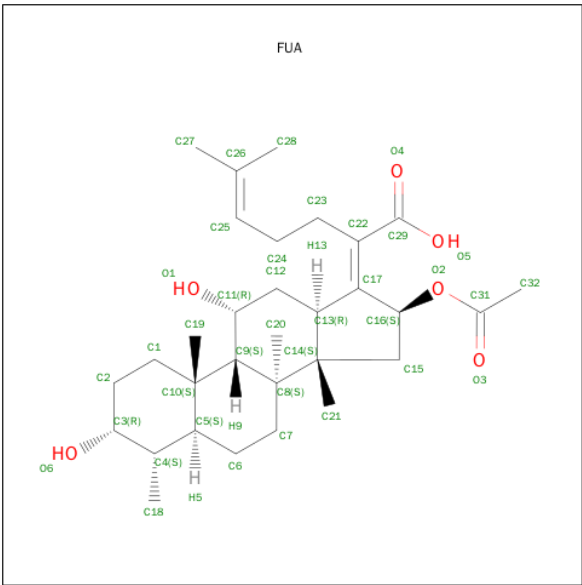
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AY	1	Total 1	Zn 1	0	0
59	BN	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0
59	C5	1	Total 1	Zn 1	0	0
59	C6	1	Total 1	Zn 1	0	0
59	A6	1	Total 1	Zn 1	0	0
59	C9	1	Total 1	Zn 1	0	0
59	DN	1	Total 1	Zn 1	0	0
59	A4	1	Total 1	Zn 1	0	0
59	A5	1	Total 1	Zn 1	0	0
59	A9	1	Total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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BZ	1	Total	C	O	0	0
			37	31	6		
61	DZ	1	Total	C	O	0	0
			37	31	6		

-
- The chemical structure of GDP (Guanosine Diphosphate) is shown. It consists of a guanine base (a purine ring system with an amino group at C2) attached to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The atoms are labeled with their respective element symbols and coordinates: N1, N2, N3, N7, N9, O6, O5, O4, O3, O2, O1, O2B, O1B, O3A, O3B, O4', O5', O6', O7', O8', O9', O10', O11', O12', O13', O14', O15', O16', O17', O18', O19', O20', O21', O22', O23', O24', O25', O26', O27', O28', O29', O30', O31', O32', O33', O34', O35', O36', O37', O38', O39', O40', O41', O42', O43', O44', O45', O46', O47', O48', O49', O50', O51', O52', O53', O54', O55', O56', O57', O58', O59', O60', O61', O62', O63', O64', O65', O66', O67', O68', O69', O70', O71', O72', O73', O74', O75', O76', O77', O78', O79', O80', O81', O82', O83', O84', O85', O86', O87', O88', O89', O90', O91', O92', O93', O94', O95', O96', O97', O98', O99', O100', O101', O102', O103', O104', O105', O106', O107', O108', O109', O110', O111', O112', O113', O114', O115', O116', O117', O118', O119', O120', O121', O122', O123', O124', O125', O126', O127', O128', O129', O130', O131', O132', O133', O134', O135', O136', O137', O138', O139', O140', O141', O142', O143', O144', O145', O146', O147', O148', O149', O150', O151', O152', O153', O154', O155', O156', O157', O158', O159', O160', O161', O162', O163', O164', O165', O166', O167', O168', O169', O170', O171', O172', O173', O174', O175', O176', O177', O178', O179', O180', O181', O182', O183', O184', O185', O186', O187', O188', O189', O190', O191', O192', O193', O194', O195', O196', O197', O198', O199', O200', O201', O202', O203', O204', O205', O206', O207', O208', O209', O210', O211', O212', O213', O214', O215', O216', O217', O218', O219', O220', O221', O222', O223', O224', O225', O226', O227', O228', O229', O230', O231', O232', O233', O234', O235', O236', O237', O238', O239', O240', O241', O242', O243', O244', O245', O246', O247', O248', O249', O250', O251', O252', O253', O254', O255', O256', O257', O258', O259', O260', O261', O262', O263', O264', O265', O266', O267', O268', O269', O270', O271', O272', O273', O274', O275', O276', O277', O278', O279', O280', O281', O282', O283', O284', O285', O286', O287', O288', O289', O290', O291', O292', O293', O294', O295', O296', O297', O298', O299', O300', O301', O302', O303', O304', O305', O306', O307', O308', O309', O310', O311', O312', O313', O314', O315', O316', O317', O318', O319', O320', O321', O322', O323', O324', O325', O326', O327', O328', O329', O330', O331', O332', O333', O334', O335', O336', O337', O338', O339', O340', O341', O342', O343', O344', O345', O346', O347', O348', O349', O350', O351', O352', O353', O354', O355', O356', O357', O358', O359', O360', O361', O362', O363', O364', O365', O366', O367', O368', O369', O370', O371', O372', O373', O374', O375', O376', O377', O378', O379', O380', O381', O382', O383', O384', O385', O386', O387', O388', O389', O390', O391', O392', O393', O394', O395', O396', O397', O398', O399', O400', O401', O402', O403', O404', O405', O406', O407', O408', O409', O410', O411', O412', O413', O414', O415', O416', O417', O418', O419', O420', O421', O422', O423', O424', O425', O426', O427', O428', O429', O430', O431', O432', O433', O434', O435', O436', O437', O438', O439', O440', O441', O442', O443', O444', O445', O446', O447', O448', O449', O450', O451', O452', O453', O454', O455', O456', O457', O458', O459', O460', O461', O462', O463', O464', O465', O466', O467', O468', O469', O470', O471', O472', O473', O474', O475', O476', O477', O478', O479', O480', O481', O482', O483', O484', O485', O486', O487', O488', O489', O490', O491', O492', O493', O494', O495', O496', O497', O498', O499', O500', O501', O502', O503', O504', O505', O506', O507', O508', O509', O510', O511', O512', O513', O514', O515', O516', O517', O518', O519', O520', O521', O522', O523', O524', O525', O526', O527', O528', O529', O530', O531', O532', O533', O534', O535', O536', O537', O538', O539', O540', O541', O542', O543', O544', O545', O546', O547', O548', O549', O550', O551', O552', O553', O554', O555', O556', O557', O558', O559', O560', O561', O562', O563', O564', O565', O566', O567', O568', O569', O570', O571', O572', O573', O574', O575', O576', O577', O578', O579', O580', O581', O582', O583', O584', O585', O586', O587', O588', O589', O590', O591', O592', O593', O594', O595', O596', O597', O598', O599', O600', O601', O602', O603', O604', O605', O606', O607', O608', O609', O610', O611', O612', O613', O614', O615', O616', O617', O618', O619', O620', O621', O622', O623', O624', O625', O626', O627', O628', O629', O630', O631', O632', O633', O634', O635', O636', O637', O638', O639', O640', O641', O642', O643', O644', O645', O646', O647', O648', O649', O650', O651', O652', O653', O654', O655', O656', O657', O658', O659', O660', O661', O662', O663', O664', O665', O666', O667', O668', O669', O670', O671', O672', O673', O674', O675', O676', O677', O678', O679', O680', O681', O682', O683', O684', O685', O686', O687', O688', O689', O690', O691', O692', O693', O694', O695', O696', O697', O698', O699', O700', O701', O702', O703', O704', O705', O706', O707', O708', O709', O710', O711', O712', O713', O714', O715', O716', O717', O718', O719', O720', O721', O722', O723', O724', O725', O726', O727', O728', O729', O730', O731', O732', O733', O734', O735', O736', O737', O738', O739', O740', O741', O742', O743', O744', O745', O746', O747', O748', O749', O750', O751', O752', O753', O754', O755', O756', O757', O758', O759', O760', O761', O762', O763', O764', O765', O766', O767', O768', O769', O770', O771', O772', O773', O774', O775', O776', O777', O778', O779', O780', O781', O782', O783', O784', O785', O786', O787', O788', O789', O790', O791', O792', O793', O794', O795', O796', O797', O798', O799', O800', O801', O802', O803', O804', O805', O806', O80

- Molecule 63 is water.

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	AO	3	Total 3	O 3	0	0
63	AP	15	Total 15	O 15	0	0
63	AQ	3	Total 3	O 3	0	0
63	AR	3	Total 3	O 3	0	0
63	AS	1	Total 1	O 1	0	0
63	AT	2	Total 2	O 2	0	0
63	AU	6	Total 6	O 6	0	0
63	AW	1	Total 1	O 1	0	0
63	AX	2	Total 2	O 2	0	0
63	AZ	1	Total 1	O 1	0	0
63	A0	7	Total 7	O 7	0	0
63	A1	3	Total 3	O 3	0	0
63	A3	1	Total 1	O 1	0	0
63	A5	2	Total 2	O 2	0	0
63	A6	1	Total 1	O 1	0	0
63	A7	3	Total 3	O 3	0	0
63	A8	11	Total 11	O 11	0	0
63	BA	205	Total 205	O 205	0	0
63	BD	3	Total 3	O 3	0	0
63	BE	3	Total 3	O 3	0	0
63	BJ	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BL	2	Total	O	0	0
			2	2		
63	BM	1	Total	O	0	0
			1	1		
63	BO	1	Total	O	0	0
			1	1		
63	BV	2	Total	O	0	0
			2	2		
63	BW	1	Total	O	0	0
			1	1		
63	BZ	3	Total	O	0	0
			3	3		
63	CA	981	Total	O	0	0
			981	981		
63	CB	9	Total	O	0	0
			9	9		
63	CD	15	Total	O	0	0
			15	15		
63	CE	9	Total	O	0	0
			9	9		
63	CF	6	Total	O	0	0
			6	6		
63	CP	13	Total	O	0	0
			13	13		
63	CQ	1	Total	O	0	0
			1	1		
63	CT	3	Total	O	0	0
			3	3		
63	CU	4	Total	O	0	0
			4	4		
63	CV	1	Total	O	0	0
			1	1		
63	CW	1	Total	O	0	0
			1	1		
63	CX	1	Total	O	0	0
			1	1		
63	CY	1	Total	O	0	0
			1	1		
63	C0	5	Total	O	0	0
			5	5		
63	C1	3	Total	O	0	0
			3	3		

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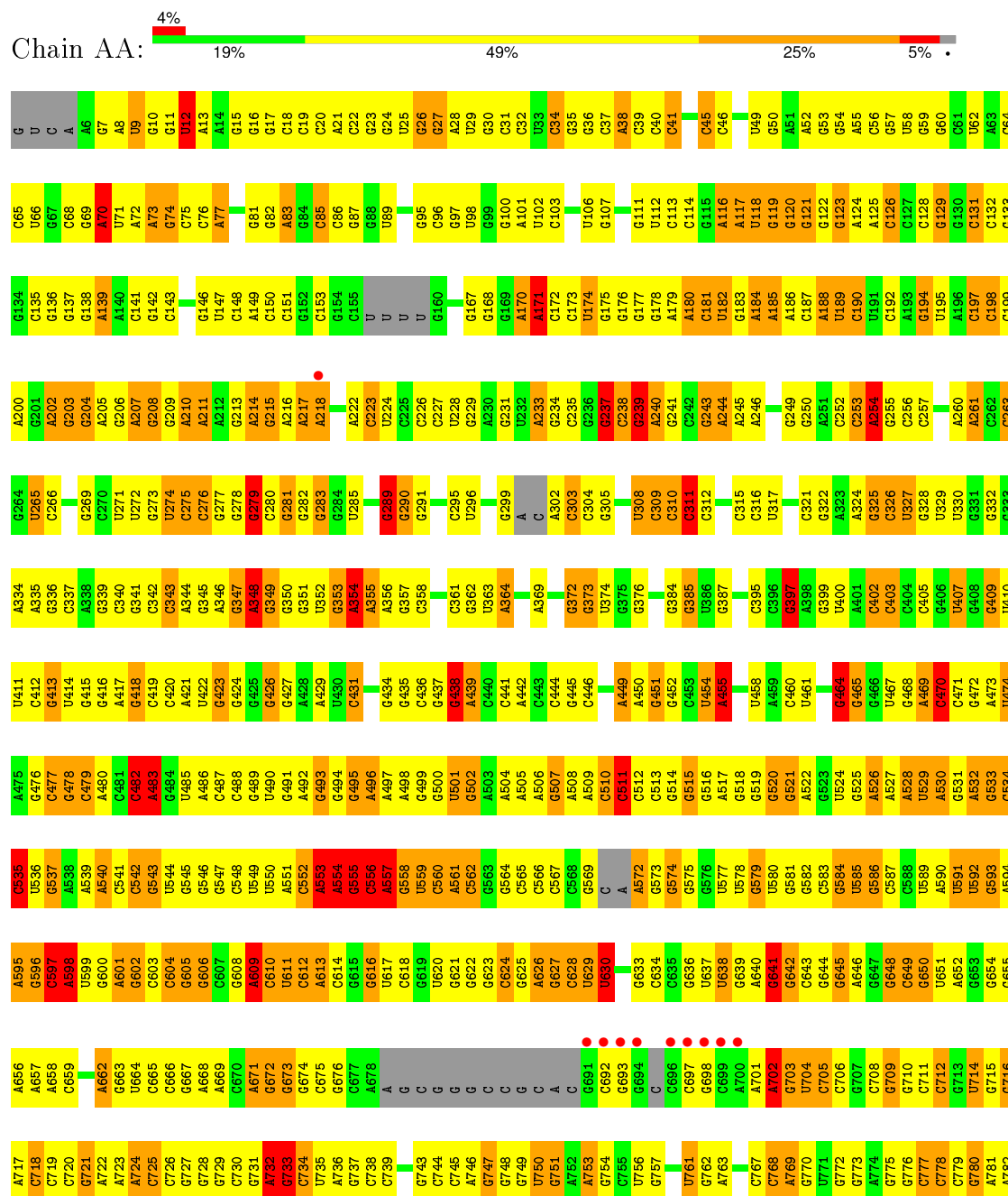
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	C3	1	Total 1	O 1	0	0
63	C5	1	Total 1	O 1	0	0
63	C7	3	Total 3	O 3	0	0
63	C8	3	Total 3	O 3	0	0
63	DA	153	Total 153	O 153	0	0
63	DE	2	Total 2	O 2	0	0
63	DH	1	Total 1	O 1	0	0
63	DJ	1	Total 1	O 1	0	0
63	DK	2	Total 2	O 2	0	0
63	DL	1	Total 1	O 1	0	0
63	DP	1	Total 1	O 1	0	0
63	DT	1	Total 1	O 1	0	0
63	DY	1	Total 1	O 1	0	0
63	DZ	2	Total 2	O 2	0	0

3 Residue-property plots

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



G1734	G1669	G1608	G1467	G1402	C1341	G1281	G1218	G1156	G1090	A1030	C969	U905	C844	C783
U1735	G1670	A1609	G1470	U1403	G1342	G1282	A1219	A1157	A1091	C1031	C996	G906	G845	C784
U1736	G1671	A1610	G1471	G1404	C1343	A1283	U1220	G1158	A1092	C1032	A972	G907	G846	C785
A1737	G1672	C1611	A1471	A1405	C1344	G1284	G1221	U1159	G1093	G1033	A973	A908	A847	G786
U1738	G1673	C1612	G1472	A1406	G1345	G1285	A1222	G1160	A1094	A1034	G974	G909	G848	U787
U1739	G1674	A1613	A1473	G1407	U1346	U1286	C1223	G1161	C1095	G1035	U975	A910	A849	G788
U1740	U1675	G1614	G1474	G1409	A1347	A1287	C1224	G1162	A1096	A1036	G976	G911	U850	G789
C1741	C1542	G1615	G1475	G1410	A1348	A1288	G1225	G1163	G1097	C1037	G977	G912	A851	G790
U1742	U1548	U1616	G1476	A1411	G1349	G1289	C1226	G1164	C1098	C1038	A978	A913	G852	G791
G1743	A1679	A1617	U1477	A1412	C1350	G1290	G1229	C	C1099	G1039	G979	C914	C853	G792
G1744	G1680	A1618	A1478	A1413	C1351	G1291	C1230	C	A1100	C980	G980	U915	U854	A793
A1745	U1619	G1619	A1479	G1414	C1352	A1292	G1231	C	G1101	C1041	C981	G916	U794	U794
G1746	G1682	G1620	A1480	G1415	A1353	A1293	G1232	C	G1102	A1042	A982	A917	G855	G795
A1747	C1683	C1621	G1481	C1416	A1354	G1294	U1233	C	A1103	G1043	G983	U918	U857	C796
A1748	A1684	U1622	G1482	G1417	G1355	U1295	A1234	C	G1104	C1044	G984	A919	U858	A797
G1749	U1685	U1623	C1483	U1418	G1356	G1296	G1235	G	U1105	U1045	G985	G920	C859	A799
U1750	U1686	G1624	A1484	A1419	G1357	G1297	G1236	A	U1106	A1046	A986	G921	U860	C801
U1751	G1687	U1625	U1485	G1420	U1358	G1298	G1237	A	U1107	A1047	G987	A922	C861	C800
U1752	A1688	A1626	G1486	C1421	U1359	A1299	G1238	A	G1108	G1048	U988	G922	C862	C802
U1753	G1689	A1627	G1487	C1422	C1360	A1300	A1239	A	G1109	G1049	G989	G926	C863	C803
G1754	U1690	G1628	G1488	U1423	C1361	U1301	G1240	U	C1110	C1050	A990	G927	C864	C804
U1755	C1691	C1629	A1491	A1424	A1362	G1302	C1241	G	U1111	C1051	G991	G928	G865	U804
C1756	G1692	A1630	A1425	A1425	A1363	C1303	G1242	A	U1112	C1052	G992	G929	A866	C805
U1757	C1693	C1631	G1492	G1426	C1364	G1304	U1243	U	A1113	C1053	G993	G930	A867	G806
U1758	G1694	A1632	C1493	G1427	G1365	G1305	U1244	C	G1114	C1054	G994	G931	A868	G807
U1759	C1695	A1633	G1494	G1428	C1366	G1306	C1245	G	A1115	A1055	G995	C932	A871	A808
G1760	G1696	U1634	G1495	C1429	A1367	C1307	G1246	G	A1116	A1056	C996	C933	C872	U809
U1761	G1697	G1635	U1496	A1430	A1368	A1308	C1247	G	G1117	G1057	G997	A934	C873	G810
U1762	G1698	U1636	G1497	G1431	C1369	U1309	G1248	G	C1118	U1058	A998	C935	U873	A811
G1763	A1699	G1637	C1498	C1432	G1370	G1310	A1249	C1185	A1119	C1059	G999	C936	U874	G812
U1770	G1700	C1638	G1499	C1433	G1371	A1311	U1250	U1186	G1120	U1060	A1000	A937	U875	C813
G1771	A1701	G1639	U1501	G1434	U1372	G1312	G1251	U1187	C1121	G1061	G1001	G938	A876	U814
C1772	A1702	G1640	G1502	G1435	C1373	G1313	G1252	A1188	C1122	G1062	A1002	G939	G877	G815
C1773	C1703	G1641	A1503	G1436	G1374	A1314	C1253	A1189	C1123	G1063	U1003	C940	G878	G816
C1774	C1704	A1642	G1504	C1437	U1375	A1315	G1254	G1190	U1126	C1064	A1004	U941	G879	G817
C1775	U1705	U1645	C1505	U1440	C1376	C1316	A1255	C1191	A1005	U1065	A942	C943	U880	G818
G1776	U1706	G1646	G1506	A1441	A1377	G1317	U1256	C1192	C1006	A1066	G1007	C944	C881	C819
C1777	C1707	C1647	A1507	U1442	G1378	A1318	G1257	C1193	U1128	A1067	G1007	C944	A882	U820
U1782	G1708	G1647	G1508	U1443	G1379	U1319	A1258	A1194	U1129	G1068	U1008	A945	G883	A821
G1783	C1709	U1648	C1509	C1444	C1380	A1320	A1259	G1195	C1009	U1069	C1009	C948	C884	G822
G1784	C1710	A1649	G1514	C1445	U1381	A1321	G1260	A1132	C1010	G1070	C1010	C948	C885	G823
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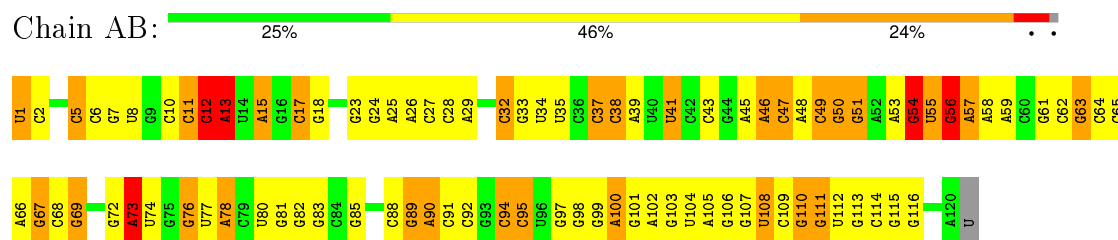
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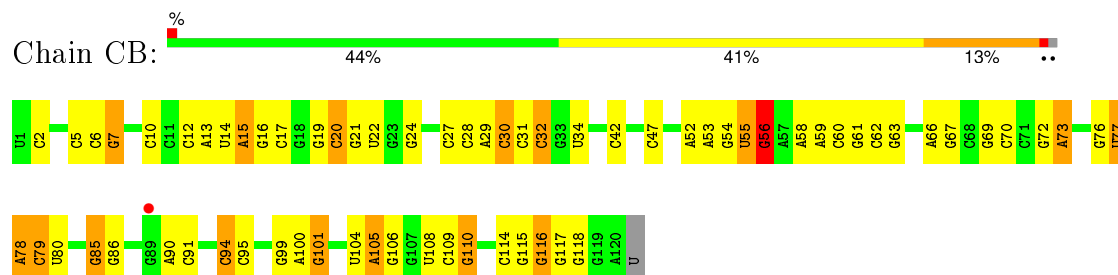
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	G2863	G	G2730	G2463	A2321	G2254	G2178	U2118	A2057	C1994	G1930
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	G2865	C	A2732	C2465	G2323	G2256	G2180	G2120	A2059	C1996	U1932
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	G2867	G2801	A2734	G2467	G2325	G2258	G2182	G2122	A2061	C1998	G1934
	G2868	G2802	G2735	G2468	A2326	G2259	G2183	G2123	A2062	C1999	G1935
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				U2510	G2368	U2301					
				U2511	G2369	G2302					
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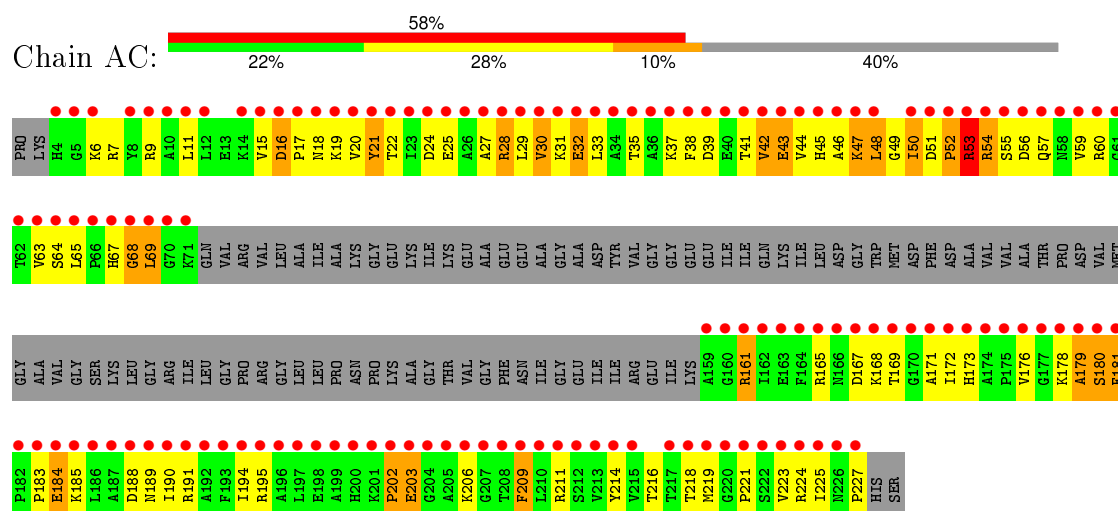
- Molecule 2: 5S Ribosomal RNA



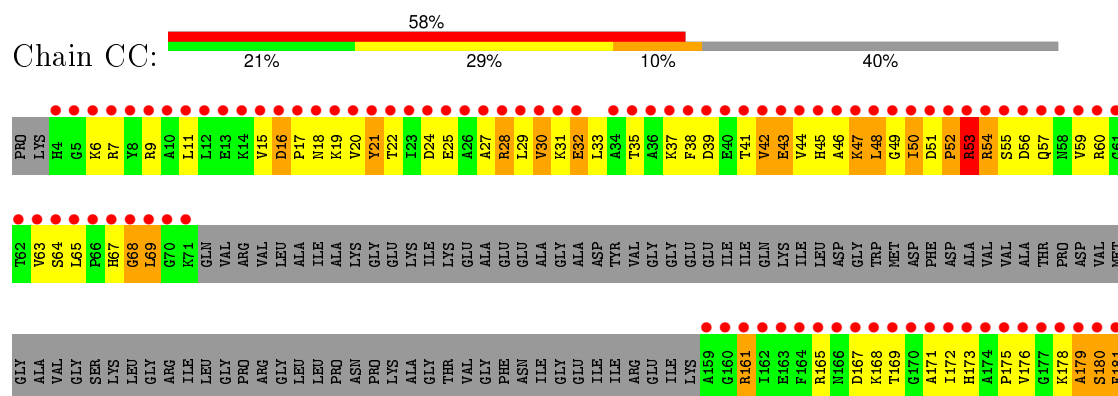
- Molecule 2: 5S Ribosomal RNA

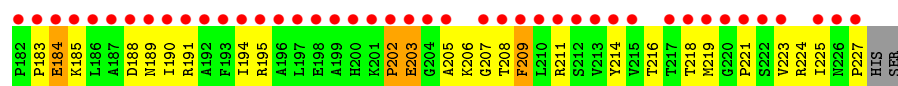


- Molecule 3: 50S ribosomal protein L1

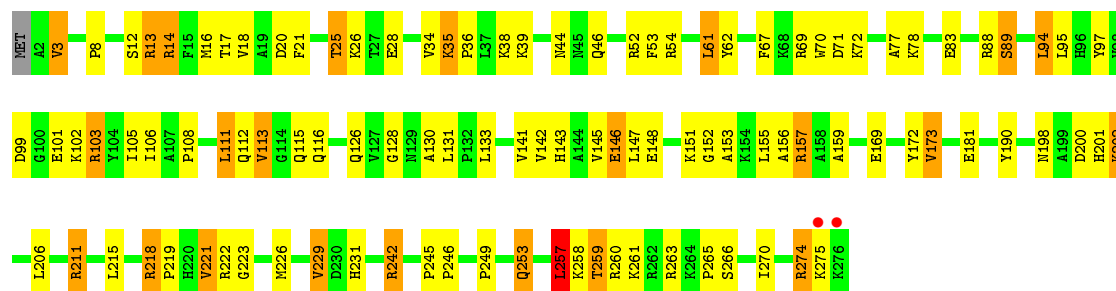


- Molecule 3: 50S ribosomal protein L1

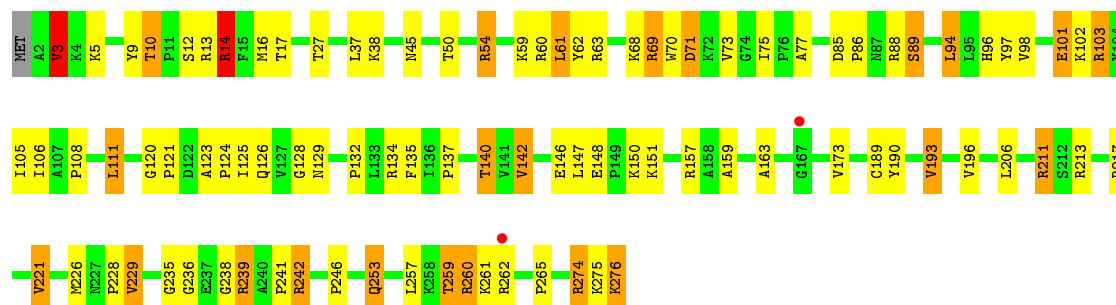




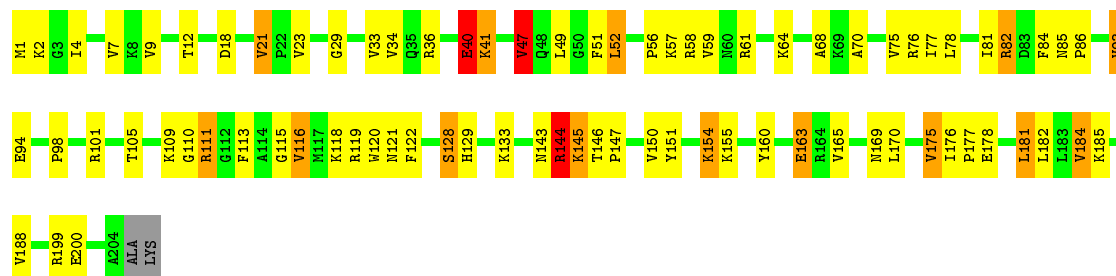
- Molecule 4: 50S ribosomal protein L2



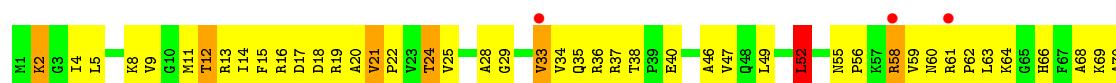
- Molecule 4: 50S ribosomal protein L2

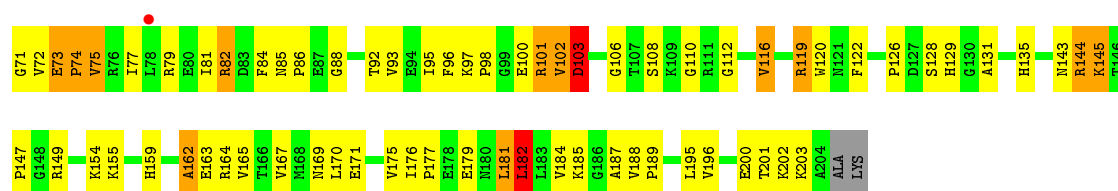


- Molecule 5: 50S ribosomal protein L3



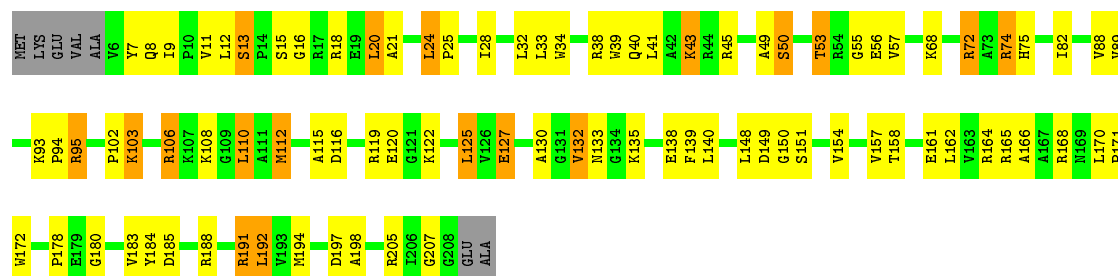
- Molecule 5: 50S ribosomal protein L3





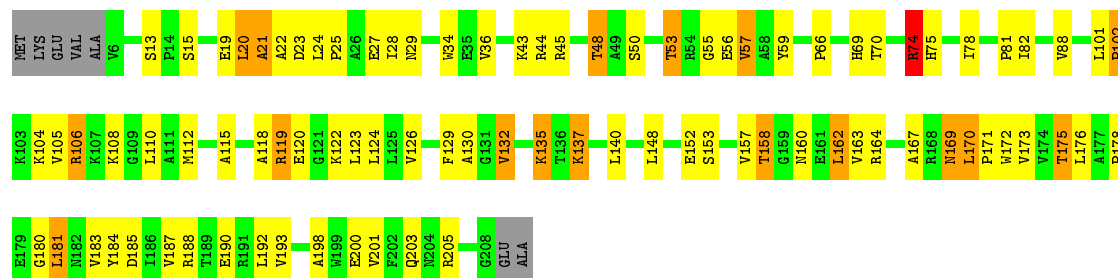
- Molecule 6: 50S ribosomal protein L4

Chain AF: 55% 33% 9% .



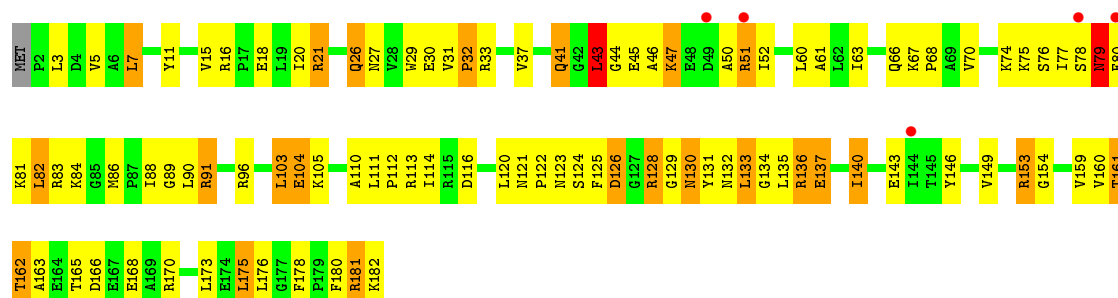
- Molecule 6: 50S ribosomal protein L4

Chain CF: 55% 33% 8% .



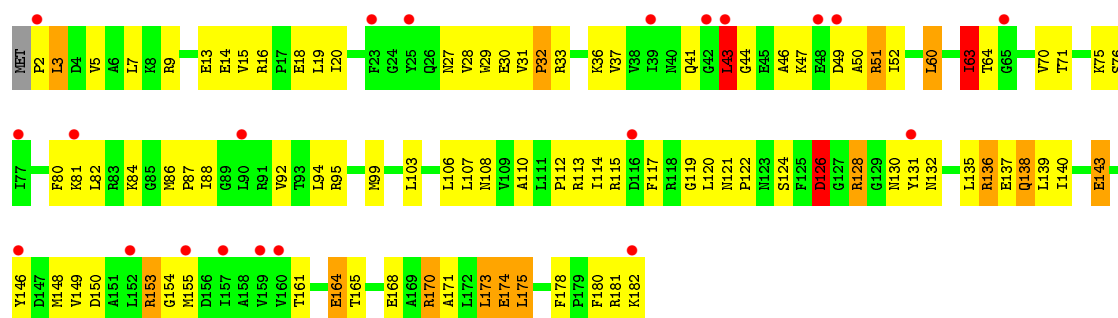
- Molecule 7: 50S ribosomal protein L5

Chain AG: 3% 46% 40% 13% ..

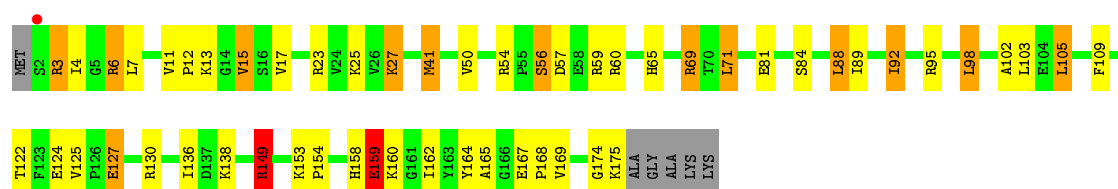


- Molecule 7: 50S ribosomal protein L5

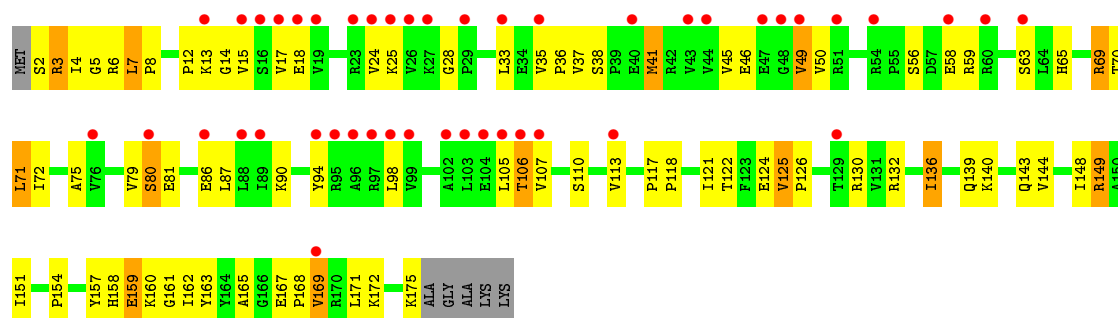
Chain CG: 12% 47% 43% 8% ..



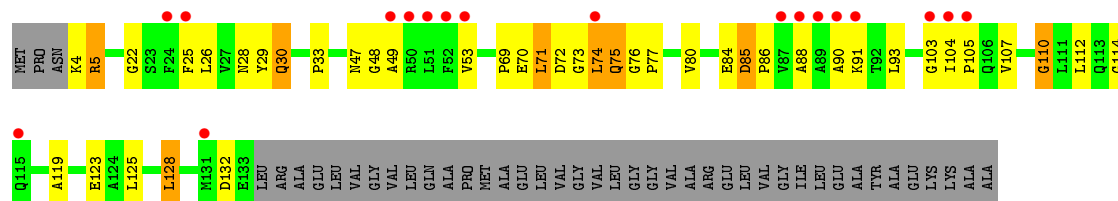
- Molecule 8: 50S ribosomal protein L6



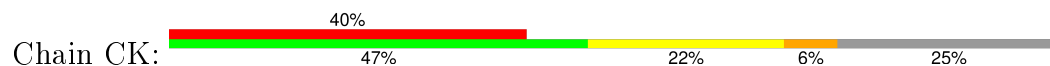
- Molecule 8: 50S ribosomal protein L6

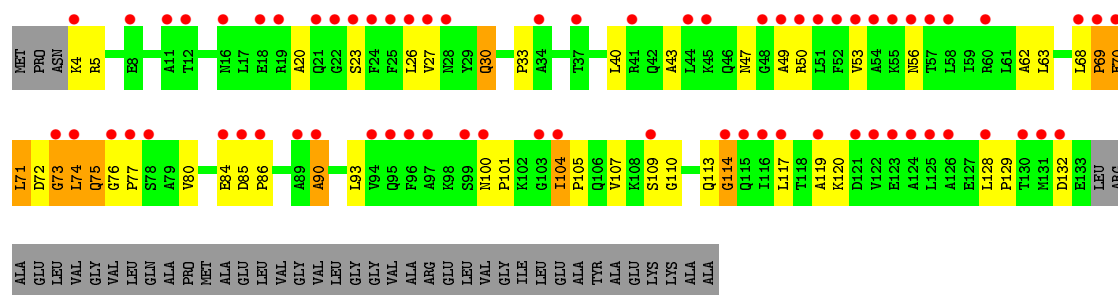


- Molecule 9: 50S ribosomal protein L10

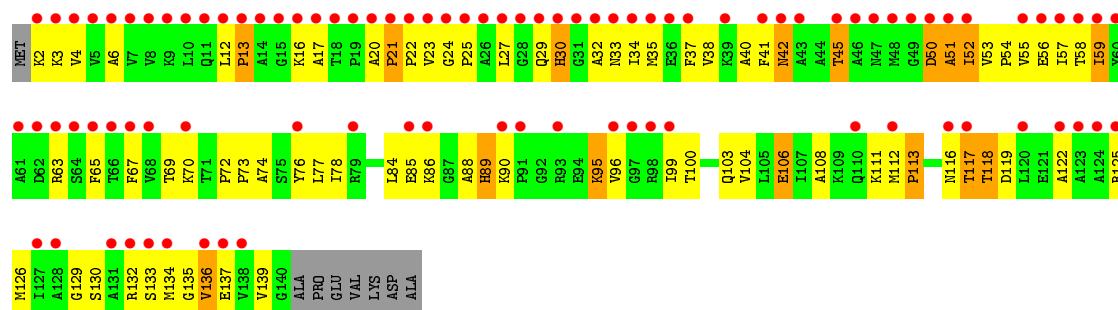
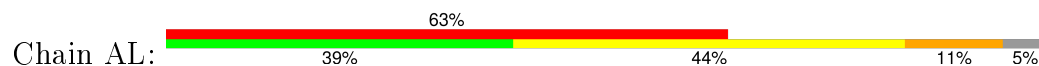


- Molecule 9: 50S ribosomal protein L10

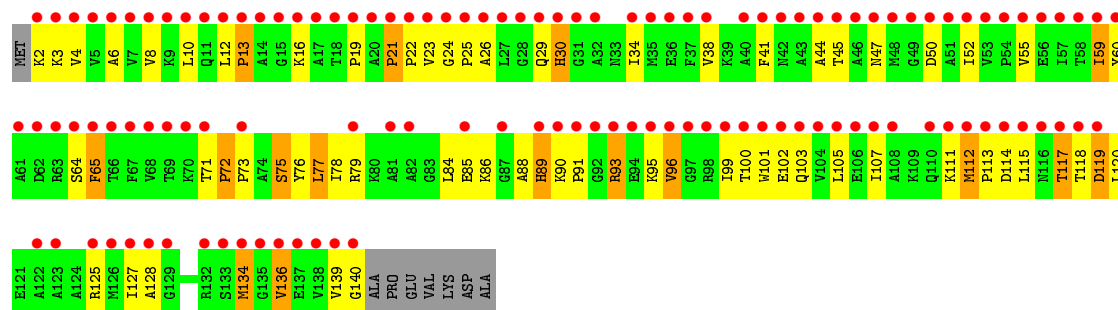
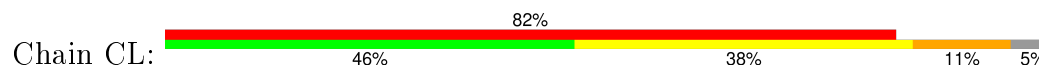




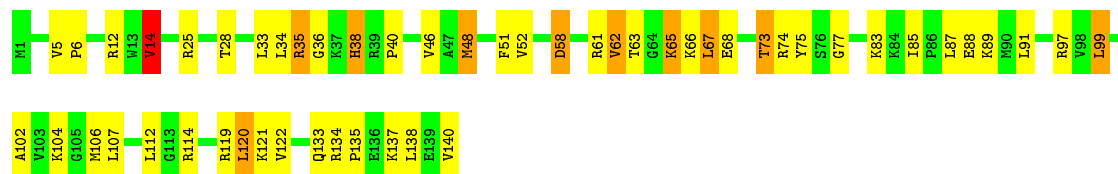
- Molecule 10: 50S ribosomal protein L11



- Molecule 10: 50S ribosomal protein L11

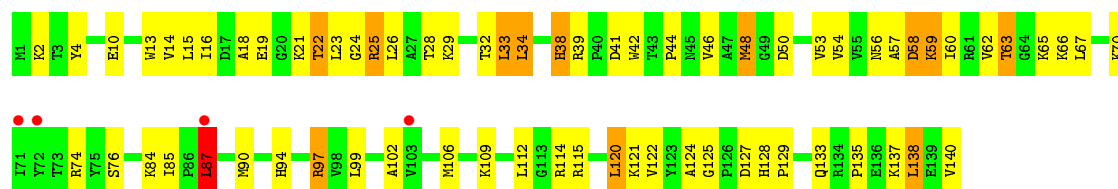


- Molecule 11: 50S ribosomal protein L13

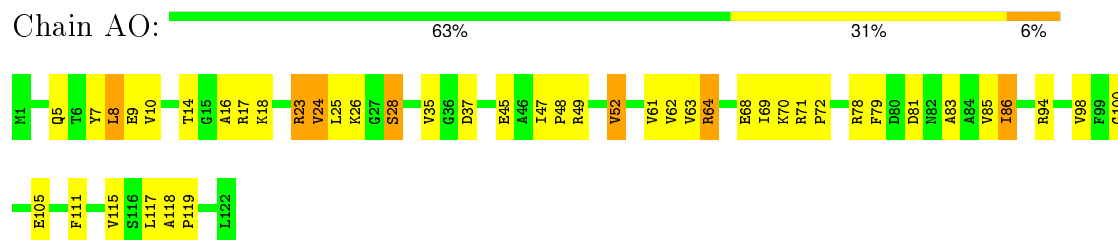


- Molecule 11: 50S ribosomal protein L13

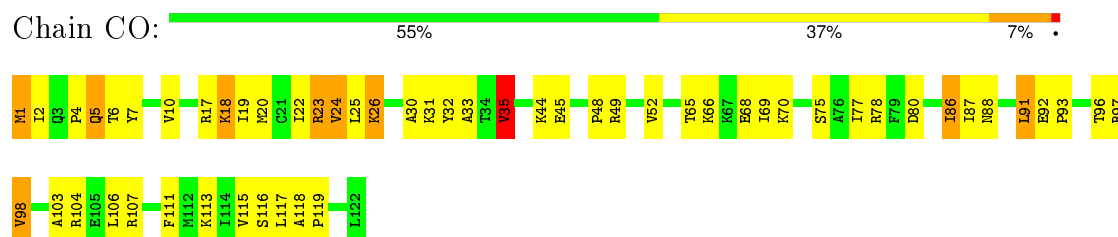




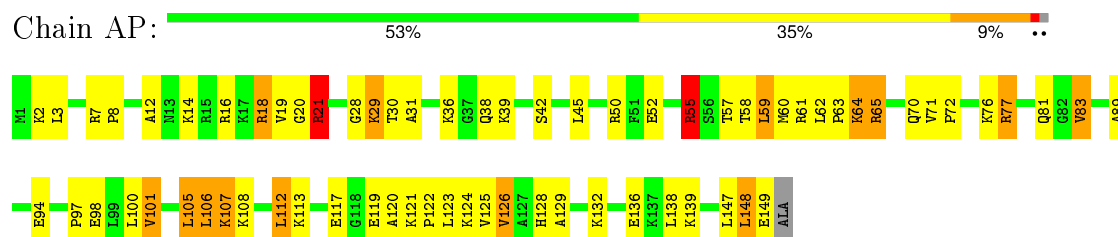
• Molecule 12: 50S ribosomal protein L14



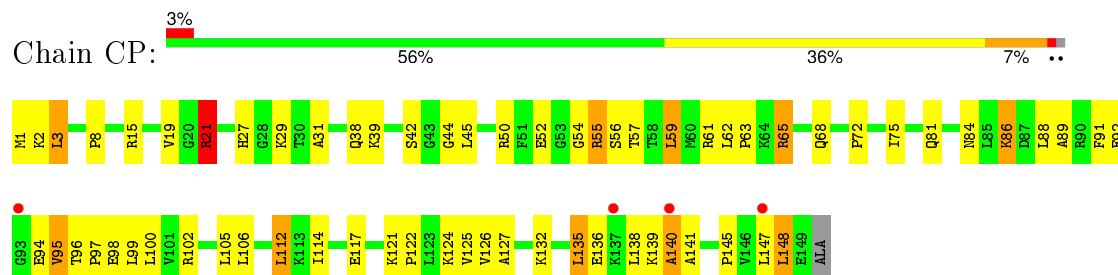
• Molecule 12: 50S ribosomal protein L14



• Molecule 13: 50S ribosomal protein L15

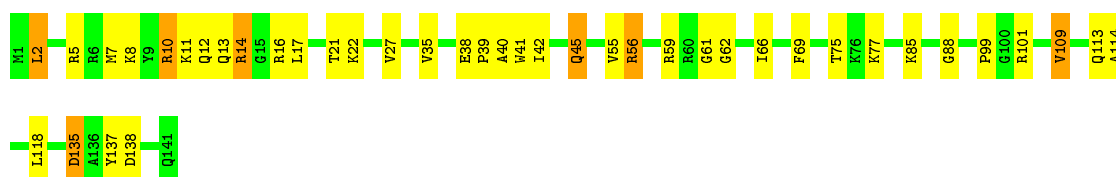


• Molecule 13: 50S ribosomal protein L15

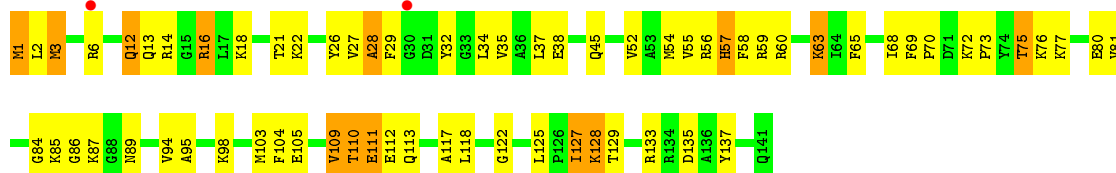


• Molecule 14: 50S ribosomal protein L16

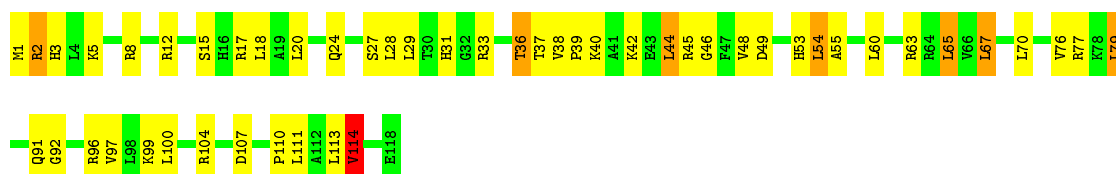




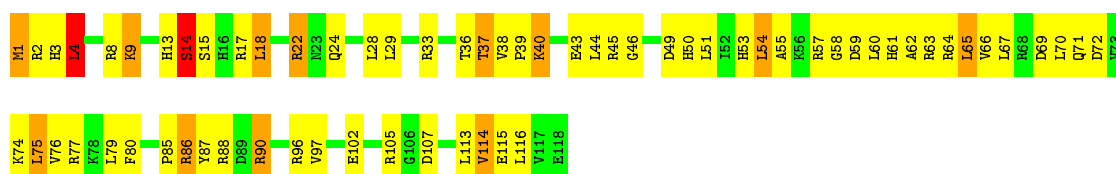
- Molecule 14: 50S ribosomal protein L16



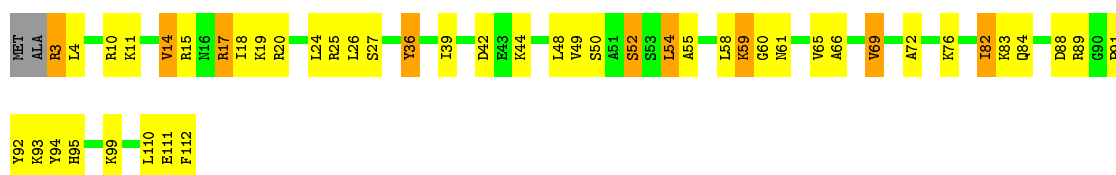
- Molecule 15: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L17

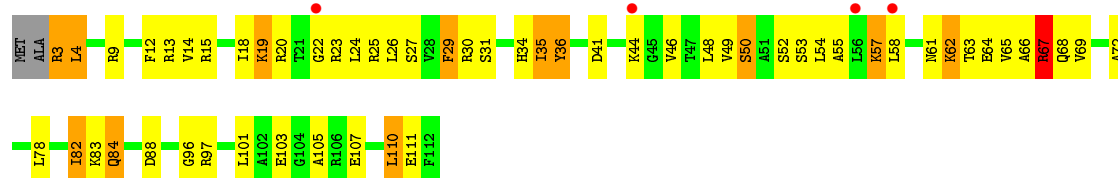


- Molecule 16: 50S ribosomal protein L18

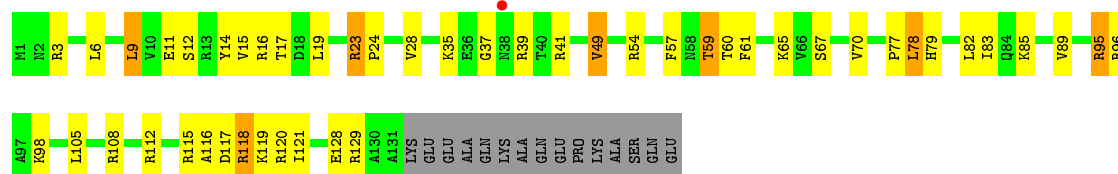


- Molecule 16: 50S ribosomal protein L18

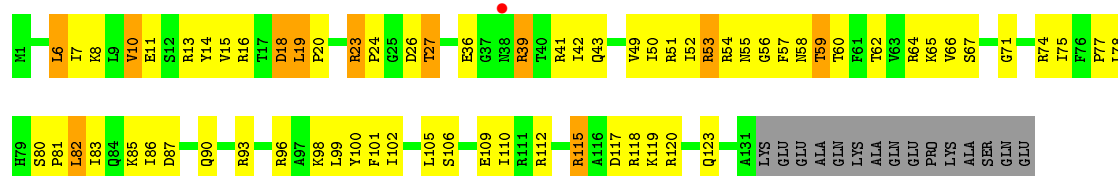
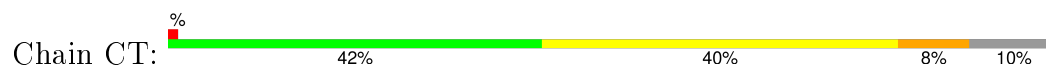




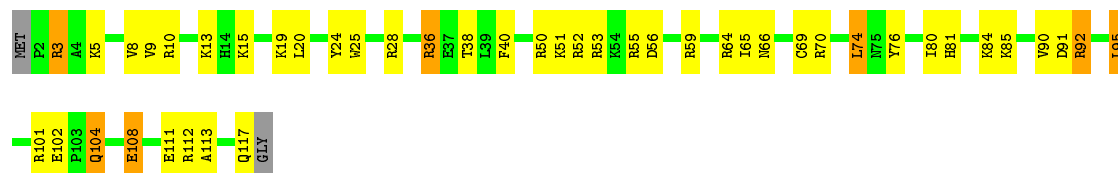
- Molecule 17: 50S ribosomal protein L19



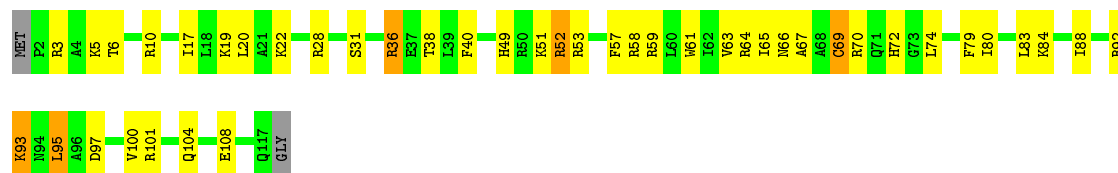
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20

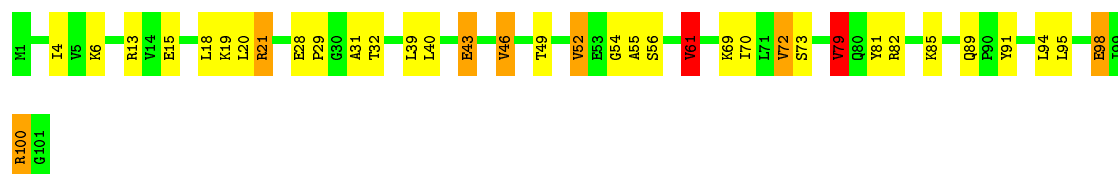


- Molecule 18: 50S ribosomal protein L20

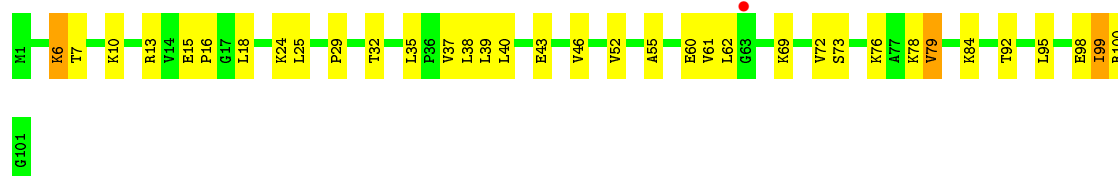


- Molecule 19: 50S ribosomal protein L21

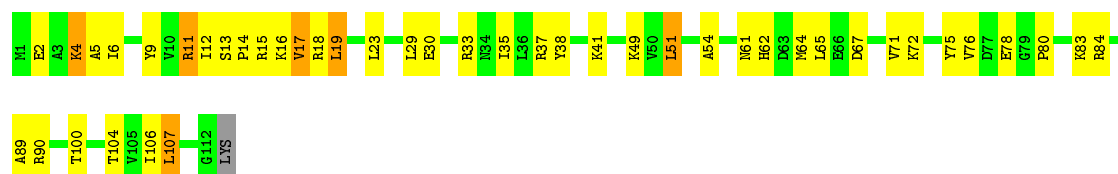




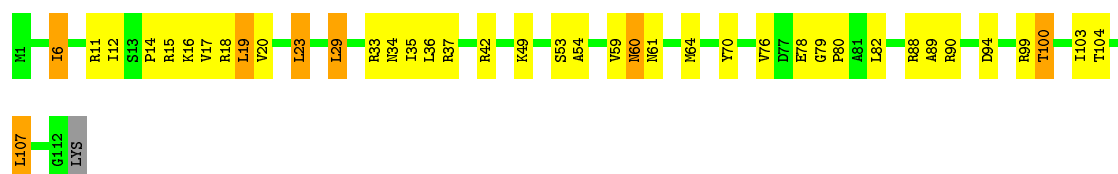
- Molecule 19: 50S ribosomal protein L21



- Molecule 20: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L22

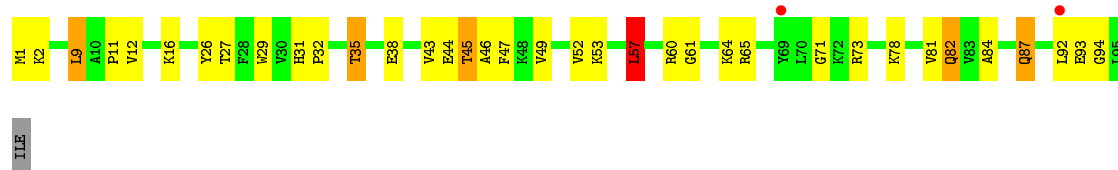


- Molecule 21: 50S ribosomal protein L23

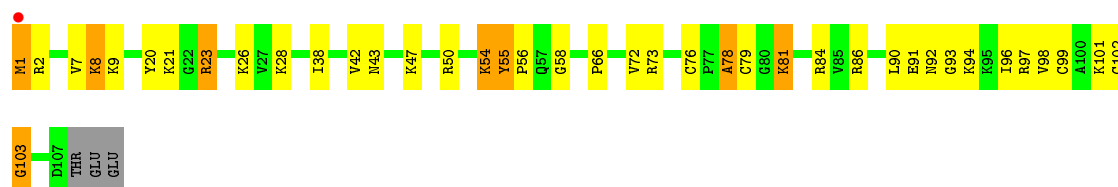


- Molecule 21: 50S ribosomal protein L23

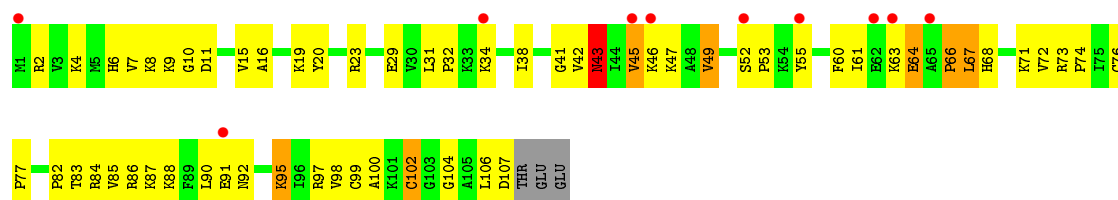
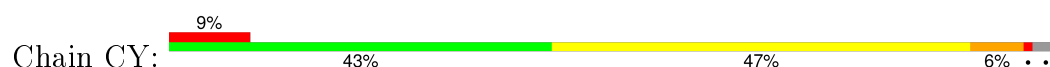




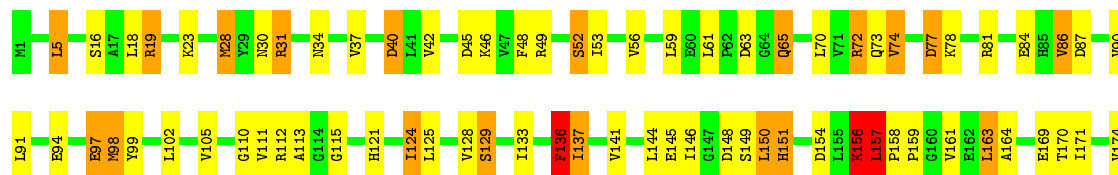
- Molecule 22: 50S ribosomal protein L24



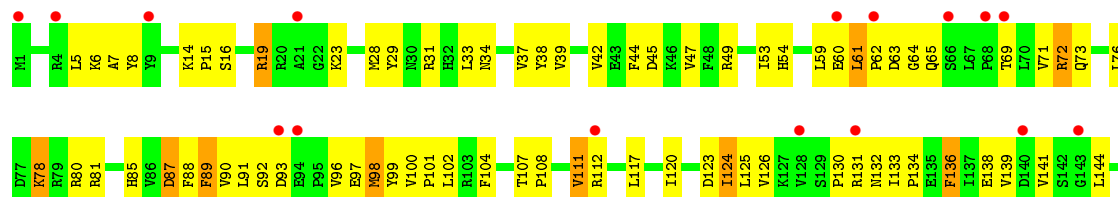
- Molecule 22: 50S ribosomal protein L24



- Molecule 23: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L25





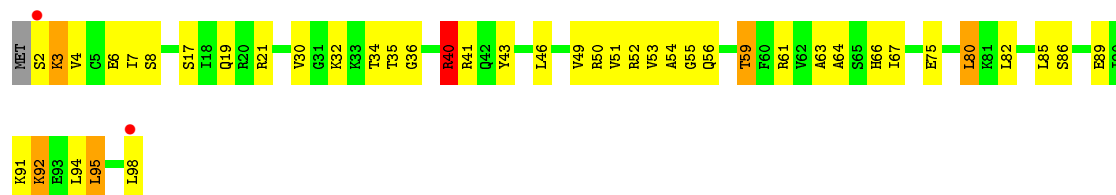
- Molecule 24: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L27



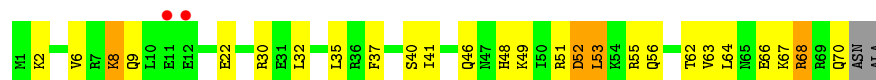
- Molecule 25: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L30

Chain A3: 



- Molecule 27: 50S ribosomal protein L30

Chain C3: 



- Molecule 28: 50S ribosomal protein L31

Chain A4: 



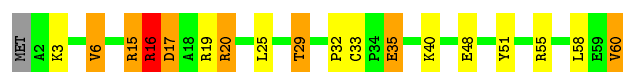
- Molecule 28: 50S ribosomal protein L31

Chain C4: 



- Molecule 29: 50S ribosomal protein L32

Chain A5: 



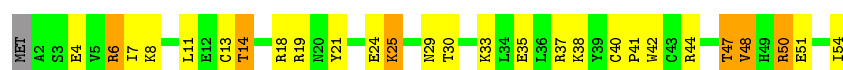
- Molecule 29: 50S ribosomal protein L32

Chain C5: 

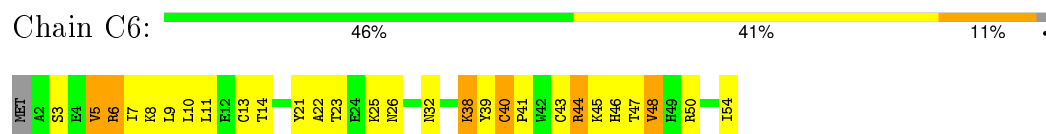


- Molecule 30: 50S ribosomal protein L33

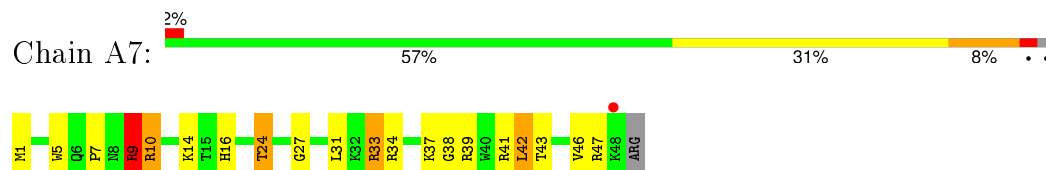
Chain A6: 



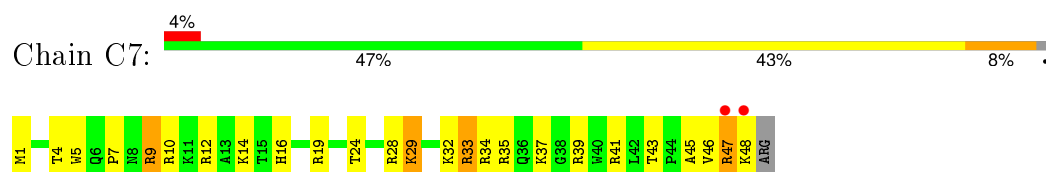
- Molecule 30: 50S ribosomal protein L33



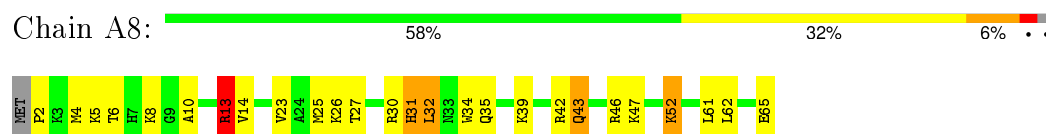
- Molecule 31: 50S ribosomal protein L34



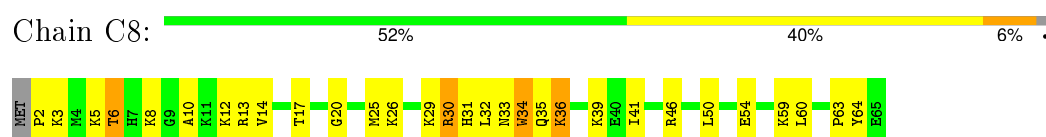
- Molecule 31: 50S ribosomal protein L34



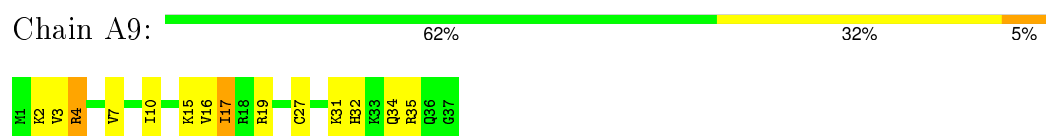
- Molecule 32: 50S ribosomal protein L35



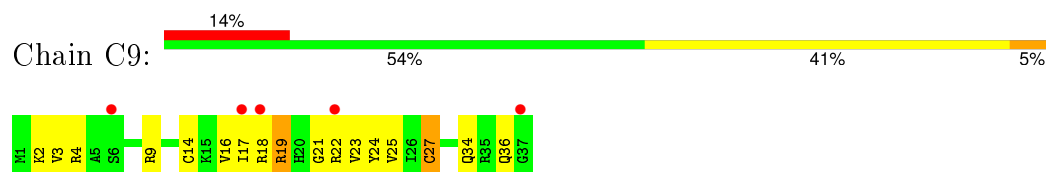
- Molecule 32: 50S ribosomal protein L35



- Molecule 33: 50S ribosomal protein L36

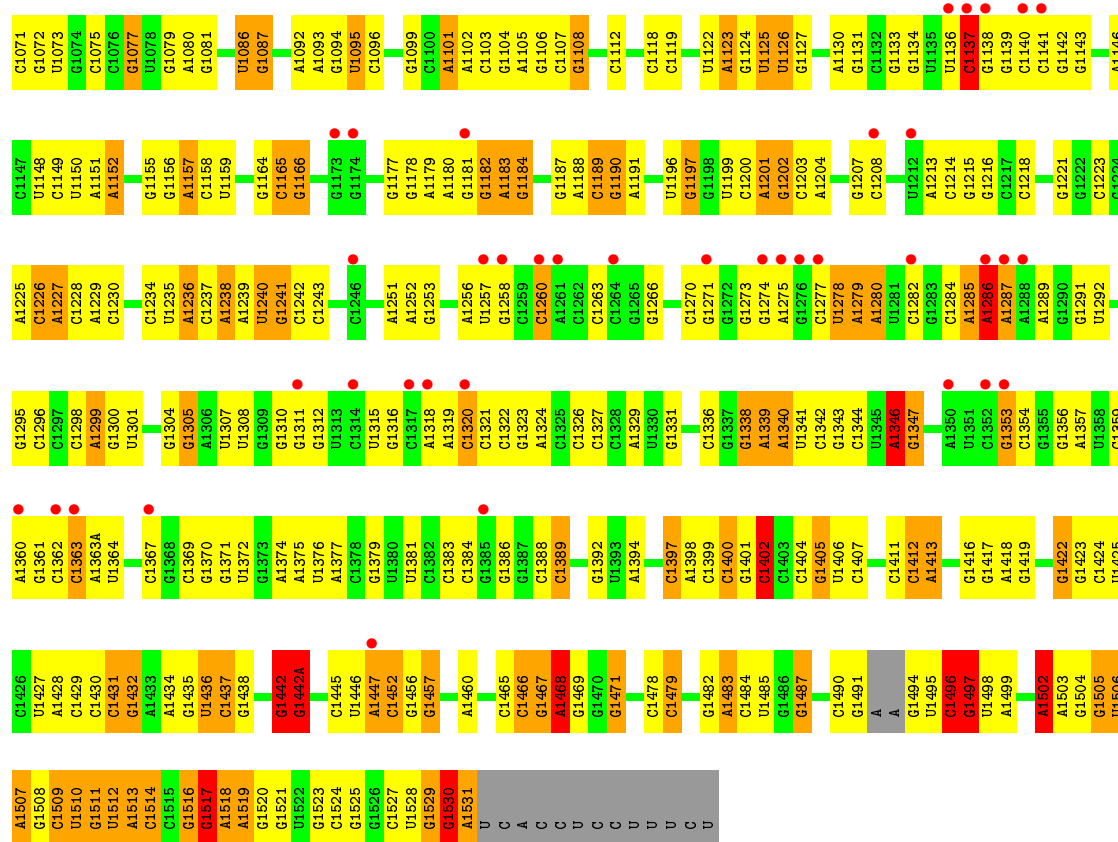


- Molecule 33: 50S ribosomal protein L36

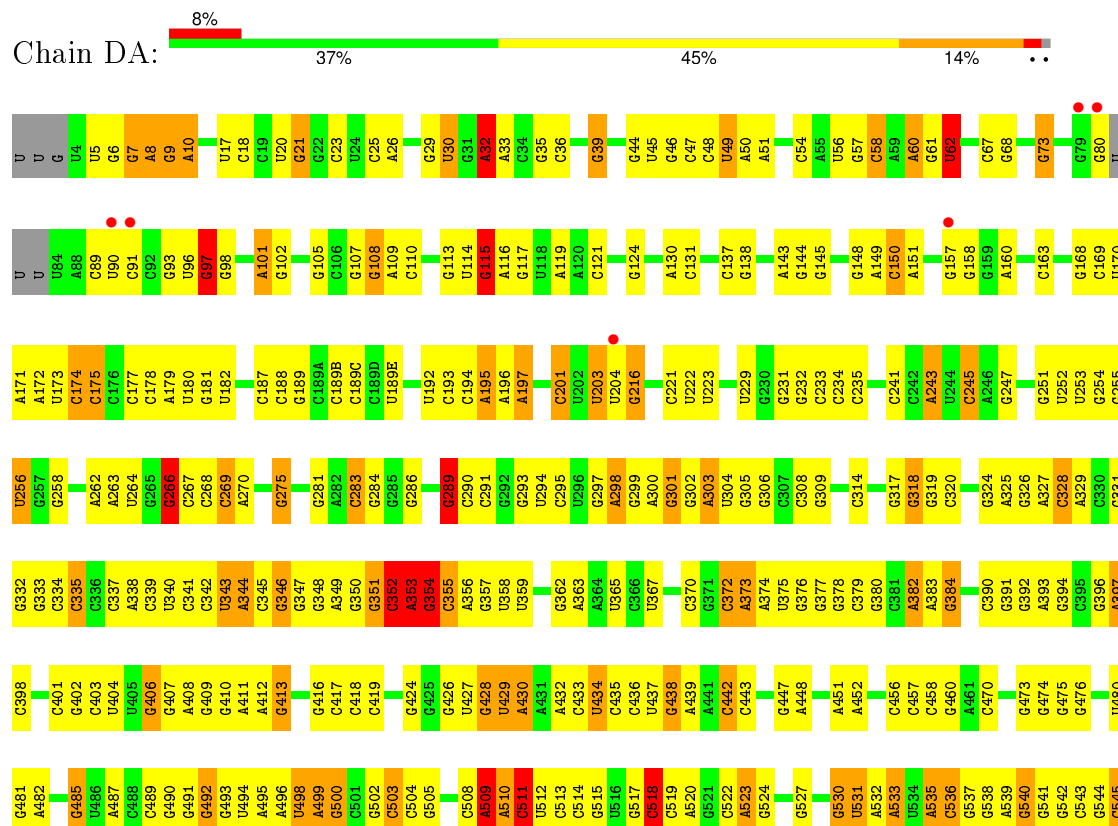


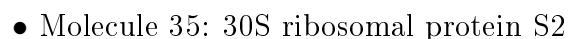
- Molecule 34: 16S Ribosomal RNA

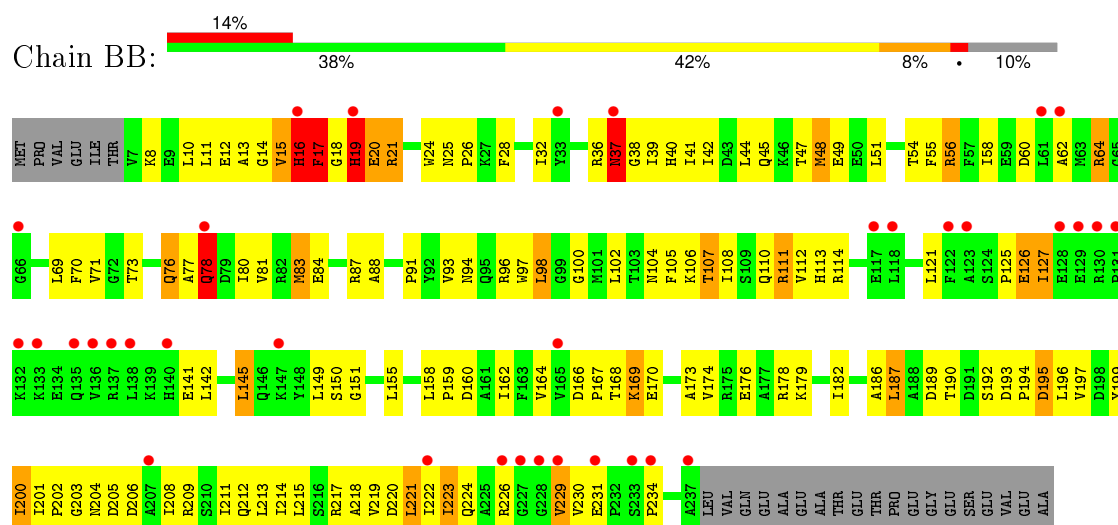




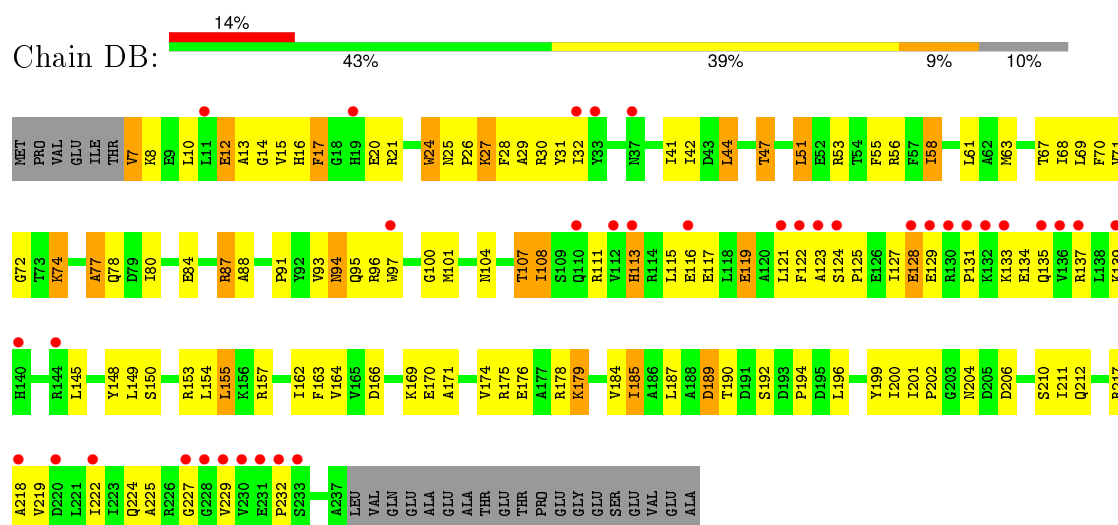
● Molecule 34: 16S Ribosomal RNA



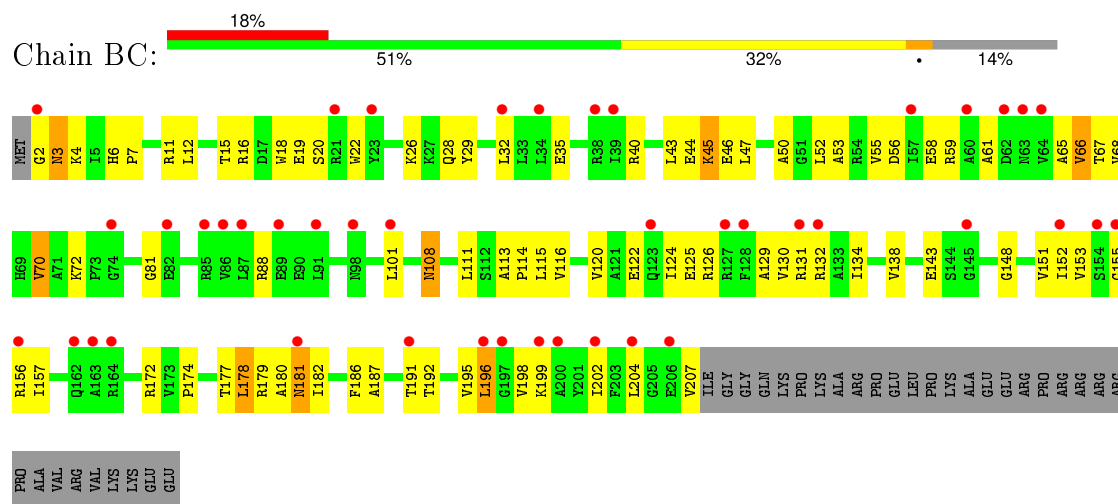




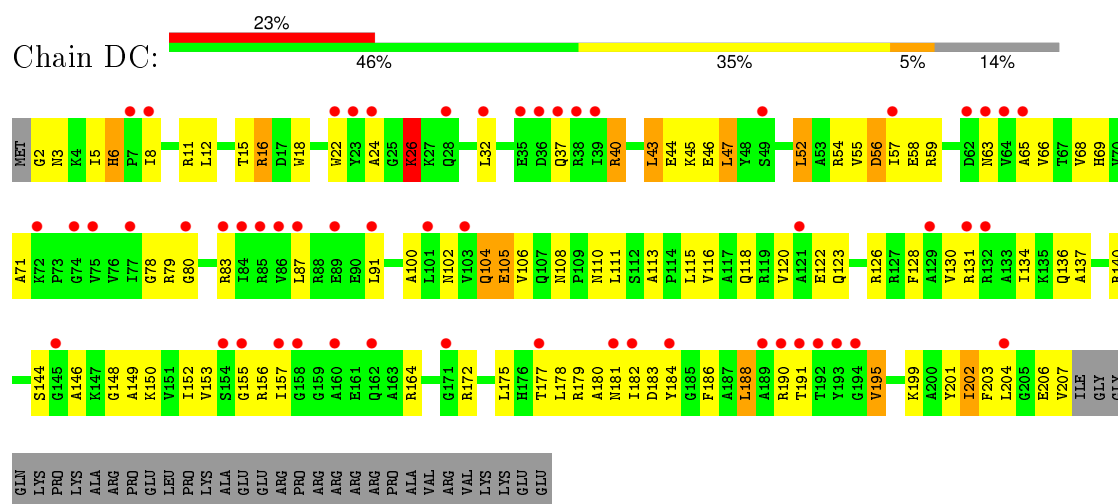
• Molecule 35: 30S ribosomal protein S2



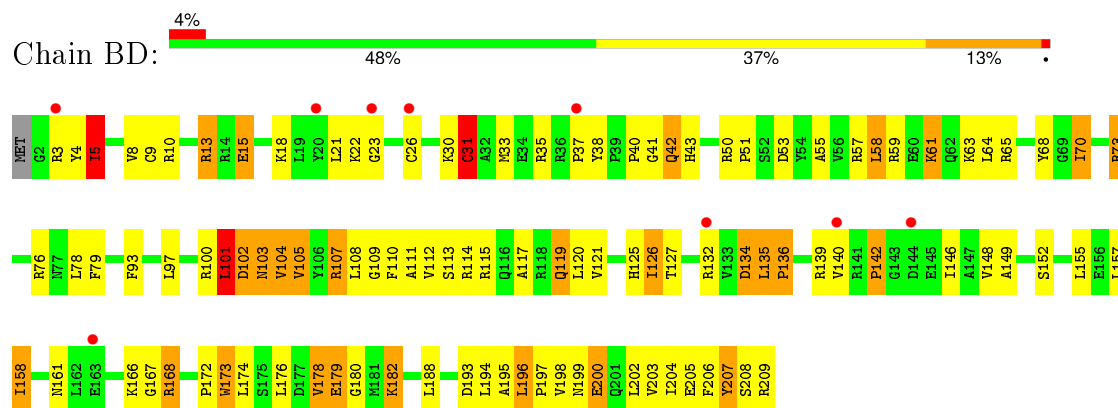
• Molecule 36: 30S ribosomal protein S3



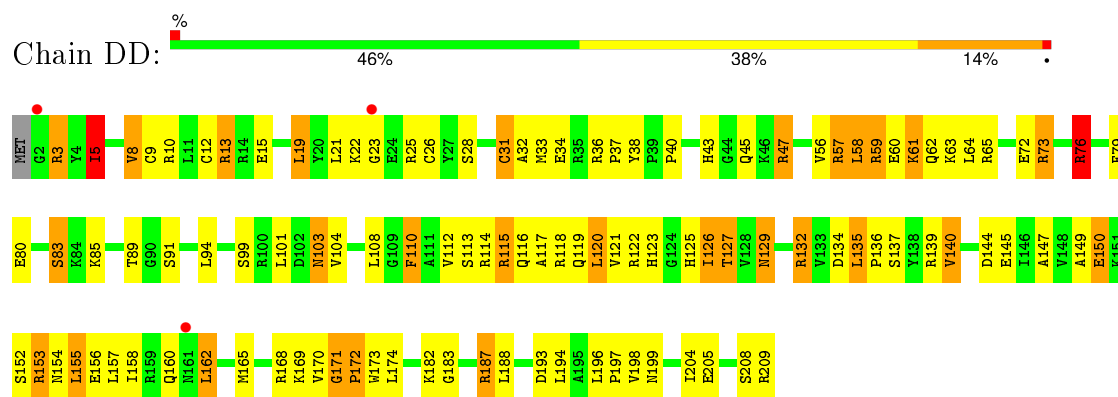
• Molecule 36: 30S ribosomal protein S3



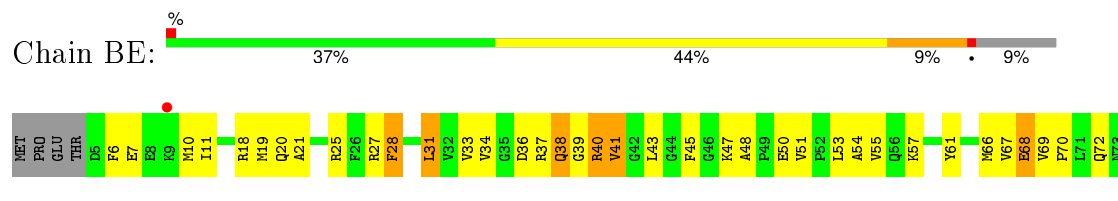
- Molecule 37: 30S ribosomal protein S4

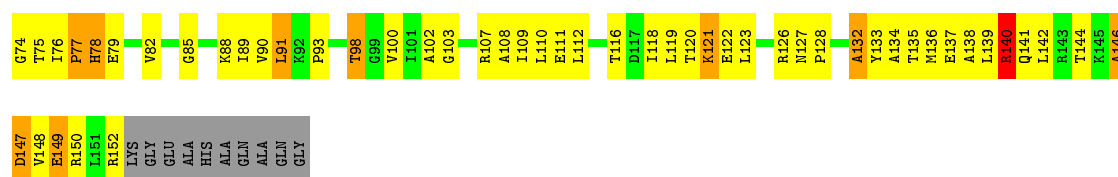


- Molecule 37: 30S ribosomal protein S4

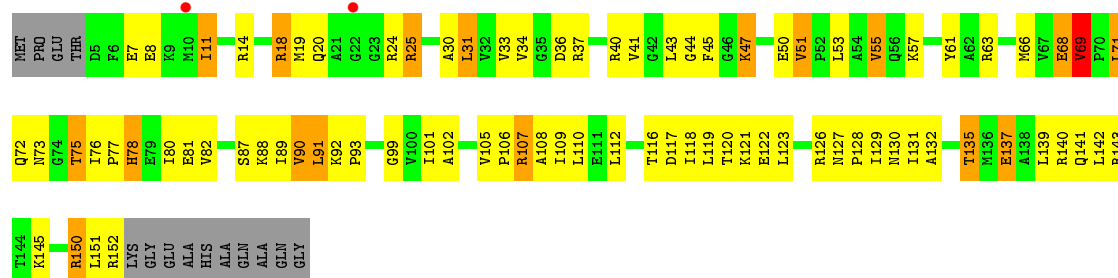


- Molecule 38: 30S ribosomal protein S5

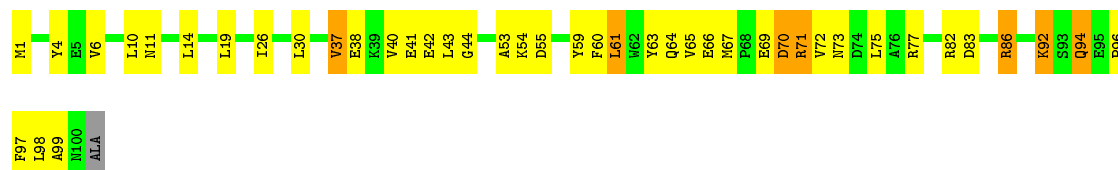




• Molecule 38: 30S ribosomal protein S5



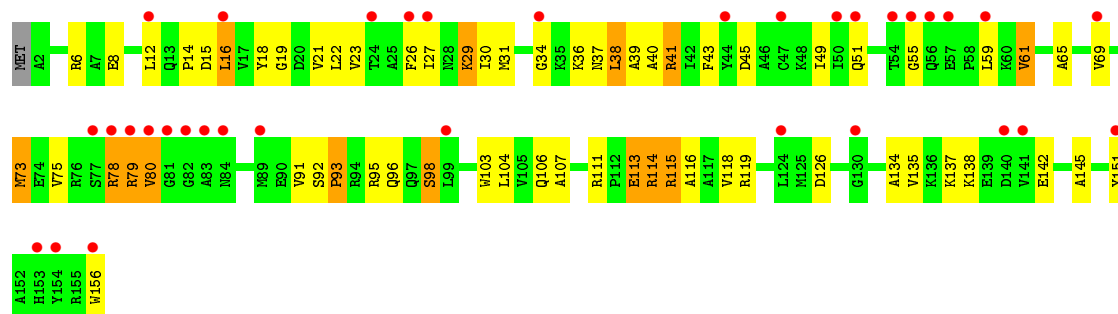
• Molecule 39: 30S ribosomal protein S6



• Molecule 39: 30S ribosomal protein S6

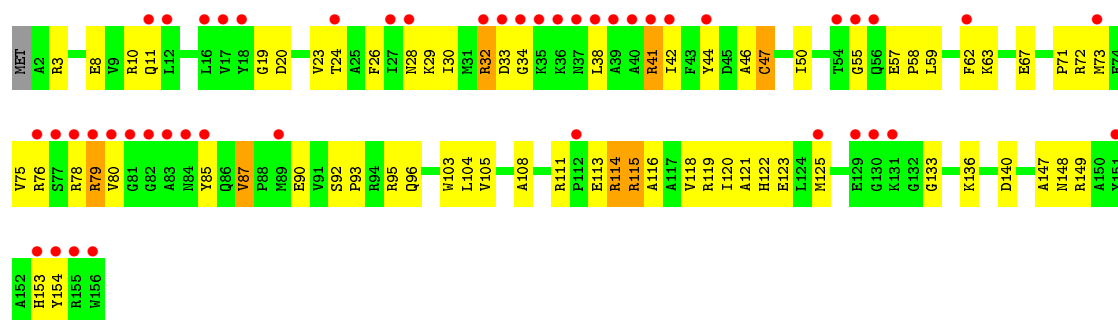


• Molecule 40: 30S ribosomal protein S7



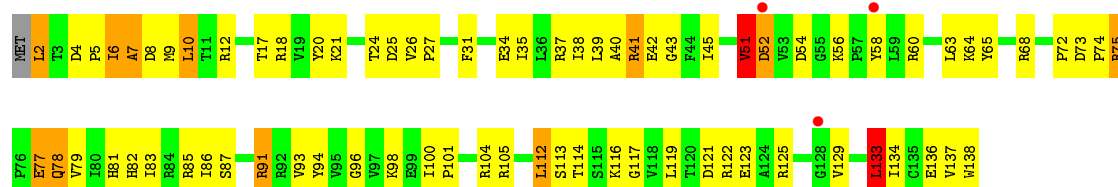
• Molecule 40: 30S ribosomal protein S7

Chain DG: 



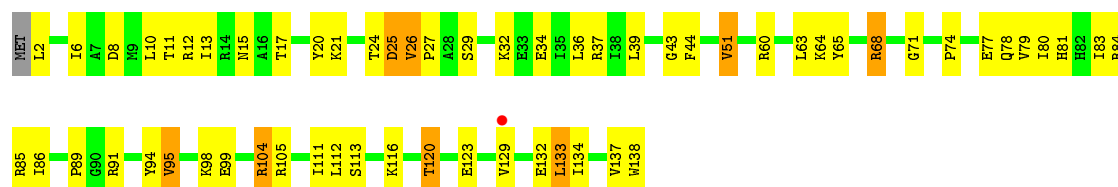
- Molecule 41: 30S ribosomal protein S8

Chain BH: 




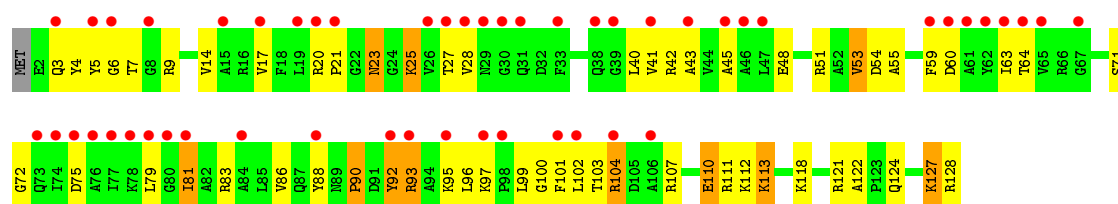
- Molecule 41: 30S ribosomal protein S8

Chain DH: 



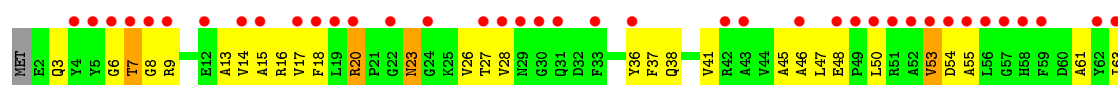
- Molecule 42: 30S ribosomal protein S9

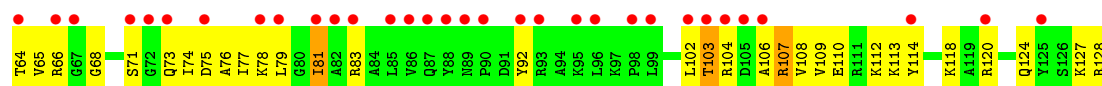
Chain BI: 



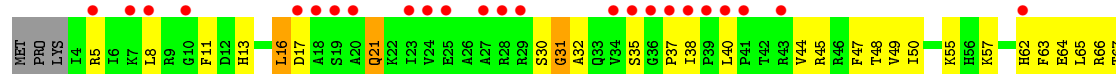
- Molecule 42: 30S ribosomal protein S9

Chain DI: 

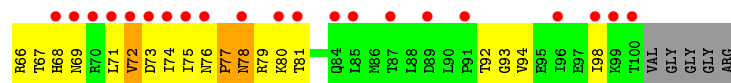
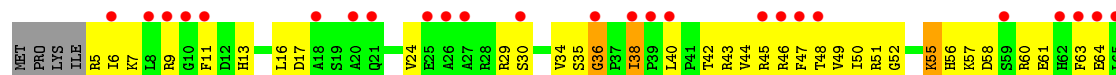




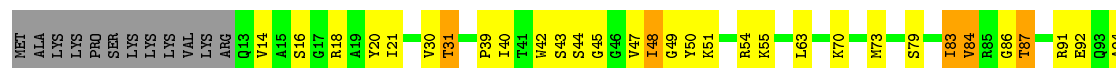
• Molecule 43: 30S ribosomal protein S10



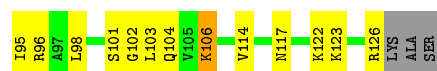
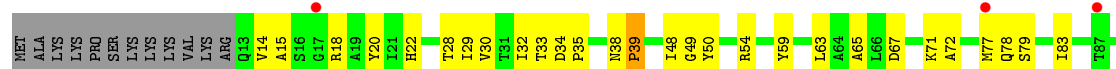
• Molecule 43: 30S ribosomal protein S10



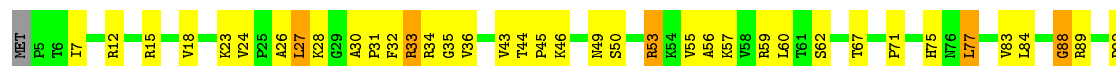
• Molecule 44: 30S ribosomal protein S11



• Molecule 44: 30S ribosomal protein S11

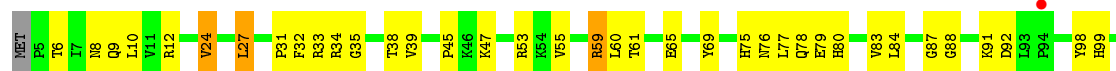


• Molecule 45: 30S ribosomal protein S12

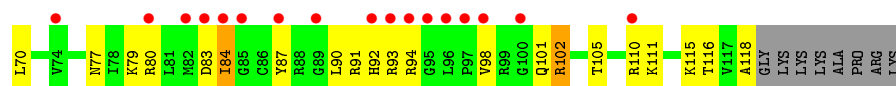
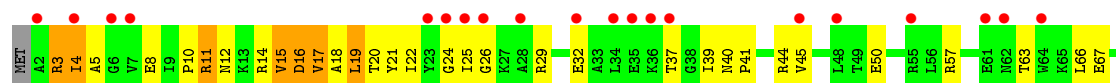




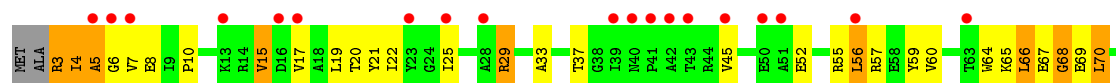
- Molecule 45: 30S ribosomal protein S12



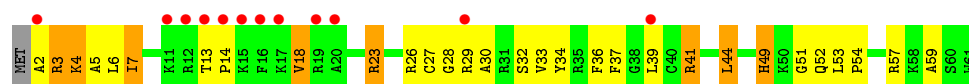
- Molecule 46: 30S ribosomal protein S13



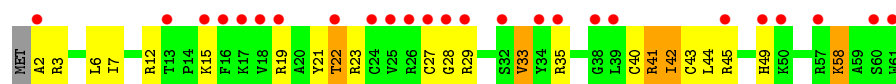
- Molecule 46: 30S ribosomal protein S13



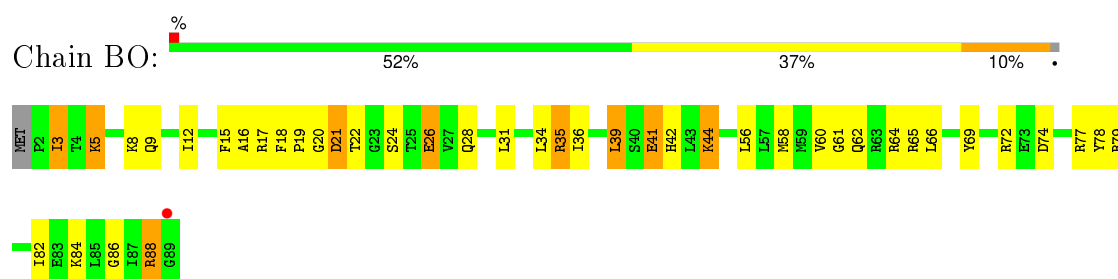
- Molecule 47: 30S ribosomal protein S14 type Z



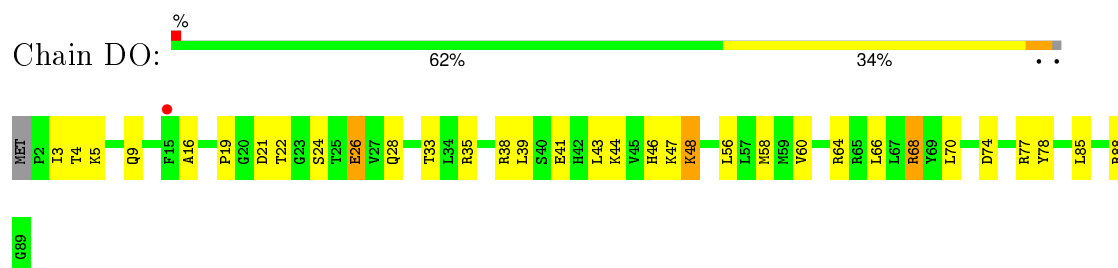
- Molecule 47: 30S ribosomal protein S14 type Z



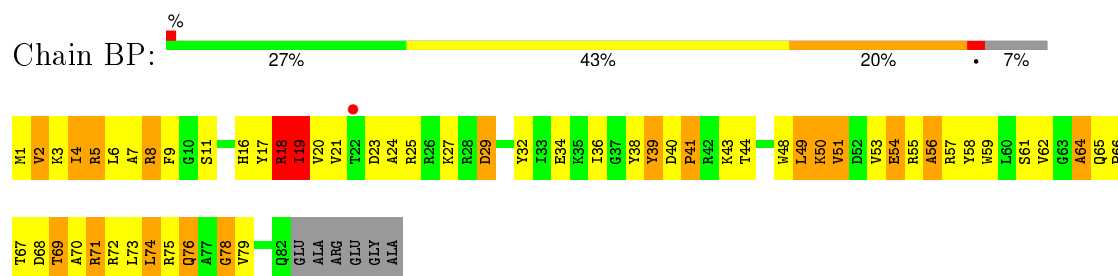
- Molecule 48: 30S ribosomal protein S15



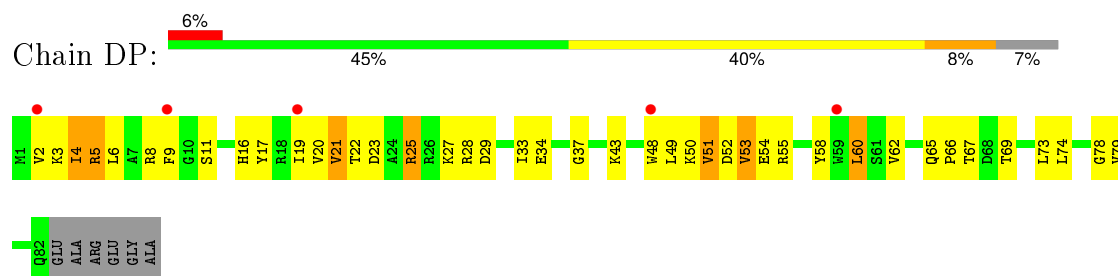
- Molecule 48: 30S ribosomal protein S15



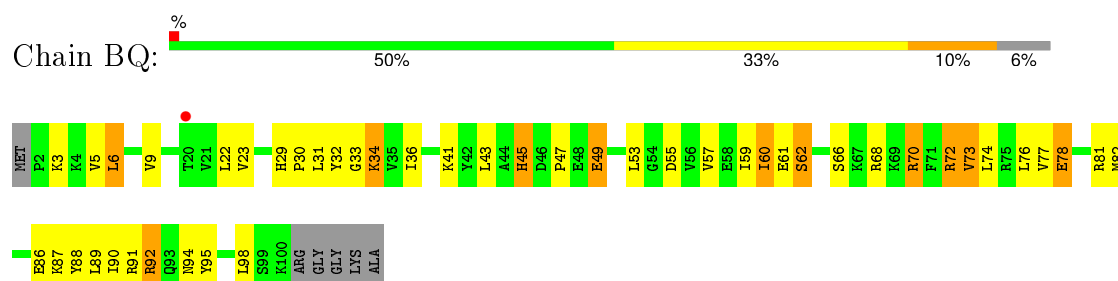
- Molecule 49: 30S ribosomal protein S16



- Molecule 49: 30S ribosomal protein S16

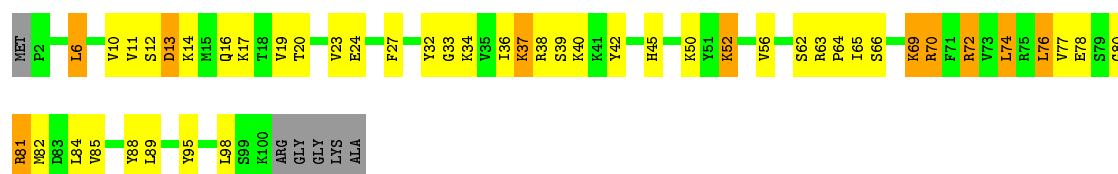


- Molecule 50: 30S ribosomal protein S17



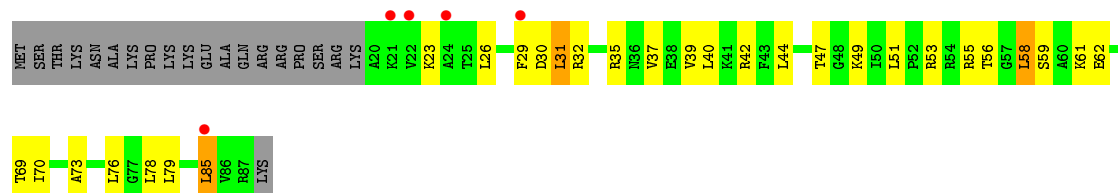
- Molecule 50: 30S ribosomal protein S17

Chain DQ: 



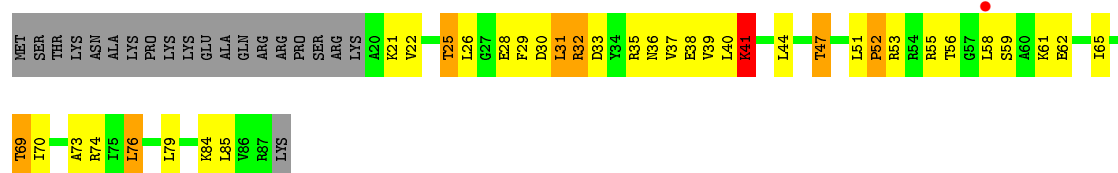
- Molecule 51: 30S ribosomal protein S18

Chain BR: 



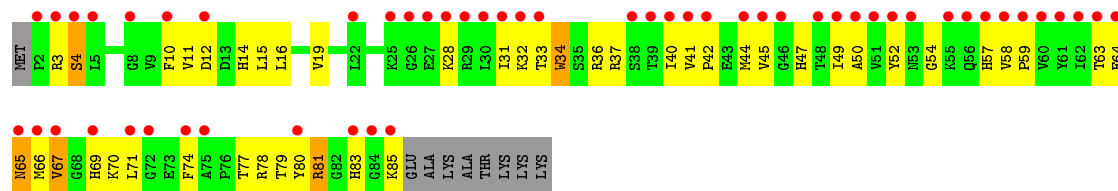
- Molecule 51: 30S ribosomal protein S18

Chain DR: 



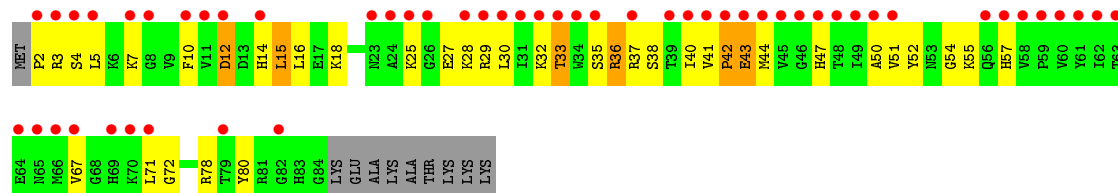
- Molecule 52: 30S ribosomal protein S19

Chain BS: 

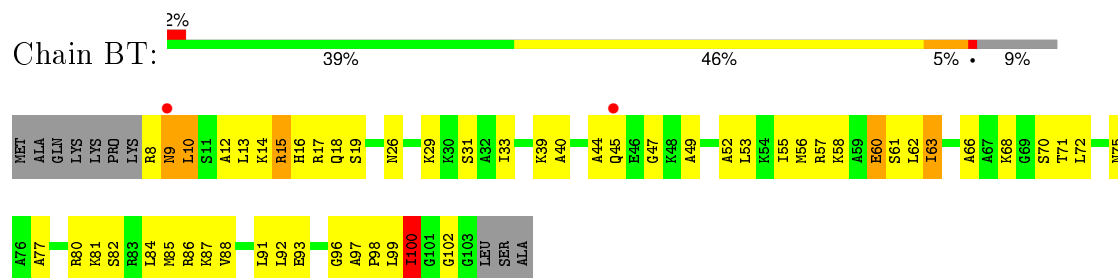


- Molecule 52: 30S ribosomal protein S19

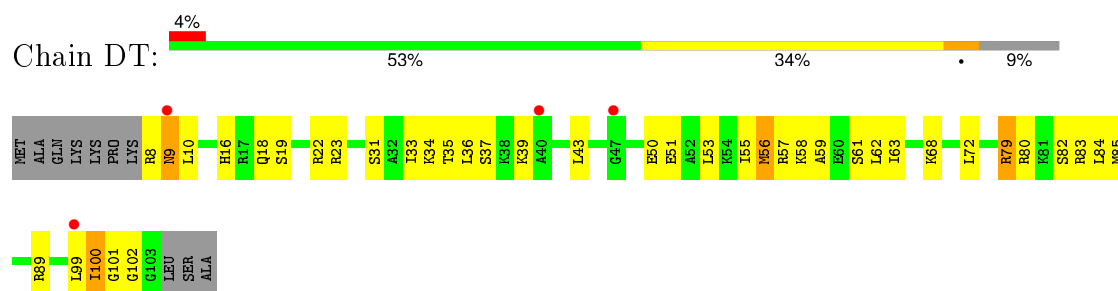
Chain DS: 



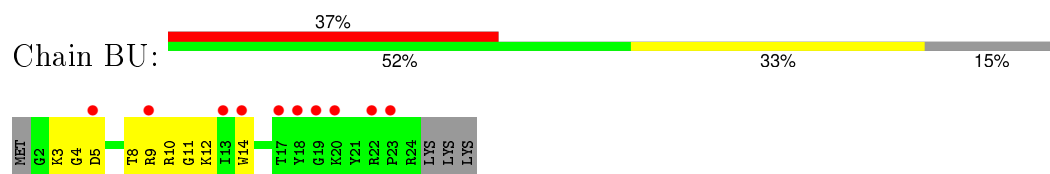
- Molecule 53: 30S ribosomal protein S20



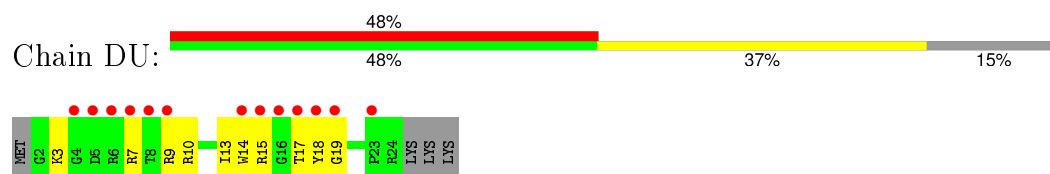
- Molecule 53: 30S ribosomal protein S20



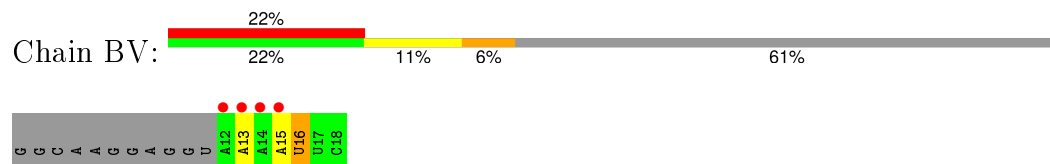
- Molecule 54: 30S ribosomal protein Thx



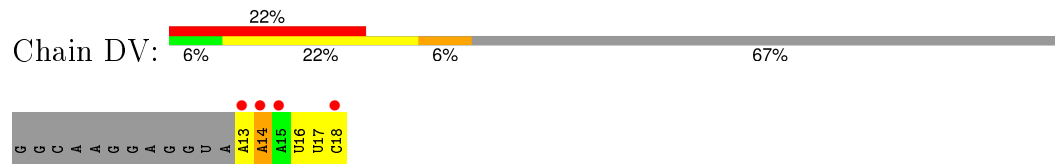
- Molecule 54: 30S ribosomal protein Thx



- Molecule 55: mRNA

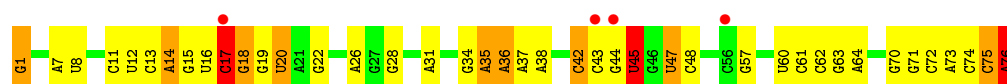


- Molecule 55: mRNA

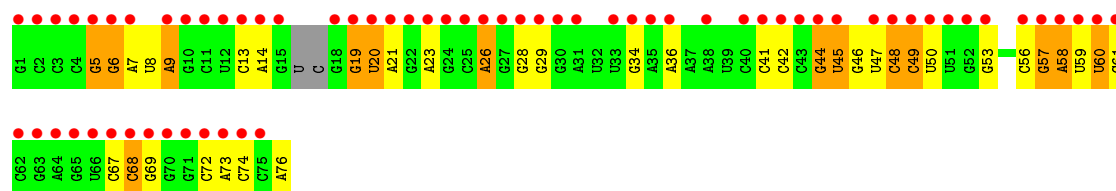


- Molecule 56: P-site tRNA

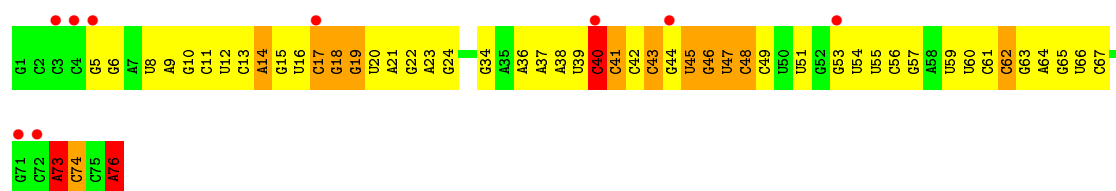




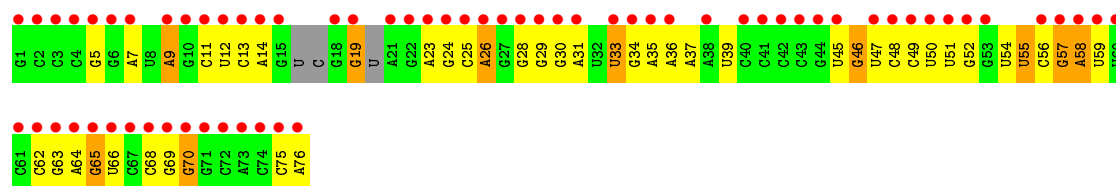
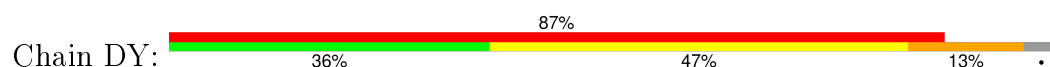
• Molecule 56: P-site tRNA



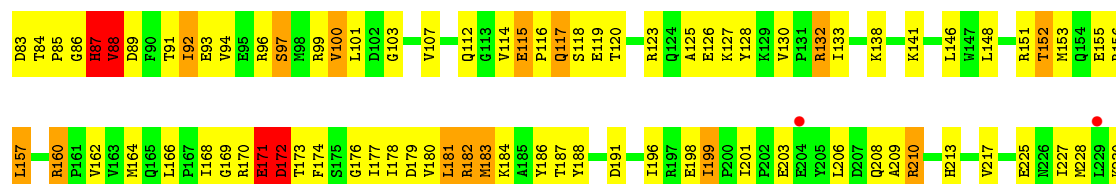
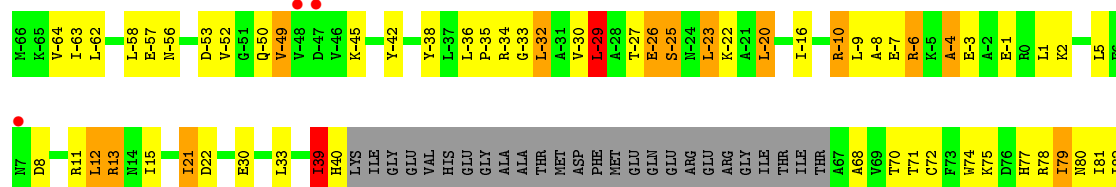
• Molecule 56: P-site tRNA

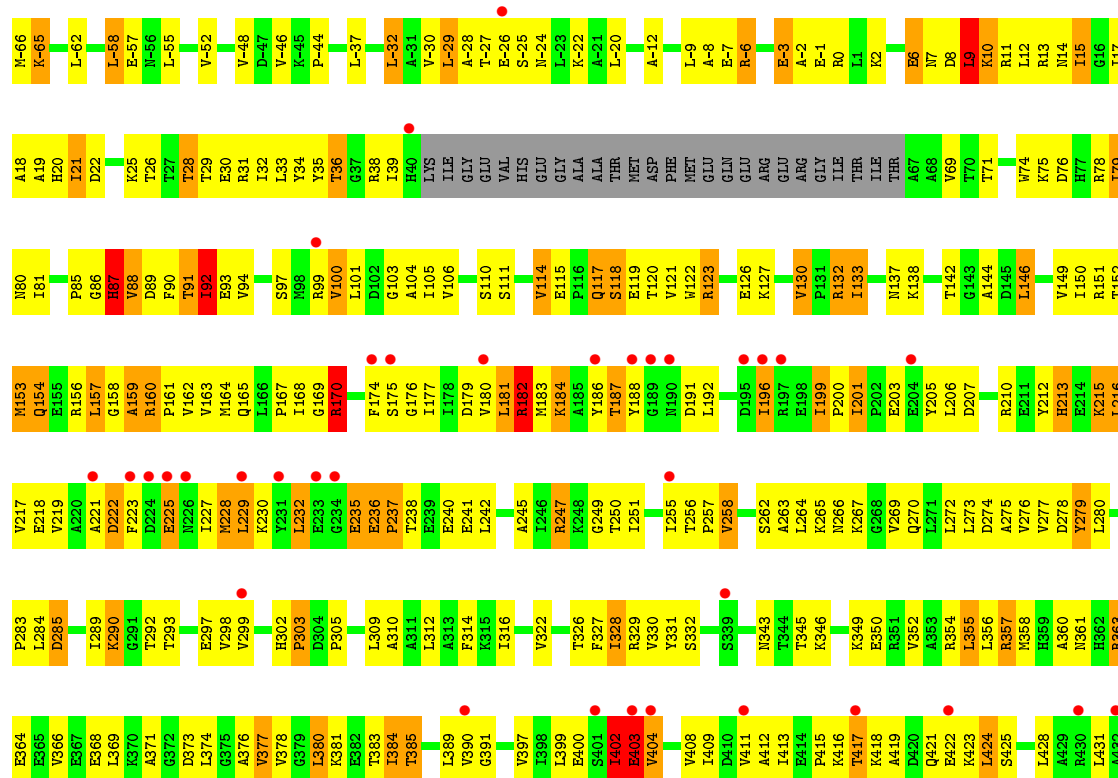


• Molecule 56: P-site tRNA



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







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.45 Å 449.00 Å 625.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.74 – 2.80 49.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.74-2.80) 99.1 (49.74-2.79)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.77 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.200 , 0.255 0.211 , 0.262	Depositor DCC
R_{free} test set	71854 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 67.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1439665 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310279	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GDP, ZN, MIA, SF4, MG, FUA, 4SU, 7MG, 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	1.51	654/68792 (1.0%)	2.24	4887/107377 (4.6%)
1	CA	1.01	71/68691 (0.1%)	1.68	1752/107219 (1.6%)
2	AB	1.21	5/2878 (0.2%)	2.01	141/4490 (3.1%)
2	CB	0.67	0/2878	1.30	18/4490 (0.4%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	1.00	4/2186 (0.2%)	1.08	8/2944 (0.3%)
4	CD	0.76	0/2192	0.92	2/2951 (0.1%)
5	AE	1.03	5/1592 (0.3%)	1.08	4/2149 (0.2%)
5	CE	0.68	0/1592	0.85	1/2149 (0.0%)
6	AF	0.96	2/1619 (0.1%)	1.07	3/2193 (0.1%)
6	CF	0.64	0/1615	0.85	1/2188 (0.0%)
7	AG	0.55	0/1450	0.77	0/1959
7	CG	0.40	0/1449	0.63	0/1958
8	AH	0.84	0/1356	0.96	3/1834 (0.2%)
8	CH	0.42	0/1356	0.64	0/1834
9	AK	0.42	0/640	0.76	1/889 (0.1%)
9	CK	0.29	0/640	0.62	0/889
10	AL	0.34	0/1044	0.58	0/1416
10	CL	0.31	0/1044	0.53	0/1416
11	AN	1.06	2/1144 (0.2%)	1.09	3/1543 (0.2%)
11	CN	0.55	0/1144	0.76	0/1543
12	AO	1.00	0/943	1.09	2/1269 (0.2%)
12	CO	0.71	0/943	0.82	0/1269
13	AP	0.89	0/1156	1.08	9/1537 (0.6%)
13	CP	0.58	0/1152	0.86	1/1533 (0.1%)
14	AQ	0.98	0/1143	1.05	4/1527 (0.3%)
14	CQ	0.62	0/1143	0.77	0/1527
15	AR	0.98	0/982	1.15	4/1312 (0.3%)
15	CR	0.62	0/982	0.95	2/1312 (0.2%)
16	AS	0.76	0/887	0.96	0/1180
16	CS	0.56	0/880	0.83	2/1172 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.87	0/1105	1.04	2/1477 (0.1%)
17	CT	0.68	0/1097	0.89	0/1468
18	AU	1.18	2/977 (0.2%)	1.19	5/1301 (0.4%)
18	CU	0.67	0/977	0.78	0/1301
19	AV	1.02	1/782 (0.1%)	1.09	1/1049 (0.1%)
19	CV	0.54	0/782	0.74	0/1049
20	AW	1.21	1/897 (0.1%)	1.19	3/1205 (0.2%)
20	CW	0.77	0/897	0.91	0/1205
21	AX	0.98	1/764 (0.1%)	0.99	2/1025 (0.2%)
21	CX	0.70	0/764	0.78	1/1025 (0.1%)
22	AY	0.92	0/819	1.00	1/1095 (0.1%)
22	CY	0.62	0/819	0.77	0/1095
23	AZ	0.77	0/1483	1.00	3/2017 (0.1%)
23	CZ	0.47	0/1483	0.71	0/2017
24	A0	0.97	0/662	1.03	0/881
24	C0	0.60	0/662	0.77	0/881
25	A1	0.94	0/762	1.04	3/1014 (0.3%)
25	C1	0.70	0/762	0.86	0/1014
26	A2	0.88	0/590	0.91	0/781
26	C2	0.60	0/590	0.75	0/781
27	A3	0.99	0/474	1.09	2/635 (0.3%)
27	C3	0.51	0/469	0.78	0/630
28	A4	0.47	0/571	0.74	0/768
28	C4	0.35	0/545	0.59	0/737
29	A5	1.22	3/469 (0.6%)	1.22	4/635 (0.6%)
29	C5	0.75	0/469	0.89	2/635 (0.3%)
30	A6	0.89	0/460	1.02	1/613 (0.2%)
30	C6	0.67	0/456	0.76	0/608
31	A7	1.11	0/426	1.21	4/561 (0.7%)
31	C7	0.86	0/426	1.03	2/561 (0.4%)
32	A8	1.00	0/525	1.04	3/691 (0.4%)
32	C8	0.72	0/525	0.85	0/691
33	A9	1.09	0/310	1.04	0/407
33	C9	0.57	0/310	0.70	0/407
34	BA	0.79	7/35976 (0.0%)	1.44	496/56145 (0.9%)
34	DA	0.70	2/36119 (0.0%)	1.31	266/56370 (0.5%)
35	BB	0.47	0/1881	0.72	0/2542
35	DB	0.39	0/1860	0.64	0/2518
36	BC	0.38	0/1576	0.57	0/2130
36	DC	0.34	0/1568	0.54	0/2122
37	BD	0.52	0/1689	0.77	0/2267
37	DD	0.51	0/1708	0.77	1/2289 (0.0%)
38	BE	0.62	0/1145	0.84	0/1543

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DE	0.54	0/1149	0.78	1/1548 (0.1%)
39	BF	0.54	0/825	0.75	0/1118
39	DF	0.54	0/833	0.77	2/1128 (0.2%)
40	BG	0.40	0/1250	0.60	0/1679
40	DG	0.33	0/1254	0.52	0/1683
41	BH	0.58	0/1108	0.80	1/1494 (0.1%)
41	DH	0.48	0/1108	0.70	0/1494
42	BI	0.38	0/1005	0.61	0/1350
42	DI	0.33	0/997	0.58	0/1343
43	BJ	0.38	0/722	0.59	0/982
43	DJ	0.34	0/727	0.57	0/988
44	BK	0.55	0/848	0.75	0/1149
44	DK	0.51	0/848	0.70	0/1149
45	BL	0.74	0/946	0.88	1/1274 (0.1%)
45	DL	0.58	0/946	0.81	0/1274
46	BM	0.39	0/933	0.62	0/1253
46	DM	0.34	0/961	0.55	0/1291
47	BN	0.39	0/501	0.68	1/664 (0.2%)
47	DN	0.35	0/501	0.56	0/664
48	BO	0.56	0/739	0.81	0/985
48	DO	0.53	0/739	0.72	0/985
49	BP	0.55	0/697	0.79	1/939 (0.1%)
49	DP	0.53	0/693	0.71	0/935
50	BQ	0.63	0/836	0.78	0/1117
50	DQ	0.57	0/836	0.73	0/1117
51	BR	0.55	0/560	0.80	1/746 (0.1%)
51	DR	0.51	0/560	0.71	0/746
52	BS	0.35	0/676	0.57	0/911
52	DS	0.31	0/661	0.61	0/893
53	BT	0.49	0/730	0.74	0/965
53	DT	0.49	0/733	0.71	0/969
54	BU	0.38	0/203	0.65	0/266
54	DU	0.31	0/203	0.57	0/266
55	BV	0.71	0/165	1.15	1/254 (0.4%)
55	DV	0.60	0/137	1.05	0/211
56	BW	0.89	1/1650 (0.1%)	1.64	41/2569 (1.6%)
56	BY	0.42	0/1602	0.95	1/2493 (0.0%)
56	DW	0.70	0/1650	1.36	20/2569 (0.8%)
56	DY	0.35	0/1579	0.86	0/2455
57	BZ	0.58	0/5792	0.81	4/7844 (0.1%)
57	DZ	0.49	0/5792	0.72	4/7844 (0.1%)
All	All	0.99	761/330005 (0.2%)	1.56	7729/491779 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	CA	0	1
17	CT	0	1
19	AV	0	1
21	AX	0	1
21	CX	0	1
23	AZ	0	1
24	A0	0	1
25	A1	0	1
28	A4	0	1
53	BT	0	1
53	DT	0	1
57	BZ	0	1
57	DZ	0	3
All	All	0	15

The worst 5 of 761 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1067	A	N9-C4	-18.69	1.26	1.37
1	AA	1188	A	N9-C4	-16.21	1.28	1.37
1	AA	990	A	N9-C4	-15.62	1.28	1.37
1	AA	354	A	N9-C4	-13.34	1.29	1.37
1	AA	1988	A	N9-C4	-12.57	1.30	1.37

The worst 5 of 7729 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1067	A	C2-N3-C4	-25.69	97.76	110.60
1	AA	1701	A	O5'-P-OP2	-25.21	80.44	110.70
1	AA	553	A	N1-C6-N6	25.19	133.71	118.60
1	AA	990	A	C5-N7-C8	-25.10	91.35	103.90
1	AA	553	A	C5-N7-C8	-23.43	92.19	103.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	A0	11	ARG	Peptide

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Mol	Chain	Res	Type	Group
25	A1	2	SER	Peptide
19	AV	54	GLY	Peptide
21	AX	93	GLU	Peptide
23	AZ	176	PRO	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	61426	0	30937	933	0
1	CA	61337	0	30928	1107	0
2	AB	2573	0	1306	39	0
2	CB	2573	0	1306	49	0
3	AC	1063	0	1089	162	0
3	CC	1063	0	1091	203	0
4	AD	2136	0	2218	72	0
4	CD	2142	0	2229	72	0
5	AE	1559	0	1618	46	0
5	CE	1559	0	1618	92	0
6	AF	1584	0	1625	58	0
6	CF	1580	0	1619	68	0
7	AG	1425	0	1443	69	0
7	CG	1424	0	1434	59	0
8	AH	1330	0	1407	40	0
8	CH	1330	0	1407	51	0
9	AK	641	0	309	13	0
9	CK	641	0	309	13	0
10	AL	1025	0	1066	54	0
10	CL	1025	0	1066	50	0
11	AN	1117	0	1184	32	0
11	CN	1117	0	1184	45	0
12	AO	933	0	996	32	0
12	CO	933	0	996	38	0
13	AP	1139	0	1223	48	0
13	CP	1135	0	1212	46	0
14	AQ	1122	0	1179	35	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CR	968	0	1033	44	0
16	AS	877	0	938	30	0
16	CS	870	0	923	43	0
17	AT	1091	0	1151	35	0
17	CT	1083	0	1136	55	0
18	AU	959	0	1019	30	0
18	CU	959	0	1018	34	0
19	AV	771	0	829	24	0
19	CV	771	0	830	16	0
20	AW	886	0	940	26	0
20	CW	886	0	940	31	0
21	AX	750	0	814	27	0
21	CX	750	0	814	27	0
22	AY	806	0	881	23	0
22	CY	806	0	881	39	0
23	AZ	1451	0	1457	56	0
23	CZ	1451	0	1457	66	0
24	A0	653	0	674	29	0
24	C0	653	0	674	22	0
25	A1	755	0	826	24	0
25	C1	755	0	826	23	0
26	A2	588	0	643	13	0
26	C2	588	0	643	19	0
27	A3	469	0	518	13	0
27	C3	464	0	514	11	0
28	A4	558	0	547	24	0
28	C4	532	0	505	14	0
29	A5	455	0	465	18	0
29	C5	455	0	465	20	0
30	A6	453	0	473	18	0
30	C6	449	0	469	13	0
31	A7	418	0	467	17	0
31	C7	418	0	467	17	0
32	A8	517	0	582	22	0
32	C8	517	0	582	28	0
33	A9	307	0	335	10	0
33	C9	307	0	335	14	0
34	BA	32141	0	16224	675	0
34	DA	32268	0	16287	690	0
35	BB	1846	0	1867	102	0
35	DB	1825	0	1828	82	0
36	BC	1552	0	1546	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DC	1544	0	1524	63	0
37	BD	1659	0	1678	93	0
37	DD	1678	0	1720	90	0
38	BE	1129	0	1185	65	0
38	DE	1133	0	1191	64	0
39	BF	812	0	804	27	0
39	DF	820	0	814	22	0
40	BG	1231	0	1238	42	0
40	DG	1235	0	1249	32	0
41	BH	1088	0	1126	62	0
41	DH	1088	0	1126	36	0
42	BI	986	0	995	41	0
42	DI	978	0	966	40	0
43	BJ	709	0	650	37	0
43	DJ	714	0	672	47	0
44	BK	833	0	836	31	0
44	DK	833	0	836	25	0
45	BL	930	0	980	37	0
45	DL	930	0	980	44	0
46	BM	923	0	970	29	0
46	DM	950	0	988	46	0
47	BN	492	0	529	29	0
47	DN	492	0	531	20	0
48	BO	728	0	760	29	0
48	DO	728	0	760	18	0
49	BP	681	0	697	51	0
49	DP	677	0	686	33	0
50	BQ	823	0	891	26	0
50	DQ	823	0	891	35	0
51	BR	555	0	618	22	0
51	DR	555	0	618	25	0
52	BS	661	0	675	34	0
52	DS	646	0	644	30	0
53	BT	728	0	798	35	0
53	DT	731	0	807	24	0
54	BU	199	0	208	5	0
54	DU	199	0	208	8	0
55	BV	148	0	76	5	0
55	DV	123	0	66	5	0
56	BW	1631	0	839	22	0
56	BY	1581	0	805	24	0
56	DW	1631	0	839	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DY	1561	0	796	40	0
57	BZ	5690	0	5783	272	0
57	DZ	5690	0	5783	322	0
58	A0	3	0	0	0	0
58	A2	2	0	0	0	0
58	A4	1	0	0	0	0
58	A5	1	0	0	0	0
58	A6	1	0	0	0	0
58	A7	3	0	0	0	0
58	A8	2	0	0	0	0
58	A9	1	0	0	0	0
58	AA	835	0	0	0	0
58	AB	23	0	0	0	0
58	AD	10	0	0	0	0
58	AE	4	0	0	0	0
58	AF	5	0	0	0	0
58	AG	2	0	0	0	0
58	AH	2	0	0	0	0
58	AN	3	0	0	0	0
58	AO	1	0	0	0	0
58	AP	2	0	0	0	0
58	AQ	3	0	0	0	0
58	AR	1	0	0	0	0
58	AU	3	0	0	0	0
58	AV	3	0	0	0	0
58	AW	4	0	0	0	0
58	AX	1	0	0	0	0
58	AY	1	0	0	0	0
58	AZ	2	0	0	0	0
58	BA	211	0	0	0	0
58	BB	1	0	0	0	0
58	BD	1	0	0	0	0
58	BE	1	0	0	0	0
58	BF	1	0	0	0	0
58	BK	1	0	0	0	0
58	BL	2	0	0	0	0
58	BM	2	0	0	0	0
58	BN	1	0	0	0	0
58	BT	1	0	0	0	0
58	BV	1	0	0	0	0
58	BW	3	0	0	0	0
58	BZ	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	C3	1	0	0	0	0
58	C5	1	0	0	0	0
58	C7	1	0	0	0	0
58	C8	1	0	0	0	0
58	CA	664	0	0	0	0
58	CB	13	0	0	0	0
58	CD	3	0	0	0	0
58	CE	6	0	0	0	0
58	CF	5	0	0	0	0
58	CG	1	0	0	0	0
58	CN	1	0	0	0	0
58	CO	2	0	0	0	0
58	CP	3	0	0	0	0
58	CQ	5	0	0	0	0
58	CR	1	0	0	0	0
58	CU	1	0	0	0	0
58	CV	2	0	0	0	0
58	CW	1	0	0	0	0
58	CY	1	0	0	0	0
58	DA	168	0	0	0	0
58	DD	1	0	0	0	0
58	DE	2	0	0	0	0
58	DF	1	0	0	0	0
58	DJ	1	0	0	0	0
58	DK	1	0	0	0	0
58	DT	1	0	0	0	0
58	DW	3	0	0	0	0
58	DZ	2	0	0	0	0
59	A4	1	0	0	0	0
59	A5	1	0	0	0	0
59	A6	1	0	0	0	0
59	A9	1	0	0	0	0
59	AY	1	0	0	0	0
59	BN	1	0	0	0	0
59	C4	1	0	0	0	0
59	C5	1	0	0	0	0
59	C6	1	0	0	0	0
59	C9	1	0	0	0	0
59	CY	1	0	0	0	0
59	DN	1	0	0	0	0
60	BD	8	0	0	1	0
60	DD	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BZ	37	0	47	11	0
61	DZ	37	0	47	17	0
62	BZ	28	0	12	5	0
62	DZ	28	0	12	9	0
63	A0	7	0	0	1	0
63	A1	3	0	0	0	0
63	A3	1	0	0	0	0
63	A5	2	0	0	0	0
63	A6	1	0	0	0	0
63	A7	3	0	0	2	0
63	A8	11	0	0	2	0
63	AA	1408	0	0	60	0
63	AB	36	0	0	1	0
63	AD	15	0	0	1	0
63	AE	19	0	0	5	0
63	AF	8	0	0	1	0
63	AG	3	0	0	1	0
63	AH	1	0	0	0	0
63	AN	2	0	0	1	0
63	AO	3	0	0	0	0
63	AP	15	0	0	0	0
63	AQ	3	0	0	0	0
63	AR	3	0	0	0	0
63	AS	1	0	0	0	0
63	AT	2	0	0	0	0
63	AU	6	0	0	0	0
63	AW	1	0	0	0	0
63	AX	2	0	0	0	0
63	AZ	1	0	0	0	0
63	BA	205	0	0	13	0
63	BD	3	0	0	0	0
63	BE	3	0	0	0	0
63	BJ	1	0	0	0	0
63	BL	2	0	0	0	0
63	BM	1	0	0	0	0
63	BO	1	0	0	0	0
63	BV	2	0	0	0	0
63	BW	1	0	0	0	0
63	BZ	3	0	0	0	0
63	C0	5	0	0	0	0
63	C1	3	0	0	0	0
63	C3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	C5	1	0	0	0	0
63	C7	3	0	0	0	0
63	C8	3	0	0	1	0
63	CA	981	0	0	65	0
63	CB	9	0	0	0	0
63	CD	15	0	0	0	0
63	CE	9	0	0	1	0
63	CF	6	0	0	0	0
63	CP	13	0	0	3	0
63	CQ	1	0	0	0	0
63	CT	3	0	0	0	0
63	CU	4	0	0	1	0
63	CV	1	0	0	0	0
63	CW	1	0	0	0	0
63	CX	1	0	0	0	0
63	CY	1	0	0	0	0
63	DA	153	0	0	11	0
63	DE	2	0	0	0	0
63	DH	1	0	0	1	0
63	DJ	1	0	0	0	0
63	DK	2	0	0	0	0
63	DL	1	0	0	0	0
63	DP	1	0	0	0	0
63	DT	1	0	0	0	0
63	DY	1	0	0	0	0
63	DZ	2	0	0	0	0
All	All	310279	0	209988	7291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 7291 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:C5'	3:AC:206:LYS:CG	1.80	1.55
1:AA:1891:G:H5''	3:AC:206:LYS:CG	1.26	1.54
1:AA:1891:G:C5'	3:AC:206:LYS:HG3	1.40	1.40
1:CA:2128:C:H5''	3:CC:219:MET:CE	1.55	1.37
1:AA:2143:G:N2	3:AC:169:THR:OG1	1.57	1.36

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	20 (7%)	4 (2%)	13	40
4	CD	273/276 (99%)	242 (89%)	26 (10%)	5 (2%)	11	34
5	AE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	19	52
5	CE	202/206 (98%)	174 (86%)	19 (9%)	9 (4%)	3	10
6	AF	201/210 (96%)	187 (93%)	11 (6%)	3 (2%)	13	40
6	CF	201/210 (96%)	186 (92%)	12 (6%)	3 (2%)	13	40
7	AG	179/182 (98%)	143 (80%)	25 (14%)	11 (6%)	2	5
7	CG	179/182 (98%)	148 (83%)	20 (11%)	11 (6%)	2	5
8	AH	172/180 (96%)	150 (87%)	20 (12%)	2 (1%)	16	47
8	CH	172/180 (96%)	148 (86%)	19 (11%)	5 (3%)	6	19
9	AK	128/173 (74%)	68 (53%)	33 (26%)	27 (21%)	0	0
9	CK	128/173 (74%)	69 (54%)	24 (19%)	35 (27%)	0	0
10	AL	137/147 (93%)	105 (77%)	23 (17%)	9 (7%)	1	4
10	CL	137/147 (93%)	95 (69%)	33 (24%)	9 (7%)	1	4
11	AN	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	62
11	CN	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	14	42
12	AO	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	11	36
12	CO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	7	24
13	AP	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	14	42
13	CP	147/150 (98%)	128 (87%)	16 (11%)	3 (2%)	9	30
14	AQ	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	14	42
14	CQ	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	8	28
15	AR	116/118 (98%)	100 (86%)	13 (11%)	3 (3%)	7	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	CR	116/118 (98%)	92 (79%)	16 (14%)	8 (7%)	1	3
16	AS	108/112 (96%)	92 (85%)	12 (11%)	4 (4%)	4	14
16	CS	108/112 (96%)	86 (80%)	17 (16%)	5 (5%)	3	9
17	AT	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	24	58
17	CT	129/146 (88%)	109 (84%)	15 (12%)	5 (4%)	4	12
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	103 (90%)	10 (9%)	1 (1%)	21	55
19	AV	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	9	30
19	CV	99/101 (98%)	87 (88%)	9 (9%)	3 (3%)	5	18
20	AW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
20	CW	110/113 (97%)	100 (91%)	10 (9%)	0	100	100
21	AX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
21	CX	93/96 (97%)	80 (86%)	11 (12%)	2 (2%)	8	28
22	AY	105/110 (96%)	91 (87%)	11 (10%)	3 (3%)	6	19
22	CY	105/110 (96%)	90 (86%)	13 (12%)	2 (2%)	10	32
23	AZ	183/206 (89%)	146 (80%)	24 (13%)	13 (7%)	1	3
23	CZ	183/206 (89%)	140 (76%)	31 (17%)	12 (7%)	1	4
24	A0	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	16	47
24	C0	81/85 (95%)	70 (86%)	11 (14%)	0	100	100
25	A1	95/98 (97%)	86 (90%)	7 (7%)	2 (2%)	9	29
25	C1	95/98 (97%)	87 (92%)	4 (4%)	4 (4%)	3	11
26	A2	68/72 (94%)	62 (91%)	5 (7%)	1 (2%)	13	40
26	C2	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	13	40
27	A3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	C3	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	A4	67/71 (94%)	41 (61%)	19 (28%)	7 (10%)	1	1
28	C4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	3	10
29	A5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
29	C5	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	11	34
30	A6	51/54 (94%)	48 (94%)	2 (4%)	1 (2%)	9	30
30	C6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	9	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	A7	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
31	C7	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	3	10
32	A8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
32	C8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	12	38
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%)	176 (77%)	42 (18%)	11 (5%)	3	9
35	DB	229/256 (90%)	177 (77%)	37 (16%)	15 (7%)	1	4
36	BC	204/239 (85%)	169 (83%)	28 (14%)	7 (3%)	5	16
36	DC	204/239 (85%)	175 (86%)	26 (13%)	3 (2%)	13	40
37	BD	206/209 (99%)	154 (75%)	34 (16%)	18 (9%)	1	2
37	DD	206/209 (99%)	161 (78%)	31 (15%)	14 (7%)	1	4
38	BE	146/162 (90%)	111 (76%)	26 (18%)	9 (6%)	2	5
38	DE	146/162 (90%)	122 (84%)	21 (14%)	3 (2%)	9	29
39	BF	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	5	17
39	DF	98/101 (97%)	82 (84%)	15 (15%)	1 (1%)	19	52
40	BG	153/156 (98%)	131 (86%)	17 (11%)	5 (3%)	5	16
40	DG	153/156 (98%)	133 (87%)	14 (9%)	6 (4%)	4	12
41	BH	135/138 (98%)	111 (82%)	18 (13%)	6 (4%)	3	10
41	DH	135/138 (98%)	122 (90%)	13 (10%)	0	100	100
42	BI	125/128 (98%)	104 (83%)	16 (13%)	5 (4%)	4	12
42	DI	125/128 (98%)	104 (83%)	18 (14%)	3 (2%)	7	25
43	BJ	95/105 (90%)	80 (84%)	12 (13%)	3 (3%)	5	17
43	DJ	94/105 (90%)	76 (81%)	9 (10%)	9 (10%)	1	1
44	BK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	4	14
44	DK	112/129 (87%)	98 (88%)	11 (10%)	3 (3%)	6	21
45	BL	120/132 (91%)	111 (92%)	7 (6%)	2 (2%)	11	36
45	DL	120/132 (91%)	103 (86%)	13 (11%)	4 (3%)	5	16
46	BM	115/126 (91%)	89 (77%)	23 (20%)	3 (3%)	7	22
46	DM	120/126 (95%)	100 (83%)	12 (10%)	8 (7%)	1	4
47	BN	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	5	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DN	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
48	BO	86/89 (97%)	72 (84%)	8 (9%)	6 (7%)	1	3
48	DO	86/89 (97%)	75 (87%)	8 (9%)	3 (4%)	4	15
49	BP	80/88 (91%)	52 (65%)	19 (24%)	9 (11%)	0	1
49	DP	80/88 (91%)	65 (81%)	12 (15%)	3 (4%)	4	13
50	BQ	97/105 (92%)	82 (84%)	9 (9%)	6 (6%)	2	5
50	DQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	5	17
51	BR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
51	DR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	5	18
52	BS	82/93 (88%)	66 (80%)	14 (17%)	2 (2%)	7	25
52	DS	81/93 (87%)	68 (84%)	8 (10%)	5 (6%)	2	5
53	BT	94/106 (89%)	77 (82%)	10 (11%)	7 (7%)	1	3
53	DT	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	5	17
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	3	9
57	BZ	726/758 (96%)	569 (78%)	106 (15%)	51 (7%)	1	3
57	DZ	726/758 (96%)	554 (76%)	121 (17%)	51 (7%)	1	3
All	All	13389/14444 (93%)	11230 (84%)	1582 (12%)	577 (4%)	3	10

5 of 577 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	42	VAL
3	AC	47	LYS
3	AC	68	GLY
3	AC	180	SER
3	AC	181	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	111/180 (62%)	104 (94%)	7 (6%)	22	53
3	CC	111/180 (62%)	103 (93%)	8 (7%)	18	45
4	AD	215/218 (99%)	181 (84%)	34 (16%)	3	9
4	CD	216/218 (99%)	179 (83%)	37 (17%)	2	7
5	AE	164/166 (99%)	130 (79%)	34 (21%)	1	4
5	CE	164/166 (99%)	130 (79%)	34 (21%)	1	4
6	AF	160/166 (96%)	128 (80%)	32 (20%)	1	5
6	CF	159/166 (96%)	124 (78%)	35 (22%)	1	3
7	AG	143/156 (92%)	114 (80%)	29 (20%)	1	4
7	CG	142/156 (91%)	111 (78%)	31 (22%)	1	3
8	AH	144/148 (97%)	121 (84%)	23 (16%)	3	9
8	CH	144/148 (97%)	124 (86%)	20 (14%)	4	13
10	AL	104/111 (94%)	83 (80%)	21 (20%)	1	4
10	CL	104/111 (94%)	84 (81%)	20 (19%)	2	5
11	AN	118/119 (99%)	97 (82%)	21 (18%)	2	6
11	CN	118/119 (99%)	92 (78%)	26 (22%)	1	3
12	AO	100/100 (100%)	88 (88%)	12 (12%)	6	19
12	CO	100/100 (100%)	82 (82%)	18 (18%)	2	6
13	AP	116/116 (100%)	90 (78%)	26 (22%)	1	3
13	CP	115/116 (99%)	95 (83%)	20 (17%)	2	7
14	AQ	111/111 (100%)	99 (89%)	12 (11%)	8	23
14	CQ	111/111 (100%)	91 (82%)	20 (18%)	2	6
15	AR	101/101 (100%)	81 (80%)	20 (20%)	1	5
15	CR	101/101 (100%)	78 (77%)	23 (23%)	1	3
16	AS	87/88 (99%)	70 (80%)	17 (20%)	2	5
16	CS	85/88 (97%)	66 (78%)	19 (22%)	1	3
17	AT	115/127 (91%)	98 (85%)	17 (15%)	4	11
17	CT	113/127 (89%)	90 (80%)	23 (20%)	1	4
18	AU	93/94 (99%)	79 (85%)	14 (15%)	3	10
18	CU	93/94 (99%)	80 (86%)	13 (14%)	4	13
19	AV	80/82 (98%)	63 (79%)	17 (21%)	1	4
19	CV	80/82 (98%)	68 (85%)	12 (15%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	AW	90/92 (98%)	77 (86%)	13 (14%)	4	12
20	CW	90/92 (98%)	82 (91%)	8 (9%)	12	34
21	AX	77/78 (99%)	69 (90%)	8 (10%)	9	25
21	CX	77/78 (99%)	69 (90%)	8 (10%)	9	25
22	AY	85/91 (93%)	71 (84%)	14 (16%)	3	8
22	CY	85/91 (93%)	69 (81%)	16 (19%)	2	6
23	AZ	156/179 (87%)	121 (78%)	35 (22%)	1	3
23	CZ	156/179 (87%)	129 (83%)	27 (17%)	2	7
24	A0	65/67 (97%)	61 (94%)	4 (6%)	23	54
24	C0	65/67 (97%)	60 (92%)	5 (8%)	16	41
25	A1	80/83 (96%)	70 (88%)	10 (12%)	6	17
25	C1	80/83 (96%)	66 (82%)	14 (18%)	2	7
26	A2	65/67 (97%)	55 (85%)	10 (15%)	3	10
26	C2	65/67 (97%)	51 (78%)	14 (22%)	1	3
27	A3	51/52 (98%)	41 (80%)	10 (20%)	1	5
27	C3	50/52 (96%)	42 (84%)	8 (16%)	3	9
28	A4	60/63 (95%)	42 (70%)	18 (30%)	0	1
28	C4	53/63 (84%)	41 (77%)	12 (23%)	1	3
29	A5	50/52 (96%)	43 (86%)	7 (14%)	4	13
29	C5	50/52 (96%)	42 (84%)	8 (16%)	3	9
30	A6	51/52 (98%)	39 (76%)	12 (24%)	1	2
30	C6	50/52 (96%)	39 (78%)	11 (22%)	1	3
31	A7	41/42 (98%)	34 (83%)	7 (17%)	2	7
31	C7	41/42 (98%)	32 (78%)	9 (22%)	1	3
32	A8	54/55 (98%)	46 (85%)	8 (15%)	4	11
32	C8	54/55 (98%)	44 (82%)	10 (18%)	2	6
33	A9	34/34 (100%)	32 (94%)	2 (6%)	24	57
33	C9	34/34 (100%)	32 (94%)	2 (6%)	24	57
35	BB	192/220 (87%)	153 (80%)	39 (20%)	1	4
35	DB	187/220 (85%)	151 (81%)	36 (19%)	2	5
36	BC	143/188 (76%)	129 (90%)	14 (10%)	10	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	DC	141/188 (75%)	116 (82%)	25 (18%)	2	7
37	BD	170/181 (94%)	143 (84%)	27 (16%)	3	9
37	DD	174/181 (96%)	137 (79%)	37 (21%)	1	4
38	BE	113/123 (92%)	89 (79%)	24 (21%)	1	4
38	DE	114/123 (93%)	92 (81%)	22 (19%)	2	5
39	BF	84/90 (93%)	68 (81%)	16 (19%)	2	5
39	DF	86/90 (96%)	75 (87%)	11 (13%)	5	16
40	BG	119/127 (94%)	102 (86%)	17 (14%)	4	12
40	DG	120/127 (94%)	99 (82%)	21 (18%)	2	7
41	BH	114/119 (96%)	96 (84%)	18 (16%)	3	9
41	DH	114/119 (96%)	92 (81%)	22 (19%)	2	5
42	BI	91/99 (92%)	75 (82%)	16 (18%)	2	7
42	DI	89/99 (90%)	76 (85%)	13 (15%)	4	11
43	BJ	66/92 (72%)	61 (92%)	5 (8%)	16	42
43	DJ	69/92 (75%)	65 (94%)	4 (6%)	25	57
44	BK	83/99 (84%)	68 (82%)	15 (18%)	2	6
44	DK	83/99 (84%)	77 (93%)	6 (7%)	18	45
45	BL	97/109 (89%)	83 (86%)	14 (14%)	4	12
45	DL	97/109 (89%)	82 (84%)	15 (16%)	3	10
46	BM	91/101 (90%)	70 (77%)	21 (23%)	1	3
46	DM	92/101 (91%)	79 (86%)	13 (14%)	4	12
47	BN	49/50 (98%)	40 (82%)	9 (18%)	2	6
47	DN	49/50 (98%)	40 (82%)	9 (18%)	2	6
48	BO	78/80 (98%)	69 (88%)	9 (12%)	7	21
48	DO	78/80 (98%)	68 (87%)	10 (13%)	5	16
49	BP	69/74 (93%)	53 (77%)	16 (23%)	1	3
49	DP	68/74 (92%)	56 (82%)	12 (18%)	2	7
50	BQ	94/97 (97%)	74 (79%)	20 (21%)	1	4
50	DQ	94/97 (97%)	85 (90%)	9 (10%)	10	29
51	BR	59/77 (77%)	48 (81%)	11 (19%)	2	6
51	DR	59/77 (77%)	47 (80%)	12 (20%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	BS	70/80 (88%)	60 (86%)	10 (14%)	4	12
52	DS	67/80 (84%)	59 (88%)	8 (12%)	6	19
53	BT	70/82 (85%)	56 (80%)	14 (20%)	1	5
53	DT	71/82 (87%)	63 (89%)	8 (11%)	7	22
54	BU	18/22 (82%)	16 (89%)	2 (11%)	8	23
54	DU	18/22 (82%)	18 (100%)	0	100	100
57	BZ	609/636 (96%)	485 (80%)	124 (20%)	1	4
57	DZ	609/636 (96%)	474 (78%)	135 (22%)	1	3
All	All	10785/11672 (92%)	8911 (83%)	1874 (17%)	2	7

5 of 1874 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
57	BZ	130	VAL
7	CG	3	LEU
53	DT	8	ARG
57	BZ	286	ILE
4	CD	71	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 175 such sidechains are listed below:

Mol	Chain	Res	Type
57	BZ	475	ASN
6	CF	169	ASN
53	DT	16	HIS
57	BZ	573	HIS
4	CD	126	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2845/2915 (97%)	527 (18%)	56 (1%)
1	CA	2839/2915 (97%)	579 (20%)	39 (1%)
2	AB	119/121 (98%)	23 (19%)	0
2	CB	119/121 (98%)	21 (17%)	0
34	BA	1491/1521 (98%)	310 (20%)	22 (1%)
34	DA	1498/1521 (98%)	303 (20%)	24 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	BV	6/18 (33%)	1 (16%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	15 (20%)	0
56	BY	71/76 (93%)	23 (32%)	2 (2%)
56	DW	74/76 (97%)	19 (25%)	2 (2%)
56	DY	69/76 (90%)	21 (30%)	1 (1%)
All	All	9210/9454 (97%)	1843 (20%)	146 (1%)

5 of 1843 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	U
1	AA	12	U
1	AA	13	A
1	AA	34	C
1	AA	45	C

5 of 146 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	748	C
1	CA	195	A
34	DA	884	U
34	BA	793	U
34	BA	1165	C

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

28 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	13,21,22	0.78	1 (7%)	18,30,33	3.92	6 (33%)
56	MIA	BW	37	56	21,31,32	1.84	3 (14%)	26,44,47	3.07	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	BW	39	56	13,21,22	1.68	1 (7%)	18,30,33	3.33	6 (33%)
56	7MG	BW	46	56	19,26,27	0.86	1 (5%)	24,39,42	3.18	7 (29%)
56	5MU	BW	54	56	12,22,23	0.48	0	14,32,35	2.03	2 (14%)
56	PSU	BW	55	56	13,21,22	1.25	1 (7%)	18,30,33	3.62	6 (33%)
56	4SU	BW	8	56	11,21,22	1.14	1 (9%)	13,30,33	1.24	1 (7%)
56	PSU	BY	32	56	13,21,22	0.92	1 (7%)	18,30,33	3.39	5 (27%)
56	MIA	BY	37	56	15,24,32	1.27	2 (13%)	16,35,47	2.16	2 (12%)
56	PSU	BY	39	56	13,21,22	1.09	1 (7%)	18,30,33	3.46	6 (33%)
56	7MG	BY	46	56	19,26,27	1.00	1 (5%)	24,39,42	3.05	6 (25%)
56	5MU	BY	54	56	12,22,23	0.34	0	14,32,35	2.40	2 (14%)
56	PSU	BY	55	56	13,21,22	1.12	1 (7%)	18,30,33	3.33	6 (33%)
56	4SU	BY	8	56	11,21,22	1.17	1 (9%)	13,30,33	1.52	2 (15%)
56	PSU	DW	32	56	13,21,22	0.60	0	18,30,33	4.03	7 (38%)
56	MIA	DW	37	56	21,31,32	2.02	2 (9%)	26,44,47	1.20	3 (11%)
56	PSU	DW	39	56	13,21,22	1.19	1 (7%)	18,30,33	3.44	7 (38%)
56	7MG	DW	46	56	19,26,27	0.94	1 (5%)	24,39,42	3.04	6 (25%)
56	5MU	DW	54	56	12,22,23	0.54	0	14,32,35	2.23	2 (14%)
56	PSU	DW	55	56	13,21,22	0.96	1 (7%)	18,30,33	3.57	6 (33%)
56	4SU	DW	8	56	11,21,22	1.23	1 (9%)	13,30,33	1.45	1 (7%)
56	PSU	DY	32	56	13,21,22	1.00	1 (7%)	18,30,33	3.45	6 (33%)
56	MIA	DY	37	56	15,24,32	1.17	2 (13%)	16,35,47	2.08	2 (12%)
56	PSU	DY	39	56	13,21,22	1.21	1 (7%)	18,30,33	3.35	5 (27%)
56	7MG	DY	46	56	19,26,27	1.06	2 (10%)	24,39,42	3.24	8 (33%)
56	5MU	DY	54	56	12,22,23	0.37	0	14,32,35	2.31	2 (14%)
56	PSU	DY	55	56	13,21,22	1.19	1 (7%)	18,30,33	3.34	6 (33%)
56	4SU	DY	8	56	11,21,22	1.28	1 (9%)	13,30,33	1.31	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	BW	32	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-	0/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/11/33/34	0/3/3/3
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	0/7/37/38	0/3/3/3
56	5MU	DW	54	56	-	0/3/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/3/25/26	0/2/2/2
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 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	DW	37	MIA	C2-S10	-7.86	1.69	1.75
56	BW	37	MIA	C2-S10	-7.15	1.69	1.75
56	BW	39	PSU	C5-C1'	-5.69	1.47	1.52
56	BW	55	PSU	C5-C1'	-3.98	1.48	1.52
56	DY	8	4SU	C4-S4	-3.81	1.60	1.67

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	37	MIA	C11-S10-C2	-13.56	93.56	102.26
56	DW	32	PSU	N1-C2-N3	-13.22	119.90	128.33
56	BW	32	PSU	N1-C2-N3	-13.10	119.97	128.33
56	BW	55	PSU	N1-C2-N3	-11.55	120.97	128.33
56	DW	55	PSU	N1-C2-N3	-11.33	121.10	128.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	37	MIA	1	0
56	BY	8	4SU	1	0
56	DW	37	MIA	2	0
56	DW	39	PSU	4	0
56	DW	46	7MG	2	0
56	DW	54	5MU	1	0
56	DW	55	PSU	2	0
56	DY	37	MIA	1	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 2058 ligands modelled in this entry, 2052 are monoatomic - leaving 6 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	$\# Z > 2$
60	SF4	BD	501	37	0,12,12	0.00	-	0,24,24	0.00	-
61	FUA	BZ	703	-	37,40,40	1.70	6 (16%)	45,64,64	1.66	7 (15%)
62	GDP	BZ	704	58	23,30,30	1.02	2 (8%)	30,47,47	1.86	6 (20%)
60	SF4	DD	501	37	0,12,12	0.00	-	0,24,24	0.00	-
61	FUA	DZ	703	-	37,40,40	1.69	6 (16%)	45,64,64	1.66	7 (15%)
62	GDP	DZ	704	58	23,30,30	1.24	2 (8%)	30,47,47	2.37	7 (23%)

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
60	SF4	BD	501	37	-	0/0/48/48	0/6/5/5
61	FUA	BZ	703	-	-	0/10/92/92	0/4/4/4
62	GDP	BZ	704	58	-	0/12/32/32	0/3/3/3
60	SF4	DD	501	37	-	0/0/48/48	0/6/5/5
61	FUA	DZ	703	-	-	0/10/92/92	0/4/4/4
62	GDP	DZ	704	58	-	0/12/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BZ	703	FUA	C23-C22	-5.99	1.39	1.51
61	DZ	703	FUA	C23-C22	-5.94	1.40	1.51
61	BZ	703	FUA	C23-C24	-4.18	1.39	1.53
61	DZ	703	FUA	C23-C24	-4.16	1.39	1.53
61	DZ	703	FUA	C24-C25	-3.83	1.39	1.50

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	DZ	704	GDP	C2'-C1'-N9	-6.55	104.29	114.29
62	BZ	704	GDP	C2'-C1'-N9	-5.04	106.59	114.29
62	DZ	704	GDP	C5-C6-N1	-4.92	116.87	123.59
61	BZ	703	FUA	C13-C12-C11	-4.54	105.80	111.95
61	DZ	703	FUA	C13-C12-C11	-4.50	105.85	111.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	BD	501	SF4	1	0
61	BZ	703	FUA	11	0
62	BZ	704	GDP	5	0
60	DD	501	SF4	2	0
61	DZ	703	FUA	17	0
62	DZ	704	GDP	9	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	2852/2915 (97%)	0.34	112 (3%)	43	31	14, 34, 139, 364	4 (0%)
1	CA	2848/2915 (97%)	0.39	126 (4%)	38	26	27, 57, 180, 356	0
2	AB	120/121 (99%)	-0.12	0	100	100	23, 50, 73, 110	0
2	CB	120/121 (99%)	0.14	1 (0%)	87	81	64, 92, 120, 168	0
3	AC	137/228 (60%)	10.45	133 (97%)	0	0	258, 289, 307, 313	0
3	CC	137/228 (60%)	11.82	133 (97%)	0	0	281, 312, 331, 336	0
4	AD	275/276 (99%)	-0.32	2 (0%)	89	84	13, 35, 59, 137	1 (0%)
4	CD	275/276 (99%)	-0.26	2 (0%)	89	84	19, 48, 74, 130	2 (0%)
5	AE	204/206 (99%)	-0.38	0	100	100	5, 33, 57, 80	3 (1%)
5	CE	204/206 (99%)	0.01	4 (1%)	68	58	21, 63, 107, 134	0
6	AF	203/210 (96%)	-0.27	0	100	100	10, 35, 78, 174	0
6	CF	203/210 (96%)	-0.26	0	100	100	21, 64, 107, 155	0
7	AG	181/182 (99%)	0.04	5 (2%)	56	44	34, 78, 134, 212	1 (0%)
7	CG	181/182 (99%)	0.73	21 (11%)	6	3	73, 112, 177, 207	0
8	AH	174/180 (96%)	-0.35	1 (0%)	90	86	26, 46, 70, 112	0
8	CH	174/180 (96%)	1.32	45 (25%)	1	0	65, 112, 161, 200	0
9	AK	130/173 (75%)	0.76	18 (13%)	4	2	48, 105, 170, 232	0
9	CK	130/173 (75%)	2.64	69 (53%)	0	0	75, 162, 204, 231	0
10	AL	139/147 (94%)	3.55	92 (66%)	0	0	96, 173, 233, 253	0
10	CL	139/147 (94%)	5.92	120 (86%)	0	0	127, 196, 252, 287	1 (0%)
11	AN	140/140 (100%)	-0.38	0	100	100	14, 28, 61, 97	1 (0%)
11	CN	140/140 (100%)	0.16	4 (2%)	55	43	32, 72, 108, 150	0
12	AO	122/122 (100%)	-0.32	0	100	100	17, 37, 63, 79	1 (0%)
12	CO	122/122 (100%)	-0.21	0	100	100	36, 59, 85, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.06	0 100 100	11, 42, 81, 107	1 (0%)
13	CP	149/150 (99%)	0.25	4 (2%) 58 45	30, 68, 117, 137	0
14	AQ	141/141 (100%)	-0.31	0 100 100	11, 34, 54, 81	0
14	CQ	141/141 (100%)	-0.16	2 (1%) 78 69	38, 71, 101, 120	0
15	AR	118/118 (100%)	-0.34	0 100 100	16, 29, 45, 56	0
15	CR	118/118 (100%)	-0.11	0 100 100	33, 56, 90, 106	0
16	AS	110/112 (98%)	-0.21	0 100 100	29, 51, 81, 94	0
16	CS	110/112 (98%)	0.36	4 (3%) 46 34	46, 85, 120, 152	0
17	AT	131/146 (89%)	-0.28	1 (0%) 87 81	24, 41, 92, 165	0
17	CT	131/146 (89%)	-0.08	1 (0%) 87 81	43, 65, 105, 143	0
18	AU	116/118 (98%)	-0.32	0 100 100	9, 22, 38, 90	1 (0%)
18	CU	116/118 (98%)	-0.04	0 100 100	27, 65, 93, 107	0
19	AV	101/101 (100%)	-0.44	0 100 100	9, 28, 50, 75	0
19	CV	101/101 (100%)	0.18	1 (0%) 84 77	36, 80, 113, 171	0
20	AW	112/113 (99%)	-0.35	0 100 100	13, 26, 43, 112	1 (0%)
20	CW	112/113 (99%)	-0.12	0 100 100	27, 50, 81, 119	0
21	AX	95/96 (98%)	-0.29	0 100 100	16, 35, 67, 99	1 (1%)
21	CX	95/96 (98%)	-0.01	2 (2%) 67 56	38, 62, 86, 107	0
22	AY	107/110 (97%)	-0.23	1 (0%) 85 79	24, 44, 87, 161	0
22	CY	107/110 (97%)	0.49	10 (9%) 11 5	46, 76, 115, 167	0
23	AZ	185/206 (89%)	-0.38	0 100 100	29, 57, 92, 148	0
23	CZ	185/206 (89%)	0.67	21 (11%) 7 3	61, 106, 149, 213	0
24	A0	83/85 (97%)	-0.06	4 (4%) 34 23	12, 35, 83, 225	1 (1%)
24	C0	83/85 (97%)	0.75	10 (12%) 6 3	42, 66, 122, 228	0
25	A1	97/98 (98%)	-0.13	2 (2%) 67 56	19, 43, 80, 101	1 (1%)
25	C1	97/98 (98%)	-0.16	1 (1%) 84 77	31, 52, 91, 125	0
26	A2	70/72 (97%)	-0.27	2 (2%) 55 43	25, 44, 69, 123	1 (1%)
26	C2	70/72 (97%)	0.01	3 (4%) 39 27	49, 71, 101, 117	0
27	A3	59/60 (98%)	-0.31	0 100 100	14, 30, 56, 101	1 (1%)
27	C3	59/60 (98%)	0.66	8 (13%) 4 2	46, 73, 112, 150	0
28	A4	69/71 (97%)	1.03	18 (26%) 1 0	59, 118, 206, 239	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.51	24 (34%) 0 0	81, 159, 207, 228	0
29	A5	59/60 (98%)	-0.29	0 100 100	8, 26, 40, 52	0
29	C5	59/60 (98%)	-0.08	0 100 100	27, 52, 90, 104	0
30	A6	53/54 (98%)	-0.41	0 100 100	23, 41, 55, 74	0
30	C6	53/54 (98%)	-0.32	0 100 100	41, 61, 80, 106	0
31	A7	48/49 (97%)	-0.23	1 (2%) 67 56	14, 24, 69, 134	1 (2%)
31	C7	48/49 (97%)	0.02	2 (4%) 40 28	26, 40, 96, 119	0
32	A8	64/65 (98%)	-0.30	0 100 100	16, 29, 45, 65	1 (1%)
32	C8	64/65 (98%)	-0.09	0 100 100	37, 52, 73, 85	0
33	A9	37/37 (100%)	-0.05	0 100 100	23, 35, 57, 68	1 (2%)
33	C9	37/37 (100%)	0.89	5 (13%) 4 2	45, 79, 96, 127	0
34	BA	1495/1521 (98%)	0.49	92 (6%) 24 15	31, 85, 186, 337	0
34	DA	1501/1521 (98%)	0.58	124 (8%) 14 7	39, 90, 196, 346	0
35	BB	231/256 (90%)	0.68	35 (15%) 3 1	43, 106, 173, 223	0
35	DB	231/256 (90%)	0.83	36 (15%) 3 1	71, 125, 176, 215	0
36	BC	206/239 (86%)	1.16	43 (20%) 1 1	56, 119, 174, 197	0
36	DC	206/239 (86%)	1.44	55 (26%) 1 0	69, 136, 182, 212	0
37	BD	208/209 (99%)	0.34	9 (4%) 39 27	44, 87, 138, 196	0
37	DD	208/209 (99%)	0.23	3 (1%) 78 69	59, 87, 136, 201	0
38	BE	148/162 (91%)	-0.06	1 (0%) 89 84	35, 73, 105, 128	0
38	DE	148/162 (91%)	0.05	2 (1%) 78 69	50, 81, 117, 182	0
39	BF	100/101 (99%)	-0.12	0 100 100	56, 86, 117, 138	0
39	DF	100/101 (99%)	-0.00	2 (2%) 68 58	48, 87, 115, 134	0
40	BG	155/156 (99%)	1.23	34 (21%) 1 1	68, 113, 183, 226	0
40	DG	155/156 (99%)	1.79	46 (29%) 1 0	72, 131, 194, 222	0
41	BH	137/138 (99%)	0.10	3 (2%) 65 54	47, 73, 99, 119	0
41	DH	137/138 (99%)	0.10	1 (0%) 89 84	57, 81, 111, 140	0
42	BI	127/128 (99%)	1.93	51 (40%) 0 0	65, 125, 167, 199	0
42	DI	127/128 (99%)	2.50	71 (55%) 0 0	91, 146, 193, 216	0
43	BJ	97/105 (92%)	1.66	35 (36%) 0 0	83, 131, 186, 215	0
43	DJ	96/105 (91%)	2.24	46 (47%) 0 0	92, 151, 200, 234	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	0.16	0 100 100	35, 79, 125, 151	0
44	DK	114/129 (88%)	0.24	3 (2%) 59 47	52, 91, 116, 177	0
45	BL	122/132 (92%)	-0.23	0 100 100	37, 60, 78, 113	0
45	DL	122/132 (92%)	-0.08	1 (0%) 87 81	46, 72, 96, 117	0
46	BM	117/126 (92%)	1.69	37 (31%) 1 0	77, 134, 182, 211	0
46	DM	122/126 (96%)	2.11	44 (36%) 0 0	94, 151, 201, 275	0
47	BN	60/61 (98%)	1.10	12 (20%) 1 1	67, 113, 146, 168	0
47	DN	60/61 (98%)	1.90	25 (41%) 0 0	98, 137, 179, 200	0
48	BO	88/89 (98%)	-0.11	1 (1%) 82 74	36, 71, 106, 121	0
48	DO	88/89 (98%)	0.03	1 (1%) 82 74	47, 71, 107, 153	0
49	BP	82/88 (93%)	0.44	1 (1%) 81 73	49, 80, 119, 171	0
49	DP	82/88 (93%)	0.50	5 (6%) 25 15	54, 78, 111, 153	0
50	BQ	99/105 (94%)	0.07	1 (1%) 84 77	44, 73, 99, 124	0
50	DQ	99/105 (94%)	0.04	0 100 100	44, 78, 104, 119	0
51	BR	68/88 (77%)	0.35	5 (7%) 17 9	42, 81, 123, 136	0
51	DR	68/88 (77%)	0.31	1 (1%) 76 68	53, 83, 128, 145	0
52	BS	84/93 (90%)	3.28	53 (63%) 0 0	97, 145, 198, 212	0
52	DS	83/93 (89%)	3.36	53 (63%) 0 0	90, 165, 216, 226	0
53	BT	96/106 (90%)	0.22	2 (2%) 67 56	62, 85, 122, 162	0
53	DT	96/106 (90%)	0.36	4 (4%) 40 28	58, 86, 135, 157	0
54	BU	23/27 (85%)	2.30	10 (43%) 0 0	62, 119, 158, 177	0
54	DU	23/27 (85%)	2.27	13 (56%) 0 0	92, 134, 173, 189	0
55	BV	7/18 (38%)	2.56	4 (57%) 0 0	53, 88, 211, 226	0
55	DV	6/18 (33%)	2.74	4 (66%) 0 0	84, 106, 214, 225	0
56	BW	69/76 (90%)	0.89	4 (5%) 26 16	38, 72, 106, 212	0
56	BY	67/76 (88%)	8.37	66 (98%) 0 0	82, 289, 329, 354	0
56	DW	69/76 (90%)	1.15	9 (13%) 5 2	54, 98, 141, 254	0
56	DY	66/76 (86%)	9.64	66 (100%) 0 0	213, 296, 333, 355	0
57	BZ	730/758 (96%)	0.19	38 (5%) 31 20	36, 79, 135, 190	0
57	DZ	730/758 (96%)	0.66	101 (13%) 4 2	36, 102, 169, 225	0
All	All	22825/23898 (95%)	0.62	2268 (9%) 9 4	5, 71, 189, 364	25 (0%)

The worst 5 of 2268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	AC	159	ALA	36.1
3	AC	57	GLN	34.3
3	CC	68	GLY	33.7
3	CC	27	ALA	33.5
3	CC	172	ILE	32.9

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
56	4SU	BY	8	20/21	0.26	0.50	-	300,300,300,300	0
56	5MU	DY	54	21/22	0.34	0.74	-	305,305,305,305	1
56	PSU	DW	39	20/21	0.87	0.35	-	93,93,93,93	3
56	7MG	DW	46	24/25	0.88	0.29	-	114,114,114,114	2
56	MIA	DW	37	29/30	0.91	0.27	-	94,94,94,94	0
56	5MU	BW	54	21/22	0.95	0.25	-	74,74,74,74	1
56	4SU	DY	8	20/21	0.17	0.51	-	275,275,275,275	0
56	PSU	BY	39	20/21	0.06	1.19	-	316,316,316,316	0
56	PSU	BW	55	20/21	0.88	0.24	-	74,74,74,74	5
56	PSU	BY	55	20/21	0.04	0.67	-	302,302,302,302	1
56	PSU	DY	32	20/21	0.18	1.61	-	268,268,268,268	0
56	PSU	DW	55	20/21	0.78	0.23	-	106,106,106,106	2
56	PSU	BY	32	20/21	0.34	0.89	-	254,254,254,254	1
56	5MU	BY	54	21/22	0.23	0.82	-	315,315,315,315	0
56	7MG	BW	46	24/25	0.94	0.20	-	63,63,63,63	5
56	PSU	DY	55	20/21	0.42	0.71	-	246,246,246,246	0
56	4SU	DW	8	20/21	0.93	0.20	-	88,88,88,88	3
56	PSU	DY	39	20/21	0.28	1.29	-	284,284,284,284	0
56	PSU	BW	39	20/21	0.95	0.25	-	65,65,65,65	3
56	PSU	BW	32	20/21	0.92	0.17	-	81,81,81,81	1
56	PSU	DW	32	20/21	0.88	0.21	-	106,106,106,106	1
56	5MU	DW	54	21/22	0.88	0.33	-	114,114,114,114	1
56	7MG	DY	46	24/25	0.52	0.53	-	302,302,302,302	0
56	7MG	BY	46	24/25	0.25	0.45	-	302,302,302,302	0
56	MIA	DY	37	22/30	0.12	1.85	-	319,319,319,319	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MIA	BW	37	29/30	0.92	0.26	-	79,79,79,79	2
56	MIA	BY	37	22/30	0.05	1.39	-	284,284,284,284	0
56	4SU	BW	8	20/21	0.94	0.15	-	51,51,51,51	6

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
58	MG	AA	3018	1/1	0.83	1.37	126.81	78,78,78,78	0
58	MG	CA	3106	1/1	0.86	0.74	100.56	55,55,55,55	0
58	MG	CA	3043	1/1	0.59	0.83	64.26	102,102,102,102	0
58	MG	AA	3135	1/1	0.94	0.66	58.03	62,62,62,62	1
58	MG	AA	3171	1/1	0.96	0.49	53.19	25,25,25,25	1
58	MG	BA	1711	1/1	0.64	0.60	47.54	71,71,71,71	0
58	MG	CA	3185	1/1	0.91	0.48	46.01	59,59,59,59	0
58	MG	CA	3467	1/1	0.87	0.64	45.66	80,80,80,80	0
58	MG	CA	3314	1/1	0.74	0.53	41.67	77,77,77,77	0
58	MG	AA	3604	1/1	0.84	0.39	37.61	38,38,38,38	1
58	MG	BA	1801	1/1	0.89	0.46	34.36	69,69,69,69	0
58	MG	CA	3088	1/1	0.76	0.53	33.45	75,75,75,75	0
58	MG	CA	3619	1/1	0.89	0.44	33.17	47,47,47,47	1
58	MG	CA	3290	1/1	0.75	0.47	32.36	75,75,75,75	0
58	MG	CA	3114	1/1	0.93	0.45	32.24	39,39,39,39	0
58	MG	CA	3073	1/1	0.84	0.60	31.06	91,91,91,91	0
58	MG	BA	1657	1/1	0.86	0.41	30.60	73,73,73,73	0
58	MG	A7	103	1/1	0.82	0.50	30.26	38,38,38,38	1
58	MG	BA	1738	1/1	0.96	0.43	30.16	56,56,56,56	0
58	MG	CA	3168	1/1	0.86	0.52	29.98	56,56,56,56	0
58	MG	CA	3218	1/1	0.95	0.50	27.35	54,54,54,54	0
58	MG	CA	3223	1/1	0.83	0.58	27.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3618	1/1	0.69	0.36	27.08	65,65,65,65	0
58	MG	CA	3498	1/1	0.94	0.49	26.75	68,68,68,68	0
58	MG	AH	3002	1/1	0.82	0.72	26.53	74,74,74,74	0
58	MG	CA	3542	1/1	0.94	0.39	26.28	68,68,68,68	0
58	MG	DA	1651	1/1	0.95	0.41	26.07	59,59,59,59	0
58	MG	CA	3230	1/1	0.93	0.42	26.04	51,51,51,51	0
58	MG	AA	3162	1/1	0.93	0.37	26.00	47,47,47,47	0
58	MG	DA	1743	1/1	0.92	0.35	25.94	72,72,72,72	0
58	MG	AB	3023	1/1	0.82	0.48	25.90	76,76,76,76	0
58	MG	AA	3211	1/1	0.92	0.57	25.62	42,42,42,42	1
58	MG	AA	3822	1/1	0.92	0.55	25.50	65,65,65,65	0
58	MG	C7	101	1/1	0.89	0.67	25.03	42,42,42,42	1
58	MG	DA	1668	1/1	0.97	0.42	24.86	62,62,62,62	0
58	MG	AA	3453	1/1	0.94	0.33	24.32	56,56,56,56	0
58	MG	BA	1664	1/1	0.88	0.39	24.13	59,59,59,59	0
58	MG	AA	3663	1/1	0.88	0.45	23.95	62,62,62,62	0
58	MG	AA	3132	1/1	0.88	0.28	23.76	27,27,27,27	1
58	MG	AA	3116	1/1	0.92	0.39	23.49	51,51,51,51	0
58	MG	AA	3768	1/1	0.72	0.40	23.47	99,99,99,99	0
58	MG	AA	3835	1/1	0.82	0.60	23.27	111,111,111,111	0
58	MG	AA	3212	1/1	0.94	0.41	23.24	34,34,34,34	1
58	MG	AA	3112	1/1	0.76	0.60	22.98	98,98,98,98	0
58	MG	CA	3441	1/1	0.91	0.35	22.41	77,77,77,77	0
58	MG	CA	3035	1/1	0.84	0.49	21.69	60,60,60,60	0
58	MG	AA	3462	1/1	0.94	0.45	21.41	71,71,71,71	0
58	MG	AA	3770	1/1	0.94	0.39	21.01	37,37,37,37	0
58	MG	BA	1629	1/1	0.91	0.49	20.83	64,64,64,64	0
58	MG	AA	3739	1/1	0.56	0.51	20.54	94,94,94,94	0
58	MG	AA	3117	1/1	0.85	0.32	20.44	30,30,30,30	1
58	MG	AA	3040	1/1	0.96	0.30	20.34	40,40,40,40	1
58	MG	CA	3588	1/1	0.95	0.35	20.31	63,63,63,63	0
58	MG	AA	3035	1/1	0.86	0.44	19.89	57,57,57,57	0
58	MG	AA	3196	1/1	0.94	0.39	19.69	52,52,52,52	0
58	MG	AA	3061	1/1	0.91	0.30	19.64	27,27,27,27	0
58	MG	DA	1684	1/1	0.85	0.54	19.53	72,72,72,72	0
58	MG	CA	3660	1/1	0.44	0.66	19.19	101,101,101,101	0
58	MG	AA	3101	1/1	0.90	0.36	19.02	52,52,52,52	0
58	MG	AA	3297	1/1	0.96	0.31	18.70	20,20,20,20	1
58	MG	AN	3001	1/1	0.31	0.89	18.66	85,85,85,85	0
58	MG	AA	3051	1/1	0.88	0.35	18.60	36,36,36,36	0
58	MG	CA	3166	1/1	0.96	0.38	18.35	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3206	1/1	0.83	0.28	18.19	39,39,39,39	0
58	MG	AU	203	1/1	0.95	0.45	18.12	62,62,62,62	0
58	MG	AA	3185	1/1	0.89	0.29	18.11	41,41,41,41	0
58	MG	AA	3221	1/1	0.88	0.34	18.07	56,56,56,56	0
58	MG	AA	3133	1/1	0.79	0.37	17.72	69,69,69,69	0
58	MG	CA	3348	1/1	0.88	0.27	17.69	54,54,54,54	0
58	MG	AA	3134	1/1	0.97	0.39	17.48	59,59,59,59	1
58	MG	CA	3182	1/1	0.97	0.36	17.45	27,27,27,27	0
58	MG	BA	1756	1/1	0.78	0.37	17.44	68,68,68,68	0
58	MG	AA	3301	1/1	0.93	0.33	17.11	23,23,23,23	0
58	MG	DA	1672	1/1	0.61	0.47	16.84	73,73,73,73	0
58	MG	DA	1606	1/1	0.67	1.00	16.78	84,84,84,84	0
58	MG	AA	3184	1/1	0.81	0.34	16.74	68,68,68,68	0
58	MG	DA	1647	1/1	0.95	0.33	16.73	58,58,58,58	0
58	MG	CA	3322	1/1	0.99	0.28	16.68	45,45,45,45	0
58	MG	AW	3003	1/1	0.88	0.45	16.57	52,52,52,52	0
58	MG	CA	3500	1/1	0.64	0.43	16.55	64,64,64,64	0
58	MG	CF	301	1/1	0.67	0.40	16.46	63,63,63,63	0
58	MG	AA	3436	1/1	0.96	0.34	16.37	38,38,38,38	0
58	MG	AA	3606	1/1	0.89	0.33	16.09	61,61,61,61	0
58	MG	CA	3028	1/1	0.97	0.55	16.00	35,35,35,35	1
58	MG	AA	3702	1/1	0.96	0.37	15.80	35,35,35,35	1
58	MG	AA	3708	1/1	0.90	0.52	15.56	53,53,53,53	1
58	MG	AA	3829	1/1	0.93	0.60	15.40	88,88,88,88	0
58	MG	AX	101	1/1	0.74	0.44	15.36	75,75,75,75	0
58	MG	AA	3168	1/1	0.80	0.38	15.05	63,63,63,63	0
58	MG	CA	3276	1/1	0.95	0.31	14.95	50,50,50,50	0
58	MG	CA	3038	1/1	0.90	0.37	14.89	48,48,48,48	0
58	MG	CA	3201	1/1	0.98	0.38	14.71	59,59,59,59	0
58	MG	AA	3525	1/1	0.95	0.33	14.67	40,40,40,40	0
58	MG	AA	3110	1/1	0.90	0.32	14.45	79,79,79,79	0
58	MG	CA	3226	1/1	0.84	0.35	14.36	69,69,69,69	0
58	MG	BA	1686	1/1	0.96	0.32	14.33	52,52,52,52	0
58	MG	AA	3267	1/1	0.91	0.42	14.05	63,63,63,63	0
58	MG	CA	3229	1/1	0.96	0.33	14.00	51,51,51,51	0
58	MG	CA	3597	1/1	0.94	0.28	13.92	39,39,39,39	0
58	MG	CU	201	1/1	0.89	0.56	13.82	64,64,64,64	0
58	MG	AA	3223	1/1	0.84	0.42	13.79	35,35,35,35	0
58	MG	AA	3823	1/1	0.97	0.24	13.46	37,37,37,37	1
58	MG	AA	3771	1/1	0.88	0.24	13.23	31,31,31,31	1
58	MG	CA	3212	1/1	0.83	0.33	13.18	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	1636	1/1	0.91	0.41	13.09	70,70,70,70	0
58	MG	AA	3819	1/1	0.92	0.26	13.05	25,25,25,25	1
58	MG	CA	3313	1/1	0.95	0.33	12.88	50,50,50,50	0
58	MG	AA	3173	1/1	0.96	0.24	12.82	60,60,60,60	0
58	MG	AA	3372	1/1	0.86	0.31	12.69	63,63,63,63	0
58	MG	CE	301	1/1	0.95	0.37	12.67	66,66,66,66	0
58	MG	CA	3428	1/1	0.93	0.29	12.49	54,54,54,54	1
58	MG	CA	3361	1/1	0.97	0.31	12.25	58,58,58,58	0
58	MG	AA	3138	1/1	0.94	0.37	12.22	50,50,50,50	0
58	MG	CA	3654	1/1	0.85	0.39	12.10	51,51,51,51	0
58	MG	CA	3661	1/1	0.91	0.26	12.01	74,74,74,74	0
58	MG	CA	3169	1/1	0.95	0.28	11.95	34,34,34,34	0
58	MG	AD	301	1/1	0.82	0.49	11.78	70,70,70,70	0
58	MG	AA	3331	1/1	0.95	0.28	11.75	34,34,34,34	0
58	MG	DA	1697	1/1	0.93	0.31	11.70	62,62,62,62	0
58	MG	AA	3400	1/1	0.98	0.36	11.68	39,39,39,39	0
58	MG	CA	3030	1/1	0.89	0.47	11.67	57,57,57,57	1
58	MG	AA	3316	1/1	0.97	0.29	11.65	60,60,60,60	0
58	MG	CA	3110	1/1	0.95	0.35	11.12	63,63,63,63	0
58	MG	AA	3179	1/1	0.97	0.31	11.04	71,71,71,71	0
58	MG	CA	3084	1/1	0.92	0.34	11.01	59,59,59,59	1
58	MG	CA	3324	1/1	0.94	0.32	10.99	40,40,40,40	0
58	MG	CA	3014	1/1	0.89	0.44	10.96	62,62,62,62	0
58	MG	CD	303	1/1	0.97	0.52	10.87	37,37,37,37	0
58	MG	AA	3420	1/1	0.93	0.23	10.86	26,26,26,26	0
58	MG	DA	1618	1/1	0.91	0.45	10.86	65,65,65,65	0
58	MG	BA	1623	1/1	0.92	0.27	10.84	65,65,65,65	0
58	MG	CF	303	1/1	0.92	0.39	10.84	62,62,62,62	0
58	MG	AA	3282	1/1	0.90	0.49	10.72	40,40,40,40	0
58	MG	CA	3137	1/1	0.89	0.36	10.65	73,73,73,73	0
58	MG	AA	3150	1/1	0.96	0.31	10.51	15,15,15,15	0
58	MG	AA	3773	1/1	0.94	0.34	10.48	30,30,30,30	1
58	MG	AA	3620	1/1	0.95	0.32	10.45	40,40,40,40	0
58	MG	CA	3455	1/1	0.95	0.27	10.29	47,47,47,47	0
58	MG	BA	1616	1/1	0.67	0.61	10.19	134,134,134,134	0
58	MG	CA	3027	1/1	0.85	0.36	10.16	44,44,44,44	0
58	MG	DA	1638	1/1	0.91	0.33	10.13	83,83,83,83	0
58	MG	AA	3210	1/1	0.95	0.33	9.99	24,24,24,24	1
58	MG	AA	3698	1/1	0.94	0.28	9.93	32,32,32,32	1
58	MG	BA	1783	1/1	0.90	0.33	9.62	69,69,69,69	0
58	MG	AH	3001	1/1	0.93	0.30	9.59	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	MG	AA	3130	1/1	0.94	0.26	9.55	37,37,37,37	0
58	MG	AA	3602	1/1	0.94	0.27	9.54	37,37,37,37	0
58	MG	CA	3375	1/1	0.92	0.32	9.52	71,71,71,71	0
58	MG	AA	3039	1/1	0.95	0.32	9.51	39,39,39,39	1
58	MG	CA	3326	1/1	0.92	0.24	9.50	34,34,34,34	0
58	MG	AA	3418	1/1	0.92	0.24	9.47	43,43,43,43	0
58	MG	CA	3607	1/1	0.84	0.28	9.46	97,97,97,97	0
58	MG	AD	302	1/1	0.87	0.38	9.43	19,19,19,19	0
58	MG	AA	3559	1/1	0.96	0.22	9.30	39,39,39,39	0
58	MG	BA	1683	1/1	0.94	0.30	9.22	69,69,69,69	0
58	MG	BA	1721	1/1	0.91	0.23	9.15	60,60,60,60	0
58	MG	CA	3163	1/1	0.90	0.34	9.12	40,40,40,40	0
58	MG	AA	3174	1/1	0.89	0.31	9.02	63,63,63,63	0
58	MG	BA	1630	1/1	0.70	0.31	9.00	63,63,63,63	0
58	MG	CA	3489	1/1	0.89	0.25	8.92	80,80,80,80	0
58	MG	DA	1649	1/1	0.71	0.85	8.91	93,93,93,93	0
58	MG	AB	3008	1/1	0.94	0.47	8.80	51,51,51,51	0
58	MG	CA	3463	1/1	0.85	0.28	8.66	49,49,49,49	0
58	MG	AA	3805	1/1	0.94	0.33	8.64	35,35,35,35	1
58	MG	AA	3249	1/1	0.87	0.34	8.63	24,24,24,24	1
58	MG	CA	3432	1/1	0.91	0.28	8.57	61,61,61,61	0
58	MG	CA	3119	1/1	0.98	0.31	8.51	128,128,128,128	0
58	MG	BA	1755	1/1	0.98	0.31	8.51	38,38,38,38	0
58	MG	CA	3213	1/1	0.90	0.27	8.46	44,44,44,44	0
58	MG	AA	3816	1/1	0.94	0.29	8.37	43,43,43,43	0
58	MG	AA	3081	1/1	0.85	0.29	8.35	40,40,40,40	0
58	MG	CA	3013	1/1	0.79	0.31	8.28	63,63,63,63	0
58	MG	AA	3617	1/1	0.89	0.23	8.25	49,49,49,49	0
58	MG	CA	3420	1/1	0.86	0.29	8.22	71,71,71,71	0
58	MG	AA	3311	1/1	0.89	0.21	8.03	33,33,33,33	0
58	MG	CA	3626	1/1	0.91	0.28	8.02	75,75,75,75	0
58	MG	AA	3354	1/1	0.83	0.31	8.01	60,60,60,60	0
58	MG	AD	309	1/1	0.74	0.30	7.94	57,57,57,57	0
58	MG	AA	3250	1/1	0.85	0.30	7.94	46,46,46,46	0
58	MG	AA	3190	1/1	0.92	0.25	7.93	45,45,45,45	0
58	MG	AA	3565	1/1	0.88	0.28	7.92	29,29,29,29	0
58	MG	DT	3001	1/1	0.87	0.53	7.92	67,67,67,67	0
58	MG	AA	3706	1/1	0.95	0.24	7.90	27,27,27,27	1
58	MG	AF	303	1/1	0.96	0.32	7.82	50,50,50,50	0
58	MG	AU	202	1/1	0.97	0.30	7.80	29,29,29,29	1
58	MG	AA	3817	1/1	0.90	0.32	7.79	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3833	1/1	0.92	0.40	7.70	49,49,49,49	0
58	MG	AA	3037	1/1	0.96	0.31	7.69	45,45,45,45	0
58	MG	AD	304	1/1	0.91	0.31	7.64	38,38,38,38	1
58	MG	AA	3381	1/1	0.94	0.27	7.64	27,27,27,27	0
58	MG	DA	1694	1/1	0.91	0.29	7.62	60,60,60,60	0
58	MG	AA	3120	1/1	0.91	0.25	7.61	46,46,46,46	0
58	MG	AU	201	1/1	0.93	0.30	7.60	44,44,44,44	0
58	MG	AA	3824	1/1	0.89	0.27	7.56	45,45,45,45	0
58	MG	CA	3221	1/1	0.86	0.27	7.45	54,54,54,54	0
58	MG	DA	1768	1/1	0.94	0.43	7.31	73,73,73,73	0
58	MG	AA	3048	1/1	0.97	0.26	7.26	34,34,34,34	0
58	MG	CA	3530	1/1	0.95	0.26	7.07	59,59,59,59	0
58	MG	CA	3124	1/1	0.93	0.26	6.82	48,48,48,48	0
58	MG	CA	3396	1/1	0.75	0.24	6.74	58,58,58,58	0
58	MG	AA	3508	1/1	0.94	0.27	6.70	49,49,49,49	0
58	MG	AA	3564	1/1	0.98	0.22	6.66	19,19,19,19	0
58	MG	AD	308	1/1	0.93	0.39	6.62	42,42,42,42	0
58	MG	AA	3507	1/1	0.97	0.25	6.57	14,14,14,14	0
58	MG	AA	3253	1/1	0.94	0.27	6.56	29,29,29,29	1
58	MG	DA	1680	1/1	0.92	0.31	6.53	62,62,62,62	0
58	MG	CA	3383	1/1	0.96	0.25	6.49	44,44,44,44	0
58	MG	AA	3113	1/1	0.91	0.32	6.48	64,64,64,64	0
58	MG	AA	3798	1/1	0.98	0.27	6.45	35,35,35,35	0
58	MG	CA	3217	1/1	0.80	0.30	6.38	52,52,52,52	0
58	MG	CA	3490	1/1	0.97	0.26	6.38	67,67,67,67	0
58	MG	AA	3240	1/1	0.95	0.34	6.37	30,30,30,30	0
58	MG	AA	3059	1/1	0.77	0.26	6.27	51,51,51,51	0
58	MG	CE	303	1/1	0.90	0.34	6.26	54,54,54,54	0
58	MG	CA	3650	1/1	0.95	0.27	6.23	27,27,27,27	0
58	MG	AA	3506	1/1	0.96	0.27	6.23	32,32,32,32	0
58	MG	CA	3190	1/1	0.91	0.37	6.20	83,83,83,83	0
58	MG	AA	3589	1/1	0.93	0.26	6.14	21,21,21,21	1
58	MG	CA	3091	1/1	0.92	0.35	6.04	111,111,111,111	0
58	MG	AA	3488	1/1	0.98	0.23	6.04	20,20,20,20	0
58	MG	CA	3330	1/1	0.94	0.24	5.99	43,43,43,43	0
58	MG	CA	3109	1/1	0.86	0.25	5.96	54,54,54,54	0
58	MG	AA	3443	1/1	0.93	0.21	5.94	65,65,65,65	0
58	MG	CA	3011	1/1	0.95	0.23	5.94	47,47,47,47	0
58	MG	CA	3127	1/1	0.97	0.25	5.90	63,63,63,63	0
58	MG	CA	3476	1/1	0.95	0.25	5.83	55,55,55,55	0
58	MG	AA	3791	1/1	0.99	0.26	5.73	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3452	1/1	0.96	0.24	5.71	61,61,61,61	0
58	MG	AA	3596	1/1	0.87	0.23	5.69	40,40,40,40	0
58	MG	AA	3247	1/1	0.87	0.31	5.64	63,63,63,63	0
58	MG	BA	1648	1/1	0.85	0.22	5.62	37,37,37,37	0
58	MG	AV	202	1/1	0.89	0.30	5.60	55,55,55,55	1
58	MG	CA	3458	1/1	0.90	0.24	5.59	49,49,49,49	0
58	MG	A8	5001	1/1	0.88	0.35	5.58	59,59,59,59	0
58	MG	CA	3603	1/1	0.80	0.25	5.56	51,51,51,51	0
58	MG	DA	1669	1/1	0.89	0.40	5.49	84,84,84,84	0
58	MG	AD	310	1/1	0.93	0.31	5.47	58,58,58,58	0
58	MG	AA	3329	1/1	0.98	0.23	5.43	17,17,17,17	0
58	MG	BA	1811	1/1	0.81	0.32	5.35	75,75,75,75	0
58	MG	AA	3034	1/1	0.90	0.29	5.34	57,57,57,57	0
58	MG	AA	3023	1/1	0.98	0.31	5.33	33,33,33,33	1
58	MG	AA	3142	1/1	0.94	0.18	5.29	26,26,26,26	1
58	MG	AA	3717	1/1	0.96	0.24	5.27	47,47,47,47	0
58	MG	AA	3014	1/1	0.91	0.20	5.19	45,45,45,45	0
58	MG	AA	3187	1/1	0.93	0.26	5.12	32,32,32,32	0
58	MG	CQ	201	1/1	0.66	0.28	5.08	62,62,62,62	0
58	MG	AA	3551	1/1	0.93	0.23	5.00	52,52,52,52	0
58	MG	AA	3036	1/1	0.92	0.19	4.95	51,51,51,51	0
58	MG	CA	3037	1/1	0.85	0.23	4.95	58,58,58,58	0
58	MG	DA	1722	1/1	0.86	0.26	4.92	65,65,65,65	0
58	MG	CA	3023	1/1	0.96	0.25	4.91	46,46,46,46	0
58	MG	AD	305	1/1	0.77	0.40	4.88	53,53,53,53	1
58	MG	AA	3439	1/1	0.97	0.23	4.80	17,17,17,17	0
58	MG	AA	3357	1/1	0.95	0.22	4.80	27,27,27,27	0
58	MG	AA	3820	1/1	0.94	0.29	4.79	40,40,40,40	0
58	MG	AA	3830	1/1	0.95	0.26	4.75	45,45,45,45	0
58	MG	AA	3395	1/1	0.96	0.21	4.74	18,18,18,18	0
58	MG	AA	3183	1/1	0.88	0.25	4.74	35,35,35,35	1
58	MG	CA	3353	1/1	0.97	0.23	4.71	48,48,48,48	0
58	MG	AA	3440	1/1	0.96	0.22	4.61	31,31,31,31	0
58	MG	AA	3806	1/1	0.81	0.25	4.61	61,61,61,61	0
58	MG	CA	3041	1/1	0.94	0.27	4.60	31,31,31,31	0
58	MG	CA	3263	1/1	0.93	0.25	4.58	57,57,57,57	0
58	MG	AA	3309	1/1	0.92	0.20	4.50	44,44,44,44	0
58	MG	CA	3086	1/1	0.94	0.24	4.50	36,36,36,36	0
58	MG	CA	3358	1/1	0.93	0.29	4.49	45,45,45,45	0
58	MG	AB	3003	1/1	0.88	0.24	4.46	51,51,51,51	0
58	MG	AA	3704	1/1	0.88	0.27	4.44	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1671	1/1	0.81	0.23	4.41	75,75,75,75	0
58	MG	BA	1723	1/1	0.89	0.31	4.37	71,71,71,71	0
58	MG	BA	1678	1/1	0.87	0.26	4.35	69,69,69,69	0
58	MG	AA	3827	1/1	0.96	0.22	4.35	40,40,40,40	0
58	MG	DA	1610	1/1	0.86	0.22	4.35	75,75,75,75	0
58	MG	CA	3409	1/1	0.91	0.24	4.25	40,40,40,40	0
58	MG	CV	202	1/1	0.91	0.28	4.23	85,85,85,85	0
58	MG	CA	3364	1/1	0.97	0.24	4.21	29,29,29,29	0
58	MG	DA	1689	1/1	0.87	0.22	4.15	58,58,58,58	0
58	MG	BA	1626	1/1	0.88	0.30	4.13	75,75,75,75	0
58	MG	AA	3711	1/1	0.93	0.29	4.11	34,34,34,34	1
58	MG	CA	3555	1/1	0.74	0.26	4.11	83,83,83,83	0
58	MG	CA	3133	1/1	0.91	0.24	4.07	69,69,69,69	0
58	MG	AA	3082	1/1	0.97	0.20	3.98	23,23,23,23	1
58	MG	AA	3102	1/1	0.97	0.19	3.92	49,49,49,49	0
58	MG	AA	3811	1/1	0.93	0.29	3.85	58,58,58,58	0
58	MG	CA	3309	1/1	0.97	0.21	3.78	29,29,29,29	0
58	MG	AA	3231	1/1	0.85	0.22	3.74	53,53,53,53	0
58	MG	AA	3442	1/1	0.81	0.30	3.61	49,49,49,49	0
58	MG	AA	3812	1/1	0.91	0.22	3.59	42,42,42,42	0
58	MG	AF	302	1/1	0.91	0.29	3.56	41,41,41,41	0
58	MG	AA	3109	1/1	0.88	0.22	3.54	50,50,50,50	0
58	MG	AA	3621	1/1	0.79	0.18	3.46	46,46,46,46	0
58	MG	AA	3020	1/1	0.96	0.20	3.40	25,25,25,25	0
58	MG	AA	3388	1/1	0.99	0.23	3.37	25,25,25,25	0
58	MG	CA	3002	1/1	0.43	0.28	3.37	114,114,114,114	0
58	MG	AE	304	1/1	0.89	0.27	3.33	30,30,30,30	0
58	MG	CA	3596	1/1	0.72	0.23	3.29	72,72,72,72	0
58	MG	AA	3012	1/1	0.80	0.23	3.26	34,34,34,34	0
58	MG	AA	3456	1/1	0.91	0.18	3.25	30,30,30,30	0
58	MG	AA	3410	1/1	0.91	0.22	3.18	30,30,30,30	0
58	MG	BA	1695	1/1	0.70	0.21	3.15	98,98,98,98	0
58	MG	CA	3491	1/1	0.91	0.20	3.15	51,51,51,51	0
58	MG	BA	1693	1/1	0.70	0.28	3.14	67,67,67,67	0
58	MG	AA	3831	1/1	0.89	0.22	3.11	65,65,65,65	0
58	MG	AA	3828	1/1	0.92	0.28	3.08	37,37,37,37	1
58	MG	AA	3735	1/1	0.67	0.23	3.01	35,35,35,35	0
58	MG	DF	3001	1/1	0.79	0.22	2.97	49,49,49,49	0
58	MG	AA	3581	1/1	0.92	0.22	2.95	40,40,40,40	0
58	MG	BA	1690	1/1	0.81	0.30	2.90	89,89,89,89	0
58	MG	BA	1763	1/1	0.91	0.27	2.90	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BT	3001	1/1	0.95	0.37	2.86	62,62,62,62	0
58	MG	AA	3726	1/1	0.92	0.19	2.82	67,67,67,67	0
58	MG	CA	3178	1/1	0.93	0.22	2.82	57,57,57,57	0
58	MG	AA	3128	1/1	0.86	0.28	2.80	59,59,59,59	0
58	MG	AA	3044	1/1	0.94	0.20	2.76	34,34,34,34	0
58	MG	CA	3328	1/1	0.86	0.26	2.76	55,55,55,55	0
58	MG	DA	1658	1/1	0.92	0.21	2.69	72,72,72,72	0
58	MG	AQ	202	1/1	0.97	0.21	2.68	31,31,31,31	0
58	MG	BA	1615	1/1	0.78	0.31	2.62	74,74,74,74	0
58	MG	AA	3272	1/1	0.74	0.45	2.62	52,52,52,52	0
58	MG	CA	3251	1/1	0.94	0.19	2.57	56,56,56,56	0
58	MG	CA	3567	1/1	0.94	0.20	2.50	56,56,56,56	0
58	MG	CA	3159	1/1	0.83	0.41	2.50	69,69,69,69	0
58	MG	CA	3392	1/1	0.85	0.21	2.49	35,35,35,35	0
58	MG	AA	3257	1/1	0.88	0.19	2.47	14,14,14,14	0
58	MG	CA	3302	1/1	0.86	0.21	2.45	68,68,68,68	0
58	MG	AA	3485	1/1	0.92	0.21	2.45	14,14,14,14	0
58	MG	AA	3832	1/1	0.97	0.22	2.43	38,38,38,38	0
58	MG	CA	3281	1/1	0.96	0.26	2.42	51,51,51,51	0
58	MG	AA	3043	1/1	0.96	0.22	2.40	31,31,31,31	0
58	MG	AA	3736	1/1	0.96	0.21	2.40	78,78,78,78	0
58	MG	AA	3815	1/1	0.98	0.17	2.31	29,29,29,29	1
58	MG	AA	3623	1/1	0.67	0.20	2.28	74,74,74,74	0
58	MG	AA	3314	1/1	0.97	0.20	2.25	28,28,28,28	0
58	MG	CA	3177	1/1	0.96	0.22	2.25	36,36,36,36	0
58	MG	C3	3001	1/1	0.95	0.33	2.13	69,69,69,69	0
58	MG	BA	1740	1/1	0.93	0.19	2.12	50,50,50,50	0
58	MG	CA	3266	1/1	0.96	0.21	2.10	69,69,69,69	0
58	MG	CA	3146	1/1	0.93	0.24	2.07	60,60,60,60	0
58	MG	CA	3340	1/1	0.88	0.22	2.07	48,48,48,48	0
58	MG	AA	3793	1/1	0.87	0.22	2.07	28,28,28,28	0
58	MG	AA	3499	1/1	0.95	0.18	2.07	51,51,51,51	1
58	MG	AA	3741	1/1	0.93	0.20	2.01	34,34,34,34	1
58	MG	AA	3519	1/1	0.87	0.19	2.00	21,21,21,21	0
58	MG	BA	1773	1/1	0.93	0.24	1.99	78,78,78,78	0
58	MG	CA	3214	1/1	0.95	0.19	1.95	40,40,40,40	0
58	MG	DA	1765	1/1	0.84	0.19	1.95	95,95,95,95	0
58	MG	CA	3362	1/1	0.93	0.19	1.92	44,44,44,44	0
58	MG	BA	1603	1/1	0.68	0.23	1.90	67,67,67,67	0
58	MG	AB	3014	1/1	0.94	0.18	1.86	67,67,67,67	0
58	MG	AA	3334	1/1	0.91	0.21	1.85	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AB	3016	1/1	0.96	0.17	1.81	34,34,34,34	0
58	MG	AA	3721	1/1	0.91	0.22	1.80	10,10,10,10	0
58	MG	AA	3518	1/1	0.87	0.22	1.79	33,33,33,33	0
58	MG	AA	3356	1/1	0.89	0.20	1.78	35,35,35,35	0
58	MG	CA	3318	1/1	0.99	0.22	1.74	33,33,33,33	0
58	MG	AA	3394	1/1	0.96	0.18	1.74	27,27,27,27	0
58	MG	BA	1752	1/1	0.97	0.21	1.73	48,48,48,48	0
58	MG	BF	3001	1/1	0.91	0.26	1.72	74,74,74,74	0
58	MG	AB	3017	1/1	0.69	0.18	1.72	77,77,77,77	0
58	MG	CV	201	1/1	0.79	0.22	1.70	100,100,100,100	0
58	MG	AA	3278	1/1	0.92	0.18	1.70	36,36,36,36	0
58	MG	AA	3543	1/1	0.83	0.20	1.66	52,52,52,52	1
58	MG	AP	201	1/1	0.96	0.21	1.62	28,28,28,28	1
58	MG	CW	201	1/1	0.94	0.26	1.58	39,39,39,39	0
58	MG	CA	3657	1/1	0.84	0.21	1.58	67,67,67,67	0
58	MG	AA	3714	1/1	0.94	0.20	1.52	56,56,56,56	0
58	MG	CA	3400	1/1	0.92	0.23	1.52	62,62,62,62	0
58	MG	CA	3521	1/1	0.93	0.20	1.48	61,61,61,61	0
58	MG	CA	3243	1/1	0.70	0.19	1.47	78,78,78,78	0
58	MG	CA	3433	1/1	0.95	0.16	1.47	71,71,71,71	0
58	MG	AA	3505	1/1	0.94	0.17	1.43	31,31,31,31	0
58	MG	BA	1700	1/1	0.85	0.24	1.43	61,61,61,61	0
58	MG	CB	3007	1/1	0.76	0.19	1.42	65,65,65,65	0
58	MG	AA	3401	1/1	0.95	0.19	1.42	33,33,33,33	0
58	MG	DA	1739	1/1	0.87	0.20	1.40	79,79,79,79	0
61	FUA	BZ	703	37/37	0.85	0.27	1.36	69,69,69,69	0
58	MG	AA	3821	1/1	0.97	0.20	1.29	41,41,41,41	1
58	MG	AA	3290	1/1	0.92	0.18	1.28	63,63,63,63	0
58	MG	AD	307	1/1	0.87	0.16	1.25	37,37,37,37	0
58	MG	DA	1682	1/1	0.95	0.20	1.24	47,47,47,47	0
58	MG	AD	303	1/1	0.88	0.17	1.24	63,63,63,63	0
58	MG	CA	3662	1/1	0.87	0.23	1.22	55,55,55,55	0
58	MG	CA	3487	1/1	0.92	0.21	1.21	70,70,70,70	0
58	MG	AA	3433	1/1	0.97	0.21	1.20	28,28,28,28	0
58	MG	AA	3181	1/1	0.92	0.18	1.19	56,56,56,56	0
58	MG	AA	3459	1/1	0.98	0.19	1.14	18,18,18,18	0
58	MG	CG	3001	1/1	0.69	0.31	1.10	83,83,83,83	0
58	MG	AA	3050	1/1	0.95	0.19	1.08	53,53,53,53	0
58	MG	CA	3655	1/1	0.98	0.23	1.03	70,70,70,70	0
58	MG	AA	3045	1/1	0.98	0.19	1.03	43,43,43,43	0
58	MG	CA	3550	1/1	0.97	0.18	1.00	33,33,33,33	0
58	MG	CA	3332	1/1	0.92	0.22	0.99	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
61	FUA	DZ	703	37/37	0.87	0.23	0.98	85,85,85,85	0
58	MG	CA	3413	1/1	0.94	0.21	0.97	39,39,39,39	0
58	MG	AA	3723	1/1	0.98	0.20	0.95	21,21,21,21	0
58	MG	AA	3511	1/1	0.92	0.21	0.91	12,12,12,12	0
58	MG	AA	3213	1/1	0.84	0.17	0.87	58,58,58,58	0
58	MG	BA	1624	1/1	0.63	0.19	0.85	87,87,87,87	0
58	MG	BK	201	1/1	0.87	0.17	0.85	57,57,57,57	0
58	MG	DE	201	1/1	0.86	0.18	0.82	84,84,84,84	0
58	MG	AA	3473	1/1	0.98	0.21	0.80	15,15,15,15	0
58	MG	DA	1720	1/1	0.47	0.19	0.76	72,72,72,72	0
58	MG	BA	1704	1/1	0.87	0.23	0.74	61,61,61,61	0
58	MG	CA	3453	1/1	0.97	0.20	0.68	39,39,39,39	0
58	MG	AA	3169	1/1	0.94	0.20	0.67	39,39,39,39	0
58	MG	BA	1662	1/1	0.85	0.17	0.65	53,53,53,53	0
58	MG	CA	3457	1/1	0.96	0.21	0.62	47,47,47,47	0
58	MG	AA	3300	1/1	0.95	0.19	0.60	50,50,50,50	0
58	MG	AA	3145	1/1	0.95	0.17	0.59	33,33,33,33	0
58	MG	AD	306	1/1	0.91	0.16	0.59	73,73,73,73	0
58	MG	AA	3622	1/1	0.96	0.17	0.59	45,45,45,45	0
58	MG	DA	1637	1/1	0.89	0.25	0.57	76,76,76,76	0
58	MG	AA	3469	1/1	0.95	0.16	0.57	43,43,43,43	0
58	MG	BA	1748	1/1	0.86	0.30	0.55	84,84,84,84	0
58	MG	CA	3267	1/1	0.88	0.17	0.53	56,56,56,56	0
58	MG	AA	3546	1/1	0.92	0.20	0.50	32,32,32,32	0
58	MG	AA	3404	1/1	0.95	0.19	0.50	19,19,19,19	0
58	MG	CA	3315	1/1	0.97	0.16	0.46	60,60,60,60	0
58	MG	AA	3389	1/1	0.99	0.19	0.46	17,17,17,17	0
58	MG	AA	3041	1/1	0.77	0.17	0.44	75,75,75,75	0
58	MG	AA	3235	1/1	0.57	0.16	0.39	64,64,64,64	0
58	MG	CF	302	1/1	0.95	0.19	0.31	56,56,56,56	0
58	MG	CA	3417	1/1	0.98	0.21	0.25	37,37,37,37	0
58	MG	AA	3007	1/1	0.91	0.16	0.25	21,21,21,21	0
58	MG	AA	3315	1/1	0.96	0.18	0.24	34,34,34,34	0
58	MG	AA	3535	1/1	0.95	0.19	0.20	15,15,15,15	0
58	MG	CF	305	1/1	0.77	0.16	0.18	51,51,51,51	0
58	MG	CA	3448	1/1	0.96	0.19	0.17	43,43,43,43	0
58	MG	CA	3564	1/1	0.99	0.19	0.14	40,40,40,40	1
58	MG	AA	3275	1/1	0.93	0.22	0.14	47,47,47,47	1
58	MG	BA	1800	1/1	0.65	0.21	0.13	84,84,84,84	0
62	GDP	DZ	704	28/28	0.93	0.17	0.13	80,80,80,80	3
58	MG	BA	1810	1/1	0.85	0.26	0.12	66,66,66,66	0
58	MG	BA	1685	1/1	0.90	0.18	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1640	1/1	0.90	0.19	0.12	55,55,55,55	0
58	MG	CA	3579	1/1	0.88	0.18	0.12	51,51,51,51	0
58	MG	AA	3540	1/1	0.97	0.19	0.05	29,29,29,29	0
58	MG	AA	3377	1/1	0.99	0.19	0.05	20,20,20,20	0
58	MG	CA	3424	1/1	0.96	0.17	0.03	55,55,55,55	0
58	MG	CA	3003	1/1	0.92	0.20	0.02	45,45,45,45	0
58	MG	BA	1702	1/1	0.78	0.18	0.00	89,89,89,89	0
58	MG	AA	3686	1/1	0.93	0.18	-0.01	73,73,73,73	0
58	MG	CA	3273	1/1	0.87	0.17	-0.02	69,69,69,69	0
58	MG	AA	3341	1/1	0.92	0.21	-0.04	15,15,15,15	0
58	MG	AA	3217	1/1	0.96	0.17	-0.09	6,6,6,6	0
58	MG	AA	3687	1/1	0.93	0.18	-0.12	45,45,45,45	0
58	MG	AA	3258	1/1	0.82	0.18	-0.14	22,22,22,22	0
58	MG	DA	1715	1/1	0.90	0.24	-0.17	76,76,76,76	0
58	MG	CA	3656	1/1	0.92	0.23	-0.19	61,61,61,61	0
58	MG	AA	3378	1/1	0.95	0.17	-0.20	19,19,19,19	0
58	MG	AA	3517	1/1	0.97	0.19	-0.21	19,19,19,19	0
58	MG	CA	3311	1/1	0.92	0.15	-0.22	48,48,48,48	0
58	MG	AA	3649	1/1	0.91	0.14	-0.27	92,92,92,92	0
58	MG	AA	3383	1/1	0.90	0.19	-0.34	54,54,54,54	0
58	MG	CA	3047	1/1	0.88	0.16	-0.37	61,61,61,61	0
58	MG	CQ	203	1/1	0.86	0.15	-0.41	67,67,67,67	0
58	MG	CA	3615	1/1	0.96	0.18	-0.44	38,38,38,38	0
58	MG	AA	3583	1/1	0.99	0.16	-0.45	13,13,13,13	0
58	MG	AA	3202	1/1	0.74	0.15	-0.46	47,47,47,47	0
58	MG	CA	3020	1/1	0.76	0.17	-0.48	63,63,63,63	0
58	MG	AA	3524	1/1	0.94	0.17	-0.48	28,28,28,28	0
58	MG	DA	1709	1/1	0.89	0.16	-0.48	72,72,72,72	0
58	MG	CA	3439	1/1	0.91	0.20	-0.49	38,38,38,38	0
58	MG	AA	3515	1/1	0.95	0.17	-0.51	20,20,20,20	0
58	MG	CA	3069	1/1	0.94	0.18	-0.52	81,81,81,81	0
58	MG	CA	3192	1/1	0.92	0.14	-0.52	58,58,58,58	0
58	MG	AA	3734	1/1	0.98	0.17	-0.55	22,22,22,22	0
58	MG	AV	201	1/1	0.98	0.19	-0.59	38,38,38,38	0
58	MG	CB	3004	1/1	0.93	0.15	-0.60	68,68,68,68	0
62	GDP	BZ	704	28/28	0.97	0.15	-0.60	53,53,53,53	1
58	MG	CA	3337	1/1	0.93	0.17	-0.60	41,41,41,41	0
58	MG	AA	3792	1/1	0.92	0.17	-0.61	45,45,45,45	0
58	MG	CA	3664	1/1	0.92	0.15	-0.63	54,54,54,54	0
58	MG	AA	3542	1/1	0.95	0.15	-0.63	63,63,63,63	0
58	MG	CA	3160	1/1	0.91	0.13	-0.68	42,42,42,42	0
58	MG	CA	3057	1/1	0.93	0.17	-0.70	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3794	1/1	0.91	0.17	-0.76	58,58,58,58	1
58	MG	DA	1630	1/1	0.81	0.16	-0.80	61,61,61,61	0
58	MG	AA	3393	1/1	0.98	0.18	-0.83	21,21,21,21	0
59	ZN	A5	101	1/1	1.00	0.12	-0.95	36,36,36,36	0
58	MG	BA	1679	1/1	0.96	0.15	-0.99	36,36,36,36	0
58	MG	AG	202	1/1	0.93	0.14	-1.02	73,73,73,73	0
58	MG	DA	1695	1/1	0.93	0.14	-1.04	66,66,66,66	0
58	MG	DA	1666	1/1	0.94	0.17	-1.05	66,66,66,66	0
58	MG	BA	1675	1/1	0.91	0.16	-1.05	57,57,57,57	0
58	MG	BA	1789	1/1	0.85	0.13	-1.06	68,68,68,68	0
58	MG	CA	3410	1/1	0.96	0.19	-1.12	31,31,31,31	0
58	MG	DA	1601	1/1	0.89	0.14	-1.12	61,61,61,61	0
58	MG	AA	3725	1/1	0.93	0.17	-1.13	39,39,39,39	0
59	ZN	C5	102	1/1	0.99	0.09	-1.17	68,68,68,68	0
58	MG	AA	3818	1/1	0.94	0.16	-1.26	19,19,19,19	0
58	MG	BM	201	1/1	0.87	0.12	-1.34	57,57,57,57	0
58	MG	CA	3105	1/1	0.61	0.12	-1.38	80,80,80,80	0
59	ZN	A4	501	1/1	0.96	0.06	-1.39	137,137,137,137	0
58	MG	AA	3009	1/1	0.94	0.14	-1.41	24,24,24,24	0
58	MG	DA	1721	1/1	0.92	0.13	-1.42	67,67,67,67	0
58	MG	AA	3571	1/1	0.89	0.15	-1.43	48,48,48,48	0
58	MG	AA	3826	1/1	0.96	0.17	-1.44	20,20,20,20	0
59	ZN	A9	501	1/1	1.00	0.10	-1.44	42,42,42,42	0
58	MG	CA	3346	1/1	0.95	0.17	-1.45	31,31,31,31	0
58	MG	CA	3427	1/1	0.86	0.14	-1.53	55,55,55,55	0
58	MG	AA	3200	1/1	0.73	0.11	-1.54	91,91,91,91	0
58	MG	CA	3227	1/1	0.96	0.15	-1.55	53,53,53,53	0
59	ZN	AY	501	1/1	0.99	0.08	-1.55	65,65,65,65	0
59	ZN	C6	501	1/1	0.99	0.10	-1.57	61,61,61,61	0
58	MG	AA	3072	1/1	0.94	0.14	-1.58	26,26,26,26	0
58	MG	AA	3099	1/1	0.87	0.13	-1.58	62,62,62,62	0
58	MG	AA	3529	1/1	0.97	0.16	-1.59	16,16,16,16	0
58	MG	AA	3619	1/1	0.96	0.15	-1.61	42,42,42,42	0
58	MG	CA	3261	1/1	0.96	0.17	-1.62	29,29,29,29	0
58	MG	DE	202	1/1	0.80	0.13	-1.66	94,94,94,94	0
58	MG	DA	1670	1/1	0.97	0.14	-1.68	75,75,75,75	0
60	SF4	DD	501	8/8	0.98	0.10	-1.70	90,90,90,90	1
58	MG	CA	3104	1/1	0.95	0.15	-1.72	48,48,48,48	0
58	MG	CA	3101	1/1	0.66	0.14	-1.73	78,78,78,78	0
58	MG	AA	3413	1/1	0.98	0.16	-1.78	20,20,20,20	0
58	MG	CA	3339	1/1	0.98	0.14	-1.78	34,34,34,34	0
58	MG	AA	3670	1/1	0.96	0.13	-1.79	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	SF4	BD	501	8/8	0.97	0.09	-1.79	80,80,80,80	0
59	ZN	C4	501	1/1	0.59	0.06	-1.85	189,189,189,189	0
58	MG	DA	1652	1/1	0.75	0.13	-1.86	71,71,71,71	0
58	MG	CA	3462	1/1	0.95	0.13	-1.89	49,49,49,49	0
58	MG	CA	3658	1/1	0.94	0.12	-1.90	50,50,50,50	0
58	MG	CA	3019	1/1	0.95	0.15	-1.92	28,28,28,28	0
58	MG	CA	3425	1/1	0.96	0.14	-1.93	53,53,53,53	0
58	MG	CA	3600	1/1	0.92	0.12	-1.93	50,50,50,50	0
58	MG	CA	3501	1/1	0.96	0.16	-1.94	45,45,45,45	1
59	ZN	A6	102	1/1	1.00	0.11	-1.96	46,46,46,46	0
58	MG	AA	3532	1/1	0.96	0.16	-2.00	25,25,25,25	0
58	MG	BA	1617	1/1	0.94	0.13	-2.01	73,73,73,73	0
58	MG	CA	3189	1/1	0.90	0.10	-2.07	68,68,68,68	0
58	MG	DA	1730	1/1	0.83	0.15	-2.09	88,88,88,88	0
58	MG	AA	3251	1/1	0.98	0.14	-2.11	42,42,42,42	0
58	MG	CA	3050	1/1	0.98	0.10	-2.12	44,44,44,44	0
59	ZN	C9	501	1/1	0.99	0.07	-2.14	94,94,94,94	0
58	MG	AA	3084	1/1	0.96	0.11	-2.15	32,32,32,32	0
58	MG	CA	3617	1/1	0.99	0.13	-2.18	31,31,31,31	0
58	MG	DA	1686	1/1	0.77	0.15	-2.19	53,53,53,53	0
58	MG	CA	3310	1/1	0.94	0.12	-2.19	48,48,48,48	0
59	ZN	DN	501	1/1	0.96	0.06	-2.29	129,129,129,129	0
58	MG	BA	1733	1/1	0.93	0.15	-2.35	62,62,62,62	0
58	MG	AA	3069	1/1	0.95	0.13	-2.38	34,34,34,34	0
58	MG	CA	3157	1/1	0.92	0.15	-2.38	55,55,55,55	0
58	MG	AA	3384	1/1	0.98	0.15	-2.39	34,34,34,34	0
58	MG	AA	3313	1/1	0.97	0.13	-2.40	35,35,35,35	0
59	ZN	BN	501	1/1	0.95	0.05	-2.50	123,123,123,123	0
58	MG	AA	3614	1/1	0.94	0.12	-2.50	56,56,56,56	0
58	MG	CA	3274	1/1	0.98	0.12	-2.53	50,50,50,50	1
58	MG	AA	3528	1/1	0.97	0.15	-2.55	28,28,28,28	0
58	MG	DA	1617	1/1	0.89	0.10	-2.56	48,48,48,48	0
58	MG	AA	3574	1/1	0.95	0.16	-2.58	30,30,30,30	1
58	MG	DA	1624	1/1	0.87	0.13	-2.61	44,44,44,44	0
59	ZN	CY	501	1/1	0.98	0.04	-2.66	93,93,93,93	0
58	MG	AA	3307	1/1	0.98	0.15	-2.67	6,6,6,6	0
58	MG	CA	3138	1/1	0.85	0.11	-2.70	63,63,63,63	0
58	MG	CA	3306	1/1	0.93	0.12	-2.72	41,41,41,41	0
58	MG	BA	1607	1/1	0.91	0.12	-2.75	62,62,62,62	0
58	MG	AA	3613	1/1	0.62	0.12	-2.76	104,104,104,104	0
58	MG	AA	3408	1/1	0.99	0.15	-2.78	20,20,20,20	0
58	MG	AA	3514	1/1	0.98	0.14	-2.82	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3322	1/1	0.98	0.13	-2.84	32,32,32,32	1
58	MG	CE	302	1/1	0.97	0.13	-2.85	47,47,47,47	0
58	MG	CA	3372	1/1	0.99	0.13	-2.92	42,42,42,42	0
58	MG	CA	3320	1/1	0.98	0.15	-3.03	30,30,30,30	0
58	MG	AB	3020	1/1	0.93	0.11	-3.07	55,55,55,55	0
58	MG	CA	3010	1/1	0.84	0.08	-3.07	41,41,41,41	0
58	MG	AA	3526	1/1	0.98	0.16	-3.08	20,20,20,20	0
58	MG	CA	3360	1/1	0.94	0.12	-3.09	49,49,49,49	0
58	MG	AA	3344	1/1	0.96	0.10	-3.10	84,84,84,84	0
58	MG	AA	3396	1/1	0.94	0.14	-3.13	22,22,22,22	0
58	MG	CA	3419	1/1	0.92	0.11	-3.24	60,60,60,60	0
58	MG	AA	3398	1/1	0.99	0.14	-3.26	15,15,15,15	0
58	MG	AA	3022	1/1	0.92	0.16	-3.28	9,9,9,9	0
58	MG	BA	1680	1/1	0.98	0.11	-3.29	53,53,53,53	0
58	MG	AA	3547	1/1	0.88	0.10	-3.29	31,31,31,31	0
58	MG	CA	3211	1/1	0.94	0.11	-3.32	40,40,40,40	0
58	MG	BA	1620	1/1	0.96	0.09	-3.42	37,37,37,37	0
58	MG	DA	1687	1/1	0.67	0.13	-3.42	100,100,100,100	0
58	MG	CA	3370	1/1	0.94	0.13	-3.43	47,47,47,47	0
58	MG	CA	3464	1/1	0.94	0.14	-3.43	46,46,46,46	0
58	MG	BA	1654	1/1	0.95	0.09	-3.46	54,54,54,54	0
58	MG	BB	3001	1/1	0.91	0.12	-3.49	75,75,75,75	0
58	MG	AG	201	1/1	0.95	0.10	-3.49	52,52,52,52	0
58	MG	AA	3750	1/1	0.91	0.13	-3.49	24,24,24,24	0
58	MG	AA	3486	1/1	0.95	0.16	-3.54	27,27,27,27	0
58	MG	AA	3572	1/1	0.93	0.14	-3.56	32,32,32,32	0
58	MG	CA	3278	1/1	0.87	0.15	-3.57	37,37,37,37	0
58	MG	CA	3488	1/1	0.91	0.10	-3.58	51,51,51,51	0
58	MG	CA	3265	1/1	0.96	0.11	-3.59	40,40,40,40	0
58	MG	CA	3560	1/1	0.98	0.13	-3.60	36,36,36,36	0
58	MG	AA	3435	1/1	0.96	0.16	-3.61	20,20,20,20	0
58	MG	AA	3324	1/1	0.96	0.12	-3.76	33,33,33,33	0
58	MG	AA	3642	1/1	0.95	0.14	-3.76	49,49,49,49	0
58	MG	AA	3387	1/1	0.99	0.14	-3.80	17,17,17,17	0
58	MG	AA	3038	1/1	0.99	0.13	-3.83	11,11,11,11	0
58	MG	CA	3584	1/1	0.95	0.13	-3.87	46,46,46,46	0
58	MG	AA	3775	1/1	0.89	0.11	-3.94	45,45,45,45	0
58	MG	BA	1674	1/1	0.94	0.05	-3.96	68,68,68,68	0
58	MG	AA	3556	1/1	0.94	0.15	-3.99	39,39,39,39	0
58	MG	AA	3054	1/1	0.94	0.14	-4.07	38,38,38,38	0
58	MG	DA	1645	1/1	0.98	0.12	-4.12	64,64,64,64	0
58	MG	CA	3282	1/1	0.98	0.12	-4.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3343	1/1	0.91	0.13	-4.18	36,36,36,36	0
58	MG	AA	3825	1/1	0.94	0.13	-4.22	17,17,17,17	1
58	MG	BA	1741	1/1	0.96	0.09	-4.33	46,46,46,46	0
58	MG	AB	3007	1/1	0.93	0.09	-4.38	45,45,45,45	0
58	MG	AA	3777	1/1	0.98	0.10	-4.50	19,19,19,19	0
58	MG	AA	3299	1/1	0.98	0.13	-4.53	20,20,20,20	0
58	MG	BA	1611	1/1	0.97	0.13	-4.71	31,31,31,31	0
58	MG	DA	1654	1/1	0.97	0.10	-4.76	30,30,30,30	0
58	MG	AA	3385	1/1	0.98	0.13	-5.03	28,28,28,28	0
58	MG	AA	3403	1/1	0.96	0.09	-5.09	28,28,28,28	0
58	MG	AA	3539	1/1	0.96	0.14	-5.15	28,28,28,28	0
58	MG	BA	1612	1/1	0.91	0.10	-5.23	75,75,75,75	0
58	MG	CA	3526	1/1	0.94	0.10	-5.34	40,40,40,40	0
58	MG	CA	3321	1/1	0.97	0.12	-5.48	31,31,31,31	0
58	MG	CA	3317	1/1	0.92	0.12	-5.54	44,44,44,44	0
58	MG	CA	3438	1/1	0.92	0.15	-5.71	46,46,46,46	0
58	MG	AA	3434	1/1	0.93	0.12	-5.77	17,17,17,17	0
58	MG	AA	3616	1/1	0.94	0.10	-5.81	28,28,28,28	0
58	MG	AA	3374	1/1	0.98	0.08	-5.89	18,18,18,18	0
58	MG	AA	3003	1/1	0.98	0.09	-6.00	20,20,20,20	0
58	MG	AA	3502	1/1	0.97	0.12	-6.14	51,51,51,51	1
58	MG	AA	3021	1/1	0.92	0.11	-6.28	40,40,40,40	0
58	MG	CA	3647	1/1	0.91	0.07	-6.69	66,66,66,66	0
58	MG	AA	3449	1/1	0.97	0.11	-6.79	15,15,15,15	0
58	MG	AA	3754	1/1	0.98	0.08	-6.82	29,29,29,29	0
58	MG	CA	3029	1/1	0.94	0.11	-6.84	33,33,33,33	0
58	MG	AA	3342	1/1	0.99	0.14	-7.04	5,5,5,5	0
58	MG	AA	3684	1/1	0.97	0.10	-7.16	29,29,29,29	0
58	MG	AA	3669	1/1	0.97	0.06	-7.28	33,33,33,33	0
58	MG	CA	3242	1/1	0.91	0.12	-7.99	41,41,41,41	0
58	MG	BA	1643	1/1	0.94	0.07	-8.03	58,58,58,58	0
58	MG	BA	1728	1/1	0.97	0.11	-8.14	52,52,52,52	0
58	MG	AA	3562	1/1	0.97	0.06	-8.28	48,48,48,48	1
58	MG	BA	1613	1/1	0.90	0.08	-9.17	101,101,101,101	0
58	MG	CA	3628	1/1	0.96	0.13	-9.52	66,66,66,66	0
58	MG	CA	3291	1/1	0.97	0.12	-9.95	27,27,27,27	0
58	MG	AA	3493	1/1	0.95	0.13	-10.19	30,30,30,30	1
58	MG	AA	3498	1/1	0.99	0.12	-10.33	37,37,37,37	0
58	MG	AA	3011	1/1	0.97	0.09	-11.13	40,40,40,40	0
58	MG	BA	1758	1/1	0.98	0.06	-12.63	57,57,57,57	0
58	MG	CA	3021	1/1	0.96	0.12	-13.57	29,29,29,29	0
58	MG	DA	1621	1/1	0.94	0.12	-15.63	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BW	503	1/1	0.89	0.15	-	45,45,45,45	0
58	MG	CA	3423	1/1	0.88	0.19	-	50,50,50,50	0
58	MG	CA	3048	1/1	0.94	0.18	-	86,86,86,86	0
58	MG	BA	1794	1/1	0.96	0.17	-	77,77,77,77	0
58	MG	CA	3454	1/1	0.92	0.18	-	81,81,81,81	0
58	MG	CA	3074	1/1	0.92	0.50	-	53,53,53,53	0
58	MG	BA	1757	1/1	0.87	0.28	-	65,65,65,65	0
58	MG	AA	3452	1/1	0.95	0.14	-	69,69,69,69	0
58	MG	AQ	203	1/1	0.94	0.43	-	41,41,41,41	0
58	MG	AA	3656	1/1	0.81	0.22	-	56,56,56,56	0
58	MG	AY	502	1/1	0.91	0.31	-	58,58,58,58	0
58	MG	AA	3146	1/1	0.95	0.23	-	33,33,33,33	1
58	MG	CA	3545	1/1	0.91	0.13	-	68,68,68,68	0
58	MG	CA	3644	1/1	0.65	0.25	-	84,84,84,84	0
58	MG	BA	1644	1/1	0.81	0.33	-	75,75,75,75	0
58	MG	AA	3164	1/1	0.89	0.23	-	58,58,58,58	0
58	MG	DA	1700	1/1	0.40	0.28	-	124,124,124,124	0
58	MG	CA	3056	1/1	0.76	0.25	-	85,85,85,85	0
58	MG	AA	3699	1/1	0.92	0.37	-	46,46,46,46	1
58	MG	DA	1702	1/1	0.95	0.10	-	65,65,65,65	0
58	MG	AA	3013	1/1	0.95	0.18	-	35,35,35,35	0
58	MG	CA	3121	1/1	0.89	0.15	-	45,45,45,45	0
58	MG	BA	1786	1/1	0.97	0.16	-	66,66,66,66	0
58	MG	CA	3236	1/1	0.78	0.45	-	87,87,87,87	0
58	MG	CA	3087	1/1	0.86	0.21	-	67,67,67,67	0
58	MG	CA	3188	1/1	0.91	0.56	-	58,58,58,58	0
58	MG	CA	3444	1/1	0.80	0.15	-	91,91,91,91	0
58	MG	CA	3365	1/1	0.97	0.20	-	48,48,48,48	0
58	MG	DA	1626	1/1	0.94	0.50	-	49,49,49,49	0
58	MG	AA	3071	1/1	0.95	0.75	-	41,41,41,41	0
58	MG	CA	3547	1/1	0.96	0.14	-	61,61,61,61	0
58	MG	AA	3359	1/1	0.79	0.19	-	51,51,51,51	0
58	MG	DA	1605	1/1	0.92	0.23	-	73,73,73,73	0
58	MG	CA	3286	1/1	0.87	0.21	-	64,64,64,64	0
58	MG	CA	3352	1/1	0.98	0.18	-	68,68,68,68	0
58	MG	AA	3005	1/1	0.92	0.21	-	62,62,62,62	0
58	MG	CA	3573	1/1	0.79	0.20	-	80,80,80,80	0
58	MG	CB	3009	1/1	0.91	0.16	-	67,67,67,67	0
58	MG	CA	3234	1/1	0.96	0.30	-	54,54,54,54	0
58	MG	DA	1690	1/1	0.89	0.53	-	82,82,82,82	0
58	MG	CA	3629	1/1	0.96	0.17	-	55,55,55,55	0
58	MG	AB	3021	1/1	0.72	0.21	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1622	1/1	0.70	1.05	-	75,75,75,75	0
58	MG	AA	3479	1/1	0.88	0.26	-	54,54,54,54	0
58	MG	AA	3705	1/1	0.98	0.24	-	24,24,24,24	1
58	MG	AA	3087	1/1	0.93	0.25	-	72,72,72,72	0
58	MG	BA	1781	1/1	0.96	0.39	-	62,62,62,62	0
58	MG	AA	3073	1/1	0.94	0.27	-	58,58,58,58	0
58	MG	CA	3553	1/1	0.79	0.21	-	81,81,81,81	0
58	MG	AB	3009	1/1	0.94	0.08	-	56,56,56,56	0
58	MG	CA	3341	1/1	0.97	0.34	-	71,71,71,71	0
58	MG	CA	3275	1/1	0.95	0.23	-	42,42,42,42	0
58	MG	BV	101	1/1	0.82	0.34	-	110,110,110,110	0
58	MG	AA	3789	1/1	0.95	0.18	-	54,54,54,54	0
58	MG	AA	3137	1/1	0.82	0.29	-	56,56,56,56	0
58	MG	DA	1633	1/1	0.87	0.49	-	73,73,73,73	0
58	MG	CE	305	1/1	0.96	0.26	-	43,43,43,43	0
58	MG	AA	3321	1/1	0.95	0.32	-	70,70,70,70	0
58	MG	AA	3157	1/1	0.98	0.11	-	34,34,34,34	0
58	MG	CA	3514	1/1	0.72	0.80	-	105,105,105,105	0
58	MG	AA	3283	1/1	0.82	0.56	-	62,62,62,62	0
58	MG	CA	3152	1/1	0.68	0.28	-	56,56,56,56	0
58	MG	AZ	301	1/1	0.73	0.34	-	98,98,98,98	0
58	MG	DA	1685	1/1	0.94	0.37	-	65,65,65,65	0
58	MG	CA	3203	1/1	0.85	0.12	-	60,60,60,60	0
58	MG	AA	3780	1/1	0.92	0.32	-	42,42,42,42	0
58	MG	AA	3254	1/1	0.96	0.19	-	42,42,42,42	0
58	MG	CA	3634	1/1	0.86	0.10	-	81,81,81,81	0
58	MG	AA	3659	1/1	0.89	0.24	-	14,14,14,14	0
58	MG	AA	3609	1/1	0.98	0.19	-	53,53,53,53	0
58	MG	CA	3225	1/1	0.85	0.47	-	65,65,65,65	0
58	MG	AA	3057	1/1	0.87	0.46	-	57,57,57,57	0
58	MG	CA	3331	1/1	0.94	0.36	-	52,52,52,52	0
58	MG	AA	3182	1/1	0.90	0.22	-	76,76,76,76	0
58	MG	CA	3518	1/1	0.88	0.32	-	86,86,86,86	0
58	MG	AA	3733	1/1	0.90	0.20	-	68,68,68,68	0
58	MG	CA	3430	1/1	0.89	0.33	-	53,53,53,53	0
58	MG	DA	1619	1/1	0.78	0.31	-	71,71,71,71	0
58	MG	AA	3167	1/1	0.96	0.14	-	65,65,65,65	0
58	MG	BA	1731	1/1	0.96	0.27	-	63,63,63,63	0
58	MG	BA	1676	1/1	0.96	0.25	-	44,44,44,44	0
58	MG	DA	1740	1/1	0.92	0.09	-	81,81,81,81	0
58	MG	CA	3296	1/1	0.97	0.32	-	42,42,42,42	0
58	MG	CP	203	1/1	0.82	0.25	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1659	1/1	0.82	0.42	-	84,84,84,84	0
58	MG	AA	3339	1/1	0.87	0.29	-	43,43,43,43	0
58	MG	AA	3246	1/1	0.69	0.41	-	72,72,72,72	0
58	MG	CA	3297	1/1	0.98	0.34	-	56,56,56,56	0
58	MG	AA	3047	1/1	0.89	0.35	-	34,34,34,34	0
58	MG	CA	3044	1/1	0.91	0.35	-	52,52,52,52	0
58	MG	AA	3495	1/1	0.93	0.17	-	59,59,59,59	0
58	MG	BA	1809	1/1	0.91	0.22	-	68,68,68,68	0
58	MG	AA	3679	1/1	0.88	0.28	-	65,65,65,65	0
58	MG	AA	3423	1/1	0.98	0.15	-	22,22,22,22	0
58	MG	BA	1775	1/1	0.72	0.21	-	75,75,75,75	0
58	MG	CA	3621	1/1	0.88	0.31	-	73,73,73,73	0
58	MG	CA	3445	1/1	0.93	0.32	-	40,40,40,40	0
58	MG	AA	3326	1/1	0.97	0.12	-	58,58,58,58	0
58	MG	DA	1703	1/1	0.95	0.29	-	74,74,74,74	0
58	MG	BA	1701	1/1	0.96	0.46	-	58,58,58,58	0
58	MG	CA	3036	1/1	0.85	0.19	-	44,44,44,44	0
58	MG	DA	1677	1/1	0.87	0.13	-	74,74,74,74	0
58	MG	AA	3067	1/1	0.97	0.41	-	55,55,55,55	0
58	MG	BA	1697	1/1	0.90	0.38	-	78,78,78,78	0
58	MG	AA	3579	1/1	0.93	0.14	-	38,38,38,38	0
58	MG	AA	3799	1/1	0.90	0.19	-	47,47,47,47	0
58	MG	CA	3529	1/1	0.96	0.08	-	57,57,57,57	0
58	MG	AA	3497	1/1	0.93	0.04	-	46,46,46,46	0
58	MG	CA	3052	1/1	0.91	0.43	-	69,69,69,69	0
58	MG	CA	3536	1/1	0.87	0.12	-	71,71,71,71	0
58	MG	AA	3744	1/1	0.67	0.29	-	86,86,86,86	0
58	MG	CA	3195	1/1	0.91	0.15	-	60,60,60,60	0
58	MG	AA	3143	1/1	0.87	0.33	-	47,47,47,47	0
58	MG	AA	3237	1/1	0.86	0.14	-	71,71,71,71	0
58	MG	AA	3380	1/1	0.93	0.14	-	15,15,15,15	0
58	MG	AA	3266	1/1	0.93	0.50	-	50,50,50,50	0
58	MG	AA	3161	1/1	0.86	0.48	-	60,60,60,60	0
58	MG	CA	3630	1/1	0.91	0.12	-	63,63,63,63	0
58	MG	CA	3480	1/1	0.88	0.29	-	55,55,55,55	0
58	MG	CA	3541	1/1	0.90	0.17	-	71,71,71,71	0
58	MG	AA	3718	1/1	0.88	0.11	-	43,43,43,43	0
58	MG	AA	3063	1/1	0.80	0.45	-	67,67,67,67	0
58	MG	AA	3634	1/1	0.91	0.32	-	62,62,62,62	0
58	MG	AA	3630	1/1	0.87	0.23	-	71,71,71,71	0
58	MG	AA	3802	1/1	0.86	0.38	-	55,55,55,55	0
58	MG	A0	102	1/1	0.87	0.23	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3118	1/1	0.90	0.62	-	64,64,64,64	0
58	MG	AF	301	1/1	0.93	0.17	-	43,43,43,43	0
58	MG	AA	3302	1/1	0.91	0.21	-	56,56,56,56	0
58	MG	BA	1706	1/1	0.94	0.43	-	62,62,62,62	0
58	MG	BA	1651	1/1	0.80	0.16	-	102,102,102,102	0
58	MG	AA	3064	1/1	0.90	0.17	-	29,29,29,29	0
58	MG	BA	1771	1/1	0.19	0.94	-	115,115,115,115	0
58	MG	CA	3175	1/1	0.99	0.28	-	42,42,42,42	0
58	MG	AA	3373	1/1	0.82	0.29	-	59,59,59,59	0
58	MG	CA	3299	1/1	0.98	0.16	-	61,61,61,61	0
58	MG	CA	3652	1/1	0.95	0.17	-	53,53,53,53	0
58	MG	AA	3160	1/1	0.94	0.17	-	57,57,57,57	0
58	MG	CA	3148	1/1	0.98	0.29	-	65,65,65,65	0
58	MG	CB	3002	1/1	0.72	0.27	-	66,66,66,66	0
58	MG	CA	3082	1/1	0.73	0.31	-	70,70,70,70	0
58	MG	AA	3763	1/1	0.96	0.36	-	65,65,65,65	0
58	MG	BA	1798	1/1	0.91	0.15	-	69,69,69,69	0
58	MG	BA	1673	1/1	0.78	0.96	-	77,77,77,77	0
58	MG	CA	3571	1/1	0.66	0.14	-	65,65,65,65	0
58	MG	AA	3238	1/1	0.93	0.35	-	61,61,61,61	0
58	MG	BA	1734	1/1	0.68	0.40	-	81,81,81,81	0
58	MG	AA	3033	1/1	0.96	0.23	-	29,29,29,29	1
58	MG	CA	3215	1/1	0.86	0.09	-	73,73,73,73	0
58	MG	DA	1748	1/1	0.92	0.16	-	78,78,78,78	0
58	MG	AA	3585	1/1	0.69	0.17	-	65,65,65,65	0
58	MG	CA	3477	1/1	0.89	0.11	-	74,74,74,74	0
58	MG	CB	3010	1/1	0.93	0.23	-	55,55,55,55	0
58	MG	DA	1712	1/1	0.93	0.14	-	81,81,81,81	0
58	MG	AA	3446	1/1	0.91	0.51	-	61,61,61,61	0
58	MG	AA	3580	1/1	0.79	0.14	-	23,23,23,23	0
58	MG	AA	3428	1/1	0.94	0.17	-	35,35,35,35	0
58	MG	CA	3659	1/1	0.95	0.11	-	77,77,77,77	0
58	MG	AA	3318	1/1	0.96	0.25	-	51,51,51,51	1
58	MG	BA	1791	1/1	0.89	0.14	-	63,63,63,63	0
58	MG	AA	3364	1/1	0.88	0.34	-	81,81,81,81	0
58	MG	AA	3232	1/1	0.91	0.30	-	79,79,79,79	0
58	MG	CA	3640	1/1	0.86	0.29	-	59,59,59,59	0
58	MG	CA	3602	1/1	0.89	0.17	-	66,66,66,66	0
58	MG	AA	3567	1/1	0.97	0.21	-	51,51,51,51	0
58	MG	DA	1691	1/1	0.76	0.20	-	85,85,85,85	0
58	MG	AA	3633	1/1	0.88	0.25	-	48,48,48,48	1
58	MG	DA	1644	1/1	0.96	0.16	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3220	1/1	0.88	0.24	-	78,78,78,78	0
58	MG	AA	3086	1/1	0.95	0.15	-	47,47,47,47	0
58	MG	CA	3531	1/1	0.91	0.21	-	51,51,51,51	0
58	MG	CA	3107	1/1	0.36	0.47	-	108,108,108,108	0
58	MG	AA	3431	1/1	0.98	0.10	-	25,25,25,25	0
58	MG	AA	3159	1/1	0.94	0.23	-	46,46,46,46	1
58	MG	AA	3628	1/1	0.89	0.28	-	80,80,80,80	0
58	MG	DA	1736	1/1	0.95	0.11	-	79,79,79,79	0
58	MG	CA	3509	1/1	0.83	0.18	-	76,76,76,76	0
58	MG	CA	3538	1/1	0.89	0.07	-	71,71,71,71	0
58	MG	AA	3749	1/1	0.98	0.14	-	14,14,14,14	0
58	MG	CA	3204	1/1	0.74	0.37	-	74,74,74,74	0
58	MG	CA	3565	1/1	0.98	0.39	-	51,51,51,51	0
58	MG	A0	103	1/1	0.93	0.12	-	37,37,37,37	0
58	MG	AA	3426	1/1	0.91	0.15	-	50,50,50,50	0
58	MG	CA	3401	1/1	0.93	0.23	-	69,69,69,69	0
58	MG	AA	3358	1/1	0.88	0.17	-	63,63,63,63	0
58	MG	AA	3214	1/1	0.93	0.16	-	34,34,34,34	0
58	MG	AA	3491	1/1	0.88	0.29	-	35,35,35,35	0
58	MG	AA	3809	1/1	0.89	0.22	-	62,62,62,62	0
58	MG	CA	3376	1/1	0.94	0.08	-	66,66,66,66	0
58	MG	BA	1694	1/1	0.86	0.07	-	80,80,80,80	0
58	MG	AA	3095	1/1	0.77	0.47	-	82,82,82,82	0
58	MG	DA	1757	1/1	0.89	0.33	-	75,75,75,75	0
58	MG	AA	3340	1/1	0.98	0.10	-	59,59,59,59	0
58	MG	AA	3647	1/1	0.91	0.21	-	72,72,72,72	0
58	MG	DA	1657	1/1	0.40	0.20	-	93,93,93,93	0
58	MG	CA	3164	1/1	0.96	0.41	-	41,41,41,41	0
58	MG	AA	3558	1/1	0.83	0.14	-	51,51,51,51	0
58	MG	AA	3441	1/1	0.93	0.18	-	51,51,51,51	1
58	MG	CA	3139	1/1	0.84	0.33	-	123,123,123,123	0
58	MG	AA	3355	1/1	0.86	0.17	-	58,58,58,58	0
58	MG	CA	3510	1/1	0.92	0.14	-	65,65,65,65	0
58	MG	BA	1646	1/1	0.83	0.80	-	75,75,75,75	0
58	MG	AA	3075	1/1	0.97	0.15	-	9,9,9,9	0
58	MG	DA	1764	1/1	0.92	0.08	-	55,55,55,55	0
58	MG	BA	1747	1/1	0.94	0.40	-	68,68,68,68	0
58	MG	AA	3607	1/1	0.97	0.09	-	30,30,30,30	0
58	MG	AA	3371	1/1	0.96	0.34	-	62,62,62,62	0
58	MG	AA	3730	1/1	0.96	0.27	-	30,30,30,30	0
58	MG	CA	3125	1/1	0.88	0.50	-	73,73,73,73	0
58	MG	CA	3651	1/1	0.86	0.24	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3134	1/1	0.55	1.10	-	86,86,86,86	0
58	MG	AA	3294	1/1	0.88	0.25	-	66,66,66,66	0
58	MG	AA	3225	1/1	0.92	0.26	-	27,27,27,27	1
58	MG	CA	3009	1/1	0.85	0.51	-	67,67,67,67	0
58	MG	AA	3320	1/1	0.95	0.19	-	24,24,24,24	0
58	MG	CA	3351	1/1	0.91	0.14	-	46,46,46,46	0
58	MG	CA	3594	1/1	0.37	0.21	-	80,80,80,80	0
58	MG	CA	3055	1/1	0.97	0.51	-	39,39,39,39	0
58	MG	DA	1653	1/1	0.90	0.19	-	60,60,60,60	0
58	MG	AA	3636	1/1	0.84	0.25	-	65,65,65,65	0
58	MG	CA	3627	1/1	0.93	0.18	-	63,63,63,63	0
58	MG	CA	3248	1/1	0.81	0.65	-	77,77,77,77	0
58	MG	CA	3636	1/1	0.82	0.19	-	80,80,80,80	0
58	MG	DA	1761	1/1	0.97	0.29	-	66,66,66,66	0
58	MG	AR	201	1/1	0.96	0.28	-	32,32,32,32	0
58	MG	DA	1719	1/1	0.92	0.12	-	74,74,74,74	0
58	MG	CA	3645	1/1	0.85	0.14	-	82,82,82,82	0
58	MG	AA	3476	1/1	0.82	0.24	-	69,69,69,69	0
58	MG	CA	3136	1/1	0.90	0.35	-	53,53,53,53	0
58	MG	AA	3070	1/1	0.89	0.40	-	60,60,60,60	0
58	MG	DA	1648	1/1	0.96	0.22	-	50,50,50,50	0
58	MG	CA	3067	1/1	0.84	0.34	-	72,72,72,72	0
58	MG	AA	3289	1/1	0.94	0.11	-	27,27,27,27	0
58	MG	AA	3584	1/1	0.96	0.08	-	65,65,65,65	0
58	MG	AB	3012	1/1	0.99	0.22	-	29,29,29,29	1
58	MG	BA	1797	1/1	0.80	0.21	-	63,63,63,63	0
58	MG	CA	3354	1/1	0.97	0.25	-	61,61,61,61	0
58	MG	CA	3200	1/1	0.89	0.47	-	54,54,54,54	0
58	MG	AA	3480	1/1	0.91	0.08	-	54,54,54,54	0
58	MG	AA	3586	1/1	0.90	0.14	-	62,62,62,62	0
58	MG	CA	3623	1/1	0.90	0.26	-	64,64,64,64	0
58	MG	CA	3240	1/1	0.91	0.15	-	64,64,64,64	0
58	MG	AA	3566	1/1	0.96	0.18	-	27,27,27,27	0
58	MG	AA	3561	1/1	0.88	0.26	-	58,58,58,58	0
58	MG	AA	3415	1/1	0.96	0.07	-	56,56,56,56	0
58	MG	CA	3012	1/1	0.97	0.26	-	59,59,59,59	0
58	MG	CA	3172	1/1	0.79	0.33	-	83,83,83,83	0
58	MG	AA	3406	1/1	0.91	0.16	-	57,57,57,57	0
58	MG	AA	3695	1/1	0.93	0.51	-	78,78,78,78	0
58	MG	AA	3001	1/1	0.96	0.10	-	37,37,37,37	0
58	MG	DA	1750	1/1	0.86	0.17	-	68,68,68,68	0
58	MG	BA	1614	1/1	0.83	0.32	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3697	1/1	0.80	0.15	-	63,63,63,63	0
58	MG	CA	3199	1/1	0.90	0.35	-	74,74,74,74	0
58	MG	AA	3330	1/1	0.97	0.13	-	69,69,69,69	0
58	MG	AA	3748	1/1	0.96	0.28	-	56,56,56,56	0
58	MG	AA	3738	1/1	0.80	0.26	-	75,75,75,75	0
58	MG	AA	3555	1/1	0.97	0.17	-	38,38,38,38	0
58	MG	AA	3197	1/1	0.96	0.38	-	37,37,37,37	0
58	MG	DA	1604	1/1	0.81	0.37	-	76,76,76,76	0
58	MG	AA	3188	1/1	0.98	0.18	-	13,13,13,13	0
58	MG	AA	3530	1/1	0.98	0.12	-	53,53,53,53	0
58	MG	BA	1805	1/1	0.64	0.18	-	83,83,83,83	0
58	MG	CA	3610	1/1	0.81	0.16	-	98,98,98,98	0
58	MG	AA	3761	1/1	0.88	0.46	-	50,50,50,50	0
58	MG	AA	3764	1/1	0.97	0.20	-	55,55,55,55	0
58	MG	DA	1763	1/1	0.85	0.20	-	77,77,77,77	0
58	MG	AA	3227	1/1	0.92	0.26	-	55,55,55,55	0
58	MG	AA	3277	1/1	0.80	0.23	-	79,79,79,79	0
58	MG	CA	3080	1/1	0.61	0.22	-	87,87,87,87	0
58	MG	CA	3103	1/1	0.85	0.49	-	62,62,62,62	0
58	MG	CA	3582	1/1	0.93	0.19	-	44,44,44,44	0
58	MG	AA	3678	1/1	0.97	0.24	-	31,31,31,31	0
58	MG	DW	501	1/1	0.91	0.26	-	74,74,74,74	0
58	MG	AA	3693	1/1	0.96	0.21	-	48,48,48,48	0
58	MG	AA	3189	1/1	0.95	0.40	-	40,40,40,40	0
58	MG	BA	1739	1/1	0.86	0.14	-	93,93,93,93	0
58	MG	CA	3018	1/1	0.78	0.32	-	64,64,64,64	0
58	MG	DA	1718	1/1	0.74	0.15	-	77,77,77,77	0
58	MG	BW	502	1/1	0.96	0.11	-	53,53,53,53	0
58	MG	CA	3556	1/1	0.86	0.08	-	48,48,48,48	0
58	MG	AA	3611	1/1	0.97	0.15	-	51,51,51,51	0
58	MG	DA	1681	1/1	0.95	0.17	-	55,55,55,55	0
58	MG	CA	3349	1/1	0.97	0.26	-	41,41,41,41	0
58	MG	CA	3347	1/1	0.93	0.13	-	59,59,59,59	0
58	MG	AA	3463	1/1	0.94	0.30	-	46,46,46,46	0
58	MG	BA	1672	1/1	0.88	0.26	-	61,61,61,61	0
58	MG	CA	3099	1/1	0.88	0.15	-	92,92,92,92	0
58	MG	BA	1790	1/1	0.86	0.10	-	72,72,72,72	0
58	MG	AA	3361	1/1	0.98	0.15	-	29,29,29,29	0
58	MG	CA	3186	1/1	0.81	0.35	-	69,69,69,69	0
58	MG	DA	1701	1/1	0.85	0.28	-	63,63,63,63	0
58	MG	AA	3668	1/1	0.93	0.19	-	40,40,40,40	0
58	MG	CA	3319	1/1	0.93	0.19	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3193	1/1	0.94	0.23	-	64,64,64,64	0
58	MG	CA	3015	1/1	0.70	0.54	-	85,85,85,85	0
58	MG	AA	3467	1/1	0.98	0.12	-	44,44,44,44	0
58	MG	CA	3591	1/1	0.95	0.14	-	83,83,83,83	0
58	MG	CA	3061	1/1	0.92	0.46	-	67,67,67,67	0
58	MG	BA	1602	1/1	0.92	0.11	-	53,53,53,53	0
58	MG	AA	3492	1/1	0.88	0.36	-	45,45,45,45	0
58	MG	AA	3046	1/1	0.96	0.23	-	34,34,34,34	0
58	MG	AA	3681	1/1	0.91	0.37	-	65,65,65,65	0
58	MG	CA	3595	1/1	0.95	0.10	-	53,53,53,53	0
58	MG	CA	3173	1/1	0.69	0.46	-	65,65,65,65	0
58	MG	AA	3287	1/1	0.97	0.40	-	47,47,47,47	0
58	MG	AA	3545	1/1	0.89	0.10	-	51,51,51,51	1
58	MG	BA	1726	1/1	0.98	0.30	-	52,52,52,52	0
58	MG	CA	3006	1/1	0.73	0.26	-	67,67,67,67	0
58	MG	CB	3008	1/1	0.89	0.12	-	59,59,59,59	0
58	MG	AA	3800	1/1	0.94	0.13	-	30,30,30,30	0
58	MG	BA	1714	1/1	0.85	0.26	-	88,88,88,88	0
58	MG	CA	3483	1/1	0.93	0.48	-	69,69,69,69	0
58	MG	BA	1806	1/1	0.70	0.28	-	81,81,81,81	0
58	MG	CA	3141	1/1	0.76	0.30	-	54,54,54,54	0
58	MG	AA	3760	1/1	0.68	0.20	-	27,27,27,27	0
58	MG	AA	3106	1/1	0.93	0.28	-	52,52,52,52	0
58	MG	AA	3527	1/1	0.95	0.18	-	26,26,26,26	0
58	MG	CA	3170	1/1	0.94	0.34	-	47,47,47,47	0
58	MG	AA	3573	1/1	0.88	0.14	-	50,50,50,50	0
58	MG	CA	3062	1/1	0.64	0.25	-	68,68,68,68	0
58	MG	AA	3363	1/1	0.93	0.34	-	28,28,28,28	0
58	MG	AA	3430	1/1	0.93	0.14	-	44,44,44,44	0
58	MG	DW	502	1/1	0.78	0.11	-	84,84,84,84	0
58	MG	CA	3469	1/1	0.86	0.13	-	69,69,69,69	0
58	MG	AA	3349	1/1	0.85	0.29	-	40,40,40,40	0
58	MG	AA	3487	1/1	0.93	0.17	-	39,39,39,39	0
58	MG	BA	1605	1/1	0.52	0.28	-	67,67,67,67	0
58	MG	CA	3031	1/1	0.82	0.08	-	76,76,76,76	0
58	MG	DD	502	1/1	0.96	0.63	-	62,62,62,62	0
58	MG	AA	3031	1/1	0.93	0.25	-	10,10,10,10	1
58	MG	CA	3562	1/1	0.96	0.21	-	76,76,76,76	0
58	MG	CA	3180	1/1	0.75	0.49	-	108,108,108,108	0
58	MG	BA	1633	1/1	0.83	0.35	-	62,62,62,62	0
58	MG	AA	3027	1/1	0.93	0.48	-	77,77,77,77	0
58	MG	AA	3370	1/1	0.94	0.28	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3066	1/1	0.97	0.29	-	50,50,50,50	0
58	MG	AA	3170	1/1	0.94	0.44	-	53,53,53,53	0
58	MG	CA	3357	1/1	0.92	0.06	-	80,80,80,80	0
58	MG	AA	3201	1/1	0.86	0.37	-	65,65,65,65	0
58	MG	AV	203	1/1	0.97	0.35	-	38,38,38,38	0
58	MG	CA	3241	1/1	0.61	0.55	-	107,107,107,107	0
58	MG	AA	3366	1/1	0.95	0.22	-	53,53,53,53	0
58	MG	CA	3268	1/1	0.95	0.30	-	69,69,69,69	0
58	MG	AZ	302	1/1	0.88	0.21	-	68,68,68,68	0
58	MG	BA	1634	1/1	0.68	0.51	-	100,100,100,100	0
58	MG	AA	3233	1/1	0.82	0.36	-	55,55,55,55	0
58	MG	AA	3513	1/1	0.97	0.11	-	35,35,35,35	0
58	MG	AA	3451	1/1	0.94	0.24	-	48,48,48,48	0
58	MG	AA	3627	1/1	0.98	0.17	-	54,54,54,54	0
58	MG	AA	3305	1/1	0.96	0.24	-	55,55,55,55	0
58	MG	CA	3416	1/1	0.98	0.17	-	48,48,48,48	0
58	MG	DA	1725	1/1	0.78	0.20	-	70,70,70,70	0
58	MG	CA	3112	1/1	0.88	0.26	-	61,61,61,61	0
58	MG	AA	3336	1/1	0.94	0.17	-	54,54,54,54	0
58	MG	BA	1699	1/1	0.94	0.17	-	75,75,75,75	0
58	MG	AA	3643	1/1	0.99	0.17	-	49,49,49,49	0
58	MG	BA	1799	1/1	0.95	0.21	-	65,65,65,65	0
58	MG	CA	3232	1/1	0.96	0.09	-	60,60,60,60	0
58	MG	CA	3004	1/1	0.87	0.42	-	64,64,64,64	0
58	MG	AA	3291	1/1	0.88	0.15	-	44,44,44,44	0
58	MG	AA	3807	1/1	0.77	0.30	-	62,62,62,62	1
58	MG	BA	1649	1/1	0.89	0.24	-	68,68,68,68	0
58	MG	AA	3756	1/1	0.96	0.16	-	40,40,40,40	1
58	MG	BA	1727	1/1	0.92	0.10	-	45,45,45,45	0
58	MG	BA	1735	1/1	0.89	0.28	-	72,72,72,72	0
58	MG	CA	3187	1/1	0.91	0.28	-	37,37,37,37	0
58	MG	AA	3516	1/1	0.97	0.17	-	18,18,18,18	0
58	MG	BA	1684	1/1	0.89	0.13	-	81,81,81,81	0
58	MG	CA	3585	1/1	0.85	0.21	-	78,78,78,78	0
58	MG	AA	3834	1/1	0.80	0.22	-	58,58,58,58	0
58	MG	AA	3575	1/1	0.96	0.12	-	69,69,69,69	0
58	MG	CA	3356	1/1	0.92	0.16	-	57,57,57,57	0
58	MG	CA	3049	1/1	0.97	0.13	-	81,81,81,81	0
58	MG	AA	3477	1/1	0.88	0.17	-	58,58,58,58	0
58	MG	AA	3369	1/1	0.96	0.24	-	27,27,27,27	0
58	MG	CA	3499	1/1	0.93	0.24	-	83,83,83,83	0
58	MG	AA	3788	1/1	0.91	0.27	-	58,58,58,58	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3207	1/1	0.94	0.18	-	22,22,22,22	1
58	MG	AA	3522	1/1	0.95	0.22	-	28,28,28,28	0
58	MG	AA	3457	1/1	0.91	0.18	-	67,67,67,67	0
58	MG	AA	3481	1/1	0.88	0.15	-	51,51,51,51	0
58	MG	AA	3582	1/1	0.96	0.41	-	66,66,66,66	0
58	MG	CA	3345	1/1	0.99	0.22	-	38,38,38,38	0
58	MG	AA	3598	1/1	0.94	0.23	-	54,54,54,54	0
58	MG	BA	1670	1/1	0.94	0.23	-	92,92,92,92	0
58	MG	BA	1708	1/1	0.76	0.20	-	79,79,79,79	0
58	MG	CA	3040	1/1	0.92	0.15	-	66,66,66,66	0
58	MG	CA	3171	1/1	0.94	0.33	-	55,55,55,55	0
58	MG	BA	1618	1/1	0.74	0.30	-	57,57,57,57	0
58	MG	CA	3460	1/1	0.70	0.47	-	109,109,109,109	0
58	MG	AA	3786	1/1	0.89	0.37	-	59,59,59,59	0
58	MG	CA	3609	1/1	0.88	0.23	-	76,76,76,76	0
58	MG	CA	3633	1/1	0.96	0.23	-	68,68,68,68	0
58	MG	AA	3242	1/1	0.90	0.27	-	72,72,72,72	0
58	MG	AA	3779	1/1	0.91	0.20	-	62,62,62,62	0
58	MG	AA	3646	1/1	0.89	0.13	-	58,58,58,58	0
58	MG	AA	3576	1/1	0.97	0.28	-	38,38,38,38	0
58	MG	BA	1639	1/1	0.92	0.37	-	49,49,49,49	0
58	MG	CA	3312	1/1	0.97	0.14	-	51,51,51,51	0
58	MG	BA	1770	1/1	0.98	0.38	-	56,56,56,56	0
58	MG	CA	3151	1/1	0.91	0.17	-	50,50,50,50	0
58	MG	AA	3444	1/1	0.89	0.27	-	63,63,63,63	0
58	MG	AA	3790	1/1	0.96	0.06	-	49,49,49,49	0
58	MG	CA	3308	1/1	0.96	0.11	-	41,41,41,41	0
58	MG	AA	3151	1/1	0.81	0.21	-	50,50,50,50	0
58	MG	AB	3018	1/1	0.93	0.14	-	84,84,84,84	0
58	MG	AA	3376	1/1	0.97	0.17	-	19,19,19,19	0
58	MG	DA	1679	1/1	0.95	0.42	-	58,58,58,58	0
58	MG	AA	3368	1/1	0.93	0.21	-	37,37,37,37	0
58	MG	AA	3650	1/1	0.92	0.07	-	60,60,60,60	0
58	MG	CA	3598	1/1	0.80	0.09	-	73,73,73,73	0
58	MG	AA	3348	1/1	0.93	0.22	-	32,32,32,32	0
58	MG	AA	3629	1/1	0.94	0.17	-	61,61,61,61	0
58	MG	AA	3122	1/1	0.82	0.28	-	54,54,54,54	0
58	MG	AA	3554	1/1	0.89	0.15	-	49,49,49,49	0
58	MG	CA	3250	1/1	0.94	0.16	-	52,52,52,52	0
58	MG	CA	3147	1/1	0.84	0.35	-	76,76,76,76	0
58	MG	DA	1665	1/1	0.91	0.49	-	61,61,61,61	0
58	MG	DA	1671	1/1	0.90	0.59	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3574	1/1	0.74	0.15	-	72,72,72,72	0
58	MG	AA	3333	1/1	0.94	0.15	-	66,66,66,66	0
58	MG	AA	3379	1/1	0.95	0.14	-	30,30,30,30	0
58	MG	AA	3653	1/1	0.88	0.15	-	68,68,68,68	0
58	MG	AA	3654	1/1	0.97	0.29	-	66,66,66,66	0
58	MG	AA	3720	1/1	0.85	0.72	-	77,77,77,77	0
58	MG	CA	3631	1/1	0.91	0.13	-	77,77,77,77	0
58	MG	AA	3203	1/1	0.91	0.33	-	46,46,46,46	1
58	MG	BA	1698	1/1	0.62	0.28	-	74,74,74,74	0
58	MG	AA	3407	1/1	0.98	0.12	-	49,49,49,49	0
58	MG	BA	1760	1/1	0.85	0.13	-	89,89,89,89	0
58	MG	AA	3347	1/1	0.97	0.10	-	38,38,38,38	0
58	MG	AA	3538	1/1	0.85	0.26	-	61,61,61,61	1
58	MG	AA	3494	1/1	0.97	0.23	-	50,50,50,50	0
58	MG	DZ	702	1/1	0.99	0.28	-	57,57,57,57	0
58	MG	CA	3338	1/1	0.97	0.17	-	63,63,63,63	0
58	MG	A2	102	1/1	0.79	0.37	-	54,54,54,54	0
58	MG	AA	3375	1/1	0.89	0.25	-	57,57,57,57	0
58	MG	CA	3022	1/1	0.96	0.20	-	38,38,38,38	0
58	MG	AA	3127	1/1	0.98	0.37	-	71,71,71,71	0
58	MG	DA	1759	1/1	0.82	0.35	-	76,76,76,76	0
58	MG	CA	3198	1/1	0.91	0.13	-	37,37,37,37	0
58	MG	DA	1655	1/1	0.96	0.42	-	58,58,58,58	0
58	MG	CA	3113	1/1	0.81	0.30	-	92,92,92,92	0
58	MG	AA	3125	1/1	0.93	0.22	-	23,23,23,23	1
58	MG	CA	3207	1/1	0.96	0.15	-	71,71,71,71	0
58	MG	AA	3470	1/1	0.96	0.16	-	29,29,29,29	0
58	MG	DA	1692	1/1	0.87	0.15	-	76,76,76,76	0
58	MG	AA	3450	1/1	0.91	0.27	-	53,53,53,53	0
58	MG	AA	3068	1/1	0.92	0.48	-	65,65,65,65	0
58	MG	AA	3610	1/1	0.50	0.18	-	51,51,51,51	1
58	MG	CA	3005	1/1	0.92	0.23	-	59,59,59,59	0
58	MG	AB	3013	1/1	0.98	0.18	-	54,54,54,54	0
58	MG	A7	101	1/1	0.85	0.16	-	49,49,49,49	1
58	MG	AA	3552	1/1	0.97	0.15	-	63,63,63,63	0
58	MG	CA	3007	1/1	0.97	0.10	-	28,28,28,28	0
58	MG	DA	1635	1/1	0.86	0.35	-	65,65,65,65	0
58	MG	AA	3114	1/1	0.93	0.21	-	17,17,17,17	0
58	MG	CA	3492	1/1	0.68	0.54	-	105,105,105,105	0
58	MG	AA	3425	1/1	0.95	0.24	-	18,18,18,18	0
58	MG	CA	3572	1/1	0.93	0.16	-	54,54,54,54	0
58	MG	CA	3046	1/1	-0.24	0.35	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3118	1/1	0.82	0.23	-	57,57,57,57	0
58	MG	AA	3521	1/1	0.98	0.16	-	29,29,29,29	0
58	MG	AA	3490	1/1	0.82	0.09	-	50,50,50,50	0
58	MG	CA	3486	1/1	0.95	0.27	-	69,69,69,69	0
58	MG	CA	3373	1/1	0.85	0.50	-	58,58,58,58	0
58	MG	DA	1662	1/1	0.80	0.23	-	64,64,64,64	0
58	MG	AA	3591	1/1	0.96	0.25	-	65,65,65,65	0
58	MG	AA	3703	1/1	0.84	0.10	-	76,76,76,76	0
58	MG	AA	3796	1/1	0.95	0.26	-	50,50,50,50	0
58	MG	AA	3256	1/1	0.97	0.16	-	21,21,21,21	1
58	MG	CA	3442	1/1	0.93	0.46	-	67,67,67,67	0
58	MG	BA	1749	1/1	0.95	0.12	-	48,48,48,48	0
58	MG	CA	3108	1/1	0.92	0.18	-	60,60,60,60	0
58	MG	AA	3808	1/1	0.93	0.20	-	28,28,28,28	1
58	MG	CA	3336	1/1	0.93	0.16	-	69,69,69,69	0
58	MG	AA	3165	1/1	0.83	0.42	-	57,57,57,57	0
58	MG	BA	1707	1/1	0.88	0.26	-	50,50,50,50	0
58	MG	AA	3746	1/1	0.94	0.15	-	64,64,64,64	0
58	MG	CA	3608	1/1	0.91	0.22	-	56,56,56,56	0
58	MG	CA	3149	1/1	0.92	0.08	-	66,66,66,66	0
58	MG	AA	3317	1/1	0.97	0.14	-	58,58,58,58	0
58	MG	BA	1636	1/1	0.96	0.40	-	64,64,64,64	0
58	MG	DA	1642	1/1	0.93	0.20	-	66,66,66,66	0
58	MG	AA	3466	1/1	0.95	0.12	-	63,63,63,63	0
58	MG	CA	3161	1/1	0.94	0.19	-	66,66,66,66	0
58	MG	CA	3570	1/1	0.86	0.21	-	77,77,77,77	0
58	MG	BA	1713	1/1	0.96	0.27	-	55,55,55,55	0
58	MG	AA	3665	1/1	0.85	0.34	-	85,85,85,85	0
58	MG	BZ	701	1/1	0.22	0.30	-	137,137,137,137	0
58	MG	CA	3515	1/1	0.85	0.20	-	79,79,79,79	0
58	MG	CA	3551	1/1	0.82	0.17	-	88,88,88,88	0
58	MG	DA	1676	1/1	0.83	0.09	-	78,78,78,78	0
58	MG	CA	3075	1/1	0.84	0.40	-	71,71,71,71	0
58	MG	DA	1646	1/1	0.95	0.34	-	62,62,62,62	0
58	MG	DA	1678	1/1	0.71	0.37	-	82,82,82,82	0
58	MG	AA	3327	1/1	0.97	0.14	-	13,13,13,13	0
58	MG	CQ	202	1/1	0.93	0.66	-	64,64,64,64	0
58	MG	AA	3219	1/1	0.92	0.29	-	58,58,58,58	0
58	MG	CA	3092	1/1	0.98	0.16	-	70,70,70,70	0
58	MG	CA	3495	1/1	0.85	0.15	-	65,65,65,65	0
58	MG	AA	3016	1/1	0.76	0.40	-	59,59,59,59	0
58	MG	CA	3174	1/1	0.78	0.54	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	1693	1/1	0.90	0.22	-	54,54,54,54	0
58	MG	AA	3382	1/1	0.82	0.17	-	36,36,36,36	1
58	MG	AA	3104	1/1	0.96	0.17	-	28,28,28,28	0
58	MG	CA	3316	1/1	0.94	0.17	-	50,50,50,50	0
58	MG	CA	3643	1/1	0.93	0.09	-	76,76,76,76	0
58	MG	CA	3581	1/1	0.92	0.12	-	81,81,81,81	0
58	MG	BA	1807	1/1	0.94	0.15	-	83,83,83,83	0
58	MG	AA	3261	1/1	0.85	0.36	-	51,51,51,51	0
58	MG	BA	1729	1/1	0.97	0.18	-	49,49,49,49	0
58	MG	DA	1622	1/1	0.89	0.54	-	77,77,77,77	0
58	MG	BA	1796	1/1	0.88	0.11	-	70,70,70,70	0
58	MG	CE	304	1/1	0.85	0.76	-	68,68,68,68	0
58	MG	BA	1762	1/1	0.90	0.07	-	52,52,52,52	1
58	MG	AA	3195	1/1	0.98	0.19	-	50,50,50,50	0
58	MG	AA	3155	1/1	0.84	0.31	-	64,64,64,64	0
58	MG	DA	1760	1/1	0.95	0.37	-	66,66,66,66	0
58	MG	AA	3058	1/1	0.90	0.20	-	35,35,35,35	0
58	MG	CA	3535	1/1	0.93	0.30	-	69,69,69,69	0
58	MG	DA	1710	1/1	0.97	0.20	-	70,70,70,70	0
58	MG	CA	3440	1/1	0.98	0.31	-	57,57,57,57	0
58	MG	AA	3810	1/1	0.91	0.24	-	54,54,54,54	0
58	MG	AA	3115	1/1	0.72	0.45	-	67,67,67,67	1
58	MG	AA	3141	1/1	0.92	0.47	-	40,40,40,40	0
58	MG	BA	1720	1/1	0.98	0.45	-	62,62,62,62	0
58	MG	AA	3192	1/1	0.18	0.65	-	76,76,76,76	0
58	MG	AA	3148	1/1	0.89	0.34	-	68,68,68,68	0
58	MG	CB	3001	1/1	0.89	0.20	-	99,99,99,99	0
58	MG	DA	1628	1/1	0.86	0.49	-	74,74,74,74	0
58	MG	AA	3060	1/1	0.88	0.69	-	65,65,65,65	0
58	MG	AA	3010	1/1	0.76	0.62	-	68,68,68,68	0
58	MG	BA	1746	1/1	0.89	0.17	-	83,83,83,83	0
58	MG	CA	3394	1/1	0.96	0.16	-	55,55,55,55	0
58	MG	DA	1659	1/1	0.91	0.08	-	64,64,64,64	0
58	MG	AA	3096	1/1	0.85	0.14	-	63,63,63,63	0
58	MG	CA	3167	1/1	0.93	0.10	-	60,60,60,60	0
58	MG	CA	3465	1/1	0.95	0.34	-	66,66,66,66	0
58	MG	BA	1724	1/1	0.81	0.20	-	64,64,64,64	0
58	MG	CA	3543	1/1	0.90	0.20	-	63,63,63,63	0
58	MG	BA	1779	1/1	0.91	0.15	-	46,46,46,46	1
58	MG	CA	3065	1/1	0.89	0.12	-	52,52,52,52	0
58	MG	AB	3019	1/1	0.93	0.18	-	65,65,65,65	0
58	MG	CA	3095	1/1	0.90	0.31	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3447	1/1	0.82	0.44	-	80,80,80,80	0
58	MG	BA	1737	1/1	0.95	0.27	-	63,63,63,63	0
58	MG	AA	3696	1/1	0.88	0.16	-	69,69,69,69	0
58	MG	AA	3269	1/1	0.77	0.46	-	84,84,84,84	0
58	MG	AA	3747	1/1	0.92	0.39	-	58,58,58,58	0
58	MG	CA	3247	1/1	0.92	0.66	-	66,66,66,66	0
58	MG	CA	3583	1/1	0.76	0.30	-	78,78,78,78	1
58	MG	CA	3344	1/1	0.95	0.08	-	87,87,87,87	0
58	MG	CA	3429	1/1	0.92	0.36	-	74,74,74,74	0
58	MG	DA	1698	1/1	0.93	0.40	-	68,68,68,68	0
58	MG	AA	3076	1/1	0.96	0.25	-	92,92,92,92	0
58	MG	AA	3391	1/1	0.96	0.15	-	45,45,45,45	0
58	MG	AA	3312	1/1	0.96	0.19	-	55,55,55,55	0
58	MG	CA	3398	1/1	0.85	0.10	-	65,65,65,65	0
58	MG	CA	3287	1/1	0.94	0.15	-	52,52,52,52	0
58	MG	DA	1738	1/1	0.94	0.59	-	80,80,80,80	0
58	MG	AA	3732	1/1	0.69	0.23	-	68,68,68,68	0
58	MG	CA	3256	1/1	0.97	0.18	-	40,40,40,40	0
58	MG	AA	3688	1/1	0.91	0.19	-	25,25,25,25	1
58	MG	AA	3700	1/1	0.95	0.22	-	35,35,35,35	0
58	MG	AA	3199	1/1	0.89	0.18	-	54,54,54,54	0
58	MG	CA	3639	1/1	0.93	0.32	-	55,55,55,55	0
58	MG	AA	3615	1/1	0.85	0.20	-	35,35,35,35	1
58	MG	DA	1767	1/1	0.90	0.14	-	74,74,74,74	0
58	MG	AA	3597	1/1	0.90	0.09	-	63,63,63,63	0
58	MG	DA	1675	1/1	0.92	0.36	-	74,74,74,74	0
58	MG	AA	3496	1/1	0.87	0.17	-	52,52,52,52	0
58	MG	BA	1709	1/1	0.51	0.21	-	104,104,104,104	0
58	MG	AA	3236	1/1	0.69	0.21	-	57,57,57,57	0
58	MG	AA	3119	1/1	0.93	0.34	-	40,40,40,40	1
58	MG	CA	3484	1/1	0.96	0.27	-	76,76,76,76	0
58	MG	AA	3280	1/1	0.88	0.34	-	47,47,47,47	0
58	MG	AA	3178	1/1	0.44	0.53	-	78,78,78,78	0
58	MG	CA	3262	1/1	0.92	0.17	-	61,61,61,61	0
58	MG	DA	1733	1/1	0.70	0.17	-	83,83,83,83	0
58	MG	DA	1747	1/1	0.87	0.17	-	70,70,70,70	0
58	MG	BA	1767	1/1	0.72	0.09	-	58,58,58,58	0
58	MG	AA	3216	1/1	0.90	0.21	-	51,51,51,51	0
58	MG	AA	3194	1/1	0.93	0.48	-	44,44,44,44	0
58	MG	BA	1667	1/1	0.39	0.21	-	89,89,89,89	0
58	MG	CA	3369	1/1	0.98	0.13	-	59,59,59,59	0
58	MG	DA	1661	1/1	0.86	0.41	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DZ	701	1/1	0.57	0.61	-	111,111,111,111	0
58	MG	AA	3782	1/1	0.94	0.27	-	74,74,74,74	0
58	MG	CA	3246	1/1	0.71	0.50	-	59,59,59,59	0
58	MG	DA	1731	1/1	0.93	0.51	-	82,82,82,82	0
58	MG	AA	3405	1/1	0.93	0.40	-	46,46,46,46	0
58	MG	CA	3305	1/1	0.98	0.18	-	62,62,62,62	0
58	MG	DA	1745	1/1	0.94	0.18	-	61,61,61,61	0
58	MG	AB	3005	1/1	0.97	0.28	-	69,69,69,69	0
58	MG	CA	3434	1/1	0.92	0.18	-	28,28,28,28	0
58	MG	AA	3601	1/1	0.97	0.39	-	47,47,47,47	0
58	MG	CR	201	1/1	0.85	0.45	-	51,51,51,51	0
58	MG	CA	3085	1/1	0.79	0.54	-	66,66,66,66	0
58	MG	CA	3143	1/1	0.92	0.71	-	57,57,57,57	0
58	MG	AA	3801	1/1	0.82	0.07	-	88,88,88,88	0
58	MG	BA	1669	1/1	0.67	0.30	-	73,73,73,73	0
58	MG	CA	3228	1/1	0.86	0.26	-	63,63,63,63	0
58	MG	AA	3549	1/1	0.97	0.08	-	54,54,54,54	0
58	MG	AA	3474	1/1	0.97	0.28	-	53,53,53,53	0
58	MG	CD	302	1/1	0.80	0.45	-	95,95,95,95	0
58	MG	BA	1635	1/1	0.96	0.23	-	72,72,72,72	0
58	MG	AA	3568	1/1	0.94	0.19	-	16,16,16,16	0
58	MG	CA	3208	1/1	0.81	0.44	-	84,84,84,84	0
58	MG	AA	3399	1/1	0.97	0.10	-	18,18,18,18	0
58	MG	CA	3391	1/1	0.97	0.05	-	63,63,63,63	0
58	MG	CA	3601	1/1	0.81	0.08	-	75,75,75,75	0
58	MG	CA	3293	1/1	0.97	0.06	-	71,71,71,71	0
58	MG	AA	3360	1/1	0.88	0.12	-	114,114,114,114	0
58	MG	DA	1758	1/1	0.94	0.16	-	71,71,71,71	0
58	MG	CA	3576	1/1	0.95	0.10	-	36,36,36,36	0
58	MG	AA	3264	1/1	0.91	0.08	-	62,62,62,62	0
58	MG	CA	3132	1/1	0.86	0.20	-	30,30,30,30	0
58	MG	CA	3549	1/1	0.93	0.06	-	57,57,57,57	0
58	MG	BA	1606	1/1	0.89	0.17	-	74,74,74,74	0
58	MG	CA	3076	1/1	0.74	0.41	-	84,84,84,84	0
58	MG	CA	3466	1/1	0.96	0.48	-	57,57,57,57	0
58	MG	CA	3561	1/1	0.58	0.19	-	95,95,95,95	0
58	MG	CA	3179	1/1	0.90	0.53	-	75,75,75,75	0
58	MG	AA	3218	1/1	0.96	0.16	-	38,38,38,38	0
58	MG	AA	3644	1/1	0.94	0.18	-	56,56,56,56	0
58	MG	AA	3310	1/1	0.90	0.26	-	58,58,58,58	0
58	MG	CA	3334	1/1	0.96	0.27	-	44,44,44,44	0
58	MG	AA	3753	1/1	0.89	0.18	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3803	1/1	0.86	0.32	-	62,62,62,62	0
58	MG	DA	1683	1/1	0.95	0.37	-	54,54,54,54	0
58	MG	AA	3065	1/1	0.87	0.54	-	48,48,48,48	0
58	MG	BA	1780	1/1	0.87	0.20	-	81,81,81,81	0
58	MG	DA	1616	1/1	0.95	0.24	-	64,64,64,64	0
58	MG	AA	3758	1/1	0.78	0.36	-	81,81,81,81	0
58	MG	CA	3115	1/1	0.91	0.23	-	76,76,76,76	0
58	MG	CA	3016	1/1	0.89	0.56	-	80,80,80,80	0
58	MG	AA	3715	1/1	0.92	0.08	-	66,66,66,66	0
58	MG	AA	3489	1/1	0.93	0.09	-	64,64,64,64	0
58	MG	CO	201	1/1	0.94	0.16	-	64,64,64,64	0
58	MG	AA	3599	1/1	0.83	0.41	-	58,58,58,58	0
58	MG	CA	3523	1/1	0.86	0.32	-	40,40,40,40	0
58	MG	CA	3001	1/1	0.75	0.40	-	73,73,73,73	0
58	MG	AA	3751	1/1	0.78	0.64	-	56,56,56,56	1
58	MG	AA	3285	1/1	0.91	0.38	-	45,45,45,45	0
58	MG	BA	1722	1/1	0.97	0.44	-	55,55,55,55	0
58	MG	DA	1728	1/1	0.90	0.16	-	63,63,63,63	0
58	MG	BL	201	1/1	0.88	0.27	-	80,80,80,80	0
58	MG	AA	3691	1/1	0.75	0.21	-	89,89,89,89	0
58	MG	CA	3155	1/1	0.73	0.25	-	86,86,86,86	0
58	MG	AA	3675	1/1	0.96	0.10	-	38,38,38,38	0
58	MG	AA	3421	1/1	0.97	0.18	-	12,12,12,12	0
58	MG	AA	3397	1/1	0.94	0.13	-	15,15,15,15	0
58	MG	AN	3002	1/1	0.97	0.16	-	27,27,27,27	0
58	MG	AA	3094	1/1	0.89	0.75	-	111,111,111,111	0
58	MG	CA	3620	1/1	0.51	0.27	-	69,69,69,69	0
58	MG	CA	3034	1/1	0.88	0.58	-	101,101,101,101	0
58	MG	AA	3509	1/1	0.96	0.16	-	49,49,49,49	0
58	MG	AA	3024	1/1	0.78	0.14	-	57,57,57,57	0
58	MG	BA	1754	1/1	0.91	0.09	-	98,98,98,98	0
58	MG	AA	3772	1/1	0.95	0.28	-	17,17,17,17	1
58	MG	CA	3238	1/1	0.90	0.26	-	59,59,59,59	0
58	MG	BA	1601	1/1	0.88	0.27	-	93,93,93,93	0
58	MG	BA	1788	1/1	0.87	0.12	-	75,75,75,75	0
58	MG	AA	3745	1/1	0.92	0.18	-	29,29,29,29	0
58	MG	CA	3497	1/1	0.94	0.32	-	73,73,73,73	0
58	MG	CA	3456	1/1	0.98	0.13	-	60,60,60,60	0
58	MG	CA	3231	1/1	0.96	0.38	-	57,57,57,57	0
58	MG	CA	3382	1/1	0.95	0.19	-	40,40,40,40	0
58	MG	CA	3525	1/1	0.93	0.30	-	83,83,83,83	0
58	MG	AA	3042	1/1	0.85	0.43	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3198	1/1	0.95	0.07	-	58,58,58,58	0
58	MG	AA	3129	1/1	0.91	0.50	-	66,66,66,66	1
58	MG	AA	3740	1/1	0.92	0.17	-	45,45,45,45	0
58	MG	C5	101	1/1	0.95	0.64	-	65,65,65,65	0
58	MG	DA	1663	1/1	0.71	0.22	-	72,72,72,72	0
58	MG	CA	3120	1/1	0.96	0.52	-	62,62,62,62	0
58	MG	DA	1754	1/1	0.57	0.37	-	81,81,81,81	0
58	MG	AA	3759	1/1	0.91	0.29	-	65,65,65,65	0
58	MG	AA	3783	1/1	0.96	0.21	-	54,54,54,54	0
58	MG	DA	1711	1/1	0.93	0.32	-	45,45,45,45	0
58	MG	AA	3288	1/1	0.92	0.17	-	24,24,24,24	0
58	MG	AA	3153	1/1	0.89	0.30	-	59,59,59,59	0
58	MG	BA	1803	1/1	0.93	0.22	-	64,64,64,64	0
58	MG	DA	1753	1/1	0.96	0.40	-	70,70,70,70	0
58	MG	BA	1628	1/1	0.89	0.56	-	55,55,55,55	0
58	MG	CA	3077	1/1	0.90	0.39	-	66,66,66,66	0
58	MG	CA	3519	1/1	0.89	0.28	-	79,79,79,79	0
58	MG	DA	1727	1/1	0.89	0.17	-	66,66,66,66	0
58	MG	AB	3001	1/1	0.76	0.57	-	87,87,87,87	0
58	MG	CA	3479	1/1	0.95	0.22	-	46,46,46,46	0
58	MG	AA	3784	1/1	0.48	0.38	-	74,74,74,74	0
58	MG	DA	1752	1/1	0.96	0.22	-	74,74,74,74	0
58	MG	CA	3418	1/1	0.88	0.27	-	41,41,41,41	0
58	MG	DA	1735	1/1	0.89	0.57	-	83,83,83,83	0
58	MG	CA	3548	1/1	0.87	0.14	-	48,48,48,48	1
58	MG	AA	3259	1/1	0.98	0.33	-	20,20,20,20	1
58	MG	AA	3512	1/1	0.93	0.34	-	60,60,60,60	0
58	MG	BA	1689	1/1	0.53	0.77	-	91,91,91,91	0
58	MG	CA	3563	1/1	0.69	0.20	-	91,91,91,91	0
58	MG	AA	3648	1/1	0.97	0.17	-	40,40,40,40	0
58	MG	CA	3323	1/1	0.88	0.23	-	67,67,67,67	0
58	MG	AA	3353	1/1	0.91	0.08	-	76,76,76,76	0
58	MG	AA	3645	1/1	0.93	0.51	-	79,79,79,79	0
58	MG	AA	3652	1/1	0.91	0.28	-	77,77,77,77	0
58	MG	DA	1744	1/1	0.89	0.10	-	79,79,79,79	0
58	MG	AA	3062	1/1	0.89	0.35	-	67,67,67,67	0
58	MG	AA	3338	1/1	0.95	0.15	-	30,30,30,30	0
58	MG	AA	3533	1/1	0.95	0.14	-	22,22,22,22	0
58	MG	BA	1619	1/1	0.91	0.19	-	52,52,52,52	0
58	MG	AA	3208	1/1	0.85	0.32	-	61,61,61,61	0
58	MG	BA	1665	1/1	0.89	0.38	-	55,55,55,55	0
58	MG	AA	3689	1/1	0.92	0.16	-	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3191	1/1	0.93	0.29	-	65,65,65,65	0
58	MG	CA	3355	1/1	0.97	0.11	-	41,41,41,41	0
58	MG	AA	3464	1/1	0.81	0.15	-	63,63,63,63	0
58	MG	DA	1751	1/1	0.72	0.26	-	81,81,81,81	0
58	MG	CA	3380	1/1	0.95	0.20	-	71,71,71,71	0
58	MG	BA	1681	1/1	0.53	1.14	-	84,84,84,84	0
58	MG	BA	1785	1/1	0.69	0.33	-	87,87,87,87	0
58	MG	AA	3701	1/1	0.86	0.46	-	43,43,43,43	1
58	MG	CA	3255	1/1	0.88	0.48	-	67,67,67,67	0
58	MG	CA	3388	1/1	0.85	0.12	-	83,83,83,83	0
58	MG	AA	3742	1/1	0.94	0.25	-	82,82,82,82	0
58	MG	DA	1674	1/1	0.94	0.40	-	62,62,62,62	0
58	MG	AA	3124	1/1	0.95	0.63	-	63,63,63,63	0
58	MG	AA	3088	1/1	0.91	0.33	-	34,34,34,34	0
58	MG	CA	3605	1/1	0.93	0.27	-	73,73,73,73	0
58	MG	AA	3553	1/1	0.93	0.17	-	40,40,40,40	0
58	MG	AA	3690	1/1	0.90	0.25	-	71,71,71,71	0
58	MG	BA	1730	1/1	0.88	0.26	-	78,78,78,78	0
58	MG	AA	3149	1/1	0.90	0.27	-	62,62,62,62	0
58	MG	DA	1708	1/1	0.90	0.10	-	87,87,87,87	0
58	MG	AA	3813	1/1	0.93	0.59	-	54,54,54,54	0
58	MG	CA	3194	1/1	0.89	0.57	-	72,72,72,72	0
58	MG	AA	3220	1/1	0.82	0.28	-	62,62,62,62	0
58	MG	DA	1762	1/1	0.80	0.08	-	73,73,73,73	0
58	MG	AA	3241	1/1	0.94	0.21	-	69,69,69,69	0
58	MG	BA	1745	1/1	0.88	0.43	-	66,66,66,66	0
58	MG	CA	3284	1/1	0.95	0.20	-	92,92,92,92	0
58	MG	AA	3685	1/1	0.93	0.20	-	47,47,47,47	0
58	MG	AA	3682	1/1	0.96	0.30	-	53,53,53,53	0
58	MG	AA	3468	1/1	0.94	0.37	-	52,52,52,52	0
58	MG	AA	3390	1/1	0.89	0.22	-	35,35,35,35	0
58	MG	CA	3244	1/1	0.72	0.67	-	78,78,78,78	0
58	MG	AA	3683	1/1	0.96	0.37	-	67,67,67,67	0
58	MG	CA	3415	1/1	0.98	0.21	-	31,31,31,31	1
58	MG	CA	3070	1/1	0.63	0.81	-	87,87,87,87	0
58	MG	AA	3510	1/1	0.95	0.36	-	58,58,58,58	0
58	MG	CA	3625	1/1	0.85	0.54	-	79,79,79,79	0
58	MG	AA	3618	1/1	0.94	0.16	-	38,38,38,38	0
58	MG	AP	202	1/1	0.88	0.18	-	40,40,40,40	0
58	MG	CA	3421	1/1	0.57	0.25	-	76,76,76,76	0
58	MG	AA	3475	1/1	0.96	0.14	-	62,62,62,62	0
58	MG	AA	3716	1/1	0.96	0.17	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3612	1/1	0.94	0.23	-	68,68,68,68	0
58	MG	AA	3710	1/1	0.79	0.27	-	75,75,75,75	0
58	MG	AA	3676	1/1	0.95	0.19	-	66,66,66,66	0
58	MG	DA	1607	1/1	0.84	0.32	-	61,61,61,61	0
58	MG	CA	3450	1/1	0.97	0.19	-	48,48,48,48	0
58	MG	AA	3177	1/1	0.94	0.34	-	61,61,61,61	0
58	MG	AA	3667	1/1	0.95	0.20	-	28,28,28,28	0
58	MG	C8	5001	1/1	0.90	0.36	-	51,51,51,51	0
58	MG	CA	3532	1/1	0.75	0.12	-	79,79,79,79	0
58	MG	BA	1725	1/1	0.90	0.11	-	59,59,59,59	0
58	MG	AA	3350	1/1	0.92	0.29	-	31,31,31,31	0
58	MG	BA	1772	1/1	0.81	0.18	-	70,70,70,70	0
58	MG	AA	3578	1/1	0.94	0.42	-	55,55,55,55	0
58	MG	AA	3478	1/1	0.98	0.16	-	40,40,40,40	0
58	MG	CA	3505	1/1	0.93	0.27	-	73,73,73,73	0
58	MG	BA	1776	1/1	0.96	0.26	-	64,64,64,64	0
58	MG	AF	305	1/1	0.94	0.22	-	55,55,55,55	0
58	MG	CA	3116	1/1	0.81	0.43	-	75,75,75,75	0
58	MG	DA	1756	1/1	0.93	0.24	-	68,68,68,68	0
58	MG	CA	3537	1/1	0.69	0.29	-	78,78,78,78	0
58	MG	AA	3461	1/1	0.87	0.50	-	66,66,66,66	0
58	MG	BA	1660	1/1	0.73	0.21	-	70,70,70,70	0
58	MG	CA	3473	1/1	0.93	0.17	-	54,54,54,54	0
58	MG	CA	3637	1/1	0.98	0.36	-	59,59,59,59	0
58	MG	CA	3335	1/1	0.73	0.18	-	62,62,62,62	0
58	MG	CA	3363	1/1	0.86	0.24	-	66,66,66,66	0
58	MG	AA	3230	1/1	0.82	0.58	-	80,80,80,80	0
58	MG	AA	3657	1/1	0.90	0.24	-	43,43,43,43	1
58	MG	AA	3328	1/1	0.94	0.17	-	18,18,18,18	0
58	MG	DA	1734	1/1	0.86	0.25	-	83,83,83,83	0
58	MG	AA	3587	1/1	0.91	0.31	-	53,53,53,53	0
58	MG	CB	3003	1/1	0.95	0.13	-	77,77,77,77	0
58	MG	DA	1742	1/1	0.96	0.33	-	79,79,79,79	0
58	MG	CA	3379	1/1	0.90	0.29	-	65,65,65,65	0
58	MG	AA	3303	1/1	0.91	0.33	-	56,56,56,56	0
58	MG	AA	3471	1/1	0.95	0.26	-	34,34,34,34	0
58	MG	CA	3481	1/1	0.58	0.34	-	91,91,91,91	0
58	MG	AB	3002	1/1	0.98	0.18	-	59,59,59,59	0
58	MG	BA	1658	1/1	0.93	0.51	-	76,76,76,76	0
58	MG	AA	3417	1/1	0.97	0.17	-	25,25,25,25	0
58	MG	AA	3265	1/1	0.87	0.50	-	77,77,77,77	0
58	MG	DA	1634	1/1	0.59	0.34	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3234	1/1	0.95	0.17	-	30,30,30,30	1
58	MG	CA	3181	1/1	0.94	0.24	-	47,47,47,47	0
58	MG	AA	3098	1/1	0.93	0.31	-	58,58,58,58	0
58	MG	CA	3653	1/1	0.78	0.39	-	95,95,95,95	0
58	MG	DA	1696	1/1	0.86	0.20	-	91,91,91,91	0
58	MG	CA	3592	1/1	0.95	0.61	-	76,76,76,76	0
58	MG	CA	3039	1/1	0.82	0.91	-	71,71,71,71	0
58	MG	AA	3204	1/1	0.72	0.39	-	57,57,57,57	0
58	MG	AA	3186	1/1	0.83	0.16	-	37,37,37,37	0
58	MG	AO	5001	1/1	0.87	0.18	-	55,55,55,55	0
58	MG	CA	3408	1/1	0.98	0.13	-	64,64,64,64	0
58	MG	AA	3308	1/1	0.81	0.13	-	30,30,30,30	0
58	MG	CA	3528	1/1	0.83	0.42	-	79,79,79,79	0
58	MG	CA	3233	1/1	0.91	0.46	-	71,71,71,71	0
58	MG	CA	3502	1/1	0.99	0.14	-	70,70,70,70	0
58	MG	AA	3176	1/1	0.90	0.31	-	50,50,50,50	0
58	MG	CA	3496	1/1	0.98	0.17	-	63,63,63,63	0
58	MG	AA	3172	1/1	0.85	0.75	-	71,71,71,71	0
58	MG	CA	3196	1/1	0.92	0.56	-	64,64,64,64	0
58	MG	AA	3484	1/1	0.92	0.23	-	35,35,35,35	0
58	MG	AA	3594	1/1	0.92	0.23	-	43,43,43,43	0
58	MG	CA	3412	1/1	0.88	0.26	-	81,81,81,81	0
58	MG	DA	1716	1/1	0.90	0.37	-	78,78,78,78	0
58	MG	CA	3539	1/1	0.95	0.43	-	73,73,73,73	0
58	MG	CA	3058	1/1	0.72	0.42	-	77,77,77,77	0
58	MG	AA	3454	1/1	0.98	0.12	-	51,51,51,51	0
58	MG	CA	3622	1/1	0.84	0.24	-	55,55,55,55	0
58	MG	AA	3337	1/1	0.97	0.24	-	10,10,10,10	0
58	MG	AA	3319	1/1	0.90	0.18	-	69,69,69,69	0
58	MG	DW	503	1/1	0.62	0.18	-	84,84,84,84	0
58	MG	AA	3108	1/1	0.76	0.48	-	125,125,125,125	0
58	MG	CA	3260	1/1	0.97	0.23	-	65,65,65,65	0
58	MG	AA	3346	1/1	0.94	0.21	-	46,46,46,46	0
58	MG	AB	3015	1/1	0.96	0.18	-	40,40,40,40	0
58	MG	CA	3131	1/1	0.80	0.21	-	62,62,62,62	0
58	MG	CA	3117	1/1	0.80	0.31	-	68,68,68,68	0
58	MG	AA	3386	1/1	0.98	0.22	-	29,29,29,29	0
58	MG	CA	3474	1/1	0.83	0.33	-	76,76,76,76	0
58	MG	AW	3004	1/1	0.89	0.32	-	65,65,65,65	0
58	MG	AA	3612	1/1	0.86	0.21	-	56,56,56,56	0
58	MG	CA	3270	1/1	0.98	0.19	-	35,35,35,35	0
58	MG	CA	3130	1/1	0.91	0.68	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3639	1/1	0.87	0.18	-	77,77,77,77	0
58	MG	BA	1743	1/1	0.95	0.18	-	52,52,52,52	0
58	MG	CA	3235	1/1	0.85	0.61	-	75,75,75,75	0
58	MG	CA	3368	1/1	0.92	0.21	-	59,59,59,59	0
58	MG	CA	3176	1/1	0.96	0.48	-	50,50,50,50	0
58	MG	CA	3402	1/1	0.93	0.12	-	70,70,70,70	0
58	MG	CA	3471	1/1	0.94	0.17	-	45,45,45,45	0
58	MG	BA	1736	1/1	0.85	0.12	-	73,73,73,73	0
58	MG	CA	3032	1/1	0.85	0.58	-	67,67,67,67	0
58	MG	CA	3300	1/1	0.80	0.40	-	86,86,86,86	0
58	MG	CA	3142	1/1	0.90	0.27	-	69,69,69,69	0
58	MG	CA	3294	1/1	0.75	0.21	-	83,83,83,83	0
58	MG	CA	3289	1/1	0.97	0.32	-	42,42,42,42	0
58	MG	AA	3776	1/1	0.94	0.12	-	40,40,40,40	0
58	MG	CA	3558	1/1	0.91	0.20	-	51,51,51,51	1
58	MG	AA	3166	1/1	0.94	0.17	-	31,31,31,31	0
58	MG	CA	3096	1/1	0.82	0.35	-	68,68,68,68	0
58	MG	AA	3465	1/1	0.94	0.21	-	39,39,39,39	0
58	MG	DA	1656	1/1	0.79	0.23	-	75,75,75,75	0
58	MG	CA	3406	1/1	0.86	0.13	-	70,70,70,70	0
58	MG	AA	3531	1/1	0.92	0.30	-	62,62,62,62	0
58	MG	CB	3006	1/1	0.85	0.13	-	83,83,83,83	0
58	MG	AA	3409	1/1	0.98	0.20	-	45,45,45,45	0
58	MG	CA	3072	1/1	0.86	0.28	-	56,56,56,56	0
58	MG	BA	1625	1/1	0.87	0.32	-	57,57,57,57	0
58	MG	AA	3640	1/1	0.72	0.44	-	77,77,77,77	0
58	MG	CA	3468	1/1	0.82	0.16	-	61,61,61,61	0
58	MG	AA	3030	1/1	0.93	0.32	-	26,26,26,26	1
58	MG	CA	3663	1/1	0.85	0.39	-	91,91,91,91	0
58	MG	CA	3504	1/1	0.88	0.08	-	62,62,62,62	0
58	MG	DA	1714	1/1	0.97	0.12	-	51,51,51,51	0
58	MG	CA	3210	1/1	0.93	0.31	-	75,75,75,75	0
58	MG	AA	3603	1/1	0.91	0.19	-	63,63,63,63	0
58	MG	CA	3552	1/1	0.97	0.14	-	69,69,69,69	0
58	MG	AW	3002	1/1	0.91	0.28	-	55,55,55,55	0
58	MG	AA	3180	1/1	0.89	0.31	-	94,94,94,94	0
58	MG	CA	3575	1/1	0.93	0.10	-	43,43,43,43	1
58	MG	AA	3008	1/1	0.95	0.17	-	19,19,19,19	0
58	MG	CA	3051	1/1	0.97	0.44	-	63,63,63,63	0
58	MG	CA	3414	1/1	0.93	0.20	-	50,50,50,50	0
58	MG	BA	1774	1/1	0.83	0.13	-	61,61,61,61	0
58	MG	BA	1642	1/1	0.85	0.42	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3729	1/1	0.84	0.11	-	38,38,38,38	0
58	MG	AA	3279	1/1	0.88	0.35	-	53,53,53,53	0
58	MG	AA	3074	1/1	0.97	0.35	-	15,15,15,15	0
58	MG	CA	3437	1/1	0.97	0.11	-	48,48,48,48	0
58	MG	AA	3306	1/1	0.81	0.19	-	47,47,47,47	0
58	MG	BA	1804	1/1	0.92	0.18	-	67,67,67,67	0
58	MG	AA	3680	1/1	0.92	0.25	-	59,59,59,59	0
58	MG	CA	3292	1/1	0.89	0.08	-	73,73,73,73	0
58	MG	CA	3054	1/1	0.88	0.14	-	71,71,71,71	0
58	MG	CA	3071	1/1	0.32	0.51	-	97,97,97,97	0
58	MG	CA	3123	1/1	0.83	0.87	-	88,88,88,88	0
58	MG	AA	3123	1/1	0.92	0.37	-	37,37,37,37	1
58	MG	AA	3766	1/1	0.60	0.20	-	72,72,72,72	0
58	MG	AA	3273	1/1	0.83	0.33	-	90,90,90,90	0
58	MG	AA	3028	1/1	0.87	0.37	-	51,51,51,51	1
58	MG	DA	1615	1/1	0.98	0.54	-	53,53,53,53	0
58	MG	CA	3422	1/1	0.95	0.26	-	55,55,55,55	0
58	MG	BA	1682	1/1	0.89	0.11	-	69,69,69,69	0
58	MG	DA	1640	1/1	0.95	0.18	-	79,79,79,79	0
58	MG	AA	3362	1/1	0.87	0.48	-	69,69,69,69	0
58	MG	AA	3774	1/1	0.86	0.23	-	80,80,80,80	0
58	MG	BA	1784	1/1	0.88	0.22	-	60,60,60,60	0
58	MG	CA	3206	1/1	0.93	0.59	-	56,56,56,56	0
58	MG	CA	3271	1/1	0.90	0.32	-	57,57,57,57	0
58	MG	CA	3079	1/1	0.94	0.34	-	57,57,57,57	0
58	MG	CA	3145	1/1	0.92	0.08	-	79,79,79,79	0
58	MG	AA	3091	1/1	0.89	0.39	-	38,38,38,38	1
58	MG	BA	1609	1/1	0.89	0.14	-	69,69,69,69	0
58	MG	CA	3649	1/1	0.78	0.35	-	85,85,85,85	0
58	MG	CD	301	1/1	0.74	0.47	-	81,81,81,81	0
58	MG	AA	3017	1/1	0.81	0.16	-	78,78,78,78	0
58	MG	AA	3737	1/1	0.94	0.15	-	29,29,29,29	0
58	MG	AA	3245	1/1	0.82	0.78	-	69,69,69,69	0
58	MG	CA	3303	1/1	0.93	0.47	-	54,54,54,54	0
58	MG	AA	3767	1/1	0.60	0.31	-	63,63,63,63	1
58	MG	AA	3077	1/1	0.92	0.34	-	50,50,50,50	0
58	MG	CA	3288	1/1	0.97	0.25	-	54,54,54,54	0
58	MG	AB	3004	1/1	0.79	0.30	-	89,89,89,89	0
58	MG	CA	3374	1/1	0.80	0.43	-	76,76,76,76	0
58	MG	CA	3042	1/1	0.60	0.73	-	95,95,95,95	0
58	MG	BA	1652	1/1	0.77	0.14	-	69,69,69,69	0
58	MG	AA	3447	1/1	0.80	0.18	-	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BM	202	1/1	0.86	0.39	-	65,65,65,65	0
58	MG	AA	3778	1/1	0.93	0.21	-	54,54,54,54	0
58	MG	BA	1691	1/1	0.86	0.56	-	74,74,74,74	0
58	MG	DA	1643	1/1	0.90	0.16	-	55,55,55,55	0
58	MG	AA	3228	1/1	0.96	0.19	-	51,51,51,51	0
58	MG	BA	1716	1/1	0.78	0.17	-	67,67,67,67	0
58	MG	AA	3154	1/1	0.91	0.35	-	46,46,46,46	0
58	MG	AA	3432	1/1	0.90	0.33	-	57,57,57,57	0
58	MG	CE	306	1/1	0.92	0.07	-	67,67,67,67	0
58	MG	AA	3605	1/1	0.86	0.28	-	68,68,68,68	0
58	MG	CB	3005	1/1	0.94	0.31	-	62,62,62,62	0
58	MG	CA	3397	1/1	0.98	0.13	-	59,59,59,59	0
58	MG	CN	5001	1/1	0.91	0.09	-	77,77,77,77	0
58	MG	CA	3154	1/1	0.80	0.31	-	72,72,72,72	0
58	MG	AA	3131	1/1	0.96	0.45	-	55,55,55,55	0
58	MG	AA	3097	1/1	0.98	0.20	-	26,26,26,26	0
58	MG	CA	3078	1/1	0.87	0.25	-	47,47,47,47	0
58	MG	BA	1715	1/1	0.74	0.21	-	83,83,83,83	0
58	MG	CA	3102	1/1	0.92	0.35	-	56,56,56,56	0
58	MG	CA	3557	1/1	0.89	0.11	-	76,76,76,76	0
58	MG	BA	1795	1/1	0.97	0.27	-	69,69,69,69	0
58	MG	AA	3205	1/1	0.85	0.46	-	64,64,64,64	0
58	MG	CA	3377	1/1	0.97	0.19	-	80,80,80,80	0
58	MG	AA	3416	1/1	0.97	0.17	-	30,30,30,30	0
58	MG	BA	1637	1/1	0.88	0.23	-	66,66,66,66	0
58	MG	AA	3392	1/1	0.96	0.17	-	42,42,42,42	0
58	MG	CA	3472	1/1	0.93	0.60	-	72,72,72,72	0
58	MG	CA	3184	1/1	0.89	0.30	-	66,66,66,66	0
58	MG	CA	3081	1/1	0.82	0.16	-	68,68,68,68	0
58	MG	AA	3692	1/1	0.97	0.18	-	53,53,53,53	0
58	MG	DA	1704	1/1	0.96	0.07	-	69,69,69,69	0
58	MG	CB	3013	1/1	0.80	0.19	-	98,98,98,98	0
58	MG	CA	3053	1/1	0.96	0.75	-	58,58,58,58	0
58	MG	CA	3350	1/1	0.79	0.09	-	85,85,85,85	0
58	MG	AA	3448	1/1	0.89	0.05	-	78,78,78,78	0
58	MG	AA	3437	1/1	0.89	0.25	-	54,54,54,54	0
58	MG	AA	3424	1/1	0.86	0.15	-	65,65,65,65	0
58	MG	AA	3262	1/1	0.97	0.38	-	70,70,70,70	0
58	MG	BA	1650	1/1	0.71	0.36	-	72,72,72,72	0
58	MG	BA	1759	1/1	0.95	0.14	-	63,63,63,63	0
58	MG	AA	3638	1/1	0.71	0.41	-	72,72,72,72	0
58	MG	AA	3624	1/1	0.93	0.15	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3608	1/1	0.86	0.18	-	73,73,73,73	0
58	MG	AA	3103	1/1	0.98	0.07	-	15,15,15,15	0
58	MG	BA	1761	1/1	0.93	0.18	-	55,55,55,55	0
58	MG	CA	3426	1/1	0.91	0.19	-	55,55,55,55	0
58	MG	BA	1808	1/1	0.93	0.14	-	50,50,50,50	0
58	MG	AA	3105	1/1	0.84	0.14	-	81,81,81,81	0
58	MG	DA	1602	1/1	0.92	0.12	-	80,80,80,80	0
58	MG	CA	3508	1/1	0.94	0.15	-	96,96,96,96	0
58	MG	CP	202	1/1	0.88	0.42	-	71,71,71,71	0
58	MG	AA	3728	1/1	0.92	0.21	-	61,61,61,61	0
58	MG	CA	3064	1/1	0.95	0.06	-	43,43,43,43	0
58	MG	CA	3578	1/1	0.85	0.26	-	80,80,80,80	0
58	MG	AA	3015	1/1	0.81	0.48	-	64,64,64,64	0
58	MG	DA	1611	1/1	0.96	0.09	-	38,38,38,38	0
58	MG	CA	3566	1/1	0.96	0.13	-	41,41,41,41	0
58	MG	AA	3156	1/1	0.95	0.34	-	33,33,33,33	1
58	MG	DA	1660	1/1	0.52	0.63	-	90,90,90,90	0
58	MG	AA	3085	1/1	0.84	0.32	-	53,53,53,53	0
58	MG	AA	3367	1/1	0.96	0.17	-	52,52,52,52	0
58	MG	AA	3274	1/1	0.92	0.29	-	55,55,55,55	0
58	MG	CA	3066	1/1	0.62	0.59	-	84,84,84,84	0
58	MG	AA	3563	1/1	0.97	0.16	-	49,49,49,49	1
58	MG	DA	1705	1/1	0.92	0.32	-	62,62,62,62	0
58	MG	AA	3422	1/1	0.88	0.10	-	71,71,71,71	0
58	MG	CA	3387	1/1	0.95	0.34	-	70,70,70,70	0
58	MG	DJ	5001	1/1	0.53	0.48	-	105,105,105,105	0
58	MG	AA	3577	1/1	0.93	0.11	-	32,32,32,32	0
58	MG	AA	3332	1/1	0.95	0.14	-	46,46,46,46	0
58	MG	AA	3298	1/1	0.93	0.08	-	59,59,59,59	0
58	MG	AA	3724	1/1	0.97	0.28	-	40,40,40,40	0
58	MG	CA	3586	1/1	0.92	0.15	-	69,69,69,69	0
58	MG	AA	3343	1/1	0.95	0.14	-	65,65,65,65	0
58	MG	AA	3402	1/1	0.96	0.30	-	33,33,33,33	0
58	MG	CA	3520	1/1	0.92	0.18	-	59,59,59,59	0
58	MG	CA	3604	1/1	0.80	0.19	-	69,69,69,69	0
58	MG	AA	3365	1/1	0.91	0.31	-	57,57,57,57	0
58	MG	AA	3472	1/1	0.96	0.21	-	24,24,24,24	0
58	MG	CA	3366	1/1	0.96	0.24	-	61,61,61,61	0
58	MG	AA	3293	1/1	0.96	0.20	-	32,32,32,32	0
58	MG	AA	3004	1/1	0.92	0.16	-	25,25,25,25	0
58	MG	AA	3672	1/1	0.79	0.35	-	25,25,25,25	1
58	MG	CA	3307	1/1	0.97	0.30	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3237	1/1	0.96	0.31	-	75,75,75,75	0
58	MG	AA	3052	1/1	0.86	0.64	-	65,65,65,65	0
58	MG	AA	3752	1/1	0.84	0.60	-	72,72,72,72	0
58	MG	AA	3352	1/1	0.89	0.25	-	51,51,51,51	0
58	MG	BA	1627	1/1	0.89	0.28	-	87,87,87,87	0
58	MG	CA	3059	1/1	0.77	0.37	-	60,60,60,60	0
58	MG	AA	3460	1/1	0.83	0.47	-	72,72,72,72	0
58	MG	CA	3257	1/1	0.94	0.48	-	57,57,57,57	0
58	MG	AA	3438	1/1	0.89	0.22	-	57,57,57,57	0
58	MG	AA	3229	1/1	0.89	0.31	-	43,43,43,43	0
58	MG	BA	1751	1/1	0.89	0.13	-	58,58,58,58	0
58	MG	DA	1620	1/1	0.81	0.14	-	58,58,58,58	0
58	MG	CA	3224	1/1	0.69	0.97	-	81,81,81,81	0
58	MG	CA	3219	1/1	0.98	0.21	-	31,31,31,31	0
58	MG	AA	3570	1/1	0.85	0.17	-	15,15,15,15	0
58	MG	CA	3589	1/1	0.85	0.07	-	79,79,79,79	0
58	MG	AA	3139	1/1	0.92	0.10	-	58,58,58,58	0
58	MG	DA	1673	1/1	0.65	0.37	-	100,100,100,100	0
58	MG	CA	3599	1/1	0.54	0.23	-	80,80,80,80	0
58	MG	AA	3804	1/1	0.93	0.40	-	68,68,68,68	0
58	MG	AA	3548	1/1	0.95	0.16	-	57,57,57,57	1
58	MG	CA	3540	1/1	0.83	0.33	-	85,85,85,85	0
58	MG	CA	3371	1/1	0.95	0.21	-	55,55,55,55	0
58	MG	CA	3144	1/1	0.90	0.32	-	67,67,67,67	0
58	MG	AA	3080	1/1	0.80	0.40	-	57,57,57,57	0
58	MG	AA	3660	1/1	0.91	0.23	-	70,70,70,70	0
58	MG	AA	3323	1/1	0.86	0.12	-	22,22,22,22	0
58	MG	CA	3068	1/1	0.78	0.26	-	57,57,57,57	0
58	MG	CA	3060	1/1	0.91	0.41	-	77,77,77,77	0
58	MG	CA	3407	1/1	0.90	0.23	-	55,55,55,55	0
58	MG	AA	3419	1/1	0.96	0.14	-	31,31,31,31	0
58	MG	AA	3757	1/1	0.90	0.12	-	55,55,55,55	0
58	MG	CA	3205	1/1	0.09	0.69	-	105,105,105,105	0
58	MG	BA	1655	1/1	0.91	0.32	-	69,69,69,69	0
58	MG	AA	3557	1/1	0.97	0.17	-	19,19,19,19	0
58	MG	DK	5001	1/1	0.93	0.27	-	100,100,100,100	0
58	MG	CA	3386	1/1	0.90	0.28	-	65,65,65,65	0
58	MG	AA	3429	1/1	0.96	0.21	-	41,41,41,41	0
58	MG	CQ	205	1/1	0.55	0.51	-	81,81,81,81	0
58	MG	CA	3249	1/1	0.95	0.19	-	46,46,46,46	0
58	MG	CB	3012	1/1	0.95	0.35	-	76,76,76,76	0
58	MG	AA	3121	1/1	0.86	0.33	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BE	3001	1/1	0.94	0.12	-	60,60,60,60	0
58	MG	CQ	204	1/1	0.85	0.31	-	61,61,61,61	0
58	MG	CA	3435	1/1	0.97	0.11	-	52,52,52,52	0
58	MG	AB	3006	1/1	0.77	0.30	-	72,72,72,72	0
58	MG	CA	3197	1/1	0.90	0.48	-	64,64,64,64	0
58	MG	BA	1766	1/1	0.75	0.36	-	86,86,86,86	0
58	MG	AA	3658	1/1	0.99	0.15	-	62,62,62,62	0
58	MG	BA	1610	1/1	0.66	0.12	-	79,79,79,79	0
58	MG	CA	3239	1/1	0.72	0.39	-	75,75,75,75	0
58	MG	CA	3590	1/1	0.71	0.17	-	95,95,95,95	0
58	MG	CA	3642	1/1	0.83	0.99	-	80,80,80,80	0
58	MG	CA	3451	1/1	0.95	0.19	-	63,63,63,63	0
58	MG	CA	3269	1/1	0.94	0.13	-	86,86,86,86	0
58	MG	BA	1764	1/1	0.85	0.33	-	63,63,63,63	0
58	MG	BA	1638	1/1	0.79	0.63	-	78,78,78,78	0
58	MG	AA	3765	1/1	0.85	0.37	-	63,63,63,63	0
58	MG	AA	3713	1/1	0.79	0.41	-	52,52,52,52	1
58	MG	CA	3327	1/1	0.94	0.25	-	53,53,53,53	0
58	MG	AA	3727	1/1	0.88	0.15	-	49,49,49,49	0
58	MG	CA	3507	1/1	0.63	0.26	-	100,100,100,100	0
58	MG	BA	1692	1/1	0.82	0.30	-	86,86,86,86	0
58	MG	CA	3632	1/1	0.85	0.17	-	79,79,79,79	0
58	MG	AA	3078	1/1	0.80	0.29	-	66,66,66,66	0
58	MG	CA	3129	1/1	0.85	0.54	-	69,69,69,69	0
58	MG	DA	1608	1/1	0.87	0.08	-	47,47,47,47	0
58	MG	BA	1631	1/1	0.89	0.11	-	48,48,48,48	0
58	MG	DA	1713	1/1	0.96	0.54	-	72,72,72,72	0
58	MG	DA	1749	1/1	0.85	0.43	-	80,80,80,80	0
58	MG	CA	3277	1/1	0.95	0.11	-	90,90,90,90	0
58	MG	BA	1792	1/1	0.95	0.19	-	75,75,75,75	0
58	MG	CA	3153	1/1	0.89	0.19	-	78,78,78,78	0
58	MG	AA	3193	1/1	0.85	0.23	-	62,62,62,62	0
58	MG	AA	3534	1/1	0.98	0.17	-	27,27,27,27	0
58	MG	AA	3286	1/1	0.94	0.21	-	52,52,52,52	0
58	MG	DA	1755	1/1	0.74	0.64	-	86,86,86,86	0
58	MG	CA	3098	1/1	0.60	0.39	-	83,83,83,83	0
58	MG	BA	1632	1/1	0.90	0.30	-	54,54,54,54	0
58	MG	DA	1625	1/1	0.92	0.55	-	73,73,73,73	0
58	MG	AA	3458	1/1	0.92	0.19	-	72,72,72,72	0
58	MG	BA	1663	1/1	0.94	0.09	-	79,79,79,79	0
58	MG	CA	3090	1/1	0.87	0.53	-	65,65,65,65	0
58	MG	AA	3536	1/1	0.94	0.10	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1661	1/1	0.73	0.99	-	82,82,82,82	0
58	MG	CA	3280	1/1	0.90	0.18	-	30,30,30,30	0
58	MG	CA	3111	1/1	0.82	0.13	-	71,71,71,71	0
58	MG	DA	1766	1/1	0.85	0.12	-	58,58,58,58	0
58	MG	CA	3359	1/1	0.93	0.19	-	42,42,42,42	0
58	MG	AA	3093	1/1	0.91	0.28	-	27,27,27,27	1
58	MG	CA	3245	1/1	0.89	0.48	-	57,57,57,57	0
58	MG	DA	1639	1/1	0.87	0.16	-	75,75,75,75	0
58	MG	CA	3298	1/1	0.94	0.15	-	68,68,68,68	0
58	MG	AA	3655	1/1	0.98	0.16	-	61,61,61,61	0
58	MG	AA	3163	1/1	0.88	0.38	-	40,40,40,40	0
58	MG	AA	3503	1/1	0.94	0.15	-	64,64,64,64	0
58	MG	CA	3534	1/1	0.84	0.18	-	79,79,79,79	0
58	MG	CA	3593	1/1	0.68	0.26	-	73,73,73,73	0
58	MG	AA	3661	1/1	0.94	0.32	-	43,43,43,43	0
58	MG	AA	3588	1/1	0.90	0.19	-	38,38,38,38	0
58	MG	AA	3292	1/1	0.90	0.13	-	74,74,74,74	0
58	MG	AA	3029	1/1	0.87	0.29	-	53,53,53,53	0
58	MG	CA	3511	1/1	0.96	0.12	-	68,68,68,68	0
58	MG	AA	3666	1/1	0.95	0.07	-	64,64,64,64	0
58	MG	CA	3089	1/1	0.72	0.41	-	80,80,80,80	0
58	MG	AA	3092	1/1	0.94	0.13	-	53,53,53,53	0
58	MG	AA	3635	1/1	0.99	0.11	-	23,23,23,23	0
58	MG	CA	3517	1/1	0.99	0.33	-	64,64,64,64	0
58	MG	DA	1729	1/1	0.88	0.13	-	57,57,57,57	0
58	MG	CA	3008	1/1	0.72	0.41	-	100,100,100,100	0
58	MG	CA	3638	1/1	0.91	0.32	-	55,55,55,55	0
58	MG	BA	1641	1/1	0.92	0.23	-	71,71,71,71	0
58	MG	CA	3527	1/1	0.47	0.13	-	78,78,78,78	0
58	MG	AA	3268	1/1	0.80	0.12	-	88,88,88,88	0
58	MG	CA	3641	1/1	0.79	0.40	-	67,67,67,67	0
58	MG	AF	304	1/1	0.92	0.32	-	62,62,62,62	0
58	MG	AA	3244	1/1	0.45	0.25	-	100,100,100,100	0
58	MG	CA	3524	1/1	0.79	0.09	-	77,77,77,77	0
58	MG	AA	3224	1/1	0.83	0.41	-	75,75,75,75	0
58	MG	BA	1765	1/1	0.97	0.11	-	61,61,61,61	0
58	MG	CA	3554	1/1	0.95	0.18	-	67,67,67,67	0
58	MG	AA	3595	1/1	0.96	0.25	-	55,55,55,55	0
58	MG	AA	3560	1/1	0.87	0.27	-	58,58,58,58	0
58	MG	BA	1787	1/1	0.88	0.24	-	90,90,90,90	0
58	MG	AA	3483	1/1	0.85	0.07	-	43,43,43,43	1
58	MG	DA	1737	1/1	0.91	0.16	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3094	1/1	0.92	0.32	-	87,87,87,87	0
58	MG	DA	1629	1/1	0.93	0.41	-	58,58,58,58	0
58	MG	CP	201	1/1	0.85	0.82	-	65,65,65,65	0
58	MG	CA	3025	1/1	0.83	0.28	-	77,77,77,77	0
58	MG	DA	1667	1/1	0.96	0.24	-	49,49,49,49	0
58	MG	AA	3140	1/1	0.93	0.31	-	50,50,50,50	0
58	MG	CA	3478	1/1	0.94	0.14	-	58,58,58,58	0
58	MG	AA	3500	1/1	0.95	0.12	-	47,47,47,47	0
58	MG	AA	3055	1/1	0.95	0.28	-	35,35,35,35	0
58	MG	CA	3045	1/1	0.88	0.41	-	67,67,67,67	0
58	MG	AN	3003	1/1	0.91	0.13	-	47,47,47,47	0
58	MG	CA	3093	1/1	0.58	0.64	-	84,84,84,84	0
58	MG	AA	3781	1/1	0.76	0.33	-	44,44,44,44	1
58	MG	CA	3156	1/1	0.93	0.32	-	68,68,68,68	0
58	MG	BA	1777	1/1	0.90	0.21	-	79,79,79,79	0
58	MG	DA	1706	1/1	0.72	0.28	-	128,128,128,128	0
58	MG	AA	3281	1/1	0.84	0.40	-	61,61,61,61	0
58	MG	AA	3625	1/1	0.88	0.21	-	60,60,60,60	0
58	MG	DA	1627	1/1	0.80	0.23	-	70,70,70,70	0
58	MG	A4	502	1/1	0.63	0.65	-	123,123,123,123	0
58	MG	AA	3263	1/1	0.88	0.80	-	80,80,80,80	0
58	MG	BL	202	1/1	0.94	0.35	-	67,67,67,67	0
58	MG	DA	1741	1/1	0.93	0.16	-	78,78,78,78	0
58	MG	BA	1769	1/1	0.97	0.28	-	63,63,63,63	0
58	MG	CA	3494	1/1	0.94	0.21	-	63,63,63,63	0
58	MG	AB	3010	1/1	0.92	0.18	-	47,47,47,47	1
58	MG	CA	3122	1/1	0.91	0.22	-	67,67,67,67	0
58	MG	CA	3516	1/1	0.96	0.12	-	62,62,62,62	0
58	MG	AA	3226	1/1	0.92	0.27	-	56,56,56,56	0
58	MG	CA	3587	1/1	0.99	0.12	-	34,34,34,34	0
58	MG	AA	3722	1/1	0.94	0.14	-	18,18,18,18	0
58	MG	CA	3026	1/1	0.97	0.25	-	81,81,81,81	0
58	MG	AA	3674	1/1	0.94	0.25	-	75,75,75,75	0
58	MG	BA	1712	1/1	0.93	0.14	-	61,61,61,61	0
58	MG	AA	3032	1/1	0.95	0.27	-	36,36,36,36	0
58	MG	AA	3662	1/1	0.89	0.22	-	59,59,59,59	0
58	MG	CA	3616	1/1	0.66	0.66	-	79,79,79,79	0
58	MG	CA	3254	1/1	0.96	0.21	-	42,42,42,42	0
58	MG	AA	3083	1/1	0.94	0.24	-	38,38,38,38	1
58	MG	AA	3243	1/1	0.98	0.24	-	24,24,24,24	1
58	MG	CA	3611	1/1	0.74	0.70	-	91,91,91,91	0
58	MG	AA	3276	1/1	0.99	0.28	-	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3446	1/1	0.95	0.18	-	63,63,63,63	0
58	MG	DA	1732	1/1	0.89	0.36	-	76,76,76,76	0
58	MG	A2	101	1/1	0.93	0.20	-	35,35,35,35	0
58	MG	AA	3270	1/1	0.77	0.24	-	54,54,54,54	0
58	MG	AA	3053	1/1	0.97	0.16	-	14,14,14,14	0
58	MG	DA	1726	1/1	0.93	0.17	-	77,77,77,77	0
58	MG	AA	3296	1/1	0.95	0.12	-	17,17,17,17	0
58	MG	AA	3252	1/1	0.73	0.55	-	66,66,66,66	0
58	MG	AA	3255	1/1	0.89	0.35	-	53,53,53,53	0
58	MG	AA	3412	1/1	0.96	0.21	-	43,43,43,43	0
58	MG	AE	302	1/1	0.99	0.23	-	18,18,18,18	0
58	MG	AB	3022	1/1	0.98	0.05	-	58,58,58,58	0
58	MG	BA	1604	1/1	0.92	0.15	-	65,65,65,65	0
58	MG	AA	3144	1/1	0.97	0.12	-	40,40,40,40	0
58	MG	CA	3033	1/1	0.65	0.87	-	89,89,89,89	0
58	MG	AA	3147	1/1	0.88	0.27	-	69,69,69,69	0
58	MG	CA	3150	1/1	0.91	0.18	-	54,54,54,54	0
58	MG	BA	1645	1/1	0.77	0.64	-	61,61,61,61	0
58	MG	CA	3459	1/1	0.97	0.18	-	48,48,48,48	0
58	MG	CA	3461	1/1	0.94	0.18	-	43,43,43,43	0
58	MG	A7	102	1/1	0.95	0.10	-	43,43,43,43	0
58	MG	AA	3632	1/1	0.93	0.14	-	76,76,76,76	0
58	MG	AB	3011	1/1	0.96	0.19	-	30,30,30,30	0
58	MG	CA	3389	1/1	0.69	0.49	-	75,75,75,75	0
58	MG	CA	3381	1/1	0.94	0.10	-	38,38,38,38	0
58	MG	AA	3191	1/1	0.94	0.26	-	42,42,42,42	0
58	MG	BA	1778	1/1	0.98	0.07	-	42,42,42,42	0
58	MG	CA	3395	1/1	0.96	0.33	-	65,65,65,65	0
58	MG	DA	1632	1/1	0.81	0.32	-	61,61,61,61	0
58	MG	AA	3482	1/1	0.98	0.15	-	65,65,65,65	0
58	MG	AA	3158	1/1	0.90	0.31	-	97,97,97,97	0
58	MG	CA	3162	1/1	0.97	0.47	-	46,46,46,46	0
58	MG	AA	3049	1/1	0.94	0.27	-	52,52,52,52	0
58	MG	CA	3503	1/1	0.83	0.17	-	62,62,62,62	0
58	MG	AA	3785	1/1	0.92	0.19	-	72,72,72,72	0
58	MG	CA	3613	1/1	0.92	0.34	-	74,74,74,74	0
58	MG	AA	3107	1/1	0.91	0.51	-	76,76,76,76	0
58	MG	CA	3279	1/1	0.94	0.16	-	34,34,34,34	0
58	MG	AA	3631	1/1	0.94	0.30	-	46,46,46,46	0
58	MG	CA	3580	1/1	0.88	0.07	-	100,100,100,100	0
58	MG	CA	3544	1/1	0.60	0.19	-	81,81,81,81	0
58	MG	CO	202	1/1	0.93	0.21	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	BA	1742	1/1	0.67	0.21	-	79,79,79,79	0
58	MG	AA	3152	1/1	0.93	0.29	-	71,71,71,71	0
58	MG	CA	3470	1/1	0.93	0.35	-	72,72,72,72	0
58	MG	AA	3427	1/1	0.96	0.11	-	33,33,33,33	0
58	MG	CA	3304	1/1	0.76	0.13	-	93,93,93,93	0
58	MG	AA	3345	1/1	0.89	0.10	-	68,68,68,68	0
58	MG	CA	3097	1/1	0.82	0.26	-	80,80,80,80	0
58	MG	AA	3411	1/1	0.80	0.23	-	47,47,47,47	0
58	MG	AA	3504	1/1	0.94	0.20	-	58,58,58,58	0
58	MG	CA	3063	1/1	0.84	0.29	-	53,53,53,53	0
58	MG	CA	3209	1/1	0.20	0.65	-	93,93,93,93	0
58	MG	AA	3455	1/1	0.91	0.33	-	58,58,58,58	0
58	MG	AA	3673	1/1	0.89	0.17	-	67,67,67,67	0
58	MG	AA	3520	1/1	0.96	0.13	-	38,38,38,38	0
58	MG	CA	3384	1/1	0.87	0.23	-	71,71,71,71	0
58	MG	AA	3731	1/1	0.91	0.19	-	42,42,42,42	0
58	MG	AA	3814	1/1	0.76	0.37	-	93,93,93,93	0
58	MG	BN	502	1/1	0.95	0.24	-	66,66,66,66	0
58	MG	CA	3606	1/1	0.91	0.42	-	65,65,65,65	0
58	MG	AA	3351	1/1	0.97	0.14	-	30,30,30,30	0
58	MG	AA	3335	1/1	0.91	0.23	-	41,41,41,41	0
58	MG	AA	3677	1/1	0.92	0.22	-	41,41,41,41	0
58	MG	AA	3709	1/1	0.98	0.19	-	29,29,29,29	1
58	MG	AA	3769	1/1	0.93	0.23	-	57,57,57,57	0
58	MG	CA	3648	1/1	0.95	0.33	-	53,53,53,53	0
58	MG	AA	3026	1/1	0.82	0.39	-	86,86,86,86	0
58	MG	CA	3569	1/1	0.94	0.26	-	79,79,79,79	0
58	MG	AA	3248	1/1	0.73	0.52	-	64,64,64,64	0
58	MG	CA	3522	1/1	0.90	0.34	-	56,56,56,56	0
58	MG	CA	3399	1/1	0.93	0.10	-	75,75,75,75	0
58	MG	AA	3592	1/1	0.90	0.25	-	52,52,52,52	0
58	MG	CA	3252	1/1	0.94	0.23	-	64,64,64,64	0
58	MG	BA	1793	1/1	0.80	0.66	-	86,86,86,86	0
58	MG	BA	1666	1/1	0.77	0.53	-	75,75,75,75	0
58	MG	DA	1723	1/1	0.97	0.30	-	66,66,66,66	0
58	MG	CA	3475	1/1	0.91	0.36	-	55,55,55,55	0
58	MG	AE	301	1/1	0.79	0.28	-	69,69,69,69	0
58	MG	AA	3025	1/1	0.93	0.39	-	35,35,35,35	1
58	MG	DA	1699	1/1	0.99	0.08	-	75,75,75,75	0
58	MG	DA	1664	1/1	0.94	0.15	-	64,64,64,64	0
58	MG	AE	303	1/1	0.97	0.25	-	41,41,41,41	0
58	MG	AA	3215	1/1	0.89	0.62	-	42,42,42,42	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	A9	502	1/1	0.88	0.28	-	60,60,60,60	0
58	MG	CA	3624	1/1	0.53	0.17	-	104,104,104,104	0
58	MG	AA	3637	1/1	0.89	0.29	-	45,45,45,45	0
58	MG	A5	102	1/1	0.89	0.34	-	60,60,60,60	0
58	MG	AA	3671	1/1	0.93	0.22	-	58,58,58,58	0
58	MG	CA	3253	1/1	0.70	0.18	-	95,95,95,95	0
58	MG	DA	1641	1/1	0.92	0.09	-	77,77,77,77	0
58	MG	CA	3126	1/1	0.79	0.28	-	93,93,93,93	0
58	MG	AA	3089	1/1	0.90	0.31	-	47,47,47,47	1
58	MG	AA	3006	1/1	0.93	0.46	-	52,52,52,52	0
58	MG	AA	3569	1/1	0.96	0.17	-	19,19,19,19	0
58	MG	CA	3449	1/1	0.95	0.10	-	66,66,66,66	0
58	MG	BA	1703	1/1	0.93	0.25	-	78,78,78,78	0
58	MG	CA	3512	1/1	0.81	0.48	-	65,65,65,65	0
58	MG	DA	1688	1/1	0.97	0.20	-	66,66,66,66	0
58	MG	CA	3333	1/1	0.94	0.32	-	75,75,75,75	0
58	MG	AA	3550	1/1	0.94	0.21	-	47,47,47,47	0
58	MG	CA	3404	1/1	0.94	0.19	-	54,54,54,54	0
58	MG	AW	3001	1/1	0.90	0.31	-	52,52,52,52	0
58	MG	DA	1612	1/1	0.82	0.39	-	72,72,72,72	0
58	MG	CA	3533	1/1	0.79	0.20	-	81,81,81,81	0
58	MG	CA	3301	1/1	0.98	0.35	-	47,47,47,47	0
58	MG	AA	3541	1/1	0.98	0.18	-	43,43,43,43	0
58	MG	BA	1608	1/1	0.89	0.50	-	60,60,60,60	0
58	MG	CA	3393	1/1	0.68	0.08	-	82,82,82,82	0
58	MG	CA	3017	1/1	0.93	0.58	-	46,46,46,46	0
58	MG	DA	1650	1/1	0.91	0.34	-	61,61,61,61	0
58	MG	CA	3158	1/1	0.70	0.32	-	70,70,70,70	0
58	MG	CA	3614	1/1	0.84	0.20	-	52,52,52,52	0
58	MG	CA	3259	1/1	0.96	0.22	-	47,47,47,47	0
58	MG	BA	1653	1/1	0.85	0.43	-	78,78,78,78	0
58	MG	AA	3797	1/1	0.96	0.26	-	15,15,15,15	1
58	MG	CA	3635	1/1	0.85	0.16	-	79,79,79,79	0
58	MG	CA	3222	1/1	0.96	0.26	-	75,75,75,75	0
58	MG	AA	3712	1/1	0.91	0.23	-	46,46,46,46	0
58	MG	A8	5002	1/1	0.97	0.24	-	31,31,31,31	0
58	MG	AA	3795	1/1	0.90	0.33	-	68,68,68,68	1
58	MG	AA	3002	1/1	0.86	0.21	-	55,55,55,55	0
58	MG	AA	3762	1/1	0.90	0.19	-	53,53,53,53	1
58	MG	AA	3271	1/1	0.93	0.36	-	69,69,69,69	0
58	MG	BA	1718	1/1	0.86	0.52	-	83,83,83,83	0
58	MG	AA	3743	1/1	0.88	0.25	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3443	1/1	0.97	0.11	-	36,36,36,36	0
58	MG	CA	3272	1/1	0.84	0.48	-	75,75,75,75	0
58	MG	BA	1744	1/1	0.88	0.10	-	37,37,37,37	0
58	MG	CA	3367	1/1	0.95	0.23	-	65,65,65,65	0
58	MG	AA	3523	1/1	0.97	0.20	-	30,30,30,30	0
58	MG	BA	1668	1/1	0.86	0.25	-	83,83,83,83	0
58	MG	CA	3264	1/1	0.98	0.18	-	59,59,59,59	0
58	MG	DA	1609	1/1	0.94	0.30	-	46,46,46,46	0
58	MG	AA	3719	1/1	0.94	0.12	-	58,58,58,58	0
58	MG	AA	3651	1/1	0.84	0.24	-	52,52,52,52	0
58	MG	CA	3482	1/1	0.90	0.24	-	70,70,70,70	0
58	MG	AA	3414	1/1	0.82	0.16	-	36,36,36,36	0
58	MG	AA	3175	1/1	0.90	0.33	-	51,51,51,51	0
58	MG	BA	1647	1/1	0.83	0.15	-	75,75,75,75	0
58	MG	AA	3593	1/1	0.94	0.21	-	25,25,25,25	1
58	MG	CY	502	1/1	0.92	0.17	-	56,56,56,56	0
58	MG	AA	3126	1/1	0.88	0.42	-	50,50,50,50	0
58	MG	BA	1687	1/1	0.88	0.33	-	72,72,72,72	0
58	MG	BA	1677	1/1	0.86	0.16	-	87,87,87,87	0
58	MG	AA	3707	1/1	0.98	0.24	-	29,29,29,29	1
58	MG	CA	3405	1/1	0.84	0.23	-	91,91,91,91	0
58	MG	AA	3787	1/1	0.97	0.25	-	53,53,53,53	0
58	MG	CA	3403	1/1	0.93	0.08	-	91,91,91,91	0
58	MG	CA	3295	1/1	0.73	0.20	-	84,84,84,84	0
58	MG	AA	3501	1/1	0.95	0.11	-	24,24,24,24	0
58	MG	AQ	201	1/1	0.77	0.51	-	62,62,62,62	0
58	MG	BA	1768	1/1	0.94	0.07	-	75,75,75,75	0
58	MG	AA	3590	1/1	0.92	0.21	-	69,69,69,69	0
58	MG	BA	1719	1/1	0.83	0.27	-	80,80,80,80	0
58	MG	BA	1656	1/1	0.86	0.13	-	90,90,90,90	0
58	MG	BD	502	1/1	0.83	0.63	-	82,82,82,82	0
58	MG	AA	3325	1/1	0.97	0.10	-	66,66,66,66	0
58	MG	DA	1724	1/1	0.91	0.31	-	61,61,61,61	0
58	MG	CA	3411	1/1	0.94	0.36	-	61,61,61,61	0
58	MG	CA	3506	1/1	0.89	0.17	-	58,58,58,58	0
58	MG	CA	3128	1/1	0.90	0.42	-	71,71,71,71	0
58	MG	CA	3342	1/1	0.98	0.17	-	45,45,45,45	0
58	MG	AA	3295	1/1	0.89	0.39	-	47,47,47,47	0
58	MG	BZ	702	1/1	0.95	0.34	-	46,46,46,46	0
58	MG	CA	3325	1/1	0.88	0.10	-	38,38,38,38	0
58	MG	CA	3165	1/1	0.92	0.17	-	62,62,62,62	0
58	MG	CA	3100	1/1	0.84	0.46	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3285	1/1	0.95	0.37	-	57,57,57,57	0
58	MG	BA	1802	1/1	0.86	0.14	-	68,68,68,68	1
58	MG	DA	1613	1/1	0.91	0.25	-	72,72,72,72	0
58	MG	AA	3600	1/1	0.81	0.25	-	60,60,60,60	0
58	MG	AA	3111	1/1	0.89	0.43	-	48,48,48,48	0
58	MG	DA	1707	1/1	0.71	0.30	-	87,87,87,87	0
58	MG	CA	3258	1/1	0.86	0.36	-	70,70,70,70	0
58	MG	AA	3100	1/1	0.87	0.27	-	53,53,53,53	0
58	MG	CA	3546	1/1	0.63	0.11	-	119,119,119,119	0
58	MG	AA	3222	1/1	0.90	0.32	-	28,28,28,28	0
58	MG	AA	3079	1/1	0.92	0.10	-	34,34,34,34	0
58	MG	CA	3436	1/1	0.95	0.12	-	75,75,75,75	0
58	MG	CA	3485	1/1	0.76	0.23	-	83,83,83,83	0
58	MG	AA	3304	1/1	0.88	0.25	-	30,30,30,30	0
58	MG	AA	3019	1/1	0.94	0.30	-	58,58,58,58	0
58	MG	A0	101	1/1	0.98	0.14	-	43,43,43,43	0
58	MG	AA	3239	1/1	0.86	0.36	-	64,64,64,64	0
58	MG	CA	3568	1/1	0.89	0.20	-	41,41,41,41	0
58	MG	CA	3083	1/1	0.66	0.75	-	90,90,90,90	0
58	MG	DA	1623	1/1	0.55	0.13	-	117,117,117,117	0
58	MG	AA	3284	1/1	0.89	0.42	-	44,44,44,44	0
58	MG	CA	3385	1/1	0.96	0.47	-	64,64,64,64	0
58	MG	AA	3641	1/1	0.98	0.22	-	41,41,41,41	0
58	MG	BA	1732	1/1	0.86	0.07	-	71,71,71,71	0
58	MG	DA	1631	1/1	0.95	0.20	-	70,70,70,70	0
58	MG	CA	3024	1/1	0.83	0.68	-	88,88,88,88	0
58	MG	AA	3260	1/1	0.75	0.39	-	71,71,71,71	0
58	MG	CA	3513	1/1	0.90	0.26	-	75,75,75,75	0
58	MG	AA	3056	1/1	0.92	0.26	-	63,63,63,63	0
58	MG	AA	3544	1/1	0.97	0.11	-	16,16,16,16	0
58	MG	BA	1621	1/1	0.93	0.41	-	49,49,49,49	0
58	MG	CB	3011	1/1	0.94	0.29	-	53,53,53,53	0
58	MG	CA	3431	1/1	0.95	0.29	-	100,100,100,100	0
58	MG	DA	1603	1/1	0.86	0.30	-	74,74,74,74	0
58	MG	BA	1705	1/1	0.48	0.21	-	92,92,92,92	0
58	MG	DA	1614	1/1	0.79	0.80	-	87,87,87,87	0
58	MG	CA	3390	1/1	0.95	0.14	-	64,64,64,64	0
58	MG	BA	1753	1/1	0.95	0.13	-	94,94,94,94	0
58	MG	BA	1717	1/1	0.96	0.18	-	44,44,44,44	0
58	MG	BA	1750	1/1	0.97	0.27	-	65,65,65,65	0
58	MG	CA	3378	1/1	0.81	0.12	-	84,84,84,84	0
58	MG	CA	3135	1/1	0.96	0.21	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	3445	1/1	0.65	0.23	-	75,75,75,75	0
58	MG	CA	3493	1/1	0.81	0.39	-	88,88,88,88	0
58	MG	AA	3694	1/1	0.89	0.15	-	45,45,45,45	0
58	MG	CA	3140	1/1	0.71	0.60	-	98,98,98,98	0
58	MG	CA	3202	1/1	0.13	0.83	-	77,77,77,77	0
58	MG	BW	501	1/1	0.93	0.27	-	48,48,48,48	0
58	MG	AA	3537	1/1	0.78	0.15	-	95,95,95,95	0
58	MG	DA	1746	1/1	0.81	0.19	-	91,91,91,91	0
58	MG	AA	3626	1/1	0.81	0.27	-	74,74,74,74	0
58	MG	A6	101	1/1	0.93	0.37	-	65,65,65,65	0
58	MG	CA	3646	1/1	0.62	0.20	-	95,95,95,95	0
58	MG	AA	3664	1/1	0.97	0.23	-	57,57,57,57	0
58	MG	CA	3559	1/1	0.98	0.26	-	52,52,52,52	1
58	MG	AA	3755	1/1	0.83	0.42	-	63,63,63,63	0
58	MG	AA	3136	1/1	0.72	0.20	-	52,52,52,52	0
58	MG	BA	1710	1/1	0.88	0.69	-	73,73,73,73	0
58	MG	CA	3283	1/1	0.89	0.19	-	60,60,60,60	0
58	MG	CA	3183	1/1	0.76	1.07	-	86,86,86,86	0
58	MG	DA	1717	1/1	0.94	0.30	-	52,52,52,52	0
58	MG	CA	3216	1/1	0.81	0.62	-	66,66,66,66	0
58	MG	BA	1782	1/1	0.91	0.19	-	50,50,50,50	0
58	MG	AA	3090	1/1	0.93	0.56	-	30,30,30,30	1
58	MG	BA	1696	1/1	0.72	0.40	-	68,68,68,68	0
58	MG	CF	304	1/1	0.98	0.36	-	65,65,65,65	0
58	MG	CA	3577	1/1	0.92	0.17	-	83,83,83,83	0
58	MG	BA	1688	1/1	0.89	0.71	-	70,70,70,70	0
58	MG	CA	3329	1/1	0.97	0.21	-	29,29,29,29	0
58	MG	AA	3209	1/1	0.93	0.33	-	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.