



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2016 – 12:36 AM EDT

PDB ID : 4WQU
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with elongation factor G trapped by the antibiotic dityromycin
Authors : Lin, J.; Gagnon, M.G.; Steitz, T.A.
Deposited on : 2014-10-22
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

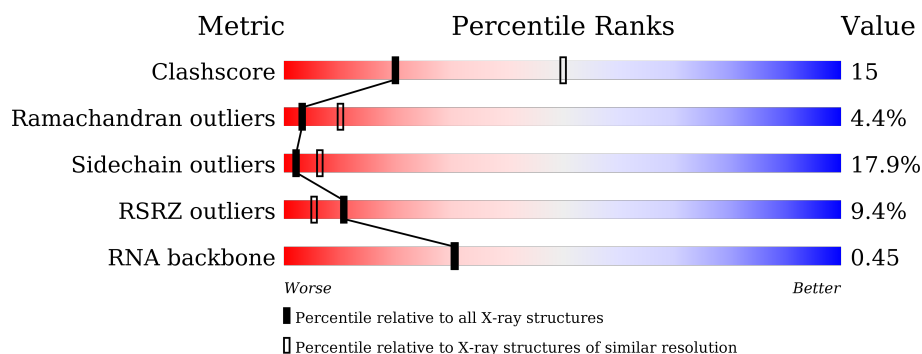
1 Overall quality at a glance

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.












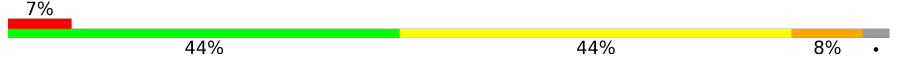
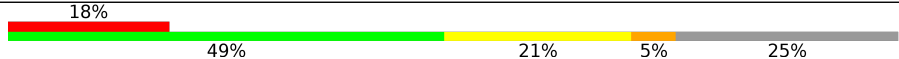
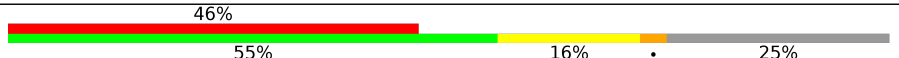

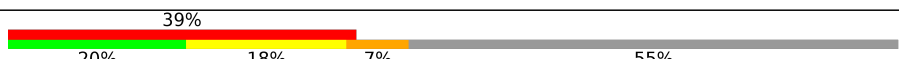




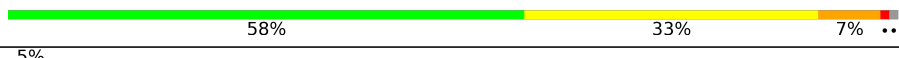


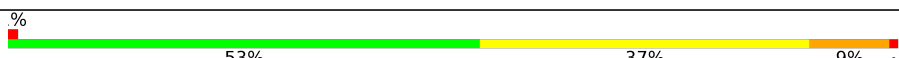



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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>3%</div> <div>24%</div> <div>47%</div> <div>23%</div> <div>..</div> </div>
1	CA	2915	<div> <div>4%</div> <div>32%</div> <div>44%</div> <div>19%</div> <div>..</div> </div>
2	AB	121	<div> <div>28%</div> <div>55%</div> <div>14%</div> <div>..</div> </div>
2	CB	121	<div> <div>%</div> <div>36%</div> <div>47%</div> <div>17%</div> <div>.</div> </div>
3	AC	228	<div> <div>54%</div> <div>22%</div> <div>28%</div> <div>10%</div> <div>40%</div> </div>
3	CC	228	<div> <div>60%</div> <div>21%</div> <div>29%</div> <div>10%</div> <div>40%</div> </div>

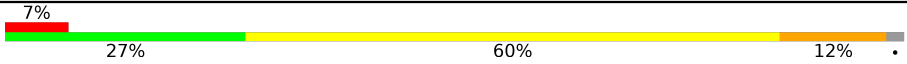



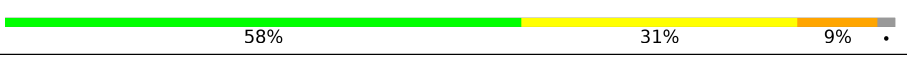
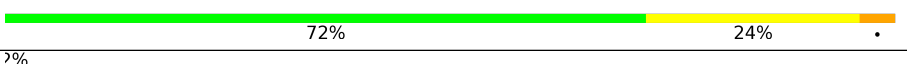
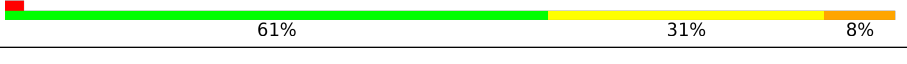

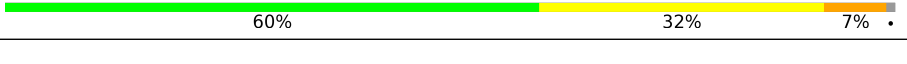


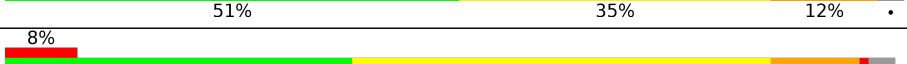
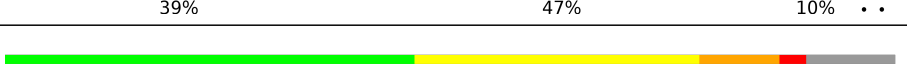
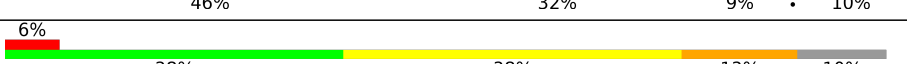


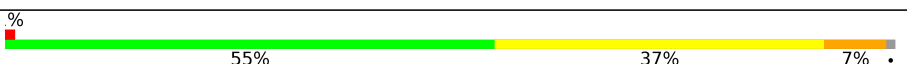
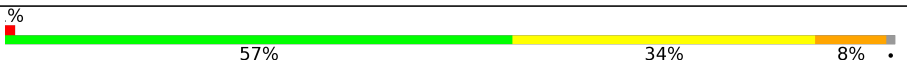
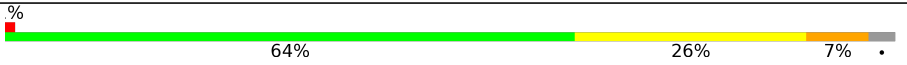


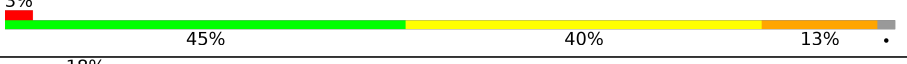

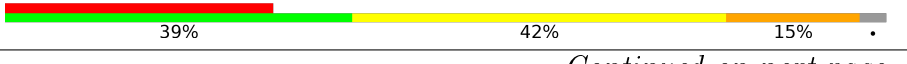

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
15	CR	118	
16	AS	112	

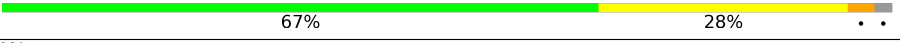

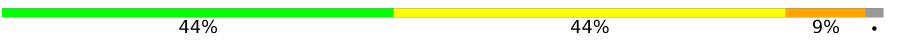







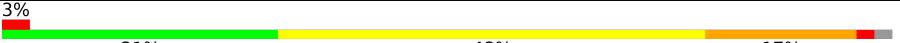
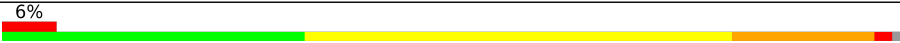
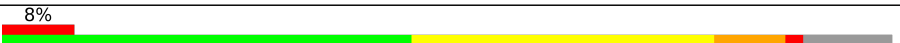
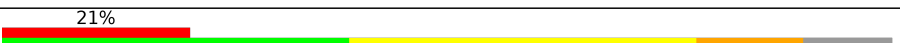


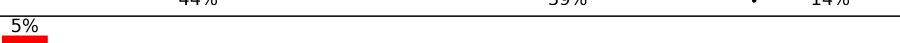
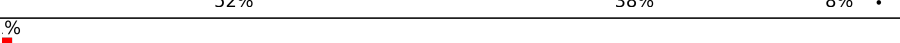







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
28	A4	71	
28	C4	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
40	DG	156	
41	BH	138	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
53	BT	106	
53	DT	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	BU	27	
54	DU	27	
55	BV	18	
55	DV	18	
56	BW	76	
56	BY	76	
56	DW	76	
56	DY	76	
57	BZ	758	
57	DZ	758	
58	BX	10	
58	DX	10	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	2QY	DX	10	-	-	X	-
59	MG	A0	101	-	-	-	X
59	MG	AA	3012	-	-	-	X
59	MG	AA	3018	-	-	-	X
59	MG	AA	3020	-	-	-	X
59	MG	AA	3023	-	-	-	X
59	MG	AA	3033	-	-	-	X
59	MG	AA	3034	-	-	-	X
59	MG	AA	3036	-	-	-	X
59	MG	AA	3038	-	-	-	X
59	MG	AA	3039	-	-	-	X
59	MG	AA	3042	-	-	-	X
59	MG	AA	3043	-	-	-	X
59	MG	AA	3044	-	-	-	X
59	MG	AA	3045	-	-	-	X
59	MG	AA	3047	-	-	-	X
59	MG	AA	3050	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3053	-	-	-	X
59	MG	AA	3060	-	-	-	X
59	MG	AA	3081	-	-	-	X
59	MG	AA	3082	-	-	-	X
59	MG	AA	3101	-	-	-	X
59	MG	AA	3102	-	-	-	X
59	MG	AA	3109	-	-	-	X
59	MG	AA	3110	-	-	-	X
59	MG	AA	3113	-	-	-	X
59	MG	AA	3117	-	-	-	X
59	MG	AA	3120	-	-	-	X
59	MG	AA	3128	-	-	-	X
59	MG	AA	3130	-	-	-	X
59	MG	AA	3131	-	-	-	X
59	MG	AA	3133	-	-	-	X
59	MG	AA	3134	-	-	-	X
59	MG	AA	3136	-	-	-	X
59	MG	AA	3137	-	-	-	X
59	MG	AA	3140	-	-	-	X
59	MG	AA	3144	-	-	-	X
59	MG	AA	3147	-	-	-	X
59	MG	AA	3152	-	-	-	X
59	MG	AA	3158	-	-	-	X
59	MG	AA	3161	-	-	-	X
59	MG	AA	3171	-	-	-	X
59	MG	AA	3172	-	-	-	X
59	MG	AA	3174	-	-	-	X
59	MG	AA	3176	-	-	-	X
59	MG	AA	3177	-	-	-	X
59	MG	AA	3179	-	-	-	X
59	MG	AA	3182	-	-	-	X
59	MG	AA	3184	-	-	-	X
59	MG	AA	3186	-	-	-	X
59	MG	AA	3188	-	-	-	X
59	MG	AA	3193	-	-	-	X
59	MG	AA	3199	-	-	-	X
59	MG	AA	3209	-	-	-	X
59	MG	AA	3213	-	-	-	X
59	MG	AA	3214	-	-	-	X
59	MG	AA	3215	-	-	-	X
59	MG	AA	3216	-	-	-	X
59	MG	AA	3217	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3224	-	-	-	X
59	MG	AA	3226	-	-	-	X
59	MG	AA	3228	-	-	-	X
59	MG	AA	3235	-	-	-	X
59	MG	AA	3241	-	-	-	X
59	MG	AA	3244	-	-	-	X
59	MG	AA	3250	-	-	-	X
59	MG	AA	3253	-	-	-	X
59	MG	AA	3254	-	-	-	X
59	MG	AA	3255	-	-	-	X
59	MG	AA	3257	-	-	-	X
59	MG	AA	3261	-	-	-	X
59	MG	AA	3280	-	-	-	X
59	MG	AA	3286	-	-	-	X
59	MG	AA	3294	-	-	-	X
59	MG	AA	3301	-	-	-	X
59	MG	AA	3307	-	-	-	X
59	MG	AA	3315	-	-	-	X
59	MG	AA	3317	-	-	-	X
59	MG	AA	3328	-	-	-	X
59	MG	AA	3335	-	-	-	X
59	MG	AA	3344	-	-	-	X
59	MG	AA	3360	-	-	-	X
59	MG	AA	3362	-	-	-	X
59	MG	AA	3384	-	-	-	X
59	MG	AA	3391	-	-	-	X
59	MG	AA	3392	-	-	-	X
59	MG	AA	3393	-	-	-	X
59	MG	AA	3398	-	-	-	X
59	MG	AA	3403	-	-	-	X
59	MG	AA	3404	-	-	-	X
59	MG	AA	3413	-	-	-	X
59	MG	AA	3421	-	-	-	X
59	MG	AA	3423	-	-	-	X
59	MG	AA	3429	-	-	-	X
59	MG	AA	3443	-	-	-	X
59	MG	AA	3466	-	-	-	X
59	MG	AA	3509	-	-	-	X
59	MG	AA	3510	-	-	-	X
59	MG	AA	3511	-	-	-	X
59	MG	AA	3515	-	-	-	X
59	MG	AA	3519	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3529	-	-	-	X
59	MG	AA	3532	-	-	-	X
59	MG	AA	3534	-	-	-	X
59	MG	AA	3543	-	-	-	X
59	MG	AA	3547	-	-	-	X
59	MG	AA	3561	-	-	-	X
59	MG	AA	3563	-	-	-	X
59	MG	AA	3565	-	-	-	X
59	MG	AA	3568	-	-	-	X
59	MG	AA	3569	-	-	-	X
59	MG	AA	3576	-	-	-	X
59	MG	AA	3593	-	-	-	X
59	MG	AA	3606	-	-	-	X
59	MG	AA	3608	-	-	-	X
59	MG	AA	3625	-	-	-	X
59	MG	AA	3653	-	-	-	X
59	MG	AA	3659	-	-	-	X
59	MG	AA	3667	-	-	-	X
59	MG	AA	3688	-	-	-	X
59	MG	AA	3690	-	-	-	X
59	MG	AA	3691	-	-	-	X
59	MG	AA	3702	-	-	-	X
59	MG	AA	3706	-	-	-	X
59	MG	AA	3708	-	-	-	X
59	MG	AA	3710	-	-	-	X
59	MG	AA	3712	-	-	-	X
59	MG	AA	3718	-	-	-	X
59	MG	AA	3721	-	-	-	X
59	MG	AA	3730	-	-	-	X
59	MG	AA	3740	-	-	-	X
59	MG	AA	3743	-	-	-	X
59	MG	AA	3766	-	-	-	X
59	MG	AA	3771	-	-	-	X
59	MG	AA	3772	-	-	-	X
59	MG	AA	3775	-	-	-	X
59	MG	AA	3793	-	-	-	X
59	MG	AA	3794	-	-	-	X
59	MG	AA	3795	-	-	-	X
59	MG	AA	3799	-	-	-	X
59	MG	AA	3803	-	-	-	X
59	MG	AA	3806	-	-	-	X
59	MG	AA	3809	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	3813	-	-	-	X
59	MG	AA	3814	-	-	-	X
59	MG	AA	3818	-	-	-	X
59	MG	AA	3820	-	-	-	X
59	MG	AA	3822	-	-	-	X
59	MG	AA	3823	-	-	-	X
59	MG	AA	3824	-	-	-	X
59	MG	AA	3825	-	-	-	X
59	MG	AA	3826	-	-	-	X
59	MG	AA	3827	-	-	-	X
59	MG	AA	3828	-	-	-	X
59	MG	AA	3829	-	-	-	X
59	MG	AA	3830	-	-	-	X
59	MG	AA	3832	-	-	-	X
59	MG	AB	3003	-	-	-	X
59	MG	AB	3020	-	-	-	X
59	MG	AD	301	-	-	-	X
59	MG	AD	304	-	-	-	X
59	MG	AD	305	-	-	-	X
59	MG	AD	307	-	-	-	X
59	MG	AD	308	-	-	-	X
59	MG	AD	309	-	-	-	X
59	MG	AD	310	-	-	-	X
59	MG	AE	305	-	-	-	X
59	MG	AF	301	-	-	-	X
59	MG	AF	304	-	-	-	X
59	MG	AH	201	-	-	-	X
59	MG	AP	201	-	-	-	X
59	MG	AQ	202	-	-	-	X
59	MG	AU	202	-	-	-	X
59	MG	AU	203	-	-	-	X
59	MG	AU	204	-	-	-	X
59	MG	AU	205	-	-	-	X
59	MG	AV	201	-	-	-	X
59	MG	AW	3003	-	-	-	X
59	MG	AX	3001	-	-	-	X
59	MG	BA	1607	-	-	-	X
59	MG	BA	1612	-	-	-	X
59	MG	BA	1615	-	-	-	X
59	MG	BA	1616	-	-	-	X
59	MG	BA	1627	-	-	-	X
59	MG	BA	1628	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	1630	-	-	-	X
59	MG	BA	1631	-	-	-	X
59	MG	BA	1641	-	-	-	X
59	MG	BA	1656	-	-	-	X
59	MG	BA	1663	-	-	-	X
59	MG	BA	1665	-	-	-	X
59	MG	BA	1672	-	-	-	X
59	MG	BA	1676	-	-	-	X
59	MG	BA	1679	-	-	-	X
59	MG	BA	1684	-	-	-	X
59	MG	BA	1687	-	-	-	X
59	MG	BA	1691	-	-	-	X
59	MG	BA	1714	-	-	-	X
59	MG	BA	1723	-	-	-	X
59	MG	BA	1725	-	-	-	X
59	MG	BA	1735	-	-	-	X
59	MG	BA	1740	-	-	-	X
59	MG	BA	1757	-	-	-	X
59	MG	BA	1758	-	-	-	X
59	MG	BA	1780	-	-	-	X
59	MG	BA	1787	-	-	-	X
59	MG	BA	1788	-	-	-	X
59	MG	C3	3001	-	-	-	X
59	MG	C5	101	-	-	-	X
59	MG	C7	101	-	-	-	X
59	MG	CA	3002	-	-	-	X
59	MG	CA	3010	-	-	-	X
59	MG	CA	3025	-	-	-	X
59	MG	CA	3026	-	-	-	X
59	MG	CA	3028	-	-	-	X
59	MG	CA	3033	-	-	-	X
59	MG	CA	3035	-	-	-	X
59	MG	CA	3036	-	-	-	X
59	MG	CA	3039	-	-	-	X
59	MG	CA	3041	-	-	-	X
59	MG	CA	3045	-	-	-	X
59	MG	CA	3054	-	-	-	X
59	MG	CA	3058	-	-	-	X
59	MG	CA	3068	-	-	-	X
59	MG	CA	3087	-	-	-	X
59	MG	CA	3090	-	-	-	X
59	MG	CA	3100	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3103	-	-	-	X
59	MG	CA	3105	-	-	-	X
59	MG	CA	3108	-	-	-	X
59	MG	CA	3113	-	-	-	X
59	MG	CA	3137	-	-	-	X
59	MG	CA	3140	-	-	-	X
59	MG	CA	3146	-	-	-	X
59	MG	CA	3157	-	-	-	X
59	MG	CA	3159	-	-	-	X
59	MG	CA	3160	-	-	-	X
59	MG	CA	3162	-	-	-	X
59	MG	CA	3163	-	-	-	X
59	MG	CA	3166	-	-	-	X
59	MG	CA	3168	-	-	-	X
59	MG	CA	3169	-	-	-	X
59	MG	CA	3182	-	-	-	X
59	MG	CA	3201	-	-	-	X
59	MG	CA	3207	-	-	-	X
59	MG	CA	3210	-	-	-	X
59	MG	CA	3212	-	-	-	X
59	MG	CA	3213	-	-	-	X
59	MG	CA	3217	-	-	-	X
59	MG	CA	3218	-	-	-	X
59	MG	CA	3221	-	-	-	X
59	MG	CA	3225	-	-	-	X
59	MG	CA	3226	-	-	-	X
59	MG	CA	3227	-	-	-	X
59	MG	CA	3229	-	-	-	X
59	MG	CA	3230	-	-	-	X
59	MG	CA	3243	-	-	-	X
59	MG	CA	3252	-	-	-	X
59	MG	CA	3277	-	-	-	X
59	MG	CA	3285	-	-	-	X
59	MG	CA	3291	-	-	-	X
59	MG	CA	3309	-	-	-	X
59	MG	CA	3314	-	-	-	X
59	MG	CA	3318	-	-	-	X
59	MG	CA	3322	-	-	-	X
59	MG	CA	3326	-	-	-	X
59	MG	CA	3330	-	-	-	X
59	MG	CA	3332	-	-	-	X
59	MG	CA	3333	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3346	-	-	-	X
59	MG	CA	3348	-	-	-	X
59	MG	CA	3353	-	-	-	X
59	MG	CA	3358	-	-	-	X
59	MG	CA	3361	-	-	-	X
59	MG	CA	3372	-	-	-	X
59	MG	CA	3375	-	-	-	X
59	MG	CA	3383	-	-	-	X
59	MG	CA	3409	-	-	-	X
59	MG	CA	3410	-	-	-	X
59	MG	CA	3413	-	-	-	X
59	MG	CA	3415	-	-	-	X
59	MG	CA	3420	-	-	-	X
59	MG	CA	3427	-	-	-	X
59	MG	CA	3428	-	-	-	X
59	MG	CA	3432	-	-	-	X
59	MG	CA	3440	-	-	-	X
59	MG	CA	3441	-	-	-	X
59	MG	CA	3442	-	-	-	X
59	MG	CA	3452	-	-	-	X
59	MG	CA	3455	-	-	-	X
59	MG	CA	3457	-	-	-	X
59	MG	CA	3458	-	-	-	X
59	MG	CA	3463	-	-	-	X
59	MG	CA	3486	-	-	-	X
59	MG	CA	3492	-	-	-	X
59	MG	CA	3499	-	-	-	X
59	MG	CA	3500	-	-	-	X
59	MG	CA	3502	-	-	-	X
59	MG	CA	3503	-	-	-	X
59	MG	CA	3526	-	-	-	X
59	MG	CA	3532	-	-	-	X
59	MG	CA	3544	-	-	-	X
59	MG	CA	3552	-	-	-	X
59	MG	CA	3557	-	-	-	X
59	MG	CA	3569	-	-	-	X
59	MG	CA	3589	-	-	-	X
59	MG	CA	3603	-	-	-	X
59	MG	CA	3618	-	-	-	X
59	MG	CA	3619	-	-	-	X
59	MG	CA	3635	-	-	-	X
59	MG	CA	3636	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	CA	3642	-	-	-	X
59	MG	CA	3650	-	-	-	X
59	MG	CA	3653	-	-	-	X
59	MG	CA	3655	-	-	-	X
59	MG	CA	3657	-	-	-	X
59	MG	CA	3658	-	-	-	X
59	MG	CA	3660	-	-	-	X
59	MG	CA	3661	-	-	-	X
59	MG	CB	3007	-	-	-	X
59	MG	CE	301	-	-	-	X
59	MG	CE	303	-	-	-	X
59	MG	CF	301	-	-	-	X
59	MG	CQ	202	-	-	-	X
59	MG	CU	201	-	-	-	X
59	MG	CV	201	-	-	-	X
59	MG	CV	202	-	-	-	X
59	MG	CW	201	-	-	-	X
59	MG	DA	1601	-	-	-	X
59	MG	DA	1609	-	-	-	X
59	MG	DA	1622	-	-	-	X
59	MG	DA	1634	-	-	-	X
59	MG	DA	1640	-	-	-	X
59	MG	DA	1641	-	-	-	X
59	MG	DA	1642	-	-	-	X
59	MG	DA	1650	-	-	-	X
59	MG	DA	1652	-	-	-	X
59	MG	DA	1655	-	-	-	X
59	MG	DA	1665	-	-	-	X
59	MG	DA	1671	-	-	-	X
59	MG	DA	1683	-	-	-	X
59	MG	DA	1745	-	-	-	X
59	MG	DA	1769	-	-	-	X
59	MG	DT	3001	-	-	-	X
61	SF4	DD	501	-	-	X	-

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 310038 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			
23	CZ	185	Total	C	N	O	S	0	0	0
			1451	927	258	264	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
24	C0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1495	Total	C	N	O	P	0	0	0
			32141	14304	5958	10384	1495			
34	DA	1501	Total	C	N	O	P	0	0	0
			32268	14361	5980	10426	1501			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	117	Total	C	N	O	S	0	0	0
			923	570	191	160	2			
46	DM	116	Total	C	N	O	S	0	0	0
			907	558	188	159	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	7	Total	C	N	O	P	0	0	0
			148	67	27	47	7			
55	DV	6	Total	C	N	O	P	0	0	0
			123	57	22	39	5			

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

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

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

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

- Molecule 58 is a protein called Dityromycin.

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

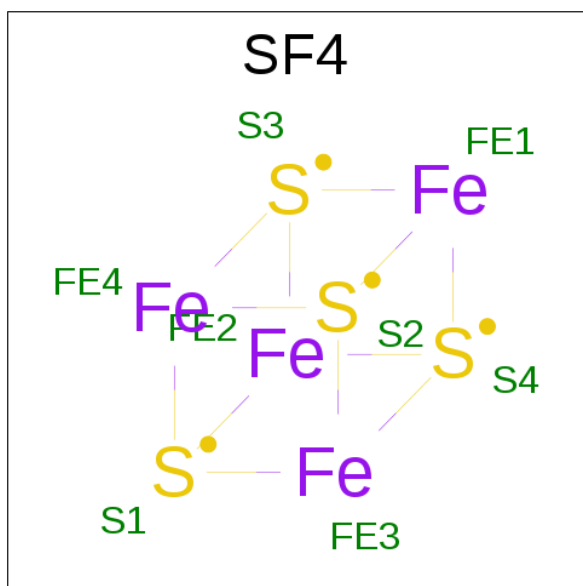
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AY	1	Total 1	Zn 1	0	0
60	BN	1	Total 1	Zn 1	0	0
60	C4	1	Total 1	Zn 1	0	0
60	C5	1	Total 1	Zn 1	0	0
60	C6	1	Total 1	Zn 1	0	0
60	A6	1	Total 1	Zn 1	0	0
60	C9	1	Total 1	Zn 1	0	0
60	DN	1	Total 1	Zn 1	0	0
60	A4	1	Total 1	Zn 1	0	0
60	A5	1	Total 1	Zn 1	0	0
60	A9	1	Total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

Continued on next page...

Continued from previous page...

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

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



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

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



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

- Molecule 63 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	BP	1	Total	O	0	0
			1	1		
63	BV	1	Total	O	0	0
			1	1		
63	BW	1	Total	O	0	0
			1	1		
63	BZ	2	Total	O	0	0
			2	2		
63	CA	983	Total	O	0	0
			983	983		
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	CN	1	Total	O	0	0
			1	1		
63	CO	1	Total	O	0	0
			1	1		
63	CP	11	Total	O	0	0
			11	11		
63	CQ	2	Total	O	0	0
			2	2		
63	CT	3	Total	O	0	0
			3	3		
63	CU	2	Total	O	0	0
			2	2		
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	2	Total	O	0	0
			2	2		
63	C0	4	Total	O	0	0
			4	4		
63	C3	2	Total	O	0	0
			2	2		

Continued on next page...

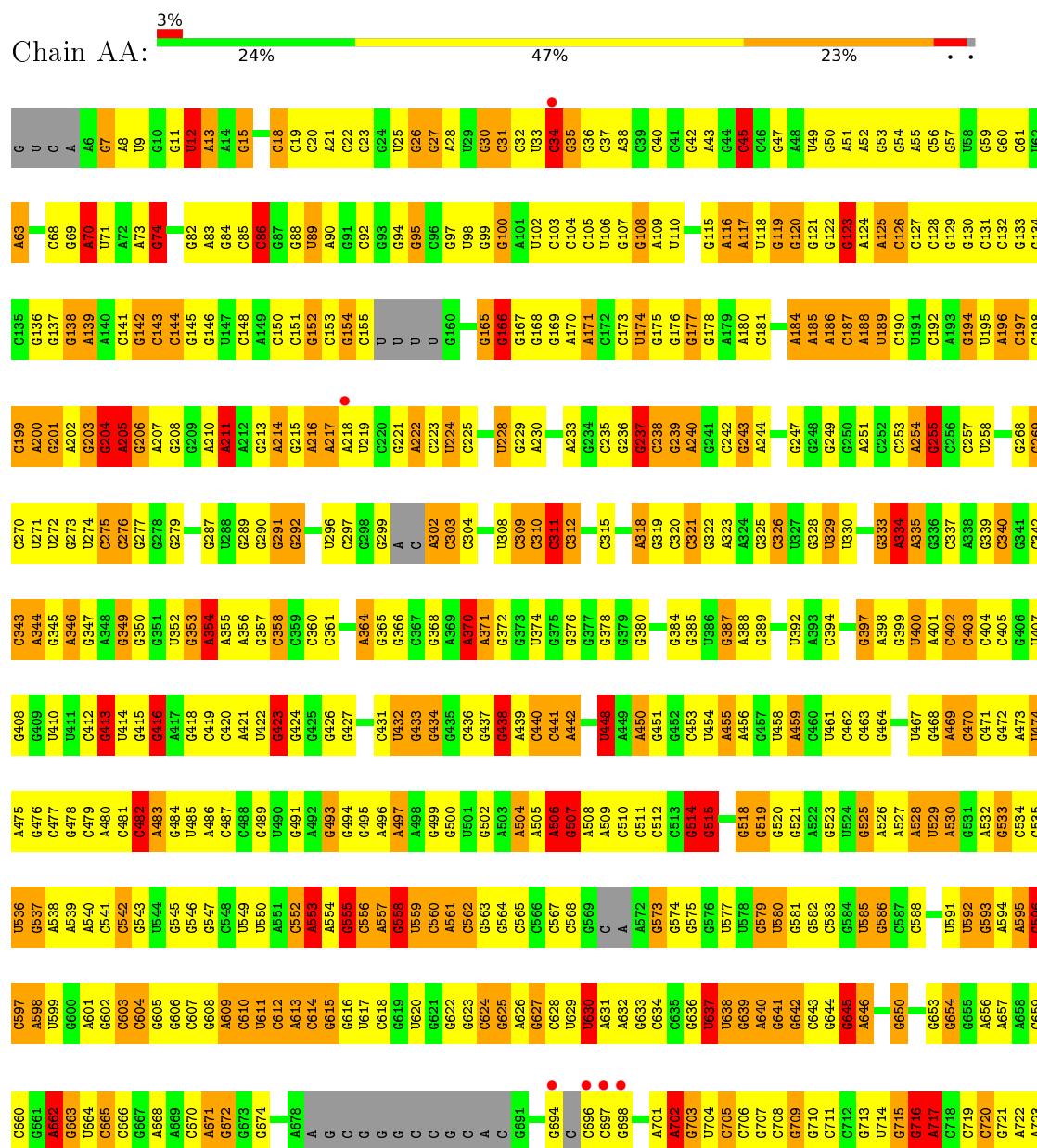
Continued from previous page...

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

3 Residue-property plots

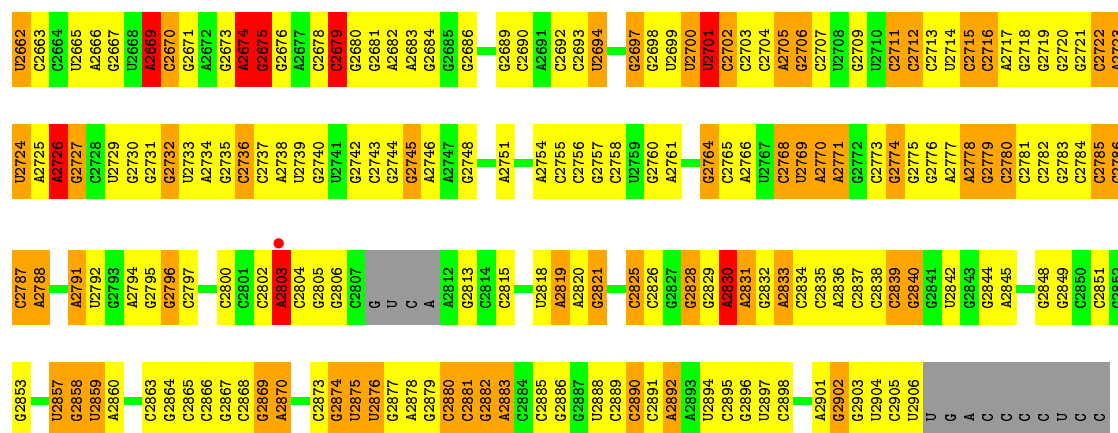
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 23S Ribosomal RNA

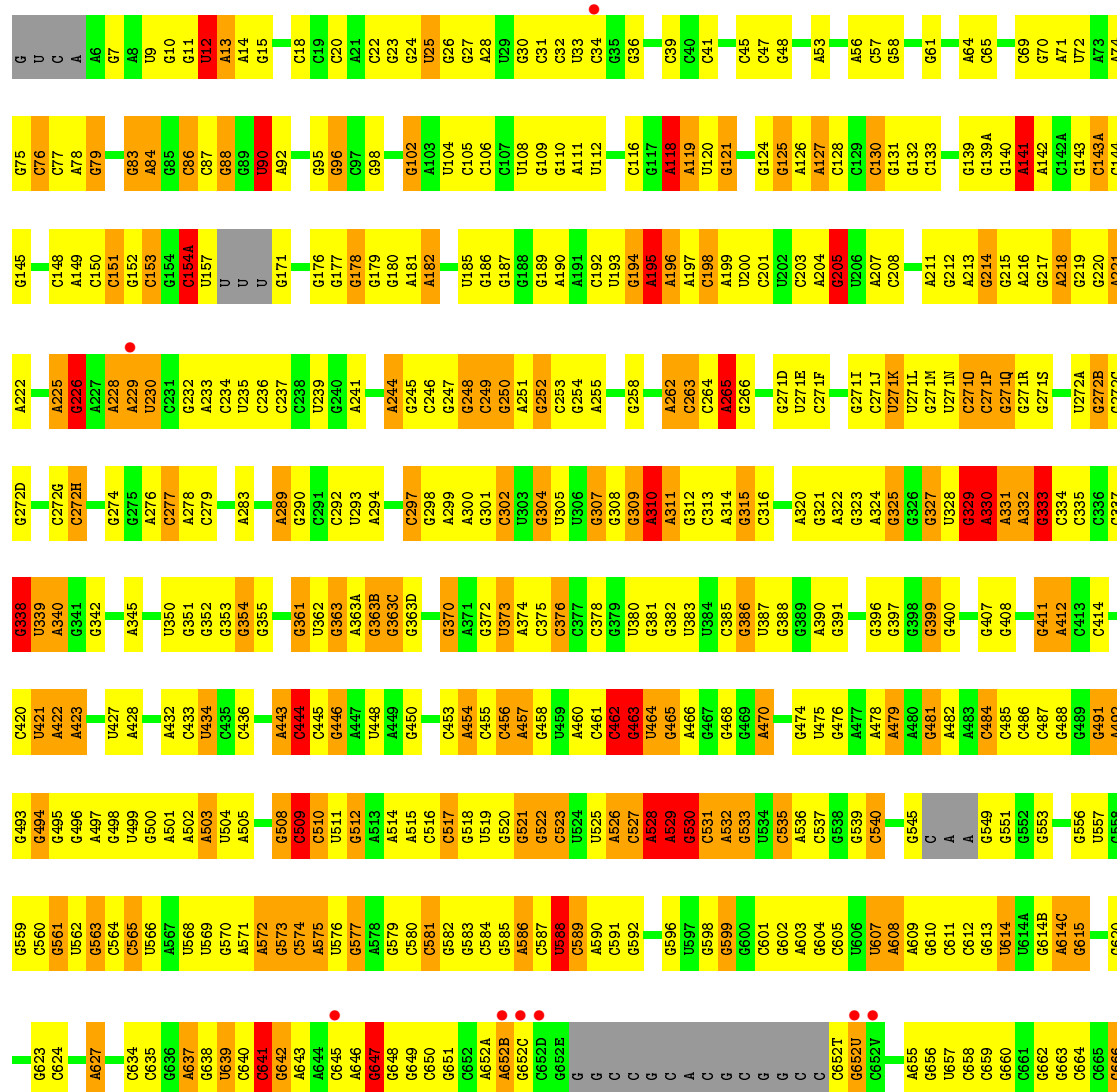




G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G3009	G3010	G3011	G3012	G3013	G3014	G3015	G3016	G3017	G3018	G3019	G3020	G3021	G3022	G3023	G3024	G3025	G3026	G3027	G3028	G3029	G3030	G3031	G3032	G3033	G3034	G3035	G3036	G3037	G3038	G3039	G3040	G3041	G3042	G3043	G3044	G3045	G3046	G3047	G3048	G3049	G3050	G3051	G3052	G3053	G3054	G3055	G3056	G3057	G3058	G3059	G3060	G3061	G3062	G3063	G3064	G3065	G3066	G3067	G3068	G3069	G3070	G3071	G3072	G3073	G3074	G3075	G3076	G3077	G3078	G3079	G3080	G3081	G3082	G3083	G3084	G3085	G3086	G3087	G3088	G3089	G3090	G3091	G3092	G3093	G3094	G3095	G3096	G3097	G3098	G3099	G3100	G3101	G3102	G3103	G3104	G3105	G3106	G3107	G3108	G3109	G3110	G3111	G3112	G3113	G3114	G3115	G3116	G3117	G3118	G3119	G3120	G3121	G3122	G3123	G3124	G3125	G3126	G3127	G3128	G3129	G3130	G3131	G3132	G3133	G3134	G3135	G3136	G3137	G3138	G3139	G3140	G3141	G3142	G3143	G3144	G3145	G3146	G3147	G3148	G3149	G3150	G3151	G3152	G3153	G3154	G3155	G3156	G3157	G3158	G3159	G3160	G3161	G3162	G3163	G3164	G3165	G3166	G3167	G3168	G3169	G3170	G3171	G3172	G3173	G3174	G3175	G3176	G3177	G3178	G3179	G3180	G3181	G3182	G3183	G3184	G3185	G3186	G3187	G3188	G3189	G3190	G3191	G3192	G3193	G3194	G3195	G3196	G3197	G3198	G3199	G3200	G3201	G3202	G3203	G3204	G3205	G3206	G3207	G3208	G3209	G3210	G3211	G3212	G3213	G3214	G3215	G3216	G3217	G3218	G3219	G3220	G3221	G3222	G3223	G3224	G3225	G3226	G3227	G3228	G3229	G3230	G3231	G3232	G3233	G3234	G3235	G3236	G3237	G3238	G3239	G3240	G3241	G3242	G3243	G3244	G3245	G3246	G3247	G3248	G3249	G3250	G3251	G3252	G3253	G3254	G3255	G3256	G3257	G3258	G3259	G3260	G3261	G3262	G3263	G3264	G3265	G3266	G3267	G3268	G3269	G3270	G3271	G3272	G3273	G3274	G3275	G3276	G3277	G3278	G3279	G3280	G3281	G3282	G3283	G3284	G3285	G3286	G3287	G3288	G3289	G3290	G3291	G3292	G3293	G3294	G3295	G3296	G3297	G3298	G3299	G3300	G3301	G3302	G3303	G3304	G3305	G3306	G3307	G3308	G3309	G3310	G3311	G3312	G3313	G3314	G3315	G3316	G3317	G3318	G3319	G3320	G3321	G3322	G3323	G3324	G3325	G3326	G3327	G3328	G3329	G3330	G3331	G3332	G3333	G3334	G3335	G3336	G3337	G3338	G3339	G3340	G3341	G3342	G3343	G3344	G3345	G3346	G3347	G3348	G3349	G3350	G3351	G3352	G3353	G3354	G3355	G3356	G3357	G3358	G3359	G3360	G3361	G3362	G3363	G3364	G3365	G3366	G3367	G3368	G3369	G3370	G3371	G3372	G3373	G3374	G3375	G3376	G3377	G3378	G3379	G3380	G3381	G3382	G3383	G3384	G3385	G3386	G3387	G3388	G3389	G3390	G3391	G3392	G3393	G3394	G3395	G3396	G3397	G3398	G3399	G3400	G3401	G3402	G3403	G3404	G3405	G3406	G3407	G3408	G3409	G3410	G3411	G3412	G3413	G3414	G3415	G3416	G3417	G3418	G3419	G3420	G3421	G3422	G3423	G3424	G3425	G3426	G3427	G3428	G3429	G3430	G3431	G3432	G3433	G3434	G3435	G3436	G3437	G3438	G3439	G3440	G3441	G3442	G3443	G3444	G3445	G3446	G3447	G3448	G3449	G3450	G3451	G3452	G3453	G3454	G3455	G3456	G3457	G3458	G3459	G3460	G3461	G3462	G3463	G3464	G3465	G3466	G3467	G3468	G3469	G3470	G3471	G3472	G3473	G3474	G3475	G3476	G3477	G3478	G3479	G3480	G3481	G3482	G3483	G3484	G3485	G3486	G3487	G3488	G3489	G3490	G3491	G3492	G3493	G3494	G3495	G3496	G3497	G3498	G3499	G3500	G3501	G3502	G3503	G3504	G3505	G3506	G3507	G3508	G3509	G3510	G3511	G3512	G3513	G3514	G3515	G3516	G3517	G3518	G3519	G3520	G3521	G3522	G3523	G3524	G3525	G3526	G3527	G3528	G3529	G3530	G3531	G3532	G3533	G3534	G3535	G3536	G3537	G3538	G3539	G3540	G3541	G3542	G3543	G3544	G3545	G3546	G3547	G3548	G3549	G3550	G3551	G3552	G3553	G3554	G3555	G3556	G3557	G3558	G3559	G3560	G3561	G3562	G3563	G3564	G3565	G3566	G3567	G3568	G3569	G3570	G3571	G3572	G3573	G3574	G3575	G3576	G3577	G3578	G3579	G3580	G3581	G3582	G3583	G3584	G3585	G3586	G3587	G3588	G3589	G3590	G3591	G3592	G3593	G3594	G3595	G3596	G3597	G3598	G3599	G3600	G3601	G3602	G3603	G3604	G3605	G3606	G3607	G3608	G3609	G3610	G3611	G3612	G3613	G3614	G3615	G3616	G3617	G3618	G3619	G3620	G3621	G3622	G3623	G3624	G3625	G3626	G3627	G3628	G3629	G3630	G3631	G3632	G3633	G3634	G3635	G3636	G3637	G3638	G3639	G3640	G3641	G3642	G3643	G3644	G3645	G3646	G3647	G3648	G3649	G3650	G3651	G3652	G3653	G3654	G3655	G3656	G3657	G3658	G3659	G3660	G3661	G3662	G3663	G3664	G3665	G3666	G3667	G3668	G3669	G3670	G3671	G3672	G3673	G3674	G3675	G3676	G3677	G3678	G3679	G3680	G3681	G3682	G3683	G3684	G3685	G3686	G3687	G3688	G3689	G3690	G3691	G3692	G3693	G3694	G3695	G3696	G3697	G3698	G3699	G3700	G3701	G3702	G3703	G3704	G3705	G3706	G3707	G3708	G3709	G3710	G3711	G3712	G3713	G3714	G3715	G3716	G3717	G3718	G3719	G3720	G3721	G3722	G3723	G3724	G3725	G3726	G3727	G3728	G3729	G3730	G3731	G3732	G3733	G3734	G3735	G3736	G3737	G3738	G3739	G3740	G3741	G3742	G3743	G3744	G3745	G3746	G3747	G3748	G3749	G3750	G3751	G3752	G3753	G3754	G3755	G3756	G3757	G3758	G3759	G3760	G3761	G3762	G3763	G3764	G3765	G3766	G3767	G3768	G3769	G3770	G3771	G3772	G3773	G3774	G3775	G3776	G3777	G3778	G3779	G3780	G3781	G3782	G3783	G3784	G3785	G3786	G3787	G3788	G3789	G3790	G3791	G3792	G3793	G3794	G3795	G3796	G3797	G3798	G3799	G3800	G3801	G3802	G3803	G3804	G3805	G3806	G3807	G3808	G3809	G3810	G3811	G3812	G3813	G3814	G3815	G3816	G3817	G3818	G3819	G3820	G3821	G3822	G3823	G3824	G3825	G3826	G3827	G3828	G3829	G3830	G3831	G3832	G3833	G3834	G3835	G3836	G3837	G3838	G3839	G3840	G3841	G3842	G3843	G3844	G3845	G3846	G3847	G3848	G3849	G3850	G3851	G3852	G3853	G3854	G3855	G3856	G3857	G3858	G3859	G3860	G3861	G3862	G3863	G3864	G3865	G3866	G3867	G3868	G3869	G3870	G3871	G3872	G3873	G3874	G3875	G3876	G3877	G3878	G3879	G3880	G3881	G3882	G3883	G3884	G3885	G3886	G3887	G3888	G3889	G3890	G3891	G3892	G3893	G3894	G3895	G3896	G3897	G3898	G3899	G3900	G3901	G3902	G3903	G3904	G3905	G3906	G3907	G3908	G3909	G3910	G3911	G3912	G3913	G3914	G3915	G3916	G3917	G3918	G3919	G3920	G3921	G3922	G3923	G3924	G3925	G3926	G3927	G3928	G3929	G3930	G3931	G3932	G3933	G3934	G3935	G3936	G3937	G3938	G3939	G3940	G3941	G3942	G3943	G3944	G3945	G3946	G3947	G3948	G3949	G3950	G3951	G3952	G3953	G3954	G3955	G3956	G3957	G3958	G3959	G3960	G3961	G3962	G3963	G3964	G3965	G3966	G3967	G3968	G3969	G3970	G3971	G3972	G3973	G397
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------

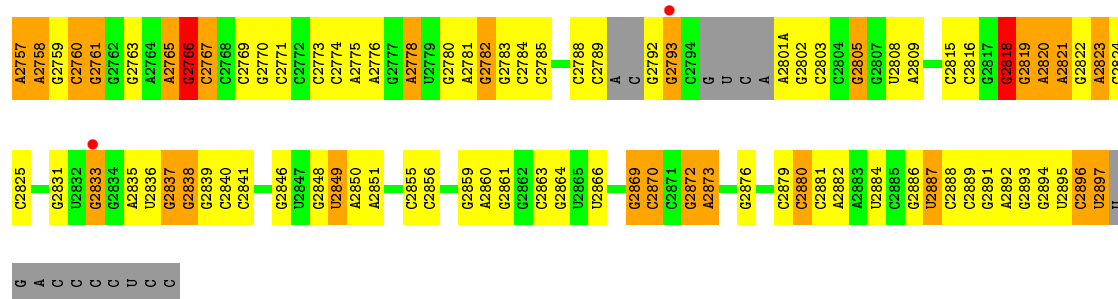


• Molecule 1: 23S Ribosomal RNA



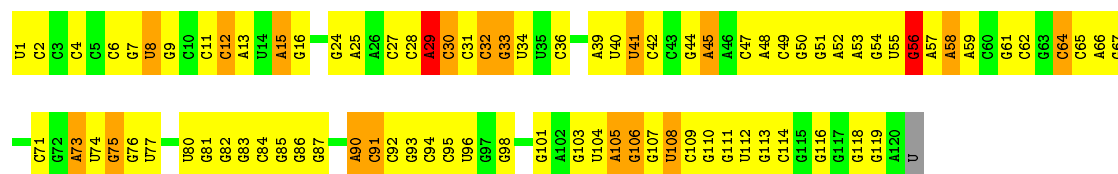


G2685	G2608	A2541	G2470	G2400	A2335	U2272	G2191	G2131	C2055	U1991	A1919	G1831	C1771	G1678	A1577
G2689	G2610	G2542	C2474	U2401	A2336	A2273	G2192	U2132	C2056	C1920	C1920	C1832	G1772	G1679	
G2690	U2611	G2543	C2475	C2404	G2340	A2274	G2193	G2133	A2057	G1921	G1921	U1833	A1773	U1679	
U2612	U2613	U2547	A2476	G2405	G2341	C2275	C2194	A2134		G1922	U1923	U1834	C1774	U1680	
G2694	U2614	G2548	A2477	U2406	C2343	C2276	C2195	A2135	G2060	U1924	U1924	G1835	U1775	G1681	
U2615	U2616	G2549	A2478	G2407	U2344	G2277	C2196	U2136	A2061	U1925	U1925	C1836	G1776	G1682	
G2617	G2618	G2550	A2479	U2408	U2345	A2278	U2197	C2137	A2062	C1926	U1926	C1837	U1777	C1683	
U2552	C2551	G2485	G2479	U2409	A2346	G2279	A2198	C2138	C2063	G1927	A1927	C1838	U1778		U1688
G2553	G2486	G2487	G2486	G2410	C2347	G2280	C2200	C2139	C2064	G1928	A1928	G1839	U1779	A1689	
U2554	G2488	G2488	G2488	G2411	U2348	C2281	C2201	G2140	C2065	G1929	G1929	G1840	A1780	A1690	
U2555	G2489	G2489	G2489	G2416	G2349	G2282	C2202	G2141	C2066	G1930	U1931	U1841	C1781	C1691	
G2557	U2491	G2492	U2492	G2417	G2350	U2283	U2203	C2142		G1931	U1931	C1842	C1782	C1692	
U2562	G2493	G2493	G2493	G2422	G2351	C2284	C2205	U2144	G2070	G1932	U1932	C1843	U1783	U1693	
U2563	U2494	G2494	G2494	U2423	G2352	C2285	G2206	C2145	A2071	G1934	C1934	C1844	A1785	G1694	
A2564	A2425	G2424	G2424	U2431	G2353	U2291	C2207	G2146	C2072	G1935	C1935	A1847	A1786	G1695	
A2565	A2426	U2426	U2426	U2432	G2354	C2292	A2208	G2147	C2073	A1936	A1936	A1848	A1787	G1696	
A2566	C2427	A2427	A2427	A2434	G2355	A2287	A2209	G2148	U2074	A1937	A1937	G1849	C1788	G1697	
A2567	U2500	G2428	G2428	G2433	U2357	G2289	U2218	G2149	U2075	A1938	A1938	G1850	A1789	A1698	
G2570	G2501	G2429	U2502	A2430	G2358	U2296	G2222	U2150		U1939	U1939	G1857	C1790	A1699	
C2571	G2503	U2504	G2504	U2431	G2359	C2297		G2151	C2078		G1949	U1864	A1791	A1700	
A2572	A2504	G2505	G2505	A2434	A2360	A2298	A2225	G2152	U2079	U1943	G1950	G1858	G1792	G1701	
G2573	G2506	G2506	G2506	A2435	A2361	C2299	C2226	G2153	G2080	U1944	U1944	G1859	C1793	G1702	
G2574	G2507	G2507	G2507	A2436	G2362	C2294	A2227	G2154	C2081	G1945	G1945	G1860	U1794	G1703	
G2575	G2508	U2509	G2509	U2437	G2363	U2295	A2228	G2155	A2082	U1946	U1946	G1861	C1795	G1704	
G2576	G2510	U2510	G2510	U2438	G2364	U2296	C2229	G2156				U1864	U1796		
A2577	G2511	G2511	G2511	U2439	G2365	C2297	U2233	G2157	U2086	G1949	G1949	U1864	C1797	G1707	
G2578	G2512	G2512	G2512	U2440	G2366	A2298	G2234	U2158	C2087	G1950	G1950	G1858	C1798	G1708	
G2581	G2513	G2513	G2513	U2441	G2367	C2299	G2235	G2159	U1951	U1952	U1952	G1866	G1799	U1709	
G2582	G2514	G2514	G2514	U2442	G2368	G2300	G2236	G2160	C2095	A1952	A1952	G1876	C1800	G1710	
G2583	G2515	G2515	G2515	U2443	G2369	U2302	G2237	G2161		G1953	G1953	A1877	G1801	C1711	
U2584	G2516	G2516	G2516	U2444	G2370	G2303	G2238	G2162	U2102	U1955	U1955	G1878	A1802		
U2585	G2517	G2517	G2517	U2445	G2371	G2304	G2239	G2163	C2103	U1956	U1956	G1883	A1803	U1720	
A2586	G2518	G2518	G2518	U2446	G2372	A2305	G2239	G2164	G2104	A1722	A1722	G1883	C1804	G1721	
A2587	G2519	G2519	G2519	U2447	G2373	G2306	G2240	G2165	C2105	C1957	C1957	U1805	U1805	A1722	
A2588	G2520	G2520	G2520	U2448	G2374	G2307	U2243	G2166	G2106	G1958	G1958	G1886	C1806	U1739	
A2589	G2521	G2521	G2521	U2449	G2375	G2307	U2244	U2167	C2107	G1959	G1959	G1887	G1807	G1740	
A2590	G2522	G2522	G2522	U2450	G2376	U2312	A2247	G2168	C2108	A1889	A1889	G1878	U1808	A1741	
A2591	G2523	G2523	G2523	U2451	G2377	C2313	A2248	A2169	U2109	C1962	C1962	U1889	A1809		
G2592	G2524	G2524	G2524	U2452	G2378	C2314	C2249	A2170	G2110	U1963	U1963	C1892	A1810	C1744	
G2593	G2525	G2525	G2525	U2453	G2379	G2315	U2249	A2171	G2111	U1964	U1964	C1893	G1811		
G2594	G2526	G2526	G2526	U2454	G2380	G2316	G2250	U2172	G2112	A1966	A1966	C1894	A1812	G1747A	
G2595	G2527	G2527	G2527	U2455	G2381	G2317	G2251	G2173	G2113	C1967	C1967	C1895	G1813		
U2596	G2528	G2528	G2528	U2456	G2382	G2318	G2252	G2174	G2114	G1968	G1968	U1898	G1814	G1753	
G2597	G2529	G2529	G2529	U2457	G2383	G2319	G2253	G2175	G2115	A1969	A1969	C1754	A1815	C1754	
A2598	A2530	G2530	A2530	U2457	G2384	A2320	G2254	A2176	G2116	A1970	A1970	U1899	G1816	C1755	
G2599	G2531	G2531	G2531	U2458	G2385	G2321	G2255	C2177	A2117	A1971	A1971	G1899	G1817	G1756	
A2600	G2532	G2532	G2532	U2459	C2386	A2322	G2256	C2178	A2118	A1972	A1972	U1899	U1818	U1757	
G2601	A2533	A2533	A2533	U2460	U2387	G2323	U2257	C2179	G2119	G1973	G1973	U1899	U1819	G1758	
A2602	G2534	G2534	G2534	U2461	G2388	G2324	G2258	U2180	G2120	C1974	C1974	U1899	U1820	A1759	
G2603	G2535	G2535	G2535	U2462	G2389	G2325	G2259	G2181	G2121	G1975	G1975	G1906	A1821	A1760	
U2604	G2536	G2536	G2536	U2463	U2390	C2326	G2260	G2182	U2122			G1907	A1822	C1761	
U2605	U2537	U2537	U2537	U2464	U2391	A2327	C2261	C2183	G2123	C2046	C2046	C1908	G1822	C1762	
G2606	G2538	G2538	G2538	U2465	A2392	A2328	U2262	G2184	G2124	G1980	G1980	C1909	G1823	A1763	
G2607	G2539	G2539	G2539	U2466	A2393	G2329	U2263	G2185	G2125	A1981	A1981	U1917	G1824	G1764	
U2608	U2540	U2540	U2540	U2467	G2394	G2330	C2264	G2186	A2126			A1913	G1826		
U2609	G2541	G2541	G2541	U2468	G2395	G2331	U2265	G2187	G2127	G1984	G1984	C1914	C1827	C1767	
U2610	G2542	G2542	G2542	U2469	G2396	U2332	U2266	C2188	C2128	G1985	G1985	U1917	G1828	U1768	
U2611	G2543	G2543	G2543	U2470	G2397	U2333	A2268	C2189	C2129			A1918	A1829	G1770	
U2612	G2544	G2544	G2544	U2471	G2398	G2334	A2269	G2190	U2130				C1830		



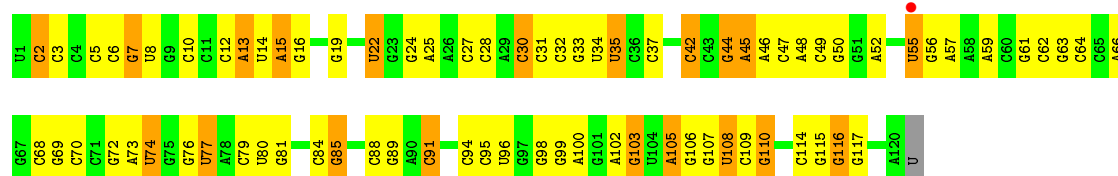
- Molecule 2: 5S Ribosomal RNA

Chain AB: 28% 55% 14% ..



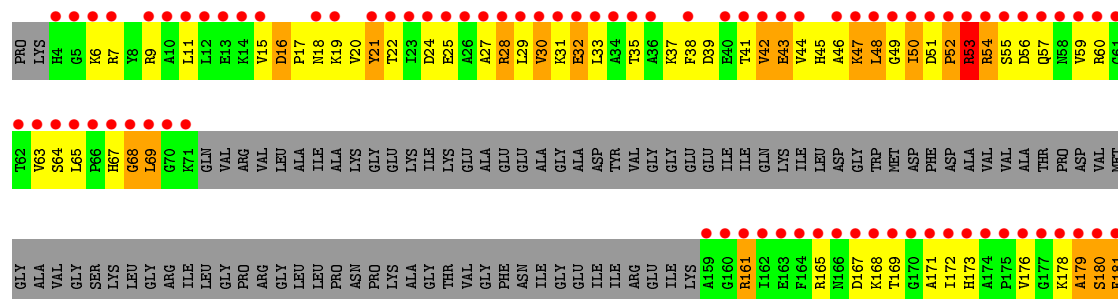
- Molecule 2: 5S Ribosomal RNA

Chain CB: 36% 47% 17% .



- Molecule 3: 50S ribosomal protein L1

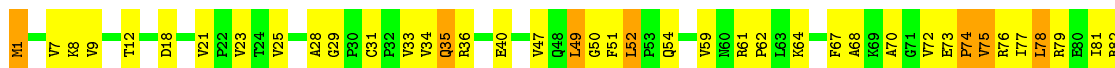
Chain AC: 22% 54% 28% 10% 40%

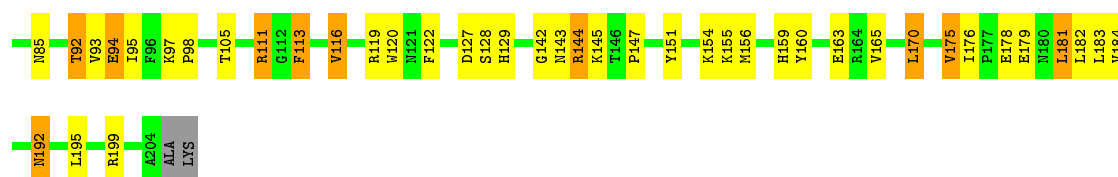


- Molecule 3: 50S ribosomal protein L1

Chain CC: 21% 60% 29% 10% 40%

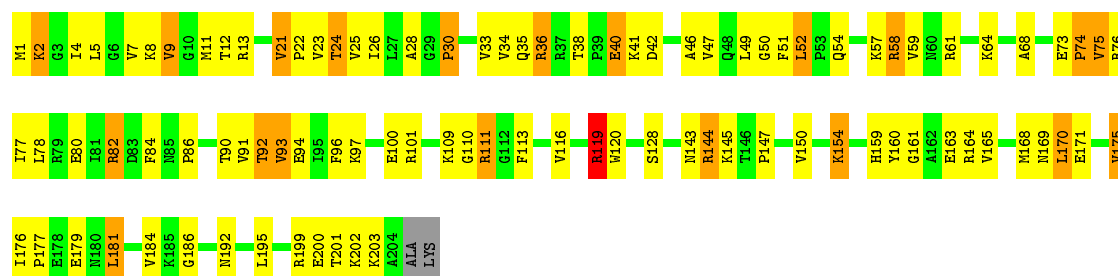






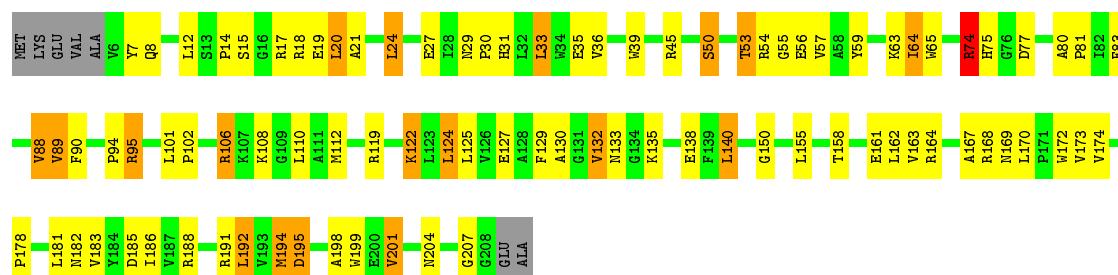
- Molecule 5: 50S ribosomal protein L3

Chain CE: 52% 36% 10% .



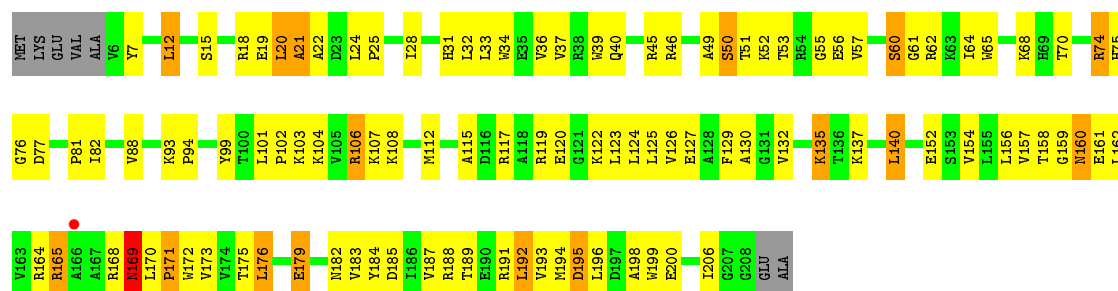
- Molecule 6: 50S ribosomal protein L4

Chain AF: 54% 33% 9% .



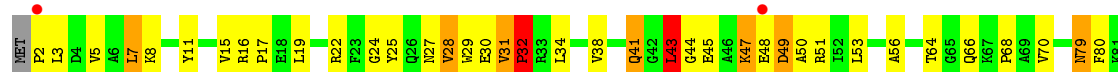
- Molecule 6: 50S ribosomal protein L4

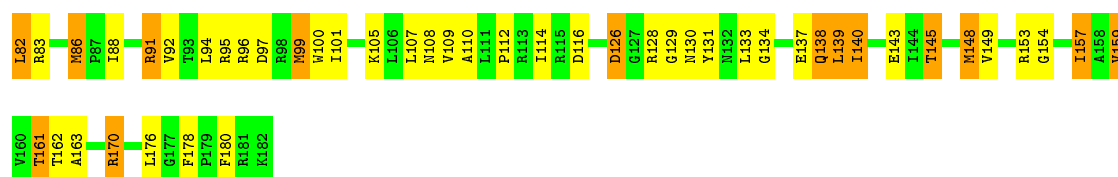
Chain CF: 46% 43% 8% .



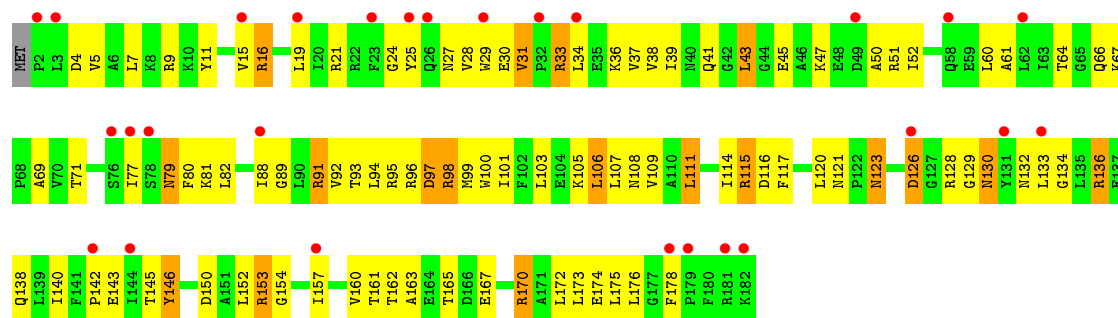
- Molecule 7: 50S ribosomal protein L5

Chain AG: 53% 34% 12% ..

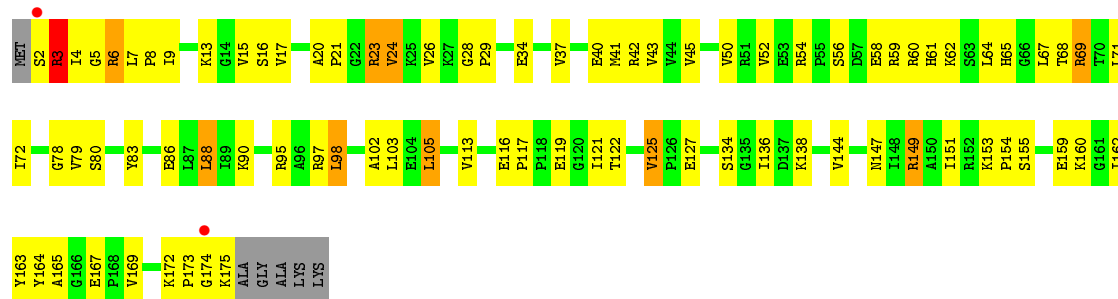




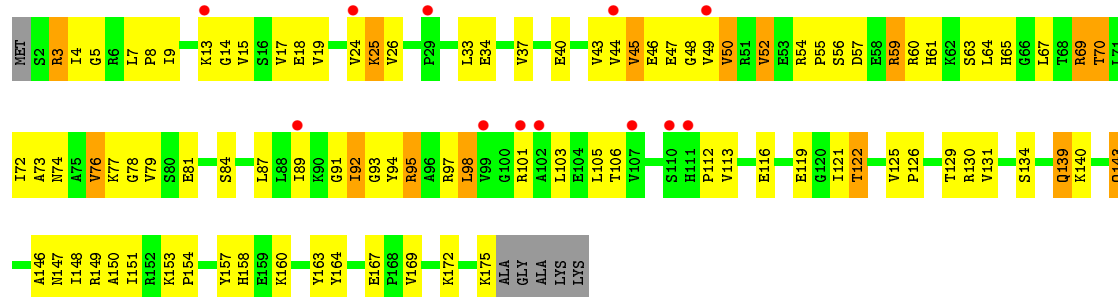
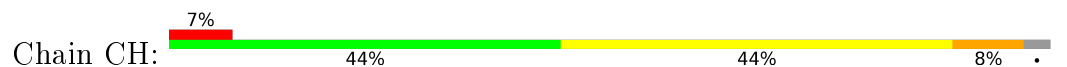
• Molecule 7: 50S ribosomal protein L5



• Molecule 8: 50S ribosomal protein L6

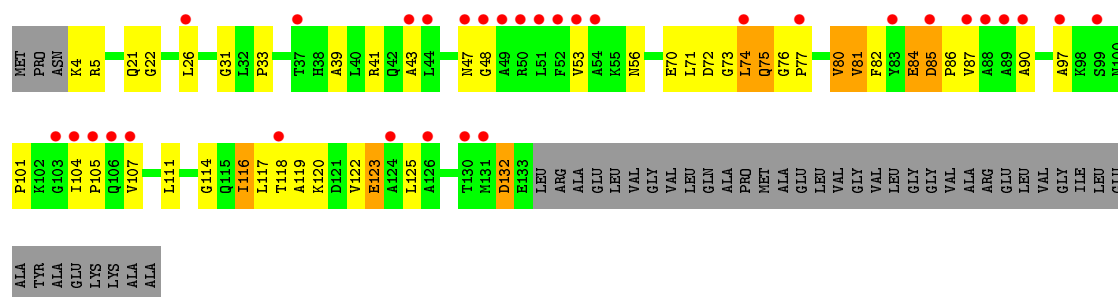


• Molecule 8: 50S ribosomal protein L6

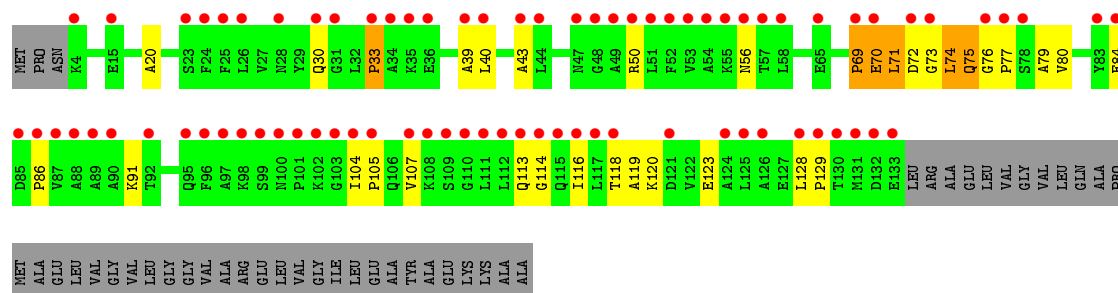


• Molecule 9: 50S ribosomal protein L10

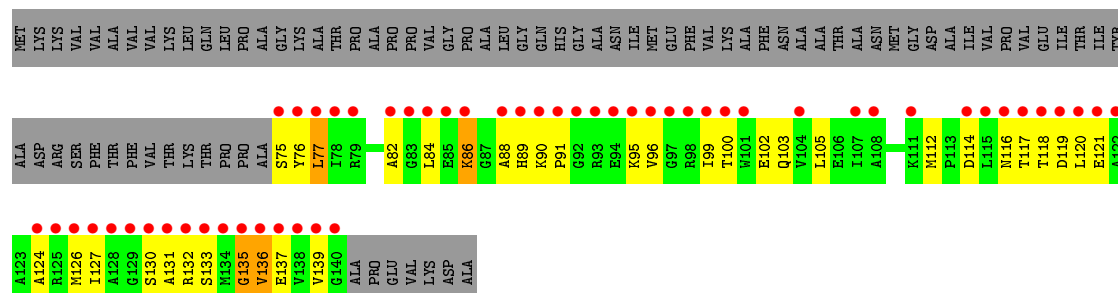
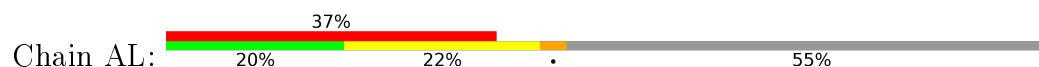




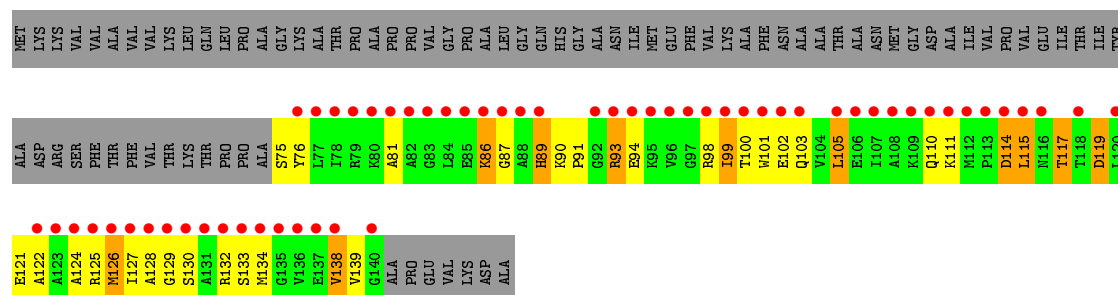
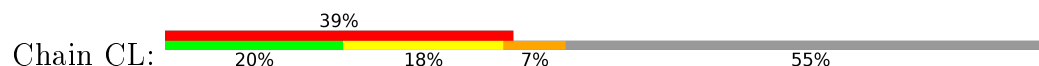
• Molecule 9: 50S ribosomal protein L10



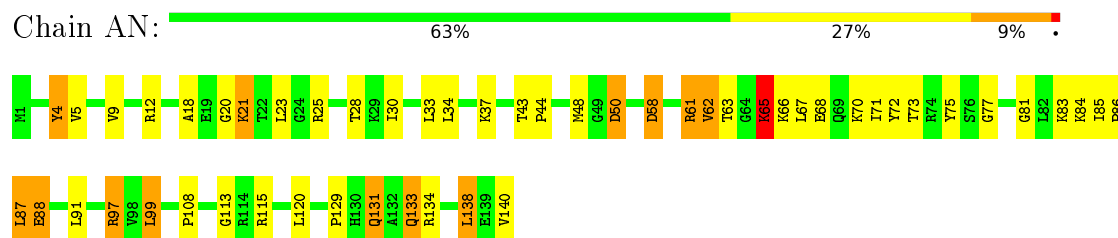
• Molecule 10: 50S ribosomal protein L11



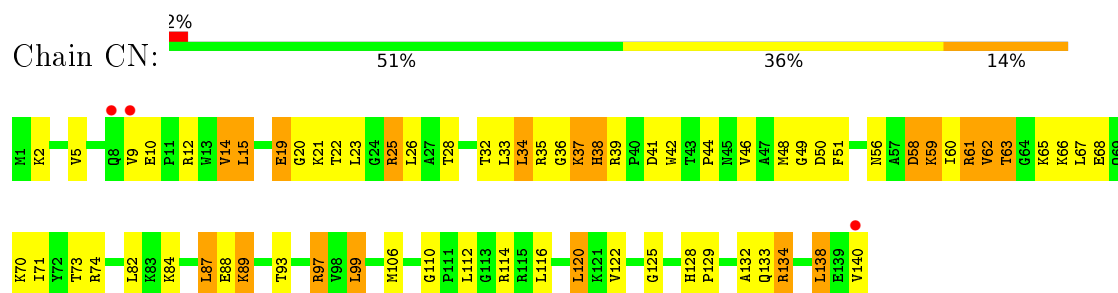
• Molecule 10: 50S ribosomal protein L11



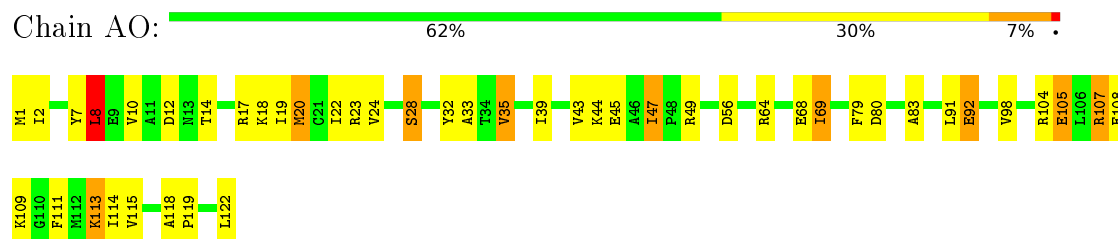
• Molecule 11: 50S ribosomal protein L13



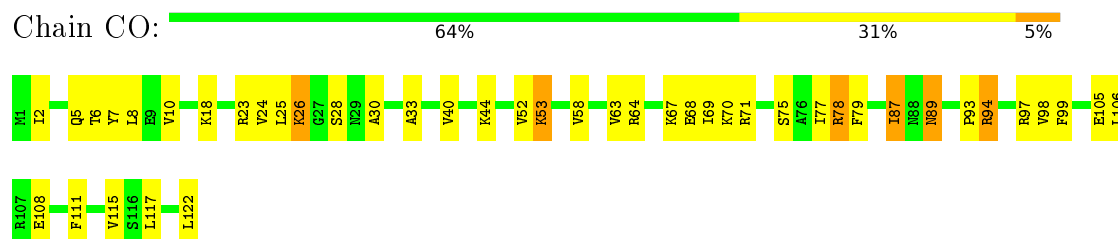
- Molecule 11: 50S ribosomal protein L13



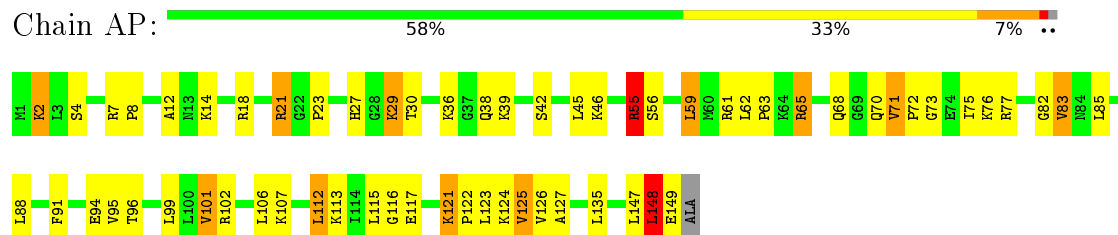
- Molecule 12: 50S ribosomal protein L14



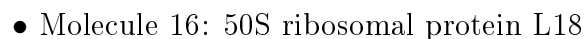
- Molecule 12: 50S ribosomal protein L14

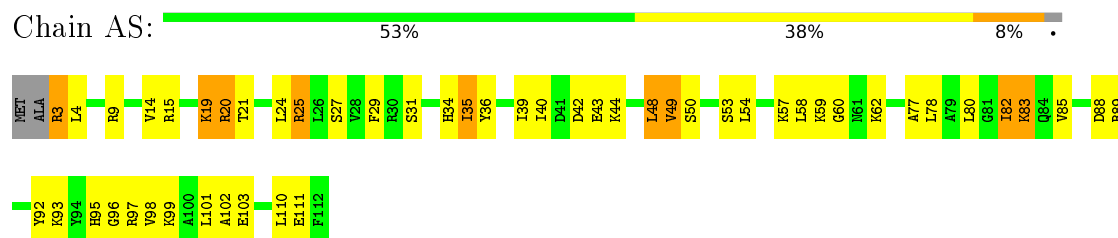


- Molecule 13: 50S ribosomal protein L15

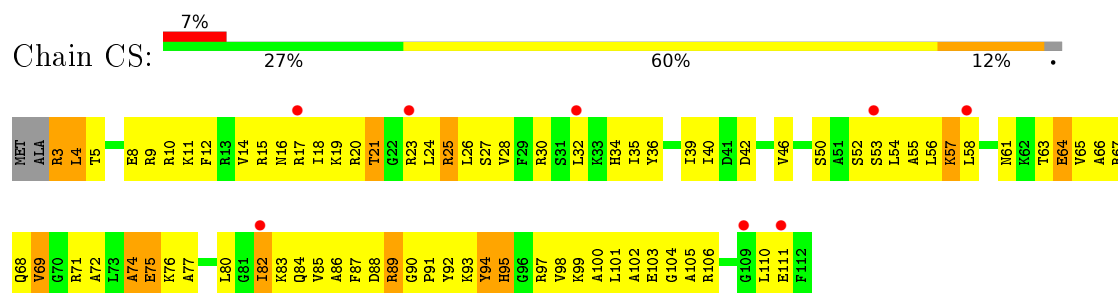


- Molecule 13: 50S ribosomal protein L15

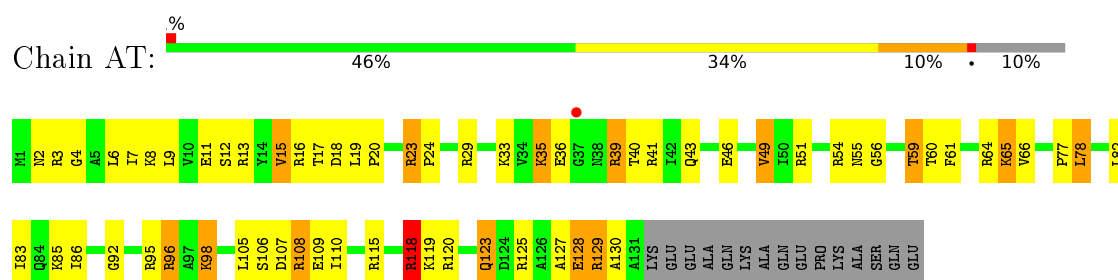


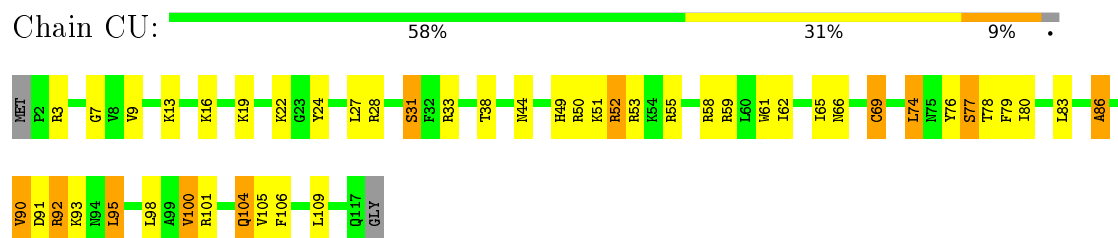


- Molecule 16: 50S ribosomal protein L18

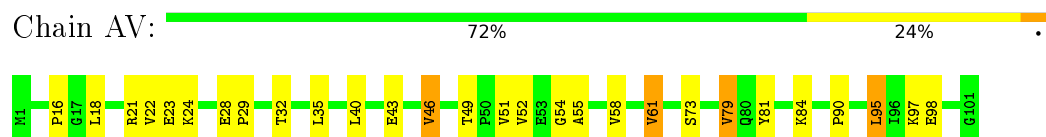


- Molecule 17: 50S ribosomal protein L19

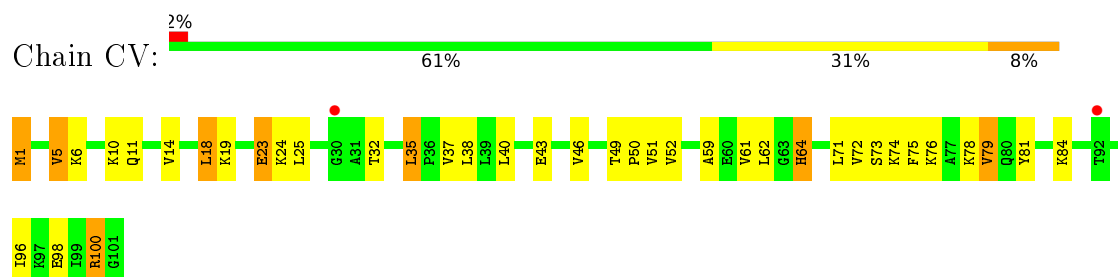




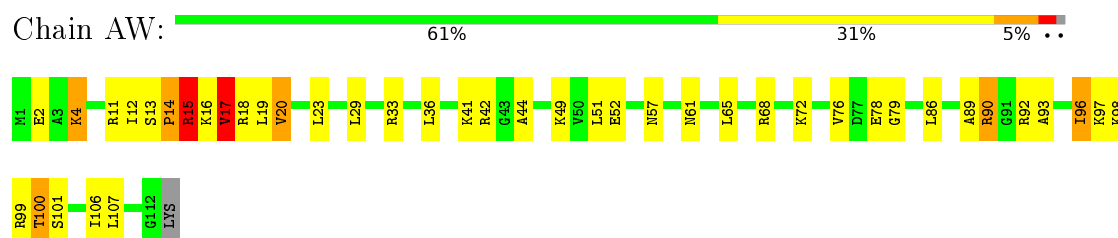
- Molecule 19: 50S ribosomal protein L21



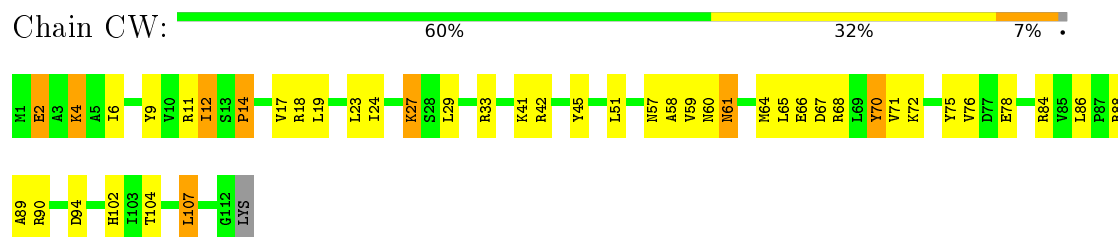
- Molecule 19: 50S ribosomal protein L21



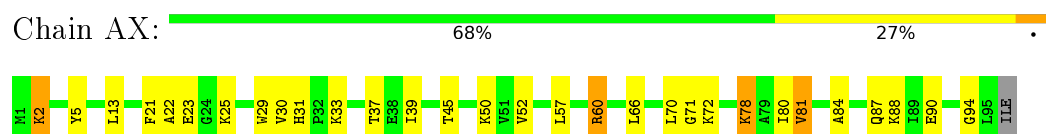
- Molecule 20: 50S ribosomal protein L22



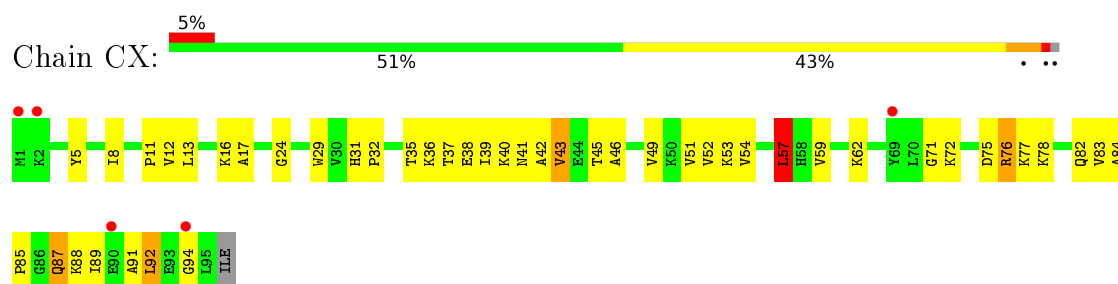
- Molecule 20: 50S ribosomal protein L22



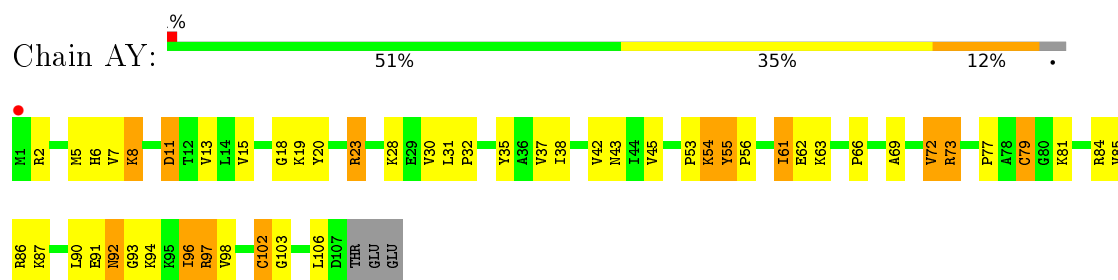
- Molecule 21: 50S ribosomal protein L23



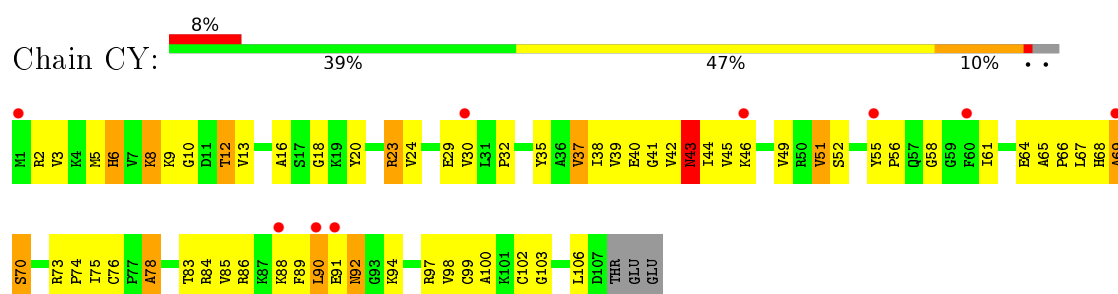
- Molecule 21: 50S ribosomal protein L23



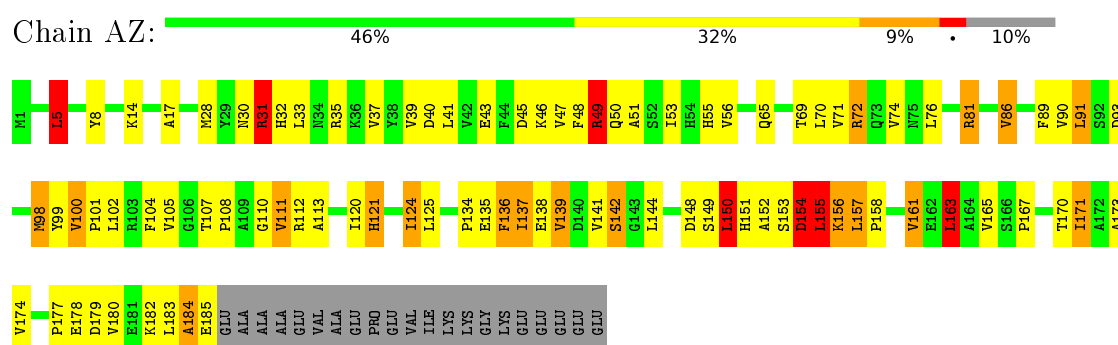
- Molecule 22: 50S ribosomal protein L24



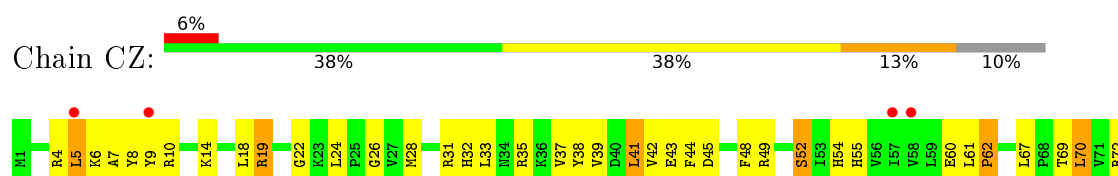
- Molecule 22: 50S ribosomal protein L24

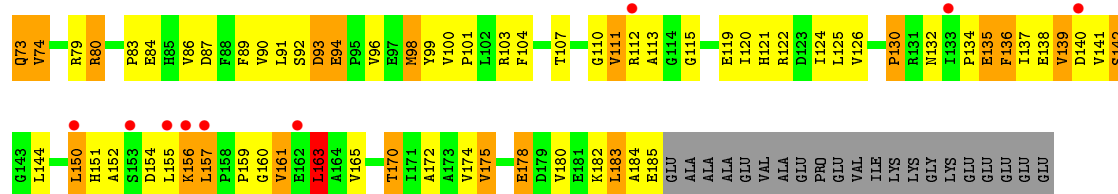


- Molecule 23: 50S ribosomal protein L25



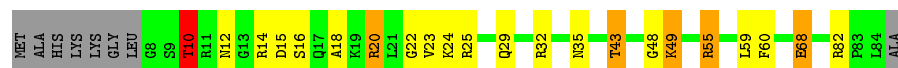
- Molecule 23: 50S ribosomal protein L25





• Molecule 24: 50S ribosomal protein L27

Chain A0: 65% 19% 6% 9%



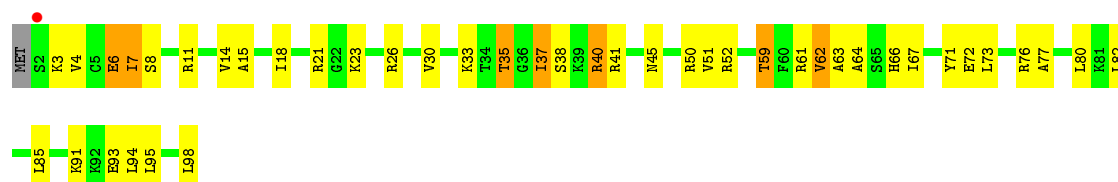
• Molecule 24: 50S ribosomal protein L27

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



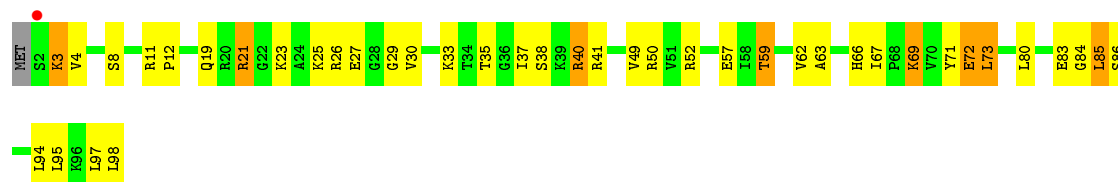
• Molecule 25: 50S ribosomal protein L28

Chain A1: % 55% 37% 7%



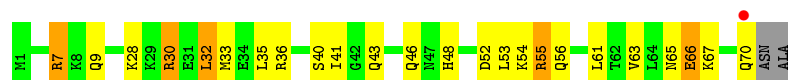
• Molecule 25: 50S ribosomal protein L28

Chain C1: % 57% 34% 8%

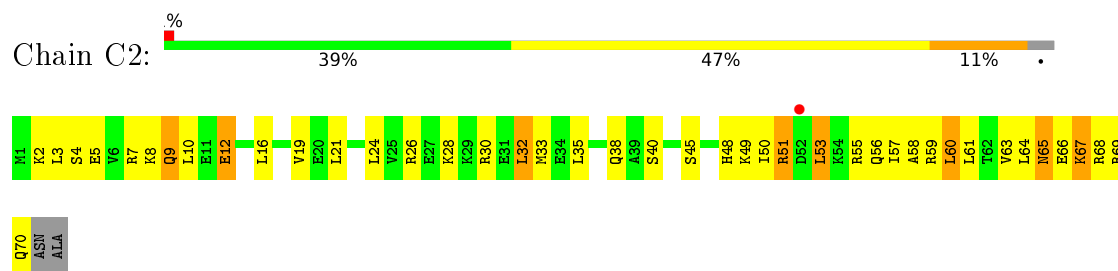


• Molecule 26: 50S ribosomal protein L29

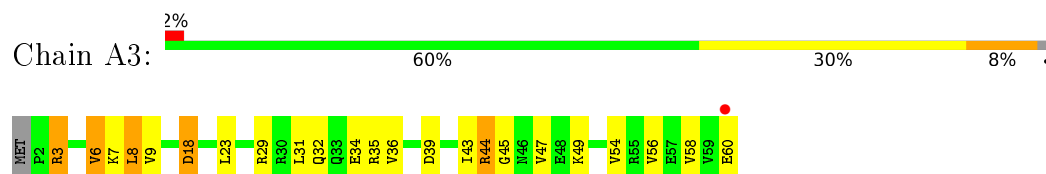
Chain A2: % 64% 26% 7%



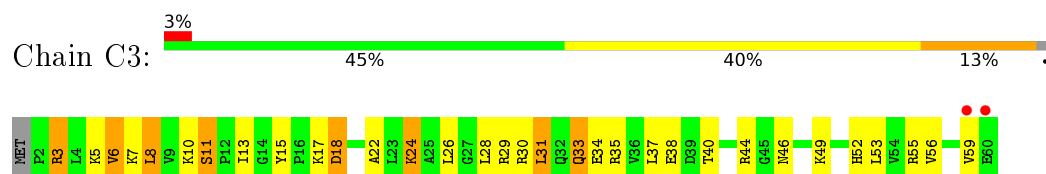
- Molecule 26: 50S ribosomal protein L29



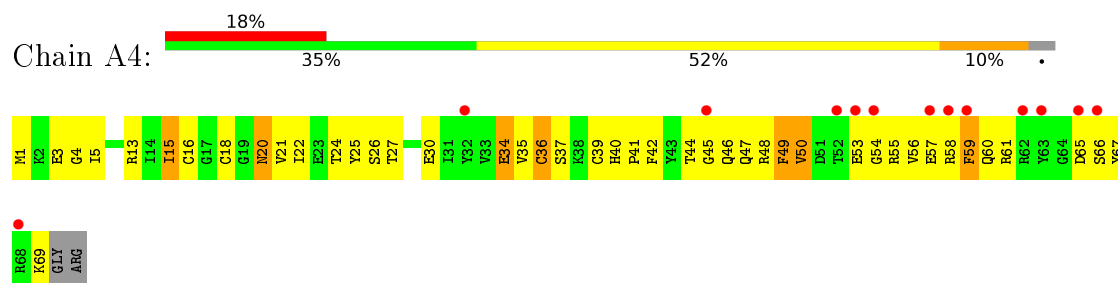
- Molecule 27: 50S ribosomal protein L30



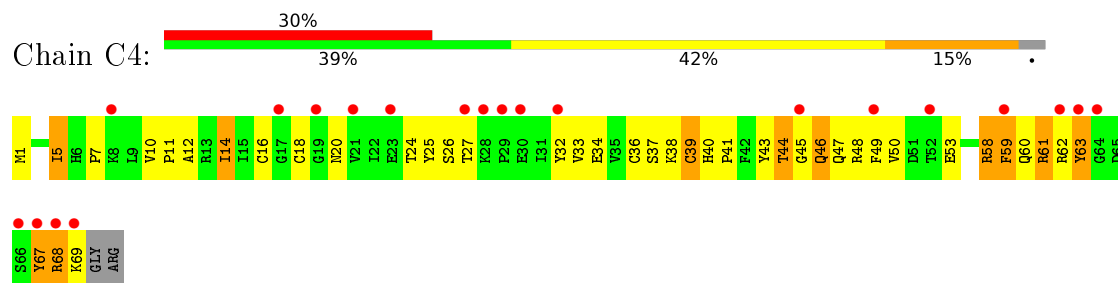
- Molecule 27: 50S ribosomal protein L30



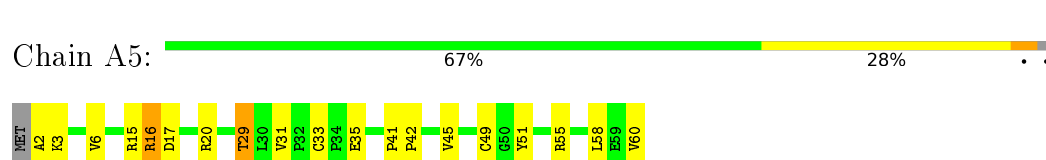
- Molecule 28: 50S ribosomal protein L31



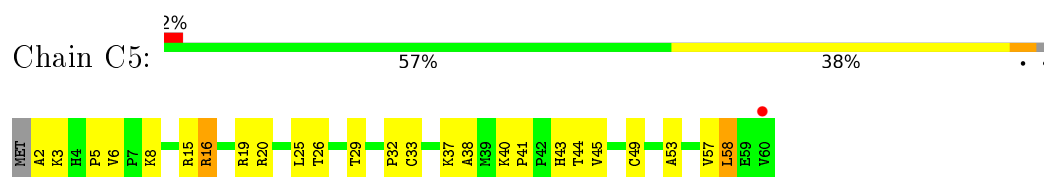
- Molecule 28: 50S ribosomal protein L31



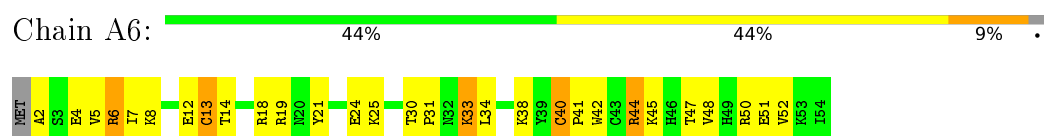
- Molecule 29: 50S ribosomal protein L32



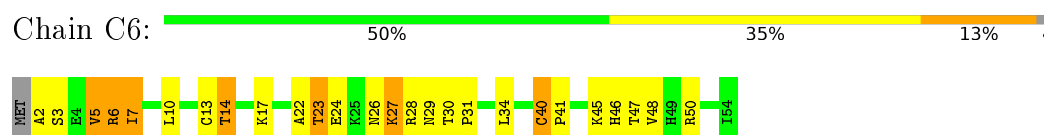
- Molecule 29: 50S ribosomal protein L32



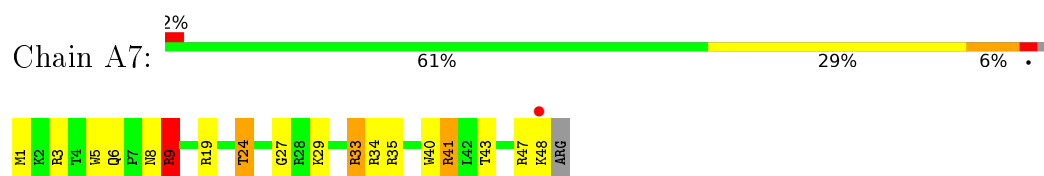
- Molecule 30: 50S ribosomal protein L33



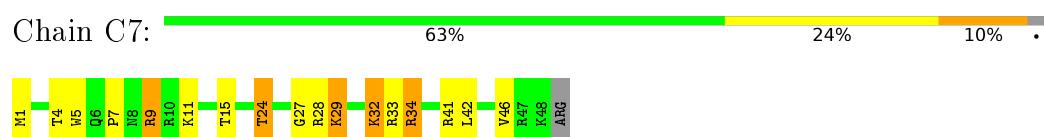
- Molecule 30: 50S ribosomal protein L33



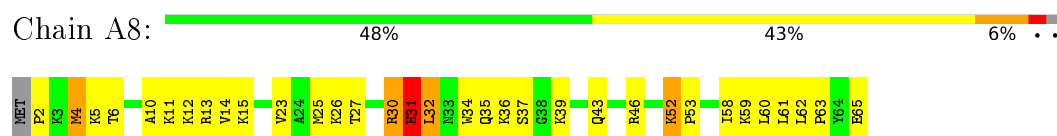
- Molecule 31: 50S ribosomal protein L34



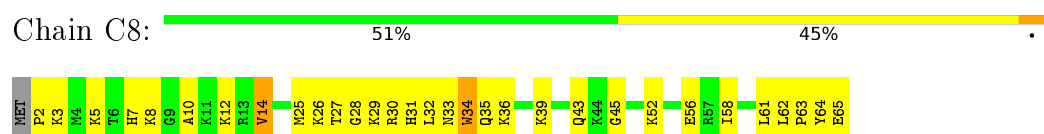
- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L35



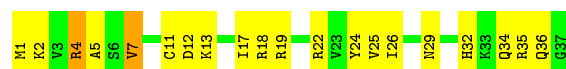
- Molecule 33: 50S ribosomal protein L36

Chain A9:  57% 38% 5%



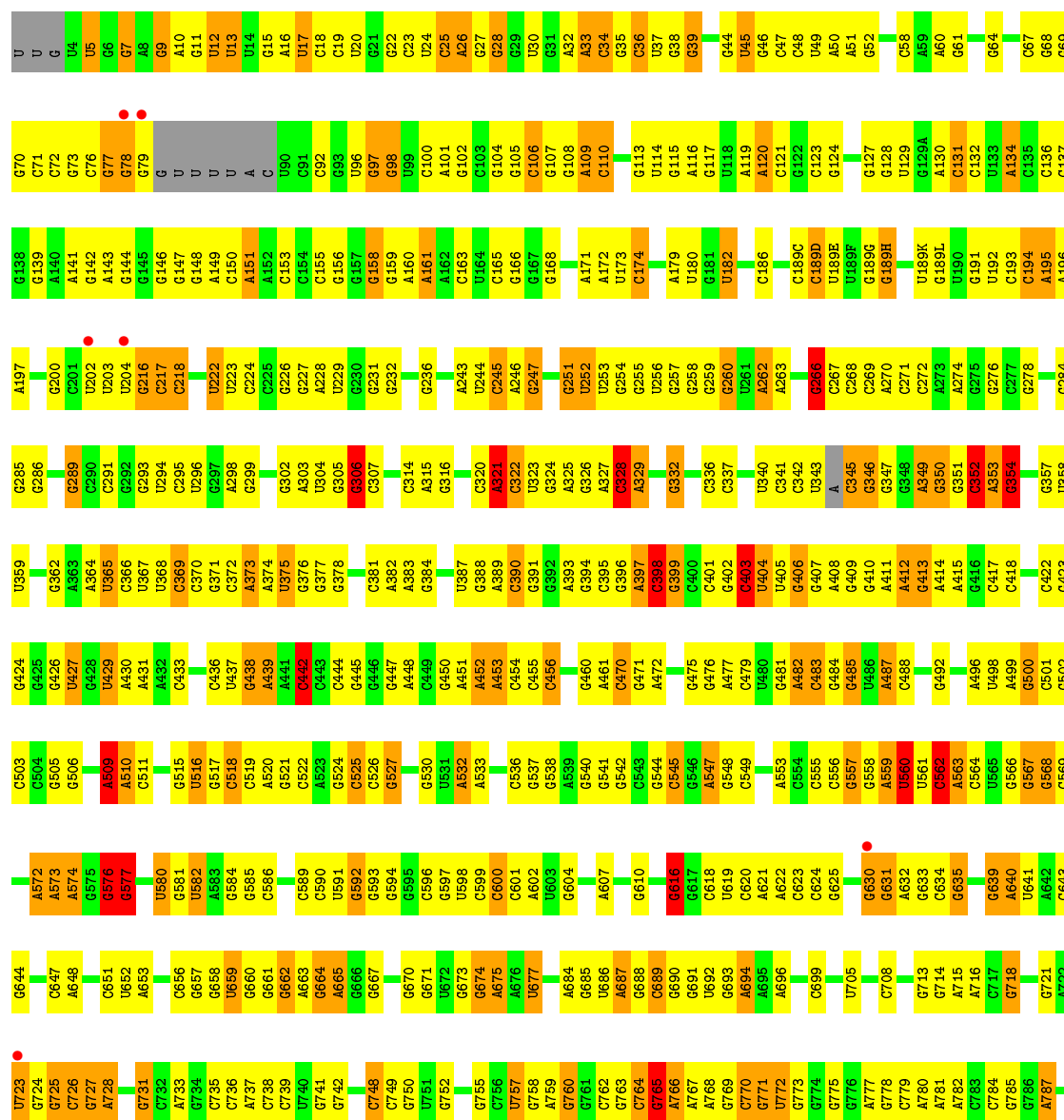
- Molecule 33: 50S ribosomal protein L36

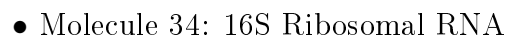
Chain C9:  46% 49% 5%

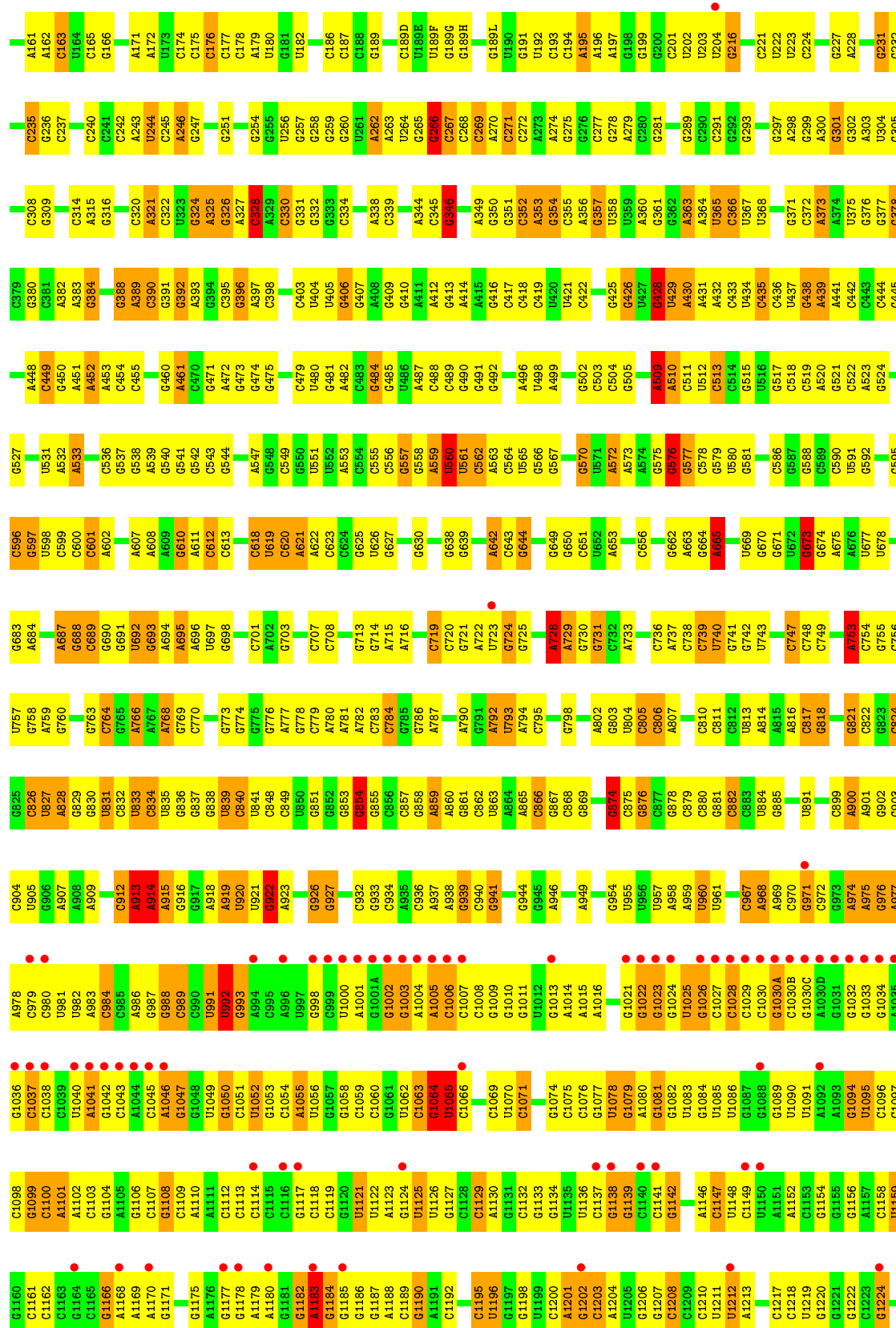


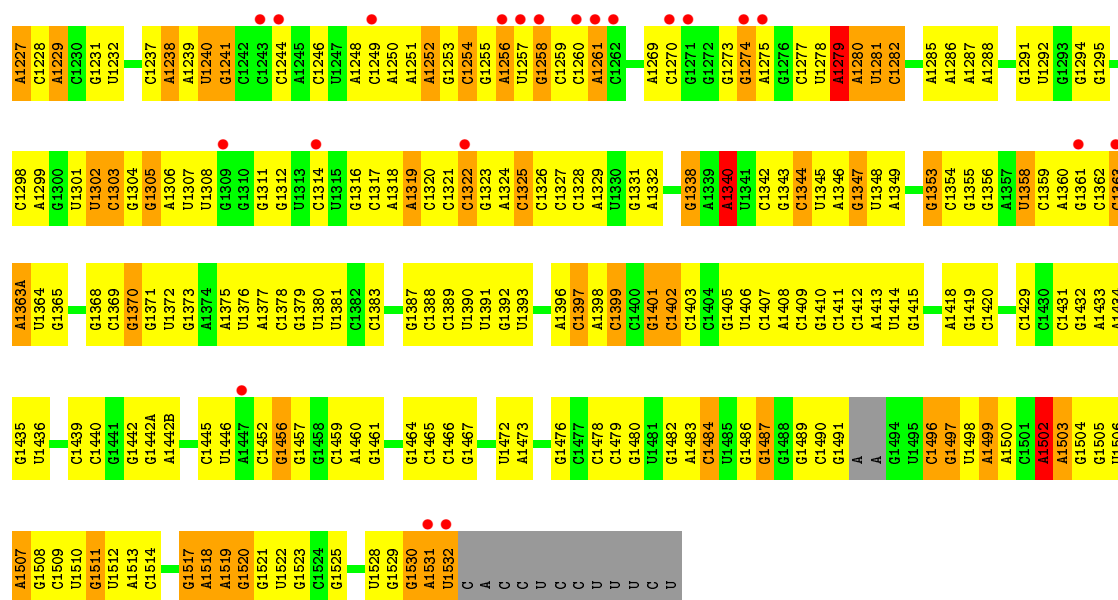
- Molecule 34: 16S Ribosomal RNA

Chain BA:  3% 31% 48% 17%

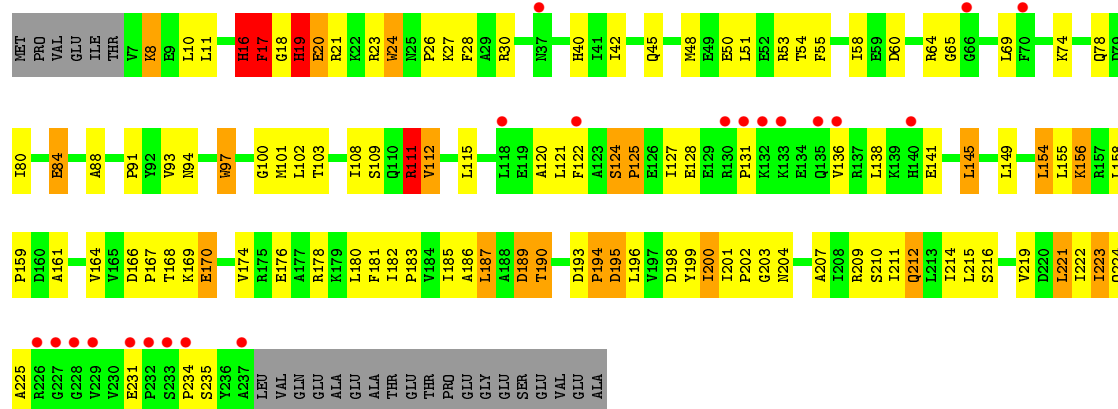




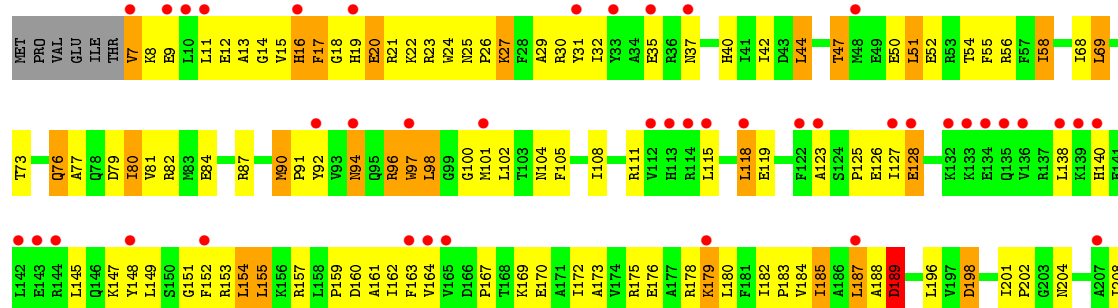




• Molecule 35: 30S ribosomal protein S2

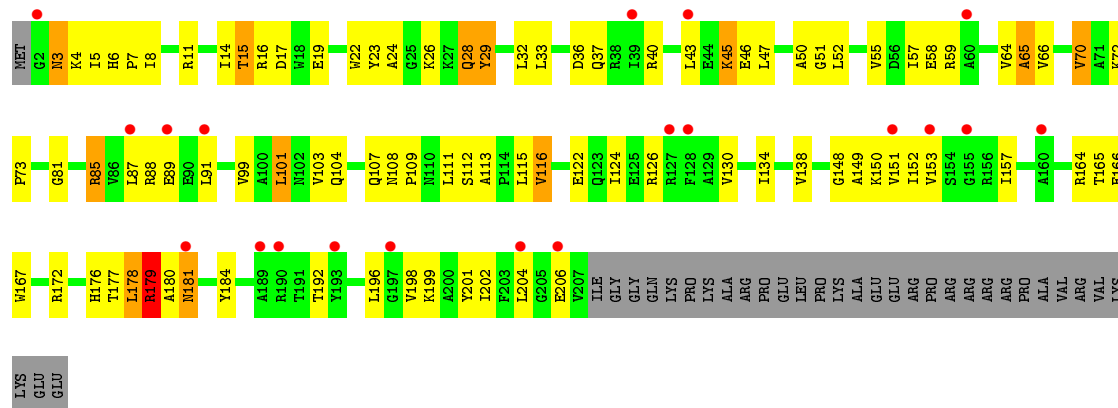


• Molecule 35: 30S ribosomal protein S2

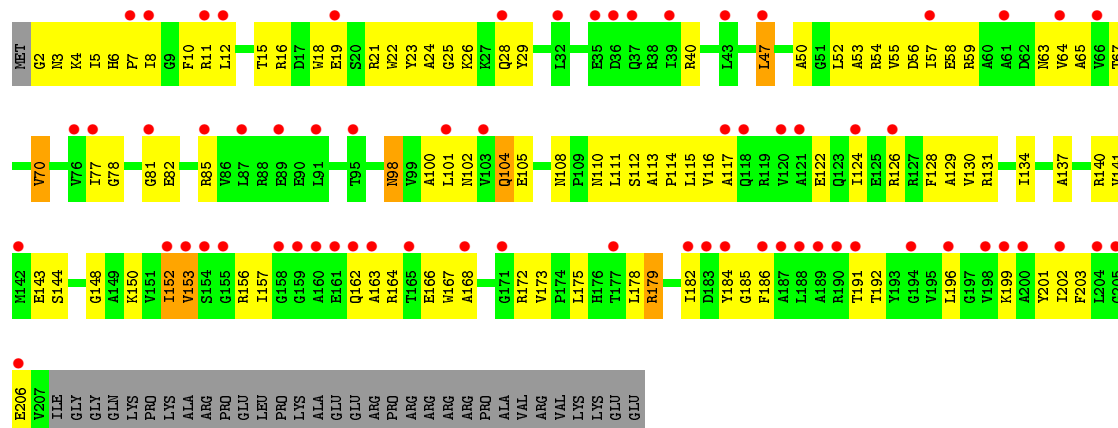




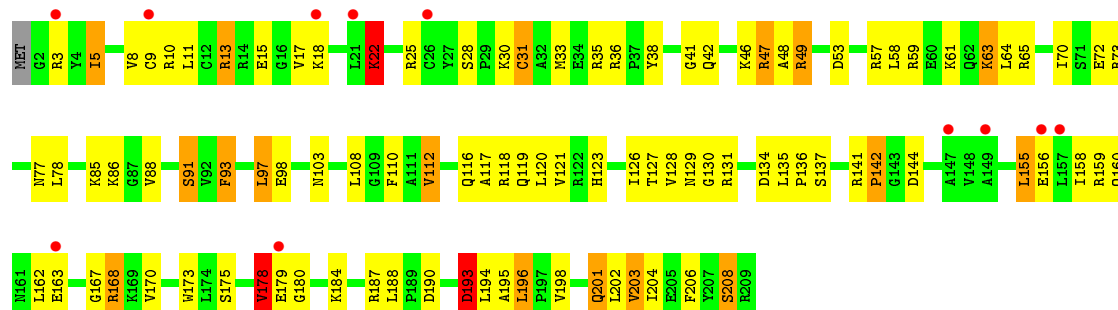
• Molecule 36: 30S ribosomal protein S3



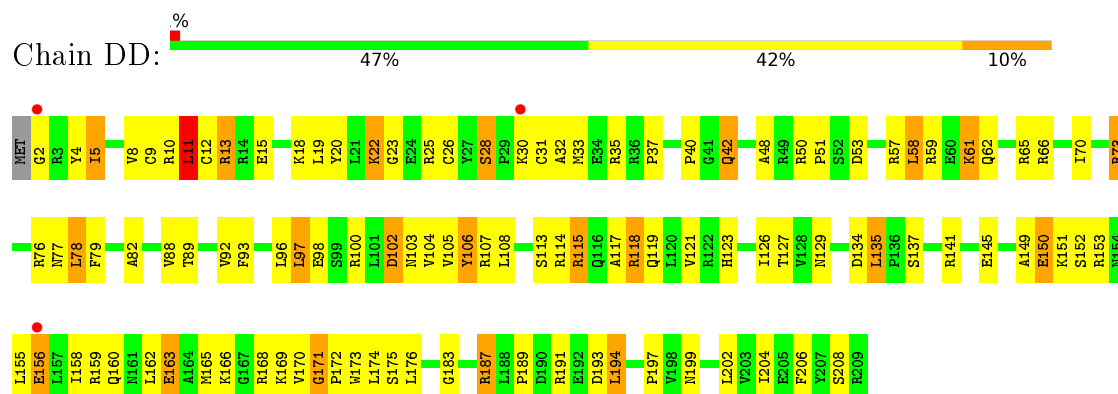
• Molecule 36: 30S ribosomal protein S3



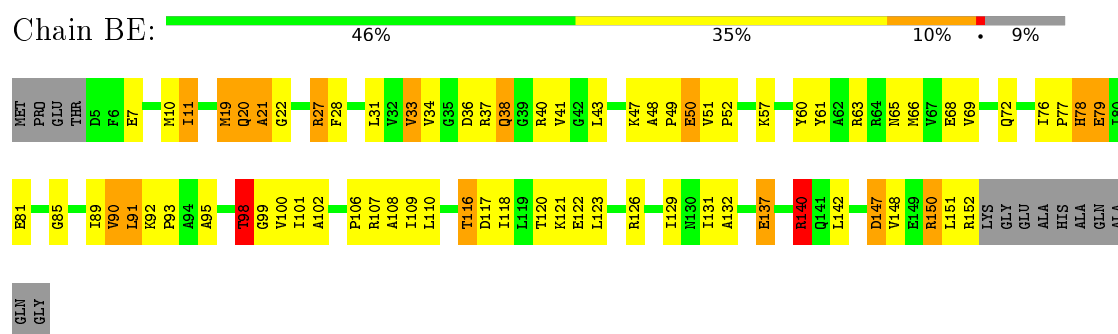
• Molecule 37: 30S ribosomal protein S4



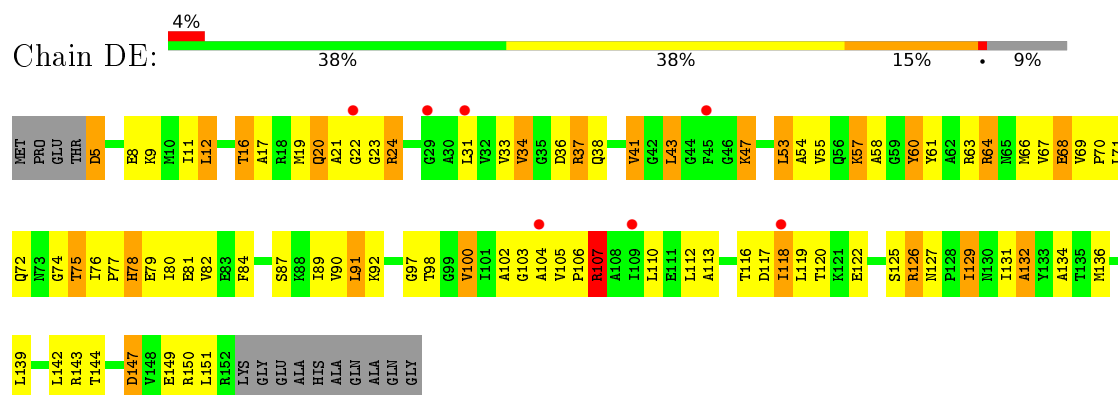
- Molecule 37: 30S ribosomal protein S4



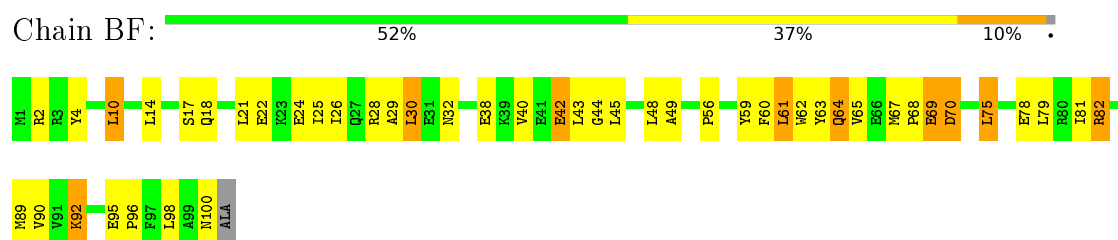
- Molecule 38: 30S ribosomal protein S5



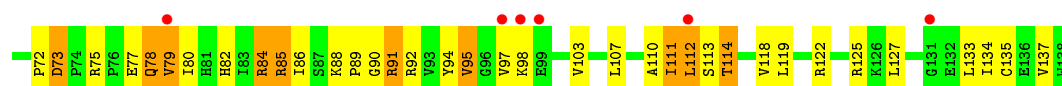
- Molecule 38: 30S ribosomal protein S5



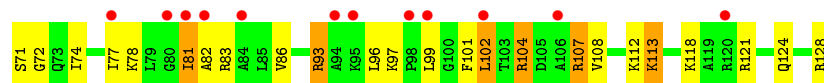
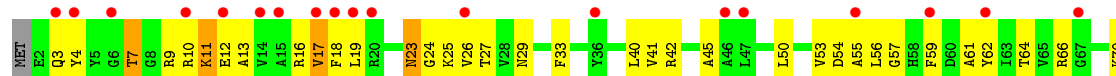
- Molecule 39: 30S ribosomal protein S6



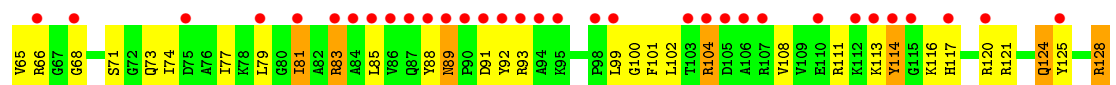
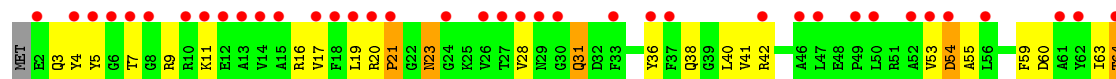
- Molecule 39: 30S ribosomal protein S6



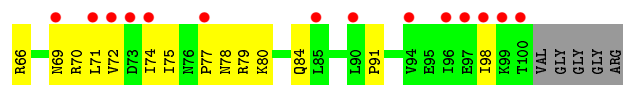
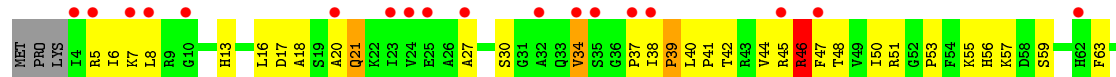
• Molecule 42: 30S ribosomal protein S9



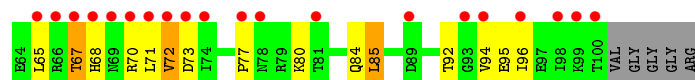
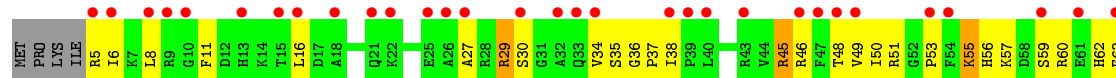
• Molecule 42: 30S ribosomal protein S9



• Molecule 43: 30S ribosomal protein S10

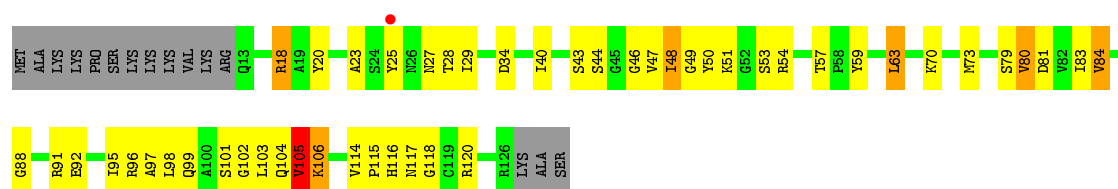


• Molecule 43: 30S ribosomal protein S10

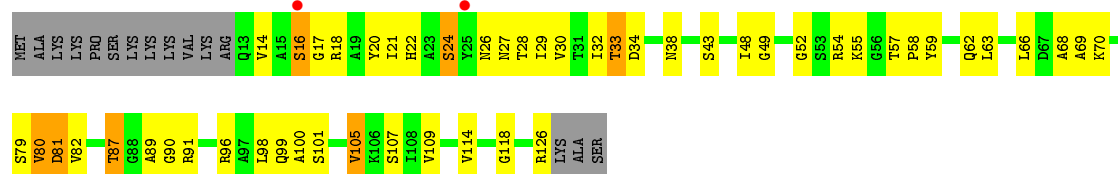


• Molecule 44: 30S ribosomal protein S11

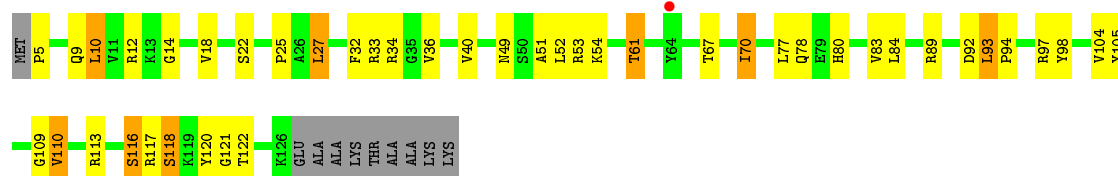




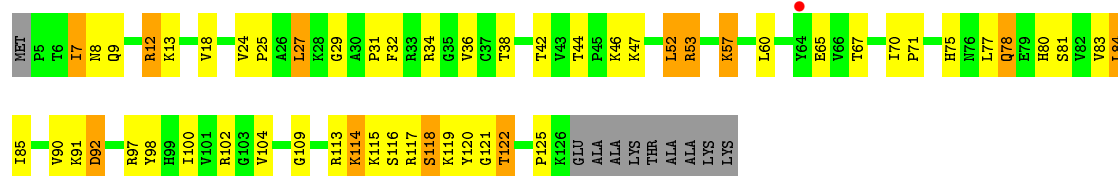
• Molecule 44: 30S ribosomal protein S11



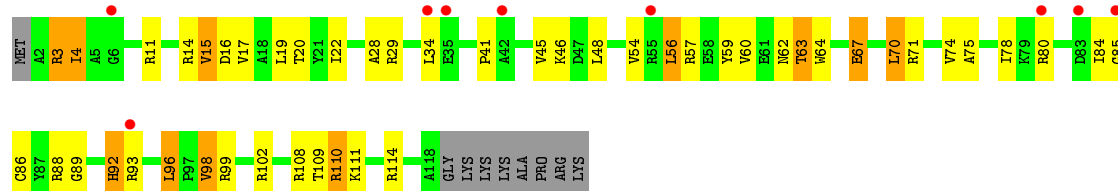
• Molecule 45: 30S ribosomal protein S12



• Molecule 45: 30S ribosomal protein S12

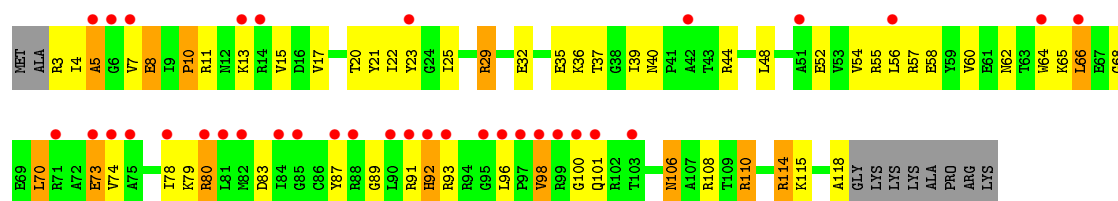


• Molecule 46: 30S ribosomal protein S13



• Molecule 46: 30S ribosomal protein S13





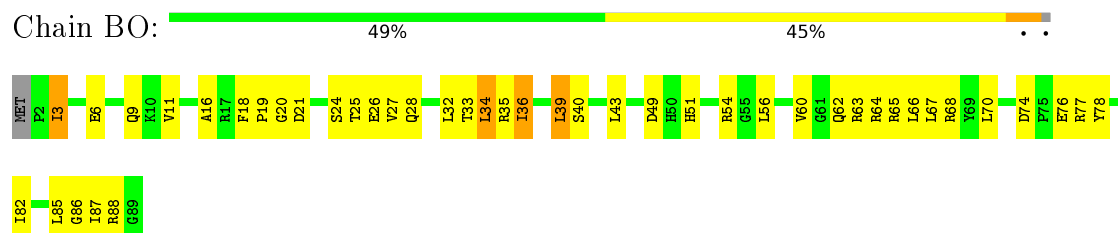
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 47: 30S ribosomal protein S14 type Z



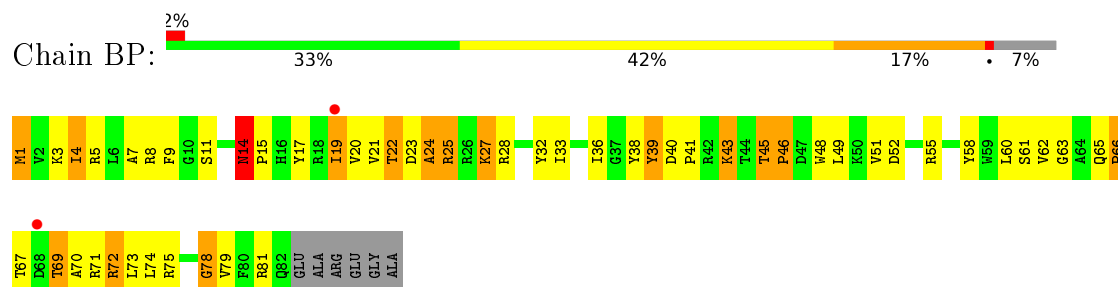
- Molecule 48: 30S ribosomal protein S15



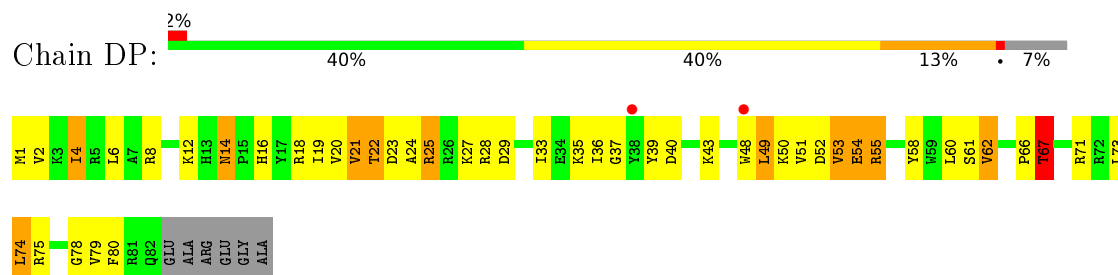
- Molecule 48: 30S ribosomal protein S15



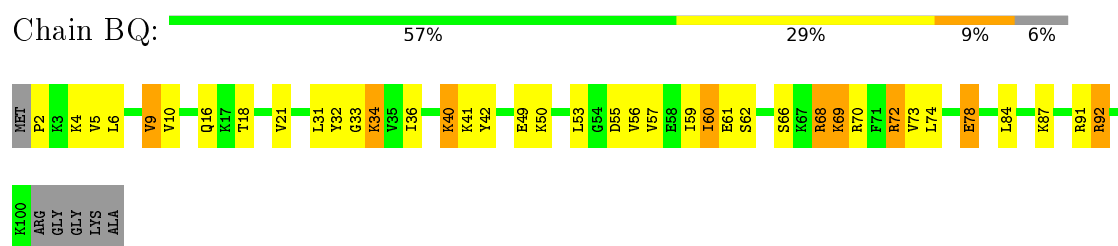
- Molecule 49: 30S ribosomal protein S16



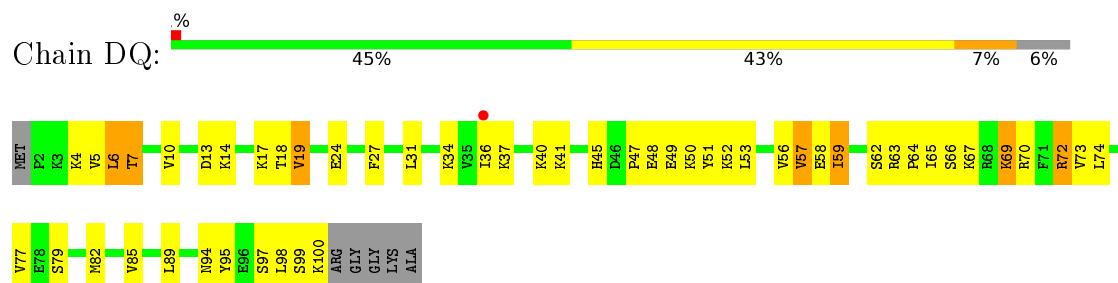
- Molecule 49: 30S ribosomal protein S16



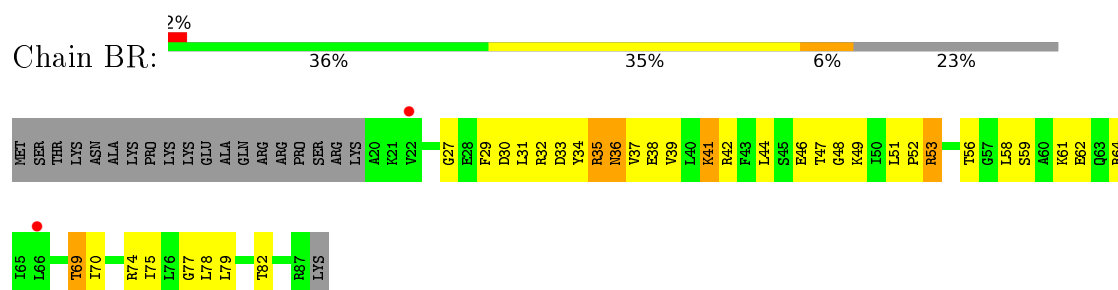
- Molecule 50: 30S ribosomal protein S17



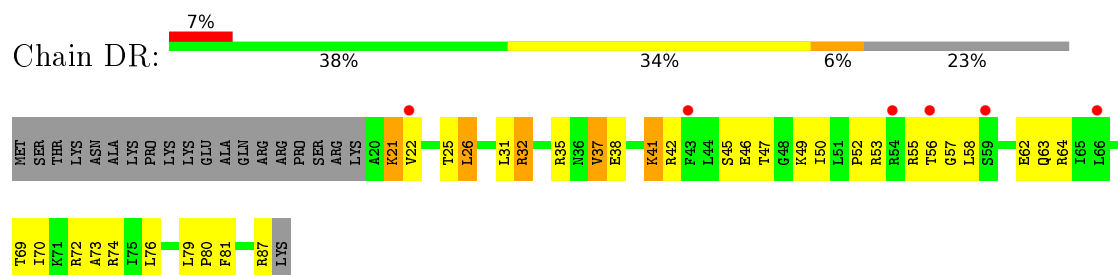
- Molecule 50: 30S ribosomal protein S17



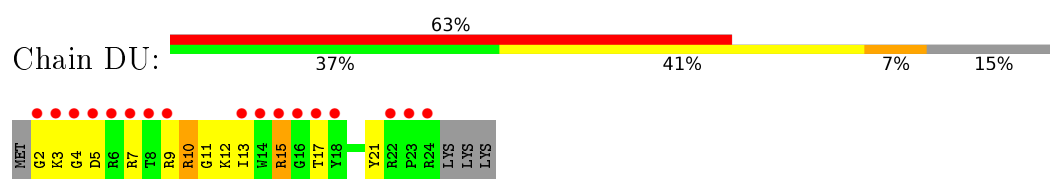
- Molecule 51: 30S ribosomal protein S18



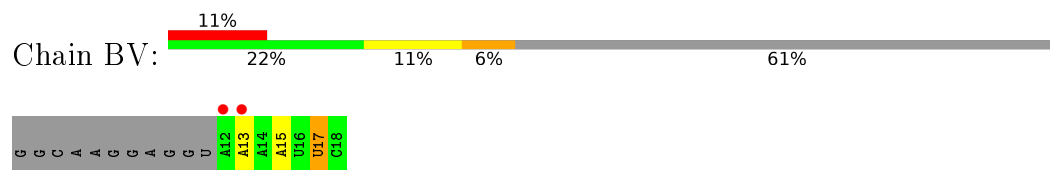
- Molecule 51: 30S ribosomal protein S18



- Molecule 54: 30S ribosomal protein Thx



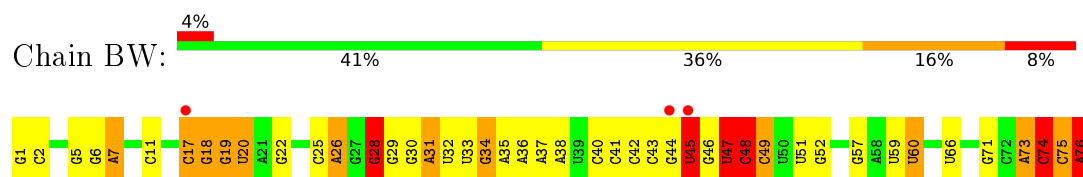
- Molecule 55: mRNA



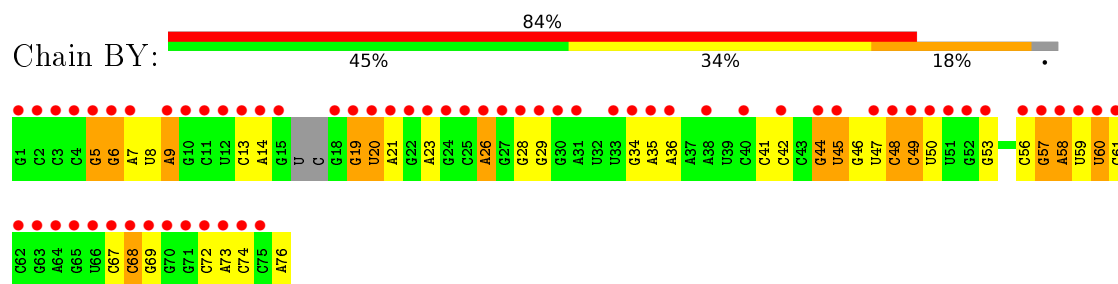
- Molecule 55: mRNA



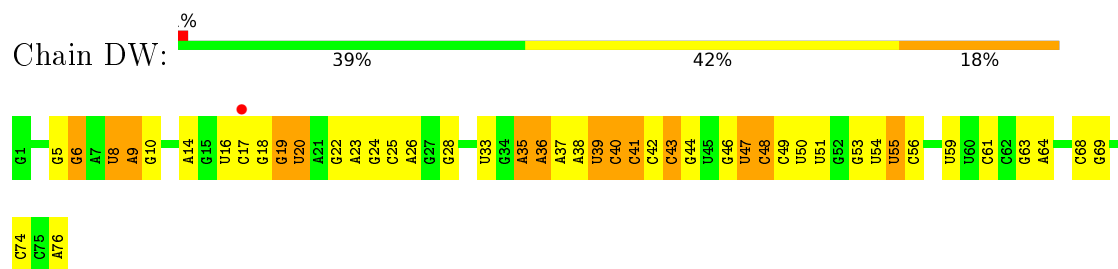
- Molecule 56: P-site tRNA



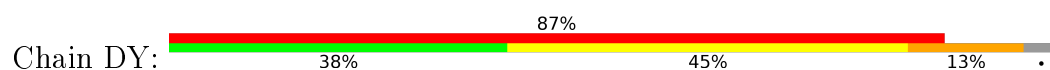
- Molecule 56: P-site tRNA

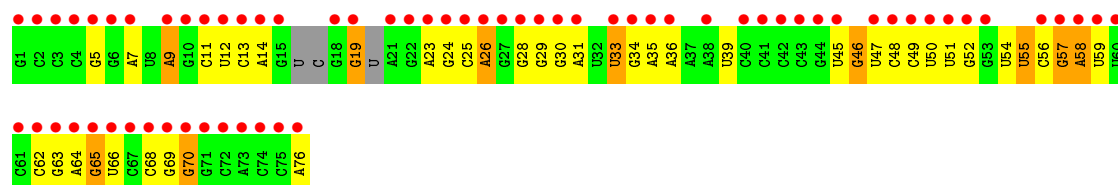


- Molecule 56: P-site tRNA

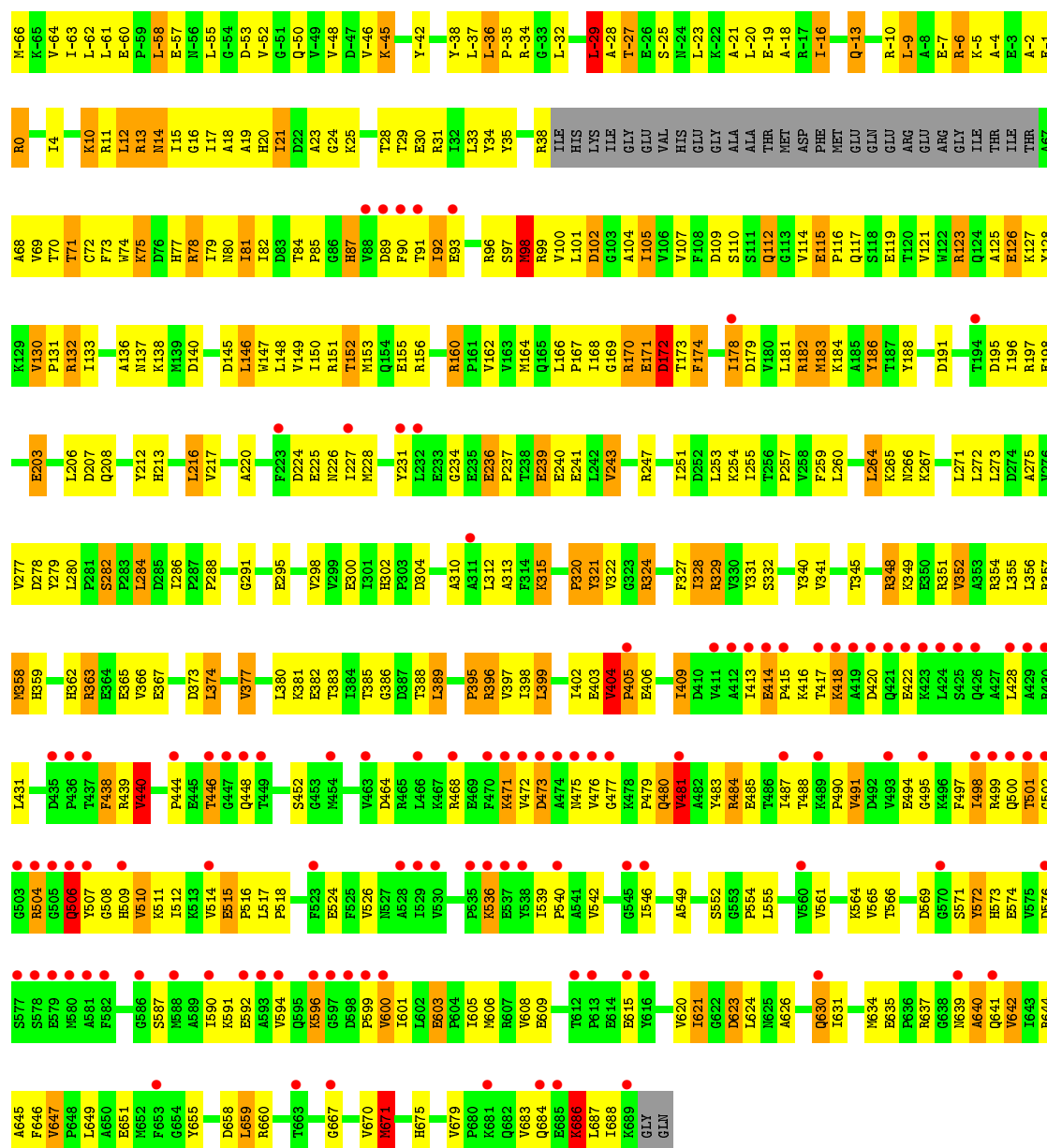


- Molecule 56: P-site tRNA



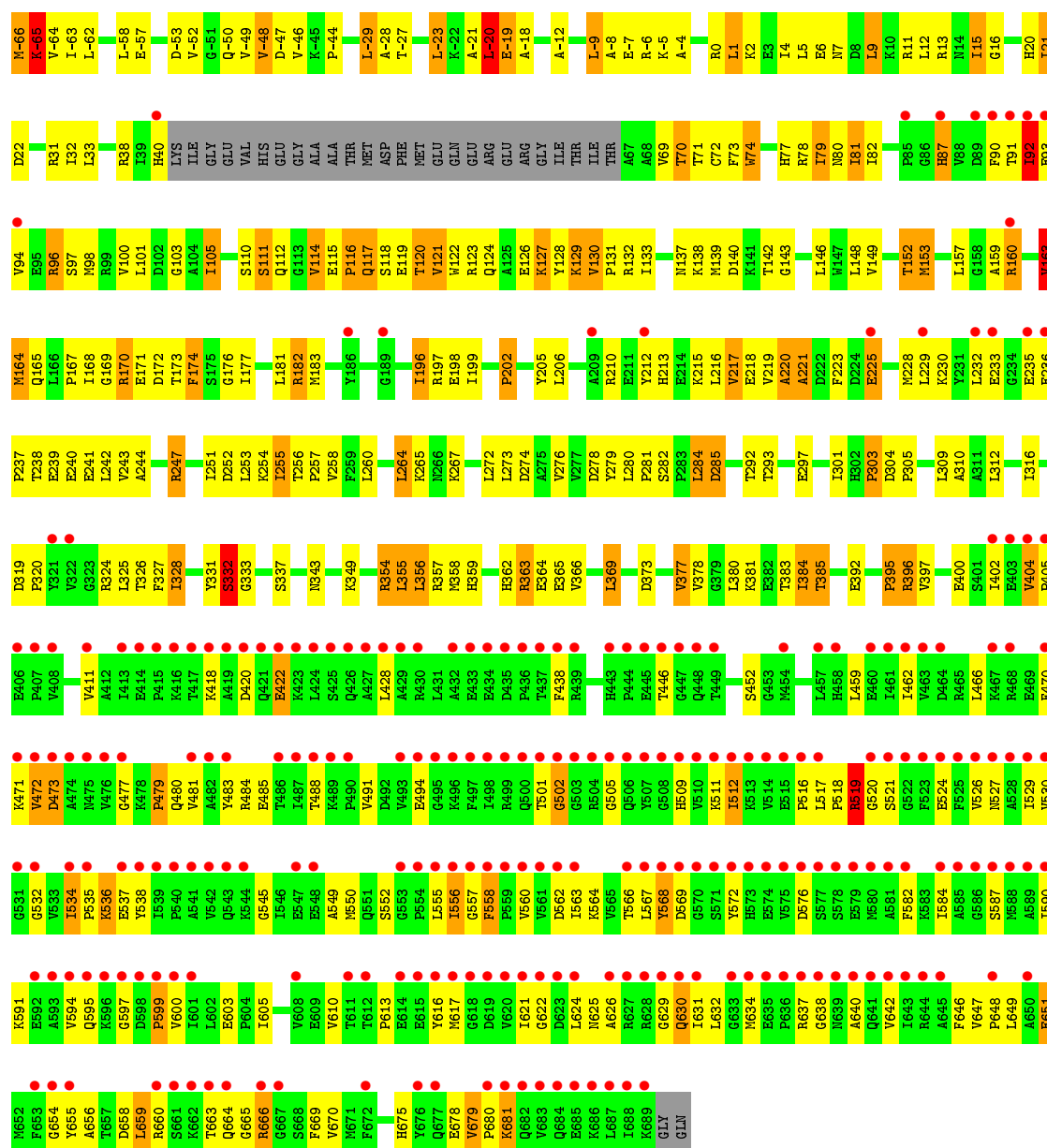


- Molecule 57: 50S ribosomal protein L9, Elongation factor G



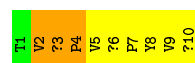
- Molecule 57: 50S ribosomal protein L9, Elongation factor G





● Molecule 58: Dityromycin

Chain BX: 10% 60% 30%



● Molecule 58: Dityromycin

Chain DX: 10% 80% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.84Å 450.58Å 623.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.80 49.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.81-2.80) 94.5 (49.80-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.209 , 0.264 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	310038	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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, 7MG, SF4, 2QZ, MG, 2QY, MVA, 004, 4SU, 2R3, 2R1, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	1.41	444/69281 (0.6%)	2.07	3848/108144 (3.6%)
1	CA	1.00	75/69179 (0.1%)	1.66	1653/107984 (1.5%)
2	AB	1.17	7/2878 (0.2%)	1.92	120/4490 (2.7%)
2	CB	0.66	0/2878	1.33	24/4490 (0.5%)
3	AC	0.34	0/1083	0.65	0/1460
3	CC	0.34	0/1083	0.65	0/1460
4	AD	0.94	2/2186 (0.1%)	1.04	5/2944 (0.2%)
4	CD	0.74	0/2192	0.95	6/2951 (0.2%)
5	AE	0.93	0/1592	1.08	2/2149 (0.1%)
5	CE	0.72	0/1592	0.91	1/2149 (0.0%)
6	AF	0.91	2/1619 (0.1%)	1.01	4/2193 (0.2%)
6	CF	0.63	0/1615	0.83	1/2188 (0.0%)
7	AG	0.60	0/1450	0.83	2/1959 (0.1%)
7	CG	0.36	0/1449	0.62	0/1958
8	AH	0.84	0/1356	0.96	1/1834 (0.1%)
8	CH	0.49	0/1356	0.67	0/1834
9	AK	0.34	0/640	0.67	0/889
9	CK	0.28	0/640	0.61	0/889
10	AL	0.31	0/503	0.54	0/673
10	CL	0.34	0/503	0.60	0/673
11	AN	0.95	0/1144	1.01	3/1543 (0.2%)
11	CN	0.61	0/1144	0.81	0/1543
12	AO	0.91	1/943 (0.1%)	1.02	3/1269 (0.2%)
12	CO	0.77	0/943	0.87	0/1269
13	AP	0.85	0/1156	1.03	4/1537 (0.3%)
13	CP	0.57	0/1152	0.87	2/1533 (0.1%)
14	AQ	0.91	0/1143	0.97	2/1527 (0.1%)
14	CQ	0.64	0/1143	0.82	1/1527 (0.1%)
15	AR	0.90	0/982	1.07	4/1312 (0.3%)
15	CR	0.65	0/982	0.88	1/1312 (0.1%)
16	AS	0.76	0/887	0.95	1/1180 (0.1%)
16	CS	0.49	0/880	0.74	0/1172

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
6	AF	0	1
19	AV	0	1
35	BB	0	1
57	DZ	0	1
58	BX	0	1
All	All	0	6

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

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

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

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

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
35	BB	93	VAL	Peptide
58	BX	3	004	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	61861	0	31172	850	0
1	CA	61771	0	31146	1166	0
2	AB	2573	0	1306	27	0
2	CB	2573	0	1306	57	0
3	AC	1063	0	1091	153	3
3	CC	1063	0	1090	186	15
4	AD	2136	0	2218	84	0
4	CD	2142	0	2229	85	0
5	AE	1559	0	1618	58	0
5	CE	1559	0	1618	76	0
6	AF	1584	0	1625	62	0
6	CF	1580	0	1619	75	0
7	AG	1425	0	1443	64	0
7	CG	1424	0	1434	82	0
8	AH	1330	0	1407	53	0
8	CH	1330	0	1407	54	0
9	AK	641	0	309	15	0
9	CK	641	0	309	9	0
10	AL	498	0	521	20	0
10	CL	498	0	521	29	0
11	AN	1117	0	1184	31	0
11	CN	1117	0	1184	38	0
12	AO	933	0	996	30	0
12	CO	933	0	996	26	0
13	AP	1139	0	1223	44	0
13	CP	1135	0	1212	57	0
14	AQ	1122	0	1179	37	0
14	CQ	1122	0	1179	54	0
15	AR	968	0	1033	32	0
15	CR	968	0	1033	37	0
16	AS	877	0	938	42	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	C1	1	0	0	0	0
59	C3	1	0	0	0	0
59	C5	1	0	0	0	0
59	C7	1	0	0	0	0
59	C8	1	0	0	0	0
59	CA	664	0	0	0	0
59	CB	13	0	0	0	0
59	CD	4	0	0	0	0
59	CE	5	0	0	0	0
59	CF	4	0	0	0	0
59	CG	1	0	0	0	0
59	CN	1	0	0	0	0
59	CO	1	0	0	0	0
59	CP	1	0	0	0	0
59	CQ	4	0	0	0	0
59	CR	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	2	0	0	0	0
59	CW	1	0	0	0	0
59	CX	1	0	0	0	0
59	DA	171	0	0	0	0
59	DD	1	0	0	0	0
59	DE	2	0	0	0	0
59	DF	1	0	0	0	0
59	DJ	1	0	0	0	0
59	DK	1	0	0	0	0
59	DT	1	0	0	0	0
59	DW	3	0	0	0	0
59	DZ	2	0	0	0	0
60	A4	1	0	0	0	0
60	A5	1	0	0	0	0
60	A6	1	0	0	0	0
60	A9	1	0	0	0	0
60	AY	1	0	0	0	0
60	BN	1	0	0	0	0
60	C4	1	0	0	0	0
60	C5	1	0	0	0	0
60	C6	1	0	0	0	0
60	C9	1	0	0	0	0
60	CY	1	0	0	0	0
60	DN	1	0	0	0	0
61	BD	8	0	0	1	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

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

The worst 5 of 18 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:BZ:502:GLY:N	3:CC:9:ARG:CD[2_655]	1.69	0.51
57:BZ:573:HIS:CE1	3:CC:13:GLU:OE1[2_655]	1.71	0.49
57:BZ:504:ARG:NH1	3:CC:9:ARG:NH2[2_655]	1.79	0.41
57:BZ:573:HIS:NE2	3:CC:13:GLU:OE1[2_655]	1.79	0.41
57:BZ:502:GLY:N	3:CC:9:ARG:CG[2_655]	1.79	0.41

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	1
3	CC	133/228 (58%)	90 (68%)	25 (19%)	18 (14%)	0	1
4	AD	273/276 (99%)	249 (91%)	19 (7%)	5 (2%)	11	34
4	CD	273/276 (99%)	234 (86%)	26 (10%)	13 (5%)	3	9
5	AE	202/206 (98%)	186 (92%)	14 (7%)	2 (1%)	19	52
5	CE	202/206 (98%)	179 (89%)	20 (10%)	3 (2%)	13	40
6	AF	201/210 (96%)	182 (90%)	18 (9%)	1 (0%)	34	69
6	CF	201/210 (96%)	177 (88%)	17 (8%)	7 (4%)	4	15
7	AG	179/182 (98%)	154 (86%)	19 (11%)	6 (3%)	5	16
7	CG	179/182 (98%)	141 (79%)	31 (17%)	7 (4%)	4	12
8	AH	172/180 (96%)	154 (90%)	15 (9%)	3 (2%)	11	36
8	CH	172/180 (96%)	144 (84%)	17 (10%)	11 (6%)	2	4
9	AK	128/173 (74%)	66 (52%)	36 (28%)	26 (20%)	0	0
9	CK	128/173 (74%)	76 (59%)	27 (21%)	25 (20%)	0	0
10	AL	64/147 (44%)	43 (67%)	17 (27%)	4 (6%)	2	4
10	CL	64/147 (44%)	42 (66%)	19 (30%)	3 (5%)	3	9
11	AN	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	26	62
11	CN	138/140 (99%)	120 (87%)	15 (11%)	3 (2%)	8	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
12	CO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	7	24
13	AP	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	14	42
13	CP	147/150 (98%)	119 (81%)	25 (17%)	3 (2%)	9	30
14	AQ	139/141 (99%)	126 (91%)	12 (9%)	1 (1%)	26	62
14	CQ	139/141 (99%)	123 (88%)	14 (10%)	2 (1%)	14	42
15	AR	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	CR	116/118 (98%)	102 (88%)	11 (10%)	3 (3%)	7	22
16	AS	108/112 (96%)	88 (82%)	16 (15%)	4 (4%)	4	14
16	CS	108/112 (96%)	83 (77%)	20 (18%)	5 (5%)	3	9
17	AT	129/146 (88%)	114 (88%)	13 (10%)	2 (2%)	12	38
17	CT	129/146 (88%)	116 (90%)	11 (8%)	2 (2%)	12	38
18	AU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
18	CU	114/118 (97%)	100 (88%)	11 (10%)	3 (3%)	7	22
19	AV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	52
19	CV	99/101 (98%)	86 (87%)	10 (10%)	3 (3%)	5	18
20	AW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
20	CW	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
21	AX	93/96 (97%)	85 (91%)	6 (6%)	2 (2%)	8	28
21	CX	93/96 (97%)	77 (83%)	11 (12%)	5 (5%)	2	7
22	AY	105/110 (96%)	93 (89%)	9 (9%)	3 (3%)	6	19
22	CY	105/110 (96%)	86 (82%)	14 (13%)	5 (5%)	3	9
23	AZ	183/206 (89%)	147 (80%)	24 (13%)	12 (7%)	1	4
23	CZ	183/206 (89%)	134 (73%)	33 (18%)	16 (9%)	1	2
24	A0	75/85 (88%)	70 (93%)	5 (7%)	0	100	100
24	C0	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	15	44
25	A1	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
25	C1	95/98 (97%)	85 (90%)	7 (7%)	3 (3%)	5	17
26	A2	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
26	C2	68/72 (94%)	60 (88%)	7 (10%)	1 (2%)	13	40
27	A3	57/60 (95%)	51 (90%)	6 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	C3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	4	15
28	A4	67/71 (94%)	46 (69%)	12 (18%)	9 (13%)	0	1
28	C4	67/71 (94%)	43 (64%)	15 (22%)	9 (13%)	0	1
29	A5	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
29	C5	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	11	34
30	A6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
30	C6	51/54 (94%)	42 (82%)	8 (16%)	1 (2%)	9	30
31	A7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
31	C7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	8	28
32	A8	62/65 (95%)	60 (97%)	1 (2%)	1 (2%)	12	38
32	C8	62/65 (95%)	54 (87%)	7 (11%)	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%)	182 (80%)	33 (14%)	14 (6%)	2	5
35	DB	229/256 (90%)	170 (74%)	41 (18%)	18 (8%)	1	2
36	BC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	2	7
36	DC	204/239 (85%)	169 (83%)	29 (14%)	6 (3%)	6	19
37	BD	206/209 (99%)	166 (81%)	28 (14%)	12 (6%)	2	5
37	DD	206/209 (99%)	171 (83%)	27 (13%)	8 (4%)	4	12
38	BE	146/162 (90%)	114 (78%)	24 (16%)	8 (6%)	2	6
38	DE	146/162 (90%)	117 (80%)	22 (15%)	7 (5%)	3	9
39	BF	98/101 (97%)	84 (86%)	11 (11%)	3 (3%)	5	17
39	DF	98/101 (97%)	90 (92%)	5 (5%)	3 (3%)	5	17
40	BG	153/156 (98%)	128 (84%)	13 (8%)	12 (8%)	1	2
40	DG	153/156 (98%)	126 (82%)	22 (14%)	5 (3%)	5	16
41	BH	135/138 (98%)	110 (82%)	22 (16%)	3 (2%)	8	28
41	DH	135/138 (98%)	114 (84%)	14 (10%)	7 (5%)	2	7
42	BI	125/128 (98%)	103 (82%)	15 (12%)	7 (6%)	2	6
42	DI	125/128 (98%)	100 (80%)	21 (17%)	4 (3%)	5	17
43	BJ	95/105 (90%)	76 (80%)	12 (13%)	7 (7%)	1	3
43	DJ	94/105 (90%)	75 (80%)	16 (17%)	3 (3%)	5	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BK	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	11	34
44	DK	112/129 (87%)	92 (82%)	16 (14%)	4 (4%)	4	14
45	BL	120/132 (91%)	108 (90%)	11 (9%)	1 (1%)	24	58
45	DL	120/132 (91%)	100 (83%)	16 (13%)	4 (3%)	5	16
46	BM	115/126 (91%)	93 (81%)	18 (16%)	4 (4%)	4	15
46	DM	114/126 (90%)	88 (77%)	17 (15%)	9 (8%)	1	2
47	BN	58/61 (95%)	46 (79%)	9 (16%)	3 (5%)	2	7
47	DN	58/61 (95%)	49 (84%)	7 (12%)	2 (3%)	5	16
48	BO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	4	15
48	DO	86/89 (97%)	72 (84%)	10 (12%)	4 (5%)	3	9
49	BP	80/88 (91%)	54 (68%)	17 (21%)	9 (11%)	0	1
49	DP	80/88 (91%)	58 (72%)	18 (22%)	4 (5%)	3	8
50	BQ	97/105 (92%)	87 (90%)	7 (7%)	3 (3%)	5	17
50	DQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
51	BR	66/88 (75%)	57 (86%)	7 (11%)	2 (3%)	5	18
51	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
52	BS	82/93 (88%)	64 (78%)	14 (17%)	4 (5%)	3	8
52	DS	81/93 (87%)	63 (78%)	15 (18%)	3 (4%)	4	14
53	BT	94/106 (89%)	78 (83%)	12 (13%)	4 (4%)	3	10
53	DT	94/106 (89%)	75 (80%)	13 (14%)	6 (6%)	2	4
54	BU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
54	DU	21/27 (78%)	17 (81%)	2 (10%)	2 (10%)	1	1
57	BZ	722/758 (95%)	563 (78%)	107 (15%)	52 (7%)	1	3
57	DZ	726/758 (96%)	537 (74%)	132 (18%)	57 (8%)	1	2
58	BX	3/10 (30%)	1 (33%)	0	2 (67%)	0	0
58	DX	3/10 (30%)	0	2 (67%)	1 (33%)	0	0
All	All	13227/14464 (91%)	10975 (83%)	1666 (13%)	586 (4%)	3	10

5 of 586 Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains ⓘ

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	A6	51/52 (98%)	37 (72%)	14 (28%)	0	1
30	C6	50/52 (96%)	43 (86%)	7 (14%)	4	13
31	A7	41/42 (98%)	35 (85%)	6 (15%)	4	11
31	C7	41/42 (98%)	35 (85%)	6 (15%)	4	11
32	A8	54/55 (98%)	43 (80%)	11 (20%)	1	4
32	C8	54/55 (98%)	48 (89%)	6 (11%)	8	23
33	A9	34/34 (100%)	30 (88%)	4 (12%)	6	19
33	C9	34/34 (100%)	30 (88%)	4 (12%)	6	19
35	BB	192/220 (87%)	157 (82%)	35 (18%)	2	6
35	DB	187/220 (85%)	148 (79%)	39 (21%)	1	4
36	BC	143/188 (76%)	127 (89%)	16 (11%)	7	22
36	DC	141/188 (75%)	113 (80%)	28 (20%)	1	5
37	BD	170/181 (94%)	136 (80%)	34 (20%)	1	5
37	DD	174/181 (96%)	143 (82%)	31 (18%)	2	6
38	BE	113/123 (92%)	86 (76%)	27 (24%)	1	2
38	DE	114/123 (93%)	82 (72%)	32 (28%)	0	1
39	BF	84/90 (93%)	70 (83%)	14 (17%)	3	8
39	DF	86/90 (96%)	74 (86%)	12 (14%)	4	13
40	BG	119/127 (94%)	99 (83%)	20 (17%)	2	8
40	DG	120/127 (94%)	104 (87%)	16 (13%)	5	14
41	BH	114/119 (96%)	90 (79%)	24 (21%)	1	4
41	DH	114/119 (96%)	86 (75%)	28 (25%)	1	2
42	BI	91/99 (92%)	78 (86%)	13 (14%)	4	12
42	DI	89/99 (90%)	73 (82%)	16 (18%)	2	6
43	BJ	66/92 (72%)	58 (88%)	8 (12%)	6	18
43	DJ	69/92 (75%)	58 (84%)	11 (16%)	3	9
44	BK	83/99 (84%)	65 (78%)	18 (22%)	1	3
44	DK	83/99 (84%)	64 (77%)	19 (23%)	1	3
45	BL	97/109 (89%)	83 (86%)	14 (14%)	4	12
45	DL	97/109 (89%)	74 (76%)	23 (24%)	1	2
46	BM	91/101 (90%)	80 (88%)	11 (12%)	6	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	DM	88/101 (87%)	75 (85%)	13 (15%)	4	11
47	BN	49/50 (98%)	38 (78%)	11 (22%)	1	3
47	DN	49/50 (98%)	42 (86%)	7 (14%)	4	12
48	BO	78/80 (98%)	70 (90%)	8 (10%)	9	26
48	DO	78/80 (98%)	66 (85%)	12 (15%)	3	10
49	BP	69/74 (93%)	54 (78%)	15 (22%)	1	3
49	DP	68/74 (92%)	51 (75%)	17 (25%)	1	2
50	BQ	94/97 (97%)	82 (87%)	12 (13%)	5	16
50	DQ	94/97 (97%)	80 (85%)	14 (15%)	4	11
51	BR	59/77 (77%)	49 (83%)	10 (17%)	2	7
51	DR	59/77 (77%)	52 (88%)	7 (12%)	6	19
52	BS	70/80 (88%)	59 (84%)	11 (16%)	3	9
52	DS	67/80 (84%)	55 (82%)	12 (18%)	2	6
53	BT	70/82 (85%)	53 (76%)	17 (24%)	1	2
53	DT	71/82 (87%)	59 (83%)	12 (17%)	2	7
54	BU	18/22 (82%)	17 (94%)	1 (6%)	26	59
54	DU	18/22 (82%)	16 (89%)	2 (11%)	8	23
57	BZ	604/636 (95%)	477 (79%)	127 (21%)	1	4
57	DZ	607/636 (95%)	509 (84%)	98 (16%)	3	9
58	BX	3/3 (100%)	3 (100%)	0	100	100
58	DX	3/3 (100%)	3 (100%)	0	100	100
All	All	10664/11678 (91%)	8760 (82%)	1904 (18%)	2	6

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

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

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

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2865/2915 (98%)	526 (18%)	51 (1%)
1	CA	2860/2915 (98%)	611 (21%)	39 (1%)
2	AB	119/121 (98%)	15 (12%)	0
2	CB	119/121 (98%)	27 (22%)	0
34	BA	1491/1521 (98%)	331 (22%)	20 (1%)
34	DA	1498/1521 (98%)	350 (23%)	22 (1%)
55	BV	6/18 (33%)	2 (33%)	0
55	DV	5/18 (27%)	1 (20%)	0
56	BW	74/76 (97%)	16 (21%)	1 (1%)
56	BY	71/76 (93%)	23 (32%)	2 (2%)
56	DW	74/76 (97%)	23 (31%)	2 (2%)
56	DY	69/76 (90%)	21 (30%)	1 (1%)
All	All	9251/9454 (97%)	1946 (21%)	138 (1%)

5 of 1946 RNA backbone outliers are listed below:

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

5 of 138 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	BA	991	U
1	CA	249	C
34	DA	991	U
34	BA	1067	A
34	BA	1530	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
56	PSU	BW	32	56	15,21,22	1.41	2 (13%)	16,30,33	2.46	4 (25%)
56	MIA	BW	37	56	22,31,32	1.76	3 (13%)	26,44,47	1.81	6 (23%)
56	PSU	BW	39	56	15,21,22	1.47	2 (13%)	16,30,33	2.24	4 (25%)
56	7MG	BW	46	56	20,26,27	1.27	2 (10%)	23,39,42	3.35	6 (26%)
56	5MU	BW	54	56	13,22,23	0.68	0	16,32,35	3.29	3 (18%)
56	PSU	BW	55	56	15,21,22	1.18	1 (6%)	16,30,33	2.29	4 (25%)
56	4SU	BW	8	56	12,21,22	0.77	0	15,30,33	1.10	1 (6%)
58	2QZ	BX	1	58	6,8,9	0.44	0	7,10,12	5.09	5 (71%)
58	2QY	BX	10	58	13,13,14	2.41	2 (15%)	12,16,18	2.21	4 (33%)
58	004	BX	3	58	9,10,11	1.16	1 (11%)	10,12,14	2.47	2 (20%)
58	MVA	BX	5	58	6,7,8	0.56	0	6,8,10	1.34	1 (16%)
58	2R1	BX	6	58	7,10,11	1.96	2 (28%)	5,13,15	2.01	2 (40%)
58	2R3	BX	8	58	13,14,15	0.67	0	15,18,20	2.14	7 (46%)
58	MVA	BX	9	58	6,7,8	0.97	1 (16%)	6,8,10	1.88	2 (33%)
56	PSU	BY	32	56	15,21,22	1.01	1 (6%)	16,30,33	2.17	3 (18%)
56	MIA	BY	37	56	17,24,32	1.24	2 (11%)	16,35,47	1.96	1 (6%)
56	PSU	BY	39	56	15,21,22	1.15	1 (6%)	16,30,33	2.32	4 (25%)
56	7MG	BY	46	56	20,26,27	1.49	2 (10%)	23,39,42	3.24	6 (26%)
56	5MU	BY	54	56	13,22,23	0.56	0	16,32,35	2.66	2 (12%)
56	PSU	BY	55	56	15,21,22	1.23	1 (6%)	16,30,33	2.24	4 (25%)
56	4SU	BY	8	56	12,21,22	0.63	0	15,30,33	1.34	2 (13%)
56	PSU	DW	32	56	15,21,22	0.84	0	16,30,33	2.23	4 (25%)
56	MIA	DW	37	56	22,31,32	1.60	3 (13%)	26,44,47	1.54	5 (19%)
56	PSU	DW	39	56	15,21,22	1.13	1 (6%)	16,30,33	2.65	4 (25%)
56	7MG	DW	46	56	20,26,27	1.33	2 (10%)	23,39,42	3.20	6 (26%)
56	5MU	DW	54	56	13,22,23	0.58	0	16,32,35	2.60	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	DW	55	56	15,21,22	1.23	1 (6%)	16,30,33	2.33	4 (25%)
56	4SU	DW	8	56	12,21,22	0.77	0	15,30,33	1.03	1 (6%)
58	2QZ	DX	1	58	6,8,9	0.48	0	7,10,12	4.79	5 (71%)
58	2QY	DX	10	58	13,13,14	2.49	2 (15%)	12,16,18	2.76	4 (33%)
58	004	DX	3	58	9,10,11	1.07	1 (11%)	10,12,14	1.34	1 (10%)
58	MVA	DX	5	58	6,7,8	1.30	1 (16%)	6,8,10	1.21	1 (16%)
58	2R1	DX	6	58	7,10,11	1.81	2 (28%)	5,13,15	2.04	2 (40%)
58	2R3	DX	8	58	13,14,15	0.63	0	15,18,20	1.67	5 (33%)
58	MVA	DX	9	58	6,7,8	1.64	1 (16%)	6,8,10	1.72	1 (16%)
56	PSU	DY	32	56	15,21,22	1.09	1 (6%)	16,30,33	2.21	4 (25%)
56	MIA	DY	37	56	17,24,32	1.15	2 (11%)	16,35,47	1.89	1 (6%)
56	PSU	DY	39	56	15,21,22	1.27	2 (13%)	16,30,33	2.28	3 (18%)
56	7MG	DY	46	56	20,26,27	1.49	3 (15%)	23,39,42	3.45	6 (26%)
56	5MU	DY	54	56	13,22,23	0.61	0	16,32,35	2.62	2 (12%)
56	PSU	DY	55	56	15,21,22	1.33	1 (6%)	16,30,33	2.18	4 (25%)
56	4SU	DY	8	56	12,21,22	0.70	0	15,30,33	1.20	1 (6%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	BY	39	56	-	0/7/25/26	0/2/2/2
56	7MG	BY	46	56	-	0/7/37/38	0/3/3/3
56	5MU	BY	54	56	-	0/3/25/26	0/2/2/2
56	PSU	BY	55	56	-	0/7/25/26	0/2/2/2
56	4SU	BY	8	56	-	0/3/25/26	0/2/2/2
56	PSU	DW	32	56	-	1/7/25/26	0/2/2/2
56	MIA	DW	37	56	-	0/11/33/34	0/3/3/3
56	PSU	DW	39	56	-	0/7/25/26	0/2/2/2
56	7MG	DW	46	56	-	0/7/37/38	0/3/3/3
56	5MU	DW	54	56	-	0/3/25/26	0/2/2/2
56	PSU	DW	55	56	-	0/7/25/26	0/2/2/2
56	4SU	DW	8	56	-	0/3/25/26	0/2/2/2
58	2QZ	DX	1	58	-	0/6/10/12	0/0/0/0
58	2QY	DX	10	58	-	0/3/8/10	0/1/1/1
58	004	DX	3	58	-	0/4/6/8	0/1/1/1
58	MVA	DX	5	58	-	0/5/8/10	0/0/0/0
58	2R1	DX	6	58	-	0/1/14/16	0/0/1/1
58	2R3	DX	8	58	-	0/10/12/14	0/1/1/1
58	MVA	DX	9	58	-	0/5/8/10	0/0/0/0
56	PSU	DY	32	56	-	0/7/25/26	0/2/2/2
56	MIA	DY	37	56	-	0/3/25/34	0/3/3/3
56	PSU	DY	39	56	-	0/7/25/26	0/2/2/2
56	7MG	DY	46	56	-	0/7/37/38	0/3/3/3
56	5MU	DY	54	56	-	0/3/25/26	0/2/2/2
56	PSU	DY	55	56	-	0/7/25/26	0/2/2/2
56	4SU	DY	8	56	-	0/3/25/26	0/2/2/2

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BW	37	MIA	C2-S10	-6.83	1.69	1.75
56	DW	37	MIA	C2-S10	-5.44	1.71	1.75
56	BW	39	PSU	C5-C1'	-4.74	1.48	1.52
56	BW	32	PSU	C5-C1'	-4.42	1.48	1.52
56	DY	55	PSU	C5-C1'	-3.83	1.48	1.52

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	54	5MU	C5-C4-N3	-9.40	117.46	125.35
56	DY	46	7MG	C5-C4-N3	-9.14	117.43	126.74
56	BY	46	7MG	C5-C4-N3	-8.91	117.66	126.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BW	46	7MG	C5-C4-N3	-8.79	117.78	126.74
56	DW	46	7MG	C5-C4-N3	-8.12	118.47	126.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

23 monomers are involved in 48 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2056 ligands modelled in this entry, 2052 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	SF4	BD	501	-	0,12,12	0.00	-	0,24,24	0.00	-
62	GDP	BZ	702	59	24,30,30	1.23	2 (8%)	26,47,47	2.32	7 (26%)
61	SF4	DD	501	37	0,12,12	0.00	-	0,24,24	0.00	-
62	GDP	DZ	703	59	24,30,30	1.21	2 (8%)	26,47,47	2.26	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	BD	501	-	-	0/0/48/48	0/6/5/5
62	GDP	BZ	702	59	-	0/12/32/32	0/3/3/3
61	SF4	DD	501	37	-	0/0/48/48	0/6/5/5
62	GDP	DZ	703	59	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	DZ	703	GDP	C5-C4	3.24	1.47	1.40
62	DZ	703	GDP	C6-C5	3.29	1.48	1.41
62	BZ	702	GDP	C5-C4	3.38	1.48	1.40
62	BZ	702	GDP	C6-C5	3.44	1.48	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	BZ	702	GDP	C5-C6-N1	-5.93	115.77	123.52
62	DZ	703	GDP	C5-C6-N1	-5.21	116.72	123.52
62	DZ	703	GDP	C2'-C1'-N9	-4.18	102.27	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	DZ	703	GDP	C6-C5-C4	-3.75	116.58	120.86
62	DZ	703	GDP	N3-C2-N1	-3.45	122.87	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	BD	501	SF4	1	0
62	BZ	702	GDP	5	0
61	DD	501	SF4	2	0
62	DZ	703	GDP	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	2872/2915 (98%)	-0.03	95 (3%)	50	38	13, 31, 166, 313	0
1	CA	2868/2915 (98%)	0.08	122 (4%)	39	27	24, 55, 177, 331	0
2	AB	120/121 (99%)	-0.39	0	100	100	24, 47, 66, 112	0
2	CB	120/121 (99%)	0.03	1 (0%)	87	81	56, 104, 146, 178	0
3	AC	137/228 (60%)	5.85	122 (89%)	0	0	89, 187, 231, 259	0
3	CC	137/228 (60%)	8.44	136 (99%)	0	0	142, 205, 249, 270	0
4	AD	275/276 (99%)	-0.44	2 (0%)	89	84	8, 30, 56, 122	0
4	CD	275/276 (99%)	-0.35	2 (0%)	89	84	13, 44, 77, 134	0
5	AE	204/206 (99%)	-0.45	0	100	100	7, 31, 60, 100	0
5	CE	204/206 (99%)	-0.29	0	100	100	16, 51, 87, 143	0
6	AF	203/210 (96%)	-0.40	0	100	100	6, 32, 76, 141	0
6	CF	203/210 (96%)	-0.18	1 (0%)	91	88	20, 66, 123, 158	0
7	AG	181/182 (99%)	-0.27	2 (1%)	82	74	34, 67, 114, 180	0
7	CG	181/182 (99%)	0.82	27 (14%)	3	2	75, 125, 183, 211	0
8	AH	174/180 (96%)	-0.45	2 (1%)	82	74	21, 46, 74, 199	0
8	CH	174/180 (96%)	0.68	12 (6%)	20	11	52, 92, 139, 174	0
9	AK	130/173 (75%)	1.29	32 (24%)	1	0	65, 131, 198, 223	0
9	CK	130/173 (75%)	2.88	79 (60%)	0	0	85, 163, 212, 233	0
10	AL	66/147 (44%)	4.23	54 (81%)	0	0	112, 182, 229, 247	0
10	CL	66/147 (44%)	5.46	58 (87%)	0	0	105, 183, 232, 263	0
11	AN	140/140 (100%)	-0.56	0	100	100	11, 28, 57, 97	0
11	CN	140/140 (100%)	-0.12	3 (2%)	67	56	35, 59, 92, 143	0
12	AO	122/122 (100%)	-0.41	0	100	100	16, 35, 66, 93	0
12	CO	122/122 (100%)	-0.30	0	100	100	30, 49, 80, 94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	149/150 (99%)	-0.33	0 100 100	8, 38, 78, 128	0
13	CP	149/150 (99%)	0.28	7 (4%) 35 24	26, 75, 123, 155	0
14	AQ	141/141 (100%)	-0.46	0 100 100	9, 32, 54, 99	0
14	CQ	141/141 (100%)	-0.26	1 (0%) 89 84	19, 63, 95, 146	0
15	AR	118/118 (100%)	-0.46	0 100 100	14, 27, 52, 76	0
15	CR	118/118 (100%)	-0.31	0 100 100	26, 49, 75, 106	0
16	AS	110/112 (98%)	-0.26	0 100 100	24, 47, 76, 86	0
16	CS	110/112 (98%)	0.66	8 (7%) 18 10	61, 96, 140, 166	0
17	AT	131/146 (89%)	-0.29	1 (0%) 87 81	20, 40, 95, 219	0
17	CT	131/146 (89%)	-0.20	1 (0%) 87 81	36, 56, 104, 152	0
18	AU	116/118 (98%)	-0.49	0 100 100	7, 22, 39, 87	0
18	CU	116/118 (98%)	-0.17	0 100 100	31, 55, 88, 107	0
19	AV	101/101 (100%)	-0.58	0 100 100	11, 27, 58, 77	0
19	CV	101/101 (100%)	-0.05	2 (1%) 68 58	29, 69, 102, 162	0
20	AW	112/113 (99%)	-0.45	0 100 100	10, 24, 49, 145	0
20	CW	112/113 (99%)	-0.20	0 100 100	26, 45, 76, 159	0
21	AX	95/96 (98%)	-0.46	0 100 100	12, 33, 64, 108	0
21	CX	95/96 (98%)	0.16	5 (5%) 30 20	37, 63, 100, 173	0
22	AY	107/110 (97%)	-0.39	1 (0%) 85 79	18, 43, 88, 120	0
22	CY	107/110 (97%)	0.57	9 (8%) 14 6	48, 81, 124, 171	0
23	AZ	185/206 (89%)	-0.43	0 100 100	28, 56, 94, 136	0
23	CZ	185/206 (89%)	0.39	13 (7%) 19 11	52, 98, 145, 175	0
24	A0	77/85 (90%)	-0.40	0 100 100	10, 31, 54, 82	0
24	C0	77/85 (90%)	0.29	4 (5%) 31 20	27, 69, 104, 127	0
25	A1	97/98 (98%)	-0.30	1 (1%) 84 77	15, 39, 80, 98	0
25	C1	97/98 (98%)	-0.15	1 (1%) 84 77	31, 56, 95, 144	0
26	A2	70/72 (97%)	-0.39	1 (1%) 78 69	15, 43, 65, 135	0
26	C2	70/72 (97%)	-0.02	1 (1%) 78 69	47, 79, 110, 151	0
27	A3	59/60 (98%)	-0.38	1 (1%) 73 63	11, 26, 53, 112	0
27	C3	59/60 (98%)	0.40	2 (3%) 49 36	31, 63, 103, 162	0
28	A4	69/71 (97%)	0.73	13 (18%) 2 1	47, 102, 188, 221	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	C4	69/71 (97%)	1.35	21 (30%) 1 0	88, 158, 196, 229	0
29	A5	59/60 (98%)	-0.49	0 100 100	11, 23, 50, 68	0
29	C5	59/60 (98%)	-0.24	1 (1%) 73 63	16, 47, 82, 121	0
30	A6	53/54 (98%)	-0.42	0 100 100	17, 36, 62, 77	0
30	C6	53/54 (98%)	-0.10	0 100 100	41, 63, 86, 104	0
31	A7	48/49 (97%)	-0.33	1 (2%) 67 56	11, 21, 54, 100	0
31	C7	48/49 (97%)	-0.21	0 100 100	23, 36, 96, 120	0
32	A8	64/65 (98%)	-0.41	0 100 100	14, 26, 39, 63	0
32	C8	64/65 (98%)	-0.19	0 100 100	27, 53, 71, 94	0
33	A9	37/37 (100%)	-0.28	0 100 100	20, 33, 64, 67	0
33	C9	37/37 (100%)	0.05	0 100 100	44, 62, 90, 101	0
34	BA	1495/1521 (98%)	0.16	50 (3%) 50 38	24, 82, 180, 330	0
34	DA	1501/1521 (98%)	0.35	94 (6%) 23 14	40, 94, 207, 307	0
35	BB	231/256 (90%)	0.52	21 (9%) 11 6	53, 104, 167, 195	0
35	DB	231/256 (90%)	1.22	54 (23%) 1 1	67, 135, 197, 228	0
36	BC	206/239 (86%)	0.74	20 (9%) 10 5	74, 114, 169, 187	0
36	DC	206/239 (86%)	1.73	66 (32%) 1 0	88, 151, 198, 221	0
37	BD	208/209 (99%)	0.28	11 (5%) 30 20	54, 91, 141, 182	0
37	DD	208/209 (99%)	0.13	3 (1%) 78 69	53, 88, 134, 199	0
38	BE	148/162 (91%)	-0.08	0 100 100	37, 72, 110, 150	0
38	DE	148/162 (91%)	0.36	7 (4%) 35 24	43, 90, 131, 177	0
39	BF	100/101 (99%)	-0.12	0 100 100	43, 81, 124, 145	0
39	DF	100/101 (99%)	0.03	2 (2%) 68 58	49, 90, 133, 146	0
40	BG	155/156 (99%)	0.62	18 (11%) 6 3	66, 100, 155, 194	0
40	DG	155/156 (99%)	1.53	39 (25%) 1 0	81, 131, 178, 214	0
41	BH	137/138 (99%)	0.12	0 100 100	45, 73, 105, 121	0
41	DH	137/138 (99%)	0.36	7 (5%) 32 21	52, 92, 126, 160	0
42	BI	127/128 (99%)	1.39	31 (24%) 1 0	59, 115, 169, 192	0
42	DI	127/128 (99%)	2.50	71 (55%) 0 0	79, 154, 192, 248	0
43	BJ	97/105 (92%)	1.61	32 (32%) 0 0	75, 123, 173, 194	0
43	DJ	96/105 (91%)	2.41	51 (53%) 0 0	77, 160, 201, 221	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BK	114/129 (88%)	-0.27	1 (0%) 85 79	30, 73, 117, 125	0
44	DK	114/129 (88%)	0.24	2 (1%) 71 61	61, 93, 139, 170	0
45	BL	122/132 (92%)	-0.20	1 (0%) 87 81	27, 61, 88, 110	0
45	DL	122/132 (92%)	0.05	1 (0%) 87 81	41, 70, 101, 142	0
46	BM	117/126 (92%)	0.54	9 (7%) 16 8	62, 108, 154, 187	0
46	DM	116/126 (92%)	1.47	35 (30%) 1 0	64, 156, 202, 235	0
47	BN	60/61 (98%)	0.80	5 (8%) 14 7	60, 110, 153, 173	0
47	DN	60/61 (98%)	1.97	28 (46%) 0 0	95, 142, 192, 210	0
48	BO	88/89 (98%)	-0.17	0 100 100	36, 69, 107, 139	0
48	DO	88/89 (98%)	0.10	0 100 100	50, 83, 115, 140	0
49	BP	82/88 (93%)	0.20	2 (2%) 62 50	46, 81, 126, 151	0
49	DP	82/88 (93%)	0.31	2 (2%) 62 50	50, 76, 108, 121	0
50	BQ	99/105 (94%)	-0.09	0 100 100	46, 72, 103, 119	0
50	DQ	99/105 (94%)	0.23	1 (1%) 84 77	47, 80, 116, 148	0
51	BR	68/88 (77%)	0.26	2 (2%) 55 43	45, 71, 115, 136	0
51	DR	68/88 (77%)	0.53	6 (8%) 12 6	58, 90, 129, 147	0
52	BS	84/93 (90%)	2.01	37 (44%) 0 0	68, 127, 168, 222	0
52	DS	83/93 (89%)	3.10	59 (71%) 0 0	98, 164, 213, 222	0
53	BT	96/106 (90%)	0.31	2 (2%) 67 56	49, 84, 117, 160	0
53	DT	96/106 (90%)	0.17	3 (3%) 52 40	48, 81, 126, 145	0
54	BU	23/27 (85%)	1.32	6 (26%) 1 0	60, 100, 114, 154	0
54	DU	23/27 (85%)	2.79	17 (73%) 0 0	78, 134, 159, 181	0
55	BV	7/18 (38%)	1.27	2 (28%) 1 0	61, 69, 175, 190	0
55	DV	6/18 (33%)	1.83	3 (50%) 0 0	89, 95, 181, 204	0
56	BW	69/76 (90%)	0.31	3 (4%) 39 27	38, 69, 118, 210	0
56	BY	67/76 (88%)	4.20	64 (95%) 0 0	76, 232, 280, 304	0
56	DW	69/76 (90%)	0.58	1 (1%) 78 69	48, 108, 151, 254	0
56	DY	66/76 (86%)	6.50	66 (100%) 0 0	145, 283, 315, 338	0
57	BZ	728/758 (96%)	0.72	113 (15%) 3 1	38, 97, 190, 248	0
57	DZ	730/758 (96%)	1.49	242 (33%) 0 0	27, 113, 212, 264	0
58	BX	3/10 (30%)	-0.16	0 100 100	83, 83, 83, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
58	DX	3/10 (30%)	0.21	0 100 100	81, 81, 81, 81	0
All	All	22705/23918 (94%)	0.38	2135 (9%) 11 5	6, 70, 189, 338	0

The worst 5 of 2135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	CC	166	ASN	26.9
3	CC	167	ASP	25.8
3	CC	179	ALA	25.2
3	AC	171	ALA	21.2
3	CC	175	PRO	19.3

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	2QZ	BX	1	9/10	0.93	0.25	-	82,82,82,82	0
56	7MG	DY	46	24/25	0.52	0.41	-	266,266,266,266	0
58	MVA	DX	9	8/9	0.94	0.25	-	81,81,81,81	0
56	MIA	DY	37	22/30	0.44	0.87	-	271,271,271,271	0
56	PSU	BY	39	20/21	0.68	0.54	-	197,197,197,197	0
58	004	BX	3	10/11	0.89	0.12	-	82,82,82,82	0
56	MIA	BW	37	29/30	0.94	0.22	-	79,79,79,79	0
56	5MU	BY	54	21/22	0.47	0.59	-	246,246,246,246	0
56	7MG	BW	46	24/25	0.89	0.19	-	76,76,76,76	3
58	004	DX	3	10/11	0.83	0.20	-	81,81,81,81	0
58	2QZ	DX	1	9/10	0.94	0.24	-	81,81,81,81	0
58	2R1	DX	6	10/11	0.83	0.15	-	81,81,81,81	0
56	PSU	BW	39	20/21	0.96	0.14	-	65,65,65,65	0
56	PSU	DY	39	20/21	0.17	1.05	-	291,291,291,291	0
56	PSU	DW	39	20/21	0.86	0.28	-	112,112,112,112	1
56	5MU	DY	54	21/22	0.38	0.84	-	303,303,303,303	0
56	PSU	DY	32	20/21	0.14	1.12	-	275,275,275,275	0
56	PSU	BW	55	20/21	0.91	0.17	-	79,79,79,79	0
58	2R3	DX	8	14/15	0.96	0.13	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	7MG	DW	46	24/25	0.87	0.23	-	124,124,124,124	0
58	2QY	DX	10	13/14	0.92	0.17	-	81,81,81,81	0
56	5MU	DW	54	21/22	0.89	0.20	-	95,95,95,95	1
56	4SU	DW	8	20/21	0.91	0.14	-	103,103,103,103	0
56	4SU	BW	8	20/21	0.96	0.15	-	60,60,60,60	1
56	MIA	DW	37	29/30	0.91	0.24	-	109,109,109,109	0
56	PSU	BY	32	20/21	0.47	0.55	-	226,226,226,226	0
56	PSU	BW	32	20/21	0.94	0.20	-	73,73,73,73	1
56	PSU	DW	55	20/21	0.88	0.19	-	92,92,92,92	0
56	7MG	BY	46	24/25	0.49	0.34	-	276,276,276,276	0
58	MVA	BX	5	8/9	0.87	0.15	-	82,82,82,82	0
56	PSU	BY	55	20/21	0.27	0.51	-	243,243,243,243	0
58	2R3	BX	8	14/15	0.92	0.14	-	82,82,82,82	0
56	5MU	BW	54	21/22	0.92	0.18	-	80,80,80,80	0
56	4SU	BY	8	20/21	0.51	0.34	-	239,239,239,239	0
56	PSU	DY	55	20/21	0.28	0.67	-	252,252,252,252	0
58	MVA	DX	5	8/9	0.95	0.37	-	81,81,81,81	0
56	4SU	DY	8	20/21	0.40	0.43	-	277,277,277,277	0
58	2QY	BX	10	13/14	0.90	0.19	-	82,82,82,82	0
58	2R1	BX	6	10/11	0.89	0.16	-	82,82,82,82	1
58	MVA	BX	9	8/9	0.89	0.31	-	82,82,82,82	0
56	PSU	DW	32	20/21	0.82	0.31	-	126,126,126,126	0
56	MIA	BY	37	22/30	0.72	0.43	-	186,186,186,186	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3018	1/1	0.82	1.45	121.71	67,67,67,67	0
59	MG	AA	3039	1/1	0.94	0.53	113.00	34,34,34,34	1
59	MG	AA	3710	1/1	0.96	0.52	67.48	29,29,29,29	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3087	1/1	0.85	0.82	59.87	68,68,68,68	0
59	MG	CA	3499	1/1	0.73	0.51	59.05	62,62,62,62	0
59	MG	AA	3136	1/1	0.97	0.65	57.11	63,63,63,63	0
59	MG	AA	3216	1/1	0.97	0.60	55.62	38,38,38,38	0
59	MG	AA	3706	1/1	0.95	0.53	50.35	41,41,41,41	1
59	MG	CA	3442	1/1	0.91	0.60	47.17	74,74,74,74	0
59	MG	AA	3137	1/1	0.95	0.63	46.59	53,53,53,53	0
59	MG	AA	3772	1/1	0.91	0.60	46.50	61,61,61,61	1
59	MG	AH	201	1/1	0.95	0.86	39.12	64,64,64,64	0
59	MG	CA	3502	1/1	0.74	0.68	39.11	90,90,90,90	0
59	MG	CA	3025	1/1	0.98	0.39	37.98	59,59,59,59	0
59	MG	CA	3146	1/1	0.63	0.96	37.45	82,82,82,82	0
59	MG	AA	3235	1/1	0.88	0.46	36.98	93,93,93,93	0
59	MG	AA	3101	1/1	0.93	0.66	36.38	68,68,68,68	0
59	MG	AA	3179	1/1	0.91	0.49	36.26	45,45,45,45	1
59	MG	C7	101	1/1	0.82	0.44	35.80	56,56,56,56	0
59	MG	CA	3157	1/1	0.92	0.55	35.67	81,81,81,81	0
59	MG	AA	3214	1/1	0.97	0.82	33.09	58,58,58,58	1
59	MG	AA	3147	1/1	0.97	0.51	32.10	40,40,40,40	1
59	MG	AA	3712	1/1	0.76	0.69	30.78	70,70,70,70	0
59	MG	AA	3174	1/1	0.94	0.46	29.53	59,59,59,59	0
59	MG	AU	202	1/1	0.96	0.45	28.81	82,82,82,82	0
59	MG	AA	3820	1/1	0.80	0.42	28.02	85,85,85,85	0
59	MG	CA	3168	1/1	0.92	0.43	28.02	58,58,58,58	0
59	MG	AA	3824	1/1	0.95	0.58	27.63	72,72,72,72	0
59	MG	AA	3140	1/1	0.71	0.59	27.61	62,62,62,62	0
59	MG	CA	3218	1/1	0.96	0.37	27.24	40,40,40,40	0
59	MG	AA	3775	1/1	0.93	0.58	27.03	25,25,25,25	1
59	MG	CA	3140	1/1	0.86	0.39	26.97	63,63,63,63	0
59	MG	CA	3162	1/1	0.96	0.40	26.79	31,31,31,31	0
59	MG	AD	301	1/1	0.90	0.72	26.54	58,58,58,58	0
59	MG	BA	1665	1/1	0.77	0.47	26.20	73,73,73,73	0
59	MG	AA	3131	1/1	0.95	0.26	25.45	63,63,63,63	0
59	MG	CA	3221	1/1	0.91	0.59	25.40	65,65,65,65	0
59	MG	CA	3503	1/1	0.88	0.35	25.39	52,52,52,52	0
59	MG	AA	3171	1/1	0.88	0.28	25.04	54,54,54,54	0
59	MG	CA	3113	1/1	0.88	0.40	24.98	38,38,38,38	0
59	MG	AA	3217	1/1	0.94	0.43	24.88	29,29,29,29	1
59	MG	C5	101	1/1	0.95	0.49	24.82	66,66,66,66	0
59	MG	AA	3060	1/1	0.97	0.33	24.68	20,20,20,20	0
59	MG	CA	3041	1/1	0.75	0.42	24.53	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3110	1/1	0.92	0.47	23.87	52,52,52,52	0
59	MG	AA	3608	1/1	0.90	0.37	23.80	60,60,60,60	0
59	MG	CA	3058	1/1	0.82	0.35	22.41	67,67,67,67	0
59	MG	AD	305	1/1	0.69	0.63	22.39	86,86,86,86	0
59	MG	AA	3133	1/1	0.92	0.33	22.28	50,50,50,50	0
59	MG	AA	3158	1/1	0.87	0.89	22.16	68,68,68,68	0
59	MG	CA	3033	1/1	0.90	0.41	21.69	55,55,55,55	0
59	MG	AA	3199	1/1	0.90	0.35	21.32	41,41,41,41	0
59	MG	CA	3658	1/1	0.93	0.39	21.21	64,64,64,64	0
59	MG	CA	3544	1/1	0.86	0.32	20.47	60,60,60,60	0
59	MG	AA	3823	1/1	0.93	0.47	19.72	39,39,39,39	0
59	MG	AA	3176	1/1	0.95	0.32	19.66	70,70,70,70	0
59	MG	CA	3028	1/1	0.96	0.63	19.54	51,51,51,51	0
59	MG	AA	3257	1/1	0.94	0.31	19.42	54,54,54,54	0
59	MG	DA	1671	1/1	0.96	0.36	19.31	56,56,56,56	0
59	MG	CA	3225	1/1	0.83	0.34	19.04	64,64,64,64	0
59	MG	AE	305	1/1	0.88	0.36	18.95	48,48,48,48	0
59	MG	AA	3113	1/1	0.96	0.32	18.91	45,45,45,45	0
59	MG	CA	3618	1/1	0.99	0.30	18.29	40,40,40,40	0
59	MG	AA	3044	1/1	0.95	0.37	18.13	52,52,52,52	0
59	MG	BA	1628	1/1	0.80	0.29	18.00	87,87,87,87	0
59	MG	CA	3432	1/1	0.84	0.27	17.81	32,32,32,32	0
59	MG	AA	3261	1/1	0.93	0.32	17.52	25,25,25,25	0
59	MG	CA	3182	1/1	0.94	0.32	17.50	38,38,38,38	0
59	MG	AA	3038	1/1	0.93	0.43	17.42	29,29,29,29	1
59	MG	DA	1769	1/1	0.76	0.44	17.25	74,74,74,74	0
59	MG	CA	3291	1/1	0.86	0.42	17.18	48,48,48,48	0
59	MG	CA	3166	1/1	0.94	0.32	17.04	27,27,27,27	0
59	MG	BA	1714	1/1	0.75	0.28	16.86	74,74,74,74	0
59	MG	CA	3226	1/1	0.85	0.34	16.58	52,52,52,52	0
59	MG	AU	204	1/1	0.97	0.37	16.54	25,25,25,25	0
59	MG	AA	3315	1/1	0.82	0.22	16.41	65,65,65,65	0
59	MG	AA	3109	1/1	0.81	0.35	16.21	56,56,56,56	0
59	MG	AA	3307	1/1	0.96	0.34	16.19	61,61,61,61	0
59	MG	CA	3440	1/1	0.95	0.32	16.14	49,49,49,49	0
59	MG	AA	3184	1/1	0.92	0.25	16.00	75,75,75,75	0
59	MG	CA	3420	1/1	0.75	0.33	15.85	69,69,69,69	0
59	MG	CA	3603	1/1	0.84	0.36	15.54	49,49,49,49	0
59	MG	CA	3441	1/1	0.94	0.24	15.51	56,56,56,56	0
59	MG	AA	3826	1/1	0.91	0.29	15.37	46,46,46,46	0
59	MG	AA	3144	1/1	0.98	0.36	14.95	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3209	1/1	0.89	0.31	14.89	62,62,62,62	0
59	MG	DA	1745	1/1	0.99	0.39	14.81	50,50,50,50	0
59	MG	AA	3213	1/1	0.87	0.64	14.46	76,76,76,76	0
59	MG	CA	3642	1/1	0.94	0.53	14.46	52,52,52,52	0
59	MG	AA	3255	1/1	0.94	0.22	14.38	38,38,38,38	0
59	MG	BA	1663	1/1	0.87	0.23	14.28	43,43,43,43	0
59	MG	AA	3403	1/1	0.96	0.34	14.15	42,42,42,42	0
59	MG	CA	3428	1/1	0.89	0.26	13.90	58,58,58,58	0
59	MG	CA	3159	1/1	0.83	0.58	13.85	69,69,69,69	0
59	MG	AA	3818	1/1	0.84	0.31	13.83	61,61,61,61	0
59	MG	CA	3230	1/1	0.97	0.33	13.68	49,49,49,49	0
59	MG	CA	3333	1/1	0.81	0.36	13.64	68,68,68,68	0
59	MG	DA	1601	1/1	0.91	0.41	13.63	74,74,74,74	0
59	MG	AA	3186	1/1	0.92	0.29	13.61	48,48,48,48	0
59	MG	AA	3043	1/1	0.91	0.30	13.58	45,45,45,45	0
59	MG	CA	3210	1/1	0.85	0.35	13.54	62,62,62,62	0
59	MG	CF	301	1/1	0.85	0.46	13.52	61,61,61,61	0
59	MG	CA	3455	1/1	0.95	0.28	13.39	49,49,49,49	0
59	MG	CA	3035	1/1	0.88	0.28	13.21	69,69,69,69	0
59	MG	AA	3828	1/1	0.94	0.38	13.15	38,38,38,38	0
59	MG	AA	3822	1/1	0.90	0.32	13.14	47,47,47,47	0
59	MG	CA	3163	1/1	0.97	0.31	13.14	30,30,30,30	0
59	MG	AA	3286	1/1	0.93	0.46	13.04	40,40,40,40	0
59	MG	AA	3809	1/1	0.82	0.29	12.99	57,57,57,57	0
59	MG	DA	1652	1/1	0.88	0.86	12.91	80,80,80,80	0
59	MG	CA	3619	1/1	0.92	0.38	12.70	40,40,40,40	0
59	MG	AA	3301	1/1	0.96	0.31	12.63	39,39,39,39	0
59	MG	CA	3160	1/1	0.96	0.40	12.50	57,57,57,57	0
59	MG	CA	3348	1/1	0.77	0.28	12.45	44,44,44,44	0
59	MG	CA	3068	1/1	0.81	0.43	12.40	66,66,66,66	0
59	MG	BA	1740	1/1	0.98	0.31	12.35	50,50,50,50	0
59	MG	AA	3280	1/1	0.90	0.29	11.95	53,53,53,53	0
59	MG	AA	3825	1/1	0.89	0.39	11.88	63,63,63,63	0
59	MG	CV	201	1/1	0.77	0.83	11.80	117,117,117,117	0
59	MG	AA	3012	1/1	0.80	0.35	11.64	49,49,49,49	0
59	MG	CA	3655	1/1	0.93	0.40	11.56	52,52,52,52	0
59	MG	CA	3375	1/1	0.95	0.34	11.31	68,68,68,68	0
59	MG	BA	1672	1/1	0.93	0.30	11.29	65,65,65,65	0
59	MG	AA	3034	1/1	0.89	0.31	11.23	49,49,49,49	0
59	MG	AD	304	1/1	0.95	0.33	11.22	41,41,41,41	0
59	MG	CA	3036	1/1	0.91	0.29	11.21	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AX	3001	1/1	0.78	0.31	11.14	52,52,52,52	0
59	MG	AA	3667	1/1	0.93	0.30	11.09	41,41,41,41	0
59	MG	AA	3740	1/1	0.85	0.29	11.08	61,61,61,61	0
59	MG	AA	3102	1/1	0.92	0.24	11.01	47,47,47,47	0
59	MG	CA	3213	1/1	0.95	0.27	10.89	51,51,51,51	0
59	MG	AA	3023	1/1	0.98	0.61	10.82	53,53,53,53	0
59	MG	CA	3207	1/1	0.92	0.28	10.68	75,75,75,75	0
59	MG	AA	3050	1/1	0.94	0.28	10.68	28,28,28,28	0
59	MG	CA	3532	1/1	0.92	0.24	10.68	49,49,49,49	0
59	MG	CA	3322	1/1	0.99	0.27	10.68	40,40,40,40	0
59	MG	BA	1691	1/1	0.59	0.44	10.51	86,86,86,86	0
59	MG	AA	3177	1/1	0.85	0.29	10.36	59,59,59,59	0
59	MG	CA	3657	1/1	0.97	0.40	10.32	41,41,41,41	0
59	MG	CA	3409	1/1	0.91	0.28	10.10	42,42,42,42	0
59	MG	CA	3326	1/1	0.96	0.24	10.04	28,28,28,28	0
59	MG	CA	3054	1/1	0.96	0.24	10.02	36,36,36,36	0
59	MG	CA	3358	1/1	0.98	0.30	10.02	36,36,36,36	0
59	MG	AA	3033	1/1	0.92	0.28	9.88	55,55,55,55	0
59	MG	AA	3803	1/1	0.89	0.34	9.72	45,45,45,45	0
59	MG	AP	201	1/1	0.96	0.31	9.47	21,21,21,21	1
59	MG	AA	3606	1/1	0.94	0.24	9.41	34,34,34,34	0
59	MG	AA	3421	1/1	0.98	0.21	9.40	28,28,28,28	0
59	MG	AA	3036	1/1	0.96	0.24	9.39	25,25,25,25	0
59	MG	BA	1630	1/1	0.87	0.31	9.32	61,61,61,61	0
59	MG	AA	3161	1/1	0.92	0.24	9.30	43,43,43,43	0
59	MG	AA	3228	1/1	0.96	0.30	9.27	32,32,32,32	0
59	MG	CU	201	1/1	0.95	0.48	9.23	74,74,74,74	0
59	MG	DA	1634	1/1	0.67	0.29	9.22	66,66,66,66	0
59	MG	AA	3423	1/1	0.96	0.21	9.21	16,16,16,16	0
59	MG	AA	3253	1/1	0.86	0.35	9.21	64,64,64,64	0
59	MG	BA	1758	1/1	0.72	0.37	9.20	76,76,76,76	0
59	MG	AA	3398	1/1	0.97	0.23	9.19	31,31,31,31	0
59	MG	CA	3650	1/1	0.98	0.25	9.18	14,14,14,14	0
59	MG	CA	3090	1/1	0.88	0.28	9.11	77,77,77,77	0
59	MG	CA	3212	1/1	0.92	0.25	9.11	84,84,84,84	0
59	MG	DA	1650	1/1	0.93	0.28	8.81	50,50,50,50	0
59	MG	CA	3500	1/1	0.89	0.24	8.74	75,75,75,75	0
59	MG	CA	3452	1/1	0.94	0.20	8.51	36,36,36,36	0
59	MG	AA	3215	1/1	0.86	0.34	8.51	59,59,59,59	0
59	MG	AA	3653	1/1	0.80	0.23	8.51	60,60,60,60	0
59	MG	AA	3130	1/1	0.98	0.24	8.46	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3172	1/1	0.93	0.22	8.43	47,47,47,47	0
59	MG	AA	3224	1/1	0.91	0.24	8.41	56,56,56,56	0
59	MG	CA	3635	1/1	0.94	0.24	8.41	48,48,48,48	0
59	MG	AA	3771	1/1	0.91	0.25	8.34	60,60,60,60	0
59	MG	CA	3415	1/1	0.98	0.26	8.26	34,34,34,34	0
59	MG	AA	3827	1/1	0.80	0.38	8.15	38,38,38,38	0
59	MG	CA	3108	1/1	0.65	0.28	8.00	78,78,78,78	0
59	MG	AA	3547	1/1	0.96	0.26	7.88	60,60,60,60	0
59	MG	AA	3832	1/1	0.93	0.41	7.69	55,55,55,55	0
59	MG	AA	3244	1/1	0.92	0.25	7.66	52,52,52,52	0
59	MG	AF	304	1/1	0.96	0.28	7.66	36,36,36,36	0
59	MG	CE	303	1/1	0.92	0.41	7.60	51,51,51,51	0
59	MG	CA	3463	1/1	0.92	0.23	7.56	56,56,56,56	0
59	MG	DA	1640	1/1	0.94	0.32	7.46	77,77,77,77	0
59	MG	BA	1780	1/1	0.93	0.37	7.46	60,60,60,60	0
59	MG	AW	3003	1/1	0.95	0.25	7.38	28,28,28,28	0
59	MG	AA	3117	1/1	0.95	0.24	7.33	25,25,25,25	1
59	MG	BA	1687	1/1	0.87	0.23	7.32	52,52,52,52	0
59	MG	AA	3128	1/1	0.81	0.46	7.28	89,89,89,89	0
59	MG	DA	1622	1/1	0.76	0.37	7.23	60,60,60,60	0
59	MG	AA	3081	1/1	0.94	0.22	7.23	56,56,56,56	0
59	MG	CA	3217	1/1	0.97	0.27	7.15	62,62,62,62	0
59	MG	AA	3814	1/1	0.74	0.58	7.13	72,72,72,72	0
59	MG	CA	3105	1/1	0.97	0.26	7.11	39,39,39,39	0
59	MG	CA	3314	1/1	0.91	0.30	7.09	57,57,57,57	0
59	MG	BA	1787	1/1	0.93	0.27	6.98	55,55,55,55	0
59	MG	AD	310	1/1	0.94	0.38	6.97	78,78,78,78	0
59	MG	CA	3457	1/1	0.82	0.27	6.93	43,43,43,43	0
59	MG	CA	3039	1/1	0.98	0.28	6.89	37,37,37,37	0
59	MG	AA	3120	1/1	0.90	0.25	6.88	33,33,33,33	0
59	MG	CA	3427	1/1	0.98	0.19	6.83	37,37,37,37	0
59	MG	CA	3486	1/1	0.72	0.24	6.74	81,81,81,81	0
59	MG	AA	3690	1/1	0.96	0.20	6.70	50,50,50,50	0
59	MG	AA	3045	1/1	0.91	0.32	6.68	55,55,55,55	0
59	MG	AA	3625	1/1	0.75	0.21	6.62	51,51,51,51	0
59	MG	AA	3534	1/1	0.97	0.19	6.62	14,14,14,14	0
59	MG	AB	3003	1/1	0.79	0.23	6.62	60,60,60,60	0
59	MG	AA	3082	1/1	0.98	0.27	6.61	60,60,60,60	0
59	MG	CE	301	1/1	0.88	0.32	6.60	53,53,53,53	0
59	MG	AA	3569	1/1	0.98	0.22	6.60	17,17,17,17	0
59	MG	AA	3799	1/1	0.99	0.33	6.52	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AV	201	1/1	0.99	0.26	6.42	42,42,42,42	0
59	MG	CA	3309	1/1	0.97	0.24	6.41	22,22,22,22	0
59	MG	CA	3410	1/1	0.94	0.22	6.33	25,25,25,25	0
59	MG	AA	3532	1/1	0.96	0.20	6.31	20,20,20,20	0
59	MG	AQ	202	1/1	0.93	0.26	6.27	35,35,35,35	0
59	MG	AA	3042	1/1	0.96	0.24	6.10	32,32,32,32	0
59	MG	AA	3254	1/1	0.94	0.26	6.08	52,52,52,52	0
59	MG	CA	3137	1/1	0.91	0.24	6.08	69,69,69,69	0
59	MG	AA	3519	1/1	0.97	0.23	6.07	27,27,27,27	0
59	MG	BA	1612	1/1	0.74	0.26	6.03	92,92,92,92	0
59	MG	CA	3458	1/1	0.90	0.22	6.03	54,54,54,54	0
59	MG	BA	1684	1/1	0.96	0.28	6.03	61,61,61,61	0
59	MG	CA	3243	1/1	0.92	0.28	5.93	58,58,58,58	0
59	MG	AD	307	1/1	0.84	0.25	5.77	56,56,56,56	0
59	MG	BA	1679	1/1	0.85	0.32	5.75	59,59,59,59	0
59	MG	AA	3152	1/1	0.98	0.25	5.58	10,10,10,10	0
59	MG	CA	3229	1/1	0.85	0.20	5.57	53,53,53,53	0
59	MG	AA	3543	1/1	0.98	0.22	5.53	32,32,32,32	0
59	MG	BA	1656	1/1	0.90	0.33	5.52	75,75,75,75	0
59	MG	AA	3830	1/1	0.97	0.27	5.45	47,47,47,47	0
59	MG	AA	3360	1/1	0.97	0.23	5.32	22,22,22,22	0
59	MG	AA	3466	1/1	0.90	0.21	5.31	76,76,76,76	0
59	MG	AA	3563	1/1	0.97	0.21	5.26	34,34,34,34	0
59	MG	BA	1725	1/1	0.97	0.25	5.24	54,54,54,54	0
59	MG	CA	3100	1/1	0.48	0.26	5.19	81,81,81,81	0
59	MG	CA	3492	1/1	0.88	0.24	5.11	59,59,59,59	0
59	MG	AA	3721	1/1	0.97	0.20	5.10	40,40,40,40	0
59	MG	CA	3169	1/1	0.98	0.22	5.08	34,34,34,34	0
59	MG	CA	3332	1/1	0.97	0.24	5.03	29,29,29,29	0
59	MG	AA	3134	1/1	0.92	0.23	5.03	62,62,62,62	0
59	MG	AU	205	1/1	0.95	0.26	4.97	45,45,45,45	0
59	MG	AA	3691	1/1	0.97	0.23	4.91	62,62,62,62	0
59	MG	AD	309	1/1	0.94	0.25	4.89	37,37,37,37	0
59	MG	AA	3404	1/1	0.96	0.20	4.82	27,27,27,27	0
59	MG	CA	3589	1/1	0.92	0.24	4.82	71,71,71,71	0
59	MG	BA	1735	1/1	0.97	0.21	4.80	41,41,41,41	0
59	MG	CA	3330	1/1	0.96	0.21	4.71	36,36,36,36	0
59	MG	CA	3252	1/1	0.95	0.19	4.69	62,62,62,62	0
59	MG	CA	3227	1/1	0.99	0.22	4.68	41,41,41,41	0
59	MG	BA	1723	1/1	0.82	0.25	4.63	70,70,70,70	0
59	MG	CA	3636	1/1	0.91	0.19	4.62	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3226	1/1	0.90	0.23	4.62	46,46,46,46	0
59	MG	AA	3510	1/1	0.95	0.24	4.58	17,17,17,17	0
59	MG	DA	1665	1/1	0.84	0.20	4.56	63,63,63,63	0
59	MG	BA	1788	1/1	0.76	0.21	4.53	79,79,79,79	0
59	MG	CW	201	1/1	0.95	0.35	4.48	46,46,46,46	0
59	MG	AA	3593	1/1	0.96	0.22	4.43	15,15,15,15	1
59	MG	AD	308	1/1	0.93	0.42	4.42	46,46,46,46	0
59	MG	CA	3103	1/1	0.97	0.20	4.38	53,53,53,53	0
59	MG	AA	3384	1/1	0.96	0.21	4.21	22,22,22,22	0
59	MG	CA	3372	1/1	0.99	0.18	4.21	35,35,35,35	0
59	MG	AA	3392	1/1	0.95	0.24	4.15	17,17,17,17	0
59	MG	AA	3317	1/1	0.97	0.17	4.13	24,24,24,24	0
59	MG	CA	3201	1/1	0.93	0.23	4.12	45,45,45,45	0
59	MG	BA	1615	1/1	0.96	0.29	4.12	62,62,62,62	0
59	MG	AA	3344	1/1	0.85	0.23	4.09	22,22,22,22	0
59	MG	CA	3285	1/1	0.94	0.20	4.08	63,63,63,63	0
59	MG	AA	3813	1/1	0.96	0.19	4.04	29,29,29,29	1
59	MG	BA	1607	1/1	0.89	0.26	3.99	64,64,64,64	0
59	MG	CA	3413	1/1	0.83	0.22	3.98	39,39,39,39	0
59	MG	CA	3010	1/1	0.96	0.19	3.88	43,43,43,43	0
59	MG	AA	3188	1/1	0.95	0.19	3.80	31,31,31,31	0
59	MG	AA	3829	1/1	0.95	0.24	3.79	47,47,47,47	0
59	MG	BA	1676	1/1	0.91	0.20	3.77	61,61,61,61	0
59	MG	AA	3515	1/1	0.97	0.22	3.76	12,12,12,12	0
59	MG	CA	3557	1/1	0.80	0.23	3.71	76,76,76,76	0
59	MG	CA	3026	1/1	0.92	0.22	3.69	32,32,32,32	1
59	MG	A0	101	1/1	0.83	0.20	3.61	69,69,69,69	0
59	MG	AA	3250	1/1	0.98	0.18	3.61	123,123,123,123	0
59	MG	AA	3193	1/1	0.95	0.20	3.59	40,40,40,40	0
59	MG	CA	3353	1/1	0.98	0.22	3.56	45,45,45,45	0
59	MG	AA	3511	1/1	0.96	0.20	3.56	14,14,14,14	0
59	MG	CB	3007	1/1	0.89	0.22	3.55	52,52,52,52	0
59	MG	AA	3241	1/1	0.64	0.21	3.54	65,65,65,65	0
59	MG	AA	3182	1/1	0.98	0.22	3.54	46,46,46,46	0
59	MG	CA	3383	1/1	0.98	0.20	3.51	30,30,30,30	0
59	MG	DA	1609	1/1	0.86	0.30	3.51	89,89,89,89	0
59	MG	AA	3795	1/1	0.89	0.25	3.37	22,22,22,22	0
59	MG	AA	3794	1/1	0.95	0.42	3.29	60,60,60,60	0
59	MG	AA	3565	1/1	0.96	0.21	3.27	44,44,44,44	0
59	MG	CA	3277	1/1	0.95	0.19	3.26	55,55,55,55	0
59	MG	C3	3001	1/1	0.92	0.40	3.19	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	1642	1/1	0.67	0.20	3.16	62,62,62,62	0
59	MG	CA	3361	1/1	0.98	0.20	3.10	43,43,43,43	0
59	MG	AB	3020	1/1	0.86	0.18	3.04	62,62,62,62	0
59	MG	CA	3552	1/1	0.95	0.18	3.02	30,30,30,30	0
59	MG	AA	3708	1/1	0.81	0.29	3.02	61,61,61,61	0
59	MG	AA	3335	1/1	0.98	0.24	3.02	15,15,15,15	0
59	MG	BA	1631	1/1	0.71	0.18	2.99	71,71,71,71	0
59	MG	CA	3526	1/1	0.93	0.21	2.98	58,58,58,58	0
59	MG	CQ	202	1/1	0.65	0.29	2.97	74,74,74,74	0
59	MG	AA	3793	1/1	0.98	0.22	2.90	7,7,7,7	0
59	MG	AA	3393	1/1	0.95	0.20	2.81	23,23,23,23	0
59	MG	AA	3576	1/1	0.90	0.18	2.81	52,52,52,52	0
59	MG	AA	3443	1/1	0.94	0.19	2.80	33,33,33,33	0
59	MG	AA	3529	1/1	0.96	0.20	2.79	30,30,30,30	0
59	MG	AA	3561	1/1	0.98	0.21	2.77	21,21,21,21	0
59	MG	AA	3047	1/1	0.88	0.19	2.75	29,29,29,29	0
59	MG	CA	3661	1/1	0.94	0.23	2.74	27,27,27,27	0
59	MG	AA	3730	1/1	0.97	0.17	2.70	75,75,75,75	0
59	MG	AF	301	1/1	0.91	0.20	2.70	35,35,35,35	1
59	MG	CA	3002	1/1	0.97	0.23	2.65	28,28,28,28	0
59	MG	AA	3718	1/1	0.93	0.21	2.64	42,42,42,42	0
59	MG	AA	3702	1/1	0.99	0.20	2.63	14,14,14,14	0
59	MG	BA	1757	1/1	0.93	0.22	2.63	43,43,43,43	0
59	MG	AA	3659	1/1	0.88	0.18	2.58	73,73,73,73	0
59	MG	AA	3053	1/1	0.99	0.18	2.56	19,19,19,19	0
59	MG	BA	1641	1/1	0.89	0.20	2.54	54,54,54,54	0
59	MG	CA	3318	1/1	0.96	0.21	2.54	24,24,24,24	0
59	MG	BA	1627	1/1	0.95	0.23	2.51	51,51,51,51	0
59	MG	CA	3660	1/1	0.93	0.20	2.51	60,60,60,60	0
59	MG	AA	3391	1/1	0.92	0.20	2.49	19,19,19,19	0
59	MG	AA	3429	1/1	0.93	0.20	2.47	31,31,31,31	0
59	MG	CA	3045	1/1	0.98	0.18	2.45	60,60,60,60	0
59	MG	AA	3806	1/1	0.95	0.18	2.45	42,42,42,42	0
59	MG	BA	1616	1/1	0.54	0.27	2.38	122,122,122,122	0
59	MG	AA	3509	1/1	0.95	0.16	2.35	40,40,40,40	0
59	MG	DT	3001	1/1	0.63	0.43	2.35	60,60,60,60	0
59	MG	AA	3688	1/1	0.96	0.15	2.33	25,25,25,25	0
59	MG	AA	3362	1/1	0.98	0.17	2.31	46,46,46,46	0
59	MG	AA	3766	1/1	0.94	0.17	2.30	54,54,54,54	0
59	MG	CA	3653	1/1	0.97	0.20	2.30	32,32,32,32	0
59	MG	DA	1655	1/1	0.63	0.24	2.26	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3568	1/1	0.97	0.19	2.25	15,15,15,15	0
59	MG	AA	3294	1/1	0.98	0.17	2.25	37,37,37,37	0
59	MG	CA	3346	1/1	0.95	0.19	2.20	30,30,30,30	0
59	MG	DA	1683	1/1	0.87	0.33	2.17	58,58,58,58	0
59	MG	AA	3413	1/1	0.94	0.19	2.14	25,25,25,25	0
59	MG	AA	3328	1/1	0.99	0.16	2.12	42,42,42,42	0
59	MG	DA	1641	1/1	0.87	0.25	2.10	74,74,74,74	0
59	MG	CA	3569	1/1	0.88	0.19	2.10	41,41,41,41	0
59	MG	AA	3020	1/1	0.98	0.18	2.09	11,11,11,11	0
59	MG	AA	3743	1/1	0.93	0.17	2.08	67,67,67,67	0
59	MG	AU	203	1/1	0.97	0.22	2.07	31,31,31,31	0
59	MG	CV	202	1/1	0.98	0.21	2.04	38,38,38,38	0
59	MG	AA	3313	1/1	0.90	0.17	1.98	39,39,39,39	0
59	MG	AA	3682	1/1	0.97	0.17	1.97	31,31,31,31	0
59	MG	CA	3448	1/1	0.92	0.21	1.95	37,37,37,37	0
59	MG	CA	3627	1/1	0.97	0.19	1.94	60,60,60,60	0
59	MG	CA	3572	1/1	0.78	0.17	1.93	70,70,70,70	0
59	MG	AA	3745	1/1	0.99	0.18	1.92	68,68,68,68	0
59	MG	AA	3407	1/1	0.98	0.20	1.92	10,10,10,10	0
59	MG	AA	3049	1/1	0.97	0.18	1.91	35,35,35,35	0
59	MG	CA	3615	1/1	0.89	0.20	1.89	28,28,28,28	0
59	MG	CA	3013	1/1	0.81	0.23	1.89	42,42,42,42	0
59	MG	DA	1661	1/1	0.92	0.18	1.84	66,66,66,66	0
59	MG	CD	304	1/1	0.94	0.30	1.76	28,28,28,28	0
59	MG	DA	1696	1/1	0.96	0.18	1.72	53,53,53,53	0
59	MG	BA	1726	1/1	0.94	0.20	1.70	46,46,46,46	0
59	MG	BA	1680	1/1	0.95	0.19	1.70	40,40,40,40	0
59	MG	CA	3264	1/1	0.88	0.19	1.69	60,60,60,60	0
59	MG	C1	101	1/1	0.94	0.19	1.63	57,57,57,57	0
59	MG	AA	3035	1/1	0.85	0.16	1.63	48,48,48,48	0
59	MG	BA	1705	1/1	0.89	0.24	1.62	53,53,53,53	0
59	MG	AA	3623	1/1	0.97	0.17	1.52	28,28,28,28	0
59	MG	CA	3232	1/1	0.95	0.17	1.49	54,54,54,54	0
59	MG	AA	3319	1/1	0.92	0.19	1.40	58,58,58,58	0
59	MG	CQ	201	1/1	0.88	0.24	1.40	72,72,72,72	0
59	MG	AU	201	1/1	0.97	0.19	1.35	25,25,25,25	0
59	MG	AA	3276	1/1	0.94	0.24	1.34	67,67,67,67	0
59	MG	BA	1815	1/1	0.85	0.23	1.34	53,53,53,53	0
59	MG	CA	3421	1/1	0.94	0.20	1.31	57,57,57,57	0
59	MG	CA	3598	1/1	0.83	0.16	1.31	65,65,65,65	0
59	MG	BA	1742	1/1	0.94	0.18	1.31	48,48,48,48	0
59	MG	BA	1671	1/1	0.89	0.21	1.28	101,101,101,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3268	1/1	0.95	0.18	1.27	52,52,52,52	0
59	MG	BA	1730	1/1	0.88	0.19	1.23	53,53,53,53	0
59	MG	CA	3523	1/1	0.98	0.14	1.23	37,37,37,37	0
59	MG	AA	3222	1/1	0.97	0.17	1.21	4,4,4,4	0
59	MG	AA	3821	1/1	0.97	0.19	1.20	38,38,38,38	0
59	MG	DA	1697	1/1	0.98	0.18	1.17	48,48,48,48	0
59	MG	AA	3815	1/1	0.97	0.17	1.16	30,30,30,30	0
59	MG	CA	3324	1/1	0.96	0.18	1.14	26,26,26,26	0
59	MG	AA	3738	1/1	0.93	0.19	1.12	24,24,24,24	0
59	MG	AA	3831	1/1	0.97	0.20	1.10	37,37,37,37	0
59	MG	AB	3016	1/1	0.97	0.14	1.07	34,34,34,34	0
59	MG	AF	303	1/1	0.98	0.21	1.05	19,19,19,19	0
59	MG	AA	3627	1/1	0.80	0.15	1.00	76,76,76,76	0
59	MG	AA	3058	1/1	0.92	0.15	0.95	22,22,22,22	0
59	MG	AA	3489	1/1	0.97	0.18	0.94	15,15,15,15	0
59	MG	CA	3614	1/1	0.93	0.24	0.92	62,62,62,62	0
59	MG	AA	3318	1/1	0.96	0.16	0.91	23,23,23,23	0
59	MG	BA	1649	1/1	0.91	0.17	0.85	35,35,35,35	0
59	MG	AA	3537	1/1	0.96	0.17	0.84	20,20,20,20	0
59	MG	CA	3417	1/1	0.89	0.21	0.82	56,56,56,56	0
59	MG	AA	3007	1/1	0.95	0.15	0.75	12,12,12,12	0
59	MG	CA	3070	1/1	0.83	0.17	0.70	60,60,60,60	0
59	MG	AA	3205	1/1	0.91	0.15	0.68	42,42,42,42	0
59	MG	AA	3528	1/1	0.98	0.16	0.64	19,19,19,19	0
59	MG	BA	1702	1/1	0.97	0.19	0.62	46,46,46,46	0
59	MG	DA	1717	1/1	0.59	0.28	0.60	95,95,95,95	0
59	MG	AA	3546	1/1	0.96	0.14	0.60	60,60,60,60	0
59	MG	CA	3392	1/1	0.84	0.19	0.54	43,43,43,43	0
59	MG	AA	3052	1/1	0.96	0.17	0.54	11,11,11,11	0
59	MG	BA	1625	1/1	0.85	0.16	0.49	86,86,86,86	0
59	MG	CA	3170	1/1	0.94	0.17	0.44	32,32,32,32	0
59	MG	AA	3245	1/1	0.94	0.18	0.42	11,11,11,11	0
59	MG	CA	3279	1/1	0.78	0.17	0.42	26,26,26,26	0
59	MG	DA	1689	1/1	0.89	0.18	0.42	56,56,56,56	0
59	MG	DA	1614	1/1	0.82	0.19	0.42	65,65,65,65	0
59	MG	CA	3132	1/1	0.94	0.17	0.40	48,48,48,48	0
59	MG	AA	3477	1/1	0.99	0.18	0.37	14,14,14,14	0
59	MG	AA	3521	1/1	0.95	0.18	0.33	19,19,19,19	0
59	MG	CA	3601	1/1	0.95	0.14	0.33	57,57,57,57	0
59	MG	AA	3518	1/1	0.94	0.17	0.28	14,14,14,14	0
59	MG	AA	3585	1/1	0.98	0.17	0.27	35,35,35,35	0
59	MG	CA	3464	1/1	0.96	0.18	0.27	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	DA	1669	1/1	0.82	0.21	0.24	65,65,65,65	0
59	MG	AD	303	1/1	0.86	0.16	0.23	50,50,50,50	0
59	MG	CA	3360	1/1	0.96	0.17	0.21	38,38,38,38	0
59	MG	BA	1760	1/1	0.92	0.17	0.18	53,53,53,53	0
59	MG	BB	3001	1/1	0.78	0.16	0.17	91,91,91,91	0
59	MG	AA	3674	1/1	0.95	0.14	0.14	30,30,30,30	0
59	MG	AD	302	1/1	0.90	0.16	0.12	17,17,17,17	0
59	MG	CA	3282	1/1	0.99	0.18	0.10	36,36,36,36	0
59	MG	CA	3296	1/1	0.83	0.15	0.09	79,79,79,79	0
59	MG	AA	3800	1/1	0.92	0.17	0.06	35,35,35,35	0
59	MG	CA	3266	1/1	0.99	0.15	0.05	36,36,36,36	0
59	MG	BA	1655	1/1	0.80	0.15	0.04	59,59,59,59	0
59	MG	CA	3310	1/1	0.89	0.17	0.02	47,47,47,47	0
59	MG	AA	3739	1/1	0.72	0.18	0.01	38,38,38,38	0
59	MG	AA	3676	1/1	0.90	0.15	-0.03	26,26,26,26	0
59	MG	AA	3587	1/1	0.98	0.15	-0.04	28,28,28,28	0
59	MG	AA	3396	1/1	0.97	0.17	-0.05	16,16,16,16	0
59	MG	AA	3463	1/1	0.98	0.16	-0.07	15,15,15,15	0
59	MG	DA	1672	1/1	0.91	0.23	-0.09	77,77,77,77	0
59	MG	DA	1747	1/1	0.95	0.14	-0.10	48,48,48,48	0
59	MG	AA	3460	1/1	0.97	0.14	-0.11	27,27,27,27	0
59	MG	AA	3753	1/1	0.98	0.15	-0.12	30,30,30,30	0
59	MG	CA	3397	1/1	0.95	0.15	-0.18	57,57,57,57	0
59	MG	CA	3357	1/1	0.94	0.12	-0.21	66,66,66,66	0
59	MG	CA	3274	1/1	0.91	0.15	-0.21	52,52,52,52	0
59	MG	CA	3419	1/1	0.89	0.15	-0.25	59,59,59,59	0
59	MG	AA	3522	1/1	0.95	0.17	-0.30	30,30,30,30	0
60	ZN	A5	501	1/1	0.99	0.13	-0.34	30,30,30,30	0
59	MG	CO	5001	1/1	0.96	0.18	-0.34	50,50,50,50	0
59	MG	AA	3390	1/1	0.97	0.16	-0.34	23,23,23,23	0
59	MG	CA	3269	1/1	0.94	0.15	-0.37	81,81,81,81	0
59	MG	AA	3523	1/1	0.98	0.16	-0.37	13,13,13,13	0
59	MG	AA	3004	1/1	0.94	0.16	-0.37	21,21,21,21	0
62	GDP	DZ	703	28/28	0.96	0.14	-0.38	66,66,66,66	1
59	MG	CA	3189	1/1	0.87	0.15	-0.38	50,50,50,50	0
59	MG	CA	3315	1/1	0.97	0.13	-0.40	47,47,47,47	0
59	MG	CF	303	1/1	0.92	0.14	-0.42	51,51,51,51	0
59	MG	AA	3436	1/1	0.98	0.18	-0.43	12,12,12,12	0
60	ZN	A6	102	1/1	0.99	0.12	-0.45	40,40,40,40	0
59	MG	AA	3744	1/1	0.88	0.16	-0.50	34,34,34,34	0
59	MG	CA	3320	1/1	0.96	0.16	-0.52	36,36,36,36	0
59	MG	AA	3438	1/1	0.99	0.15	-0.53	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3303	1/1	0.99	0.15	-0.54	24,24,24,24	0
59	MG	DA	1680	1/1	0.93	0.18	-0.54	56,56,56,56	0
59	MG	CA	3177	1/1	0.93	0.15	-0.55	29,29,29,29	0
59	MG	CA	3085	1/1	0.99	0.17	-0.56	25,25,25,25	0
59	MG	DA	1625	1/1	0.92	0.15	-0.58	50,50,50,50	0
59	MG	DE	201	1/1	0.92	0.17	-0.61	84,84,84,84	0
59	MG	CA	3104	1/1	0.94	0.16	-0.61	80,80,80,80	0
59	MG	BA	1696	1/1	0.84	0.16	-0.65	98,98,98,98	0
59	MG	AA	3399	1/1	0.96	0.16	-0.66	16,16,16,16	0
59	MG	AA	3512	1/1	0.99	0.16	-0.67	38,38,38,38	0
59	MG	DA	1700	1/1	0.93	0.16	-0.69	61,61,61,61	0
59	MG	AD	306	1/1	0.90	0.14	-0.69	65,65,65,65	0
62	GDP	BZ	702	28/28	0.97	0.12	-0.70	57,57,57,57	0
59	MG	CA	3664	1/1	0.94	0.14	-0.71	48,48,48,48	0
60	ZN	A9	501	1/1	1.00	0.12	-0.72	42,42,42,42	0
59	MG	CA	3433	1/1	0.99	0.12	-0.72	82,82,82,82	0
59	MG	CA	3012	1/1	0.95	0.16	-0.73	65,65,65,65	0
59	MG	CA	3370	1/1	0.94	0.14	-0.76	41,41,41,41	0
59	MG	CA	3339	1/1	0.97	0.14	-0.76	24,24,24,24	0
59	MG	AA	3001	1/1	0.94	0.15	-0.78	25,25,25,25	0
59	MG	DA	1723	1/1	0.93	0.13	-0.79	53,53,53,53	0
59	MG	CA	3299	1/1	0.96	0.15	-0.79	64,64,64,64	0
59	MG	DA	1771	1/1	0.83	0.12	-0.83	60,60,60,60	0
60	ZN	C4	501	1/1	0.92	0.11	-0.83	194,194,194,194	0
59	MG	CA	3223	1/1	0.89	0.15	-0.87	59,59,59,59	0
59	MG	CA	3311	1/1	0.99	0.14	-0.87	50,50,50,50	0
59	MG	CA	3300	1/1	0.96	0.13	-0.89	47,47,47,47	0
59	MG	AA	3445	1/1	0.87	0.14	-0.91	23,23,23,23	0
59	MG	BA	1750	1/1	0.84	0.21	-0.92	55,55,55,55	0
59	MG	AA	3411	1/1	0.98	0.15	-0.97	12,12,12,12	0
59	MG	AA	3305	1/1	0.96	0.17	-1.00	25,25,25,25	0
59	MG	AA	3112	1/1	0.95	0.14	-1.01	61,61,61,61	0
60	ZN	AY	501	1/1	0.99	0.10	-1.01	61,61,61,61	0
59	MG	CA	3317	1/1	0.88	0.14	-1.02	49,49,49,49	0
59	MG	AA	3539	1/1	0.97	0.15	-1.03	34,34,34,34	0
60	ZN	C9	501	1/1	0.98	0.09	-1.04	75,75,75,75	0
59	MG	BA	1748	1/1	0.92	0.14	-1.06	63,63,63,63	0
59	MG	AA	3490	1/1	0.94	0.16	-1.06	27,27,27,27	0
59	MG	DA	1703	1/1	0.89	0.21	-1.07	89,89,89,89	0
59	MG	CF	304	1/1	0.97	0.14	-1.07	65,65,65,65	0
59	MG	AA	3600	1/1	0.98	0.15	-1.12	25,25,25,25	0
60	ZN	C5	102	1/1	0.97	0.10	-1.16	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1686	1/1	0.98	0.15	-1.19	36,36,36,36	0
59	MG	CA	3004	1/1	0.96	0.14	-1.24	49,49,49,49	0
59	MG	AA	3452	1/1	0.98	0.14	-1.28	14,14,14,14	0
59	MG	BA	1766	1/1	0.96	0.15	-1.28	62,62,62,62	0
59	MG	CA	3562	1/1	0.95	0.14	-1.32	29,29,29,29	0
59	MG	BA	1603	1/1	0.83	0.11	-1.34	61,61,61,61	0
59	MG	AA	3386	1/1	0.96	0.12	-1.35	45,45,45,45	0
59	MG	AA	3727	1/1	0.97	0.14	-1.36	23,23,23,23	0
59	MG	AA	3551	1/1	0.85	0.12	-1.39	39,39,39,39	0
59	MG	BE	3001	1/1	0.93	0.11	-1.45	78,78,78,78	0
59	MG	AA	3282	1/1	0.90	0.12	-1.45	33,33,33,33	0
60	ZN	DN	501	1/1	0.96	0.08	-1.46	117,117,117,117	0
59	MG	CA	3337	1/1	0.95	0.14	-1.47	20,20,20,20	0
59	MG	CA	3462	1/1	0.92	0.12	-1.49	63,63,63,63	0
59	MG	CA	3490	1/1	0.80	0.13	-1.51	50,50,50,50	0
59	MG	AA	3575	1/1	0.85	0.14	-1.52	35,35,35,35	0
60	ZN	C6	501	1/1	0.97	0.10	-1.53	66,66,66,66	0
61	SF4	BD	501	8/8	0.98	0.10	-1.54	78,78,78,78	0
59	MG	CA	3453	1/1	0.90	0.16	-1.54	35,35,35,35	0
59	MG	CA	3048	1/1	0.94	0.10	-1.54	47,47,47,47	0
59	MG	BN	503	1/1	0.91	0.14	-1.57	62,62,62,62	0
59	MG	CA	3663	1/1	0.89	0.12	-1.58	64,64,64,64	0
60	ZN	BN	501	1/1	0.93	0.10	-1.58	132,132,132,132	0
59	MG	DA	1711	1/1	0.96	0.13	-1.59	60,60,60,60	0
59	MG	CA	3321	1/1	0.95	0.14	-1.59	28,28,28,28	0
59	MG	AA	3397	1/1	0.97	0.14	-1.62	13,13,13,13	0
60	ZN	CY	501	1/1	0.97	0.06	-1.62	101,101,101,101	0
59	MG	DA	1648	1/1	0.99	0.12	-1.66	40,40,40,40	0
59	MG	BA	1700	1/1	0.85	0.14	-1.68	52,52,52,52	0
59	MG	AB	3014	1/1	0.98	0.12	-1.69	56,56,56,56	0
59	MG	BA	1613	1/1	0.85	0.12	-1.73	76,76,76,76	0
59	MG	BK	201	1/1	0.93	0.10	-1.75	44,44,44,44	0
59	MG	BA	1754	1/1	0.92	0.13	-1.76	49,49,49,49	0
59	MG	AA	3624	1/1	0.91	0.12	-1.81	42,42,42,42	0
59	MG	CA	3498	1/1	0.97	0.12	-1.83	49,49,49,49	0
59	MG	CA	3192	1/1	0.90	0.11	-1.83	45,45,45,45	0
59	MG	AA	3762	1/1	0.95	0.14	-1.85	23,23,23,23	0
59	MG	AA	3401	1/1	0.99	0.15	-1.85	21,21,21,21	0
59	MG	DE	202	1/1	0.85	0.08	-1.86	100,100,100,100	0
59	MG	AA	3779	1/1	0.97	0.12	-1.89	22,22,22,22	0
59	MG	CA	3178	1/1	0.93	0.13	-1.95	54,54,54,54	0
59	MG	AA	3416	1/1	0.98	0.15	-2.01	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	ZN	A4	501	1/1	0.94	0.07	-2.02	117,117,117,117	0
59	MG	CA	3009	1/1	0.95	0.10	-2.02	27,27,27,27	0
59	MG	DA	1768	1/1	0.94	0.07	-2.04	59,59,59,59	0
59	MG	AA	3236	1/1	0.94	0.14	-2.07	57,57,57,57	0
59	MG	BA	1795	1/1	0.94	0.10	-2.09	59,59,59,59	0
59	MG	BA	1746	1/1	0.92	0.12	-2.15	33,33,33,33	0
59	MG	CA	3594	1/1	0.91	0.11	-2.15	73,73,73,73	0
59	MG	CX	5001	1/1	0.90	0.14	-2.16	65,65,65,65	0
59	MG	AG	201	1/1	0.97	0.07	-2.18	38,38,38,38	0
59	MG	BA	1617	1/1	0.93	0.12	-2.19	118,118,118,118	0
59	MG	CA	3079	1/1	0.91	0.10	-2.20	41,41,41,41	0
59	MG	CG	3001	1/1	0.96	0.10	-2.27	65,65,65,65	0
59	MG	AA	3190	1/1	0.94	0.13	-2.30	24,24,24,24	0
59	MG	CA	3592	1/1	0.98	0.14	-2.30	64,64,64,64	0
61	SF4	DD	501	8/8	0.98	0.10	-2.32	82,82,82,82	1
59	MG	AA	3084	1/1	0.96	0.10	-2.35	23,23,23,23	0
59	MG	CA	3214	1/1	0.98	0.11	-2.37	22,22,22,22	0
59	MG	CA	3123	1/1	0.96	0.09	-2.39	29,29,29,29	0
59	MG	AA	3502	1/1	0.94	0.13	-2.46	29,29,29,29	1
59	MG	CB	3004	1/1	0.93	0.13	-2.47	55,55,55,55	0
59	MG	AA	3725	1/1	0.96	0.15	-2.47	13,13,13,13	0
59	MG	AA	3578	1/1	0.97	0.13	-2.48	28,28,28,28	0
59	MG	BA	1611	1/1	0.92	0.13	-2.58	31,31,31,31	0
59	MG	CA	3561	1/1	0.94	0.14	-2.59	41,41,41,41	1
59	MG	CA	3017	1/1	0.97	0.14	-2.60	30,30,30,30	0
59	MG	AA	3099	1/1	0.95	0.10	-2.64	53,53,53,53	0
59	MG	CA	3283	1/1	0.94	0.12	-2.64	31,31,31,31	0
59	MG	CE	305	1/1	0.95	0.04	-2.69	58,58,58,58	0
59	MG	AG	202	1/1	0.95	0.06	-2.76	54,54,54,54	0
59	MG	CA	3528	1/1	0.82	0.10	-2.76	38,38,38,38	0
59	MG	BM	201	1/1	0.96	0.04	-2.77	62,62,62,62	0
59	MG	AA	3497	1/1	0.97	0.13	-2.80	44,44,44,44	0
59	MG	CA	3425	1/1	0.97	0.12	-2.84	50,50,50,50	0
59	MG	CA	3211	1/1	0.97	0.09	-2.89	29,29,29,29	0
59	MG	AA	3382	1/1	0.96	0.12	-2.89	37,37,37,37	0
59	MG	DA	1621	1/1	0.89	0.09	-2.92	42,42,42,42	0
59	MG	AA	3673	1/1	0.93	0.11	-2.92	38,38,38,38	0
59	MG	AA	3021	1/1	0.95	0.13	-2.95	33,33,33,33	0
59	MG	AA	3320	1/1	0.97	0.14	-3.01	37,37,37,37	0
59	MG	CA	3064	1/1	0.97	0.09	-3.02	48,48,48,48	0
59	MG	DA	1722	1/1	0.79	0.13	-3.03	77,77,77,77	0
59	MG	AA	3218	1/1	0.94	0.09	-3.17	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3617	1/1	0.97	0.13	-3.21	41,41,41,41	0
59	MG	CA	3275	1/1	0.94	0.10	-3.34	61,61,61,61	0
59	MG	AA	3069	1/1	0.90	0.10	-3.35	28,28,28,28	0
59	MG	CA	3489	1/1	0.94	0.10	-3.39	39,39,39,39	0
59	MG	DA	1657	1/1	0.96	0.10	-3.49	23,23,23,23	0
59	MG	AA	3203	1/1	0.92	0.07	-3.49	59,59,59,59	0
59	MG	BT	3001	1/1	0.96	0.12	-3.52	46,46,46,46	0
59	MG	BA	1681	1/1	0.96	0.10	-3.57	53,53,53,53	0
59	MG	AA	3777	1/1	0.98	0.12	-3.63	41,41,41,41	0
59	MG	CA	3019	1/1	0.97	0.11	-3.65	22,22,22,22	0
59	MG	AA	3757	1/1	0.95	0.07	-3.66	14,14,14,14	0
59	MG	DA	1685	1/1	0.95	0.10	-3.68	46,46,46,46	0
59	MG	CA	3262	1/1	0.96	0.12	-3.71	11,11,11,11	0
59	MG	AB	3007	1/1	0.96	0.07	-3.76	39,39,39,39	0
59	MG	CA	3652	1/1	0.98	0.14	-3.81	23,23,23,23	0
59	MG	AA	3017	1/1	0.90	0.11	-3.89	61,61,61,61	0
59	MG	AA	3022	1/1	0.95	0.13	-3.90	5,5,5,5	0
59	MG	AA	3037	1/1	0.98	0.11	-3.96	4,4,4,4	0
59	MG	CA	3018	1/1	0.94	0.08	-3.96	41,41,41,41	0
59	MG	AA	3406	1/1	0.97	0.09	-4.17	20,20,20,20	0
59	MG	AA	3262	1/1	0.96	0.15	-4.26	15,15,15,15	0
59	MG	BA	1621	1/1	0.93	0.12	-4.27	51,51,51,51	0
59	MG	CA	3595	1/1	0.90	0.10	-4.27	70,70,70,70	0
59	MG	CA	3364	1/1	0.97	0.10	-4.37	22,22,22,22	0
59	MG	BA	1794	1/1	0.90	0.07	-4.45	38,38,38,38	0
59	MG	AA	3326	1/1	0.97	0.10	-4.49	36,36,36,36	1
59	MG	AA	3380	1/1	0.99	0.12	-4.55	18,18,18,18	0
59	MG	CA	3027	1/1	0.97	0.06	-4.56	31,31,31,31	0
59	MG	AA	3009	1/1	0.91	0.09	-4.60	22,22,22,22	0
59	MG	CA	3438	1/1	0.98	0.14	-4.61	24,24,24,24	0
59	MG	AA	3345	1/1	0.99	0.13	-4.71	6,6,6,6	0
59	MG	AA	3621	1/1	0.96	0.07	-4.87	17,17,17,17	0
59	MG	CA	3056	1/1	0.93	0.09	-4.95	63,63,63,63	0
59	MG	BA	1743	1/1	0.97	0.06	-4.98	41,41,41,41	0
59	MG	AA	3506	1/1	0.97	0.10	-4.99	48,48,48,48	0
59	MG	CA	3306	1/1	0.98	0.08	-5.29	24,24,24,24	0
59	MG	CA	3468	1/1	0.97	0.06	-5.45	53,53,53,53	0
59	MG	CA	3292	1/1	0.99	0.09	-5.45	12,12,12,12	0
59	MG	DA	1628	1/1	0.96	0.09	-5.50	39,39,39,39	0
59	MG	AA	3350	1/1	0.96	0.08	-5.52	36,36,36,36	0
59	MG	CA	3604	1/1	0.92	0.09	-5.53	62,62,62,62	0
59	MG	BA	1813	1/1	0.90	0.07	-5.72	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3011	1/1	0.99	0.08	-6.11	16,16,16,16	0
59	MG	CA	3342	1/1	0.98	0.11	-6.13	33,33,33,33	0
59	MG	CA	3138	1/1	0.97	0.04	-6.18	86,86,86,86	0
59	MG	AA	3473	1/1	0.97	0.07	-6.20	53,53,53,53	0
59	MG	AA	3654	1/1	0.91	0.06	-6.26	67,67,67,67	0
59	MG	DA	1750	1/1	0.94	0.09	-6.41	67,67,67,67	0
59	MG	AA	3620	1/1	0.94	0.12	-6.44	22,22,22,22	0
59	MG	AA	3377	1/1	0.98	0.06	-6.61	20,20,20,20	0
59	MG	AA	3560	1/1	0.95	0.13	-6.97	29,29,29,29	0
59	MG	AA	3388	1/1	0.96	0.08	-7.36	28,28,28,28	0
59	MG	AA	3072	1/1	0.98	0.08	-7.52	19,19,19,19	0
59	MG	AA	3338	1/1	0.98	0.08	-9.30	28,28,28,28	0
59	MG	AA	3770	1/1	0.97	0.13	-9.77	43,43,43,43	0
59	MG	CA	3491	1/1	0.96	0.06	-10.09	44,44,44,44	0
59	MG	CA	3581	1/1	0.85	0.12	-10.24	38,38,38,38	0
59	MG	AA	3387	1/1	0.94	0.08	-10.26	29,29,29,29	0
59	MG	AA	3589	1/1	0.93	0.08	-10.71	55,55,55,55	0
59	MG	CA	3644	1/1	0.83	0.21	-	66,66,66,66	0
59	MG	AB	3018	1/1	0.94	0.23	-	69,69,69,69	0
59	MG	AA	3488	1/1	0.98	0.20	-	36,36,36,36	0
59	MG	AA	3494	1/1	0.95	0.09	-	34,34,34,34	0
59	MG	AA	3373	1/1	0.91	0.17	-	48,48,48,48	0
59	MG	AA	3311	1/1	0.98	0.14	-	2,2,2,2	0
59	MG	BA	1812	1/1	0.49	0.20	-	79,79,79,79	0
59	MG	AA	3048	1/1	0.95	0.16	-	28,28,28,28	0
59	MG	AB	3022	1/1	0.95	0.13	-	61,61,61,61	0
59	MG	CA	3343	1/1	0.91	0.12	-	32,32,32,32	0
59	MG	AA	3437	1/1	0.98	0.18	-	17,17,17,17	0
59	MG	CA	3259	1/1	0.92	0.27	-	80,80,80,80	0
59	MG	BA	1652	1/1	0.86	0.12	-	59,59,59,59	0
59	MG	CA	3549	1/1	0.92	0.16	-	70,70,70,70	0
59	MG	AA	3157	1/1	0.87	0.49	-	91,91,91,91	0
59	MG	CA	3504	1/1	0.94	0.13	-	79,79,79,79	0
59	MG	AA	3453	1/1	0.97	0.24	-	39,39,39,39	0
59	MG	BA	1668	1/1	0.80	0.16	-	69,69,69,69	0
59	MG	BA	1620	1/1	0.91	0.17	-	52,52,52,52	0
59	MG	AA	3479	1/1	0.84	0.23	-	55,55,55,55	0
59	MG	CA	3304	1/1	0.70	0.12	-	67,67,67,67	0
59	MG	AA	3776	1/1	0.83	0.12	-	69,69,69,69	0
59	MG	AA	3722	1/1	0.91	0.13	-	37,37,37,37	0
59	MG	CA	3155	1/1	0.32	0.24	-	112,112,112,112	0
59	MG	AA	3714	1/1	0.84	0.23	-	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3006	1/1	0.95	0.35	-	52,52,52,52	0
59	MG	DA	1737	1/1	0.87	0.20	-	69,69,69,69	0
59	MG	AA	3234	1/1	0.92	0.30	-	36,36,36,36	0
59	MG	AA	3003	1/1	0.98	0.06	-	8,8,8,8	0
59	MG	AN	3003	1/1	0.88	0.08	-	55,55,55,55	0
59	MG	BA	1803	1/1	0.86	0.12	-	64,64,64,64	0
59	MG	AA	3626	1/1	0.84	0.18	-	35,35,35,35	0
59	MG	AA	3432	1/1	0.98	0.23	-	42,42,42,42	0
59	MG	AA	3426	1/1	0.97	0.17	-	20,20,20,20	0
59	MG	CA	3021	1/1	0.90	0.44	-	69,69,69,69	0
59	MG	BA	1677	1/1	0.98	0.17	-	28,28,28,28	0
59	MG	AB	3012	1/1	0.98	0.15	-	23,23,23,23	1
59	MG	AA	3125	1/1	0.97	0.17	-	22,22,22,22	1
59	MG	AA	3267	1/1	0.90	0.35	-	53,53,53,53	0
59	MG	CA	3319	1/1	0.87	0.14	-	65,65,65,65	0
59	MG	CA	3273	1/1	0.84	0.35	-	58,58,58,58	0
59	MG	AA	3325	1/1	0.95	0.16	-	70,70,70,70	0
59	MG	CA	3362	1/1	0.96	0.12	-	43,43,43,43	0
59	MG	CA	3553	1/1	0.74	0.18	-	90,90,90,90	0
59	MG	DA	1673	1/1	0.98	0.14	-	82,82,82,82	0
59	MG	BA	1777	1/1	0.97	0.28	-	71,71,71,71	0
59	MG	AA	3656	1/1	0.84	0.24	-	80,80,80,80	0
59	MG	DA	1617	1/1	0.89	0.18	-	64,64,64,64	0
59	MG	AB	3006	1/1	0.84	0.19	-	57,57,57,57	0
59	MG	AA	3769	1/1	0.72	0.17	-	63,63,63,63	0
59	MG	DA	1603	1/1	0.83	0.11	-	72,72,72,72	0
59	MG	DA	1733	1/1	0.57	0.35	-	92,92,92,92	0
59	MG	AA	3486	1/1	0.91	0.22	-	67,67,67,67	0
59	MG	AA	3449	1/1	0.92	0.23	-	50,50,50,50	0
59	MG	AA	3817	1/1	0.81	0.19	-	75,75,75,75	0
59	MG	CA	3508	1/1	0.92	0.18	-	52,52,52,52	0
59	MG	AA	3619	1/1	0.87	0.12	-	47,47,47,47	0
59	MG	AA	3232	1/1	0.91	0.26	-	58,58,58,58	0
59	MG	AA	3418	1/1	0.89	0.13	-	74,74,74,74	0
59	MG	AA	3630	1/1	0.91	0.35	-	72,72,72,72	0
59	MG	AA	3571	1/1	0.72	0.35	-	94,94,94,94	0
59	MG	AA	3183	1/1	0.90	0.36	-	58,58,58,58	0
59	MG	AA	3289	1/1	0.94	0.44	-	53,53,53,53	0
59	MG	CA	3600	1/1	0.79	0.51	-	86,86,86,86	0
59	MG	AA	3671	1/1	0.95	0.23	-	19,19,19,19	0
59	MG	AA	3264	1/1	0.87	0.41	-	51,51,51,51	0
59	MG	DA	1721	1/1	0.95	0.10	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3626	1/1	0.89	0.19	-	61,61,61,61	0
59	MG	CA	3174	1/1	0.91	0.53	-	50,50,50,50	0
59	MG	CA	3637	1/1	0.97	0.48	-	61,61,61,61	0
59	MG	CA	3539	1/1	0.90	0.19	-	90,90,90,90	0
59	MG	CA	3450	1/1	0.90	0.11	-	54,54,54,54	0
59	MG	AA	3163	1/1	0.93	0.25	-	72,72,72,72	0
59	MG	DA	1715	1/1	0.78	0.29	-	79,79,79,79	0
59	MG	AA	3655	1/1	0.88	0.34	-	55,55,55,55	0
59	MG	AA	3367	1/1	0.94	0.18	-	60,60,60,60	0
59	MG	AA	3415	1/1	0.99	0.24	-	62,62,62,62	0
59	MG	CA	3515	1/1	0.92	0.21	-	54,54,54,54	0
59	MG	CA	3303	1/1	0.95	0.36	-	43,43,43,43	0
59	MG	BA	1669	1/1	0.86	0.38	-	66,66,66,66	0
59	MG	CA	3096	1/1	0.33	0.24	-	125,125,125,125	0
59	MG	CA	3101	1/1	0.58	1.14	-	84,84,84,84	0
59	MG	CA	3265	1/1	0.95	0.30	-	61,61,61,61	0
59	MG	BL	202	1/1	0.96	0.18	-	54,54,54,54	0
59	MG	CA	3449	1/1	0.97	0.07	-	55,55,55,55	0
59	MG	DA	1649	1/1	0.96	0.34	-	69,69,69,69	0
59	MG	AA	3359	1/1	0.94	0.18	-	31,31,31,31	0
59	MG	CA	3081	1/1	0.83	0.32	-	63,63,63,63	0
59	MG	DA	1687	1/1	0.95	0.43	-	56,56,56,56	0
59	MG	CA	3647	1/1	0.86	0.15	-	85,85,85,85	0
59	MG	BA	1805	1/1	0.93	0.24	-	71,71,71,71	0
59	MG	DA	1666	1/1	0.89	0.20	-	53,53,53,53	0
59	MG	CA	3172	1/1	0.83	0.35	-	81,81,81,81	0
59	MG	BW	501	1/1	0.94	0.23	-	47,47,47,47	0
59	MG	AA	3514	1/1	0.93	0.18	-	42,42,42,42	0
59	MG	CA	3276	1/1	0.85	0.19	-	44,44,44,44	0
59	MG	AA	3602	1/1	0.90	0.16	-	51,51,51,51	0
59	MG	AA	3402	1/1	0.99	0.13	-	27,27,27,27	0
59	MG	AA	3553	1/1	0.98	0.05	-	43,43,43,43	0
59	MG	CA	3161	1/1	0.92	0.25	-	57,57,57,57	0
59	MG	CA	3380	1/1	0.99	0.21	-	59,59,59,59	0
59	MG	CA	3190	1/1	0.94	0.23	-	66,66,66,66	0
59	MG	AA	3713	1/1	0.97	0.21	-	27,27,27,27	0
59	MG	CA	3278	1/1	0.91	0.12	-	58,58,58,58	0
59	MG	CA	3194	1/1	0.76	0.24	-	52,52,52,52	0
59	MG	AA	3223	1/1	0.97	0.12	-	15,15,15,15	0
59	MG	DA	1761	1/1	0.85	0.31	-	72,72,72,72	0
59	MG	CA	3037	1/1	0.80	0.73	-	57,57,57,57	0
59	MG	BA	1782	1/1	0.93	0.19	-	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	DA	1718	1/1	0.67	0.32	-	101,101,101,101	0
59	MG	CA	3554	1/1	0.97	0.10	-	66,66,66,66	0
59	MG	BA	1632	1/1	0.96	0.08	-	48,48,48,48	0
59	MG	AA	3749	1/1	0.92	0.17	-	73,73,73,73	0
59	MG	AA	3164	1/1	0.86	0.64	-	71,71,71,71	0
59	MG	CA	3077	1/1	0.80	0.24	-	42,42,42,42	0
59	MG	CA	3571	1/1	0.97	0.27	-	45,45,45,45	0
59	MG	BA	1690	1/1	0.82	0.40	-	71,71,71,71	0
59	MG	CA	3608	1/1	0.84	0.31	-	50,50,50,50	1
59	MG	AA	3166	1/1	0.91	0.42	-	40,40,40,40	0
59	MG	A0	105	1/1	0.90	0.08	-	30,30,30,30	0
59	MG	CA	3573	1/1	0.89	0.11	-	65,65,65,65	0
59	MG	DA	1744	1/1	0.93	0.22	-	66,66,66,66	0
59	MG	AA	3249	1/1	0.85	0.17	-	59,59,59,59	0
59	MG	DA	1616	1/1	0.90	0.23	-	51,51,51,51	0
59	MG	CA	3368	1/1	0.92	0.16	-	44,44,44,44	0
59	MG	AE	304	1/1	0.86	0.19	-	52,52,52,52	0
59	MG	CA	3312	1/1	0.93	0.18	-	38,38,38,38	0
59	MG	AA	3496	1/1	0.97	0.37	-	31,31,31,31	0
59	MG	CA	3006	1/1	0.97	0.08	-	22,22,22,22	0
59	MG	AF	302	1/1	0.88	0.11	-	41,41,41,41	0
59	MG	AA	3409	1/1	0.83	0.08	-	60,60,60,60	0
59	MG	DA	1678	1/1	0.92	0.29	-	66,66,66,66	0
59	MG	DW	503	1/1	0.91	0.22	-	85,85,85,85	0
59	MG	CA	3247	1/1	0.92	0.29	-	39,39,39,39	0
59	MG	CA	3095	1/1	0.86	0.32	-	58,58,58,58	0
59	MG	DA	1647	1/1	0.94	0.15	-	51,51,51,51	0
59	MG	AA	3032	1/1	0.96	0.32	-	59,59,59,59	0
59	MG	AA	3819	1/1	0.94	0.50	-	57,57,57,57	0
59	MG	DA	1726	1/1	0.92	0.30	-	60,60,60,60	0
59	MG	CA	3386	1/1	0.97	0.21	-	50,50,50,50	0
59	MG	CA	3565	1/1	0.47	0.19	-	95,95,95,95	0
59	MG	AA	3444	1/1	0.87	0.25	-	66,66,66,66	0
59	MG	CA	3446	1/1	0.98	0.19	-	33,33,33,33	0
59	MG	CA	3209	1/1	0.98	0.13	-	73,73,73,73	0
59	MG	AA	3485	1/1	0.89	0.11	-	48,48,48,48	0
59	MG	AA	3090	1/1	0.91	0.39	-	53,53,53,53	0
59	MG	CA	3154	1/1	0.69	0.21	-	64,64,64,64	0
59	MG	CA	3514	1/1	0.79	0.43	-	64,64,64,64	0
59	MG	CA	3509	1/1	0.89	0.12	-	83,83,83,83	0
59	MG	CA	3524	1/1	0.91	0.25	-	52,52,52,52	0
59	MG	AA	3729	1/1	0.98	0.20	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3640	1/1	0.98	0.30	-	43,43,43,43	0
59	MG	AA	3185	1/1	0.96	0.16	-	76,76,76,76	0
59	MG	CA	3089	1/1	0.75	0.49	-	87,87,87,87	0
59	MG	CA	3122	1/1	0.81	0.72	-	58,58,58,58	0
59	MG	AA	3187	1/1	0.95	0.30	-	56,56,56,56	0
59	MG	AA	3059	1/1	0.95	0.37	-	40,40,40,40	0
59	MG	AA	3277	1/1	0.72	0.66	-	99,99,99,99	0
59	MG	AA	3304	1/1	0.93	0.16	-	47,47,47,47	0
59	MG	AA	3225	1/1	0.78	0.15	-	73,73,73,73	0
59	MG	BA	1761	1/1	0.97	0.17	-	62,62,62,62	0
59	MG	BA	1727	1/1	0.85	0.09	-	77,77,77,77	0
59	MG	BA	1604	1/1	0.74	0.19	-	63,63,63,63	0
59	MG	DA	1719	1/1	0.95	0.39	-	61,61,61,61	0
59	MG	AA	3456	1/1	0.93	0.14	-	56,56,56,56	0
59	MG	DA	1607	1/1	0.92	0.10	-	86,86,86,86	0
59	MG	CA	3106	1/1	0.96	0.14	-	66,66,66,66	0
59	MG	AA	3156	1/1	0.89	0.43	-	49,49,49,49	0
59	MG	AB	3023	1/1	0.96	0.35	-	54,54,54,54	0
59	MG	CA	3125	1/1	0.82	0.33	-	78,78,78,78	0
59	MG	AA	3469	1/1	0.96	0.12	-	32,32,32,32	0
59	MG	AA	3169	1/1	0.85	0.34	-	35,35,35,35	0
59	MG	DA	1730	1/1	0.90	0.26	-	71,71,71,71	0
59	MG	CA	3451	1/1	0.95	0.21	-	62,62,62,62	0
59	MG	CA	3328	1/1	0.88	0.20	-	35,35,35,35	0
59	MG	AA	3704	1/1	0.94	0.20	-	49,49,49,49	0
59	MG	BA	1747	1/1	0.96	0.20	-	65,65,65,65	0
59	MG	AA	3306	1/1	0.96	0.25	-	52,52,52,52	0
59	MG	DA	1638	1/1	0.88	0.30	-	80,80,80,80	0
59	MG	BA	1745	1/1	0.94	0.20	-	46,46,46,46	0
59	MG	DA	1667	1/1	0.89	0.06	-	66,66,66,66	0
59	MG	CA	3564	1/1	0.97	0.14	-	80,80,80,80	0
59	MG	CA	3127	1/1	0.56	0.42	-	94,94,94,94	0
59	MG	C0	101	1/1	0.96	0.18	-	59,59,59,59	0
59	MG	AA	3540	1/1	0.99	0.09	-	36,36,36,36	0
59	MG	CA	3253	1/1	0.94	0.18	-	70,70,70,70	0
59	MG	AA	3334	1/1	0.97	0.14	-	63,63,63,63	0
59	MG	CA	3599	1/1	0.84	0.08	-	70,70,70,70	0
59	MG	AA	3097	1/1	0.98	0.21	-	22,22,22,22	0
59	MG	A0	102	1/1	0.83	0.09	-	56,56,56,56	0
59	MG	AA	3029	1/1	0.96	0.23	-	28,28,28,28	0
59	MG	AA	3055	1/1	0.89	0.29	-	65,65,65,65	0
59	MG	AA	3389	1/1	0.96	0.16	-	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3420	1/1	0.95	0.15	-	25,25,25,25	1
59	MG	CA	3298	1/1	0.90	0.37	-	57,57,57,57	0
59	MG	BA	1642	1/1	0.90	0.15	-	60,60,60,60	0
59	MG	CA	3043	1/1	0.92	0.42	-	61,61,61,61	0
59	MG	A0	103	1/1	0.85	0.10	-	70,70,70,70	0
59	MG	CR	201	1/1	0.90	0.27	-	34,34,34,34	0
59	MG	AA	3556	1/1	0.81	0.33	-	66,66,66,66	0
59	MG	CA	3239	1/1	0.91	0.17	-	69,69,69,69	0
59	MG	CA	3550	1/1	0.78	0.09	-	62,62,62,62	1
59	MG	AA	3191	1/1	0.90	0.11	-	16,16,16,16	0
59	MG	DD	502	1/1	0.96	0.49	-	50,50,50,50	0
59	MG	CA	3376	1/1	0.86	0.10	-	78,78,78,78	0
59	MG	DA	1759	1/1	0.93	0.17	-	53,53,53,53	0
59	MG	CA	3352	1/1	0.84	0.18	-	79,79,79,79	0
59	MG	AA	3584	1/1	0.89	0.13	-	17,17,17,17	0
59	MG	AA	3146	1/1	0.99	0.08	-	29,29,29,29	0
59	MG	BA	1786	1/1	0.58	0.22	-	82,82,82,82	0
59	MG	CA	3529	1/1	0.92	0.07	-	68,68,68,68	0
59	MG	CA	3281	1/1	0.95	0.23	-	21,21,21,21	0
59	MG	AA	3741	1/1	0.99	0.11	-	21,21,21,21	0
59	MG	BA	1749	1/1	0.95	0.32	-	61,61,61,61	0
59	MG	AA	3505	1/1	0.98	0.15	-	30,30,30,30	0
59	MG	AR	201	1/1	0.88	0.17	-	28,28,28,28	0
59	MG	CA	3416	1/1	0.95	0.14	-	44,44,44,44	0
59	MG	AA	3201	1/1	0.96	0.09	-	53,53,53,53	0
59	MG	CA	3060	1/1	0.82	0.41	-	72,72,72,72	0
59	MG	DA	1639	1/1	0.55	0.56	-	69,69,69,69	0
59	MG	CA	3469	1/1	0.95	0.22	-	61,61,61,61	0
59	MG	DA	1714	1/1	0.96	0.16	-	68,68,68,68	0
59	MG	AA	3030	1/1	0.94	0.28	-	24,24,24,24	1
59	MG	CA	3086	1/1	0.90	0.26	-	85,85,85,85	0
59	MG	BA	1739	1/1	0.90	0.20	-	62,62,62,62	0
59	MG	CA	3228	1/1	0.98	0.36	-	59,59,59,59	0
59	MG	AA	3369	1/1	0.97	0.12	-	47,47,47,47	0
59	MG	CA	3069	1/1	0.85	0.73	-	81,81,81,81	0
59	MG	AA	3475	1/1	0.99	0.25	-	45,45,45,45	0
59	MG	AA	3327	1/1	0.86	0.17	-	31,31,31,31	0
59	MG	AA	3129	1/1	0.96	0.18	-	34,34,34,34	1
59	MG	A9	502	1/1	0.95	0.25	-	41,41,41,41	0
59	MG	CA	3355	1/1	0.96	0.14	-	35,35,35,35	0
59	MG	CA	3116	1/1	0.87	0.33	-	52,52,52,52	0
59	MG	AA	3684	1/1	0.95	0.26	-	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BZ	701	1/1	0.96	0.20	-	49,49,49,49	0
59	MG	CA	3206	1/1	0.97	0.42	-	44,44,44,44	0
59	MG	AA	3080	1/1	0.92	0.51	-	61,61,61,61	0
59	MG	AA	3493	1/1	0.95	0.10	-	77,77,77,77	0
59	MG	AA	3143	1/1	0.89	0.23	-	48,48,48,48	0
59	MG	AA	3566	1/1	0.96	0.05	-	56,56,56,56	0
59	MG	AA	3337	1/1	0.94	0.16	-	75,75,75,75	0
59	MG	CA	3525	1/1	0.98	0.29	-	23,23,23,23	0
59	MG	CA	3046	1/1	0.89	0.29	-	68,68,68,68	0
59	MG	AA	3526	1/1	0.99	0.20	-	19,19,19,19	0
59	MG	AA	3535	1/1	0.97	0.14	-	48,48,48,48	0
59	MG	CA	3459	1/1	0.98	0.09	-	28,28,28,28	0
59	MG	CA	3235	1/1	0.86	0.28	-	78,78,78,78	0
59	MG	AA	3342	1/1	0.97	0.23	-	51,51,51,51	0
59	MG	DA	1676	1/1	0.97	0.15	-	74,74,74,74	0
59	MG	AA	3204	1/1	0.93	0.34	-	54,54,54,54	0
59	MG	AA	3057	1/1	0.85	0.18	-	46,46,46,46	0
59	MG	CB	3013	1/1	0.63	0.16	-	100,100,100,100	0
59	MG	AA	3647	1/1	0.96	0.11	-	43,43,43,43	0
59	MG	CA	3187	1/1	0.91	0.23	-	37,37,37,37	0
59	MG	BA	1653	1/1	0.96	0.10	-	56,56,56,56	0
59	MG	AA	3508	1/1	0.95	0.18	-	43,43,43,43	0
59	MG	BA	1635	1/1	0.82	0.52	-	65,65,65,65	0
59	MG	DA	1646	1/1	0.88	0.13	-	57,57,57,57	0
59	MG	AA	3812	1/1	0.95	0.18	-	41,41,41,41	0
59	MG	CA	3476	1/1	0.93	0.17	-	38,38,38,38	0
59	MG	AA	3442	1/1	0.97	0.14	-	23,23,23,23	0
59	MG	CA	3444	1/1	0.91	0.10	-	67,67,67,67	0
59	MG	DA	1734	1/1	0.94	0.14	-	65,65,65,65	0
59	MG	AA	3095	1/1	0.85	0.33	-	75,75,75,75	0
59	MG	AA	3065	1/1	0.87	0.59	-	62,62,62,62	0
59	MG	CA	3256	1/1	0.86	0.30	-	65,65,65,65	0
59	MG	CA	3075	1/1	0.62	0.68	-	90,90,90,90	0
59	MG	AA	3083	1/1	0.85	0.37	-	61,61,61,61	0
59	MG	AA	3024	1/1	0.93	0.13	-	48,48,48,48	0
59	MG	CA	3308	1/1	0.98	0.10	-	39,39,39,39	0
59	MG	CA	3566	1/1	0.83	0.35	-	30,30,30,30	1
59	MG	CA	3488	1/1	0.85	0.15	-	88,88,88,88	0
59	MG	AP	202	1/1	0.88	0.19	-	44,44,44,44	0
59	MG	AA	3077	1/1	0.92	0.28	-	43,43,43,43	0
59	MG	DA	1713	1/1	0.91	0.18	-	49,49,49,49	0
59	MG	AA	3675	1/1	0.81	0.15	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1618	1/1	0.92	0.31	-	52,52,52,52	0
59	MG	AA	3781	1/1	0.91	0.20	-	72,72,72,72	0
59	MG	AA	3558	1/1	0.82	0.08	-	48,48,48,48	0
59	MG	CA	3531	1/1	0.95	0.09	-	47,47,47,47	0
59	MG	CA	3145	1/1	0.81	0.43	-	76,76,76,76	0
59	MG	DA	1637	1/1	0.92	0.40	-	68,68,68,68	0
59	MG	AA	3093	1/1	0.84	1.07	-	92,92,92,92	0
59	MG	BA	1755	1/1	0.38	0.14	-	86,86,86,86	0
59	MG	AA	3104	1/1	0.95	0.33	-	54,54,54,54	0
59	MG	DA	1702	1/1	0.89	0.13	-	63,63,63,63	0
59	MG	AA	3439	1/1	0.98	0.28	-	37,37,37,37	0
59	MG	AA	3010	1/1	0.84	0.45	-	46,46,46,46	0
59	MG	DA	1681	1/1	0.86	0.37	-	70,70,70,70	0
59	MG	AA	3597	1/1	0.98	0.12	-	33,33,33,33	0
59	MG	CA	3051	1/1	0.92	0.76	-	57,57,57,57	0
59	MG	AA	3103	1/1	0.99	0.03	-	5,5,5,5	0
59	MG	AA	3379	1/1	0.97	0.26	-	23,23,23,23	0
59	MG	AA	3538	1/1	0.96	0.15	-	15,15,15,15	0
59	MG	CA	3020	1/1	0.90	0.19	-	47,47,47,47	0
59	MG	CA	3062	1/1	0.96	0.30	-	38,38,38,38	0
59	MG	BA	1629	1/1	0.91	0.29	-	61,61,61,61	0
59	MG	AB	3008	1/1	0.82	0.38	-	52,52,52,52	0
59	MG	AA	3284	1/1	0.91	0.59	-	60,60,60,60	0
59	MG	AA	3689	1/1	0.95	0.09	-	35,35,35,35	0
59	MG	AA	3628	1/1	0.94	0.23	-	70,70,70,70	0
59	MG	CA	3065	1/1	0.87	0.55	-	56,56,56,56	0
59	MG	CA	3391	1/1	0.92	0.07	-	51,51,51,51	0
59	MG	AA	3634	1/1	0.85	0.19	-	76,76,76,76	0
59	MG	DA	1710	1/1	0.94	0.24	-	104,104,104,104	0
59	MG	CA	3040	1/1	0.61	0.49	-	79,79,79,79	0
59	MG	CA	3245	1/1	0.92	0.41	-	62,62,62,62	0
59	MG	DA	1635	1/1	0.90	0.29	-	75,75,75,75	0
59	MG	AE	303	1/1	0.98	0.21	-	19,19,19,19	0
59	MG	AA	3068	1/1	0.87	0.58	-	73,73,73,73	0
59	MG	BA	1614	1/1	0.79	0.14	-	72,72,72,72	0
59	MG	CA	3632	1/1	0.89	0.18	-	74,74,74,74	0
59	MG	AA	3221	1/1	0.94	0.16	-	30,30,30,30	0
59	MG	AA	3603	1/1	0.85	0.63	-	76,76,76,76	0
59	MG	AA	3041	1/1	0.85	0.28	-	37,37,37,37	0
59	MG	CA	3611	1/1	0.96	0.16	-	59,59,59,59	0
59	MG	AQ	204	1/1	0.94	0.23	-	86,86,86,86	0
59	MG	AA	3347	1/1	0.89	0.12	-	88,88,88,88	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3242	1/1	0.63	0.29	-	85,85,85,85	0
59	MG	BA	1638	1/1	0.65	0.21	-	66,66,66,66	0
59	MG	BA	1801	1/1	0.94	0.09	-	65,65,65,65	0
59	MG	AA	3159	1/1	0.97	0.27	-	55,55,55,55	0
59	MG	CA	3517	1/1	0.76	0.16	-	62,62,62,62	0
59	MG	CA	3257	1/1	0.89	0.16	-	35,35,35,35	0
59	MG	CA	3429	1/1	0.94	0.27	-	59,59,59,59	0
59	MG	AA	3735	1/1	0.99	0.14	-	25,25,25,25	0
59	MG	AA	3308	1/1	0.90	0.23	-	18,18,18,18	0
59	MG	BA	1688	1/1	0.99	0.44	-	61,61,61,61	0
59	MG	AA	3066	1/1	0.77	0.14	-	51,51,51,51	0
59	MG	CE	302	1/1	0.96	0.14	-	64,64,64,64	0
59	MG	BA	1695	1/1	0.86	0.08	-	83,83,83,83	0
59	MG	AA	3495	1/1	0.95	0.16	-	35,35,35,35	0
59	MG	BA	1640	1/1	0.98	0.44	-	52,52,52,52	0
59	MG	CA	3605	1/1	0.80	0.21	-	70,70,70,70	0
59	MG	BA	1768	1/1	0.89	0.10	-	64,64,64,64	0
59	MG	AA	3541	1/1	0.66	0.12	-	74,74,74,74	0
59	MG	AA	3170	1/1	0.94	0.19	-	54,54,54,54	0
59	MG	BA	1648	1/1	0.82	0.11	-	74,74,74,74	0
59	MG	CA	3584	1/1	0.96	0.15	-	32,32,32,32	0
59	MG	AA	3240	1/1	0.64	0.17	-	69,69,69,69	0
59	MG	AA	3737	1/1	0.95	0.16	-	54,54,54,54	0
59	MG	AA	3312	1/1	0.96	0.10	-	23,23,23,23	0
59	MG	AA	3353	1/1	0.96	0.22	-	39,39,39,39	0
59	MG	CA	3066	1/1	0.90	0.17	-	69,69,69,69	0
59	MG	AA	3381	1/1	0.98	0.17	-	16,16,16,16	0
59	MG	AA	3070	1/1	0.82	0.42	-	81,81,81,81	0
59	MG	CD	301	1/1	0.96	0.43	-	43,43,43,43	0
59	MG	AA	3663	1/1	0.98	0.20	-	11,11,11,11	0
59	MG	CA	3396	1/1	0.92	0.23	-	39,39,39,39	0
59	MG	CA	3129	1/1	0.89	0.60	-	64,64,64,64	0
59	MG	AY	502	1/1	0.91	0.29	-	60,60,60,60	0
59	MG	AA	3732	1/1	0.78	0.29	-	70,70,70,70	0
59	MG	AA	3370	1/1	0.94	0.16	-	47,47,47,47	0
59	MG	CA	3345	1/1	0.92	0.17	-	46,46,46,46	0
59	MG	CA	3024	1/1	0.95	0.29	-	100,100,100,100	0
59	MG	AA	3168	1/1	0.89	0.32	-	47,47,47,47	0
59	MG	CA	3388	1/1	0.78	0.15	-	90,90,90,90	0
59	MG	CA	3403	1/1	0.92	0.07	-	70,70,70,70	0
59	MG	BA	1662	1/1	0.86	0.75	-	70,70,70,70	0
59	MG	BA	1751	1/1	0.98	0.12	-	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3480	1/1	0.95	0.22	-	50,50,50,50	0
59	MG	CA	3171	1/1	0.90	0.38	-	56,56,56,56	0
59	MG	CA	3609	1/1	0.92	0.16	-	52,52,52,52	0
59	MG	AA	3139	1/1	0.89	0.35	-	60,60,60,60	0
59	MG	AA	3607	1/1	0.90	0.14	-	60,60,60,60	1
59	MG	CA	3121	1/1	0.95	0.14	-	49,49,49,49	0
59	MG	CA	3082	1/1	0.75	0.77	-	76,76,76,76	0
59	MG	DA	1688	1/1	0.93	0.25	-	51,51,51,51	0
59	MG	AA	3783	1/1	0.90	0.47	-	53,53,53,53	1
59	MG	DA	1752	1/1	0.95	0.17	-	52,52,52,52	0
59	MG	DA	1630	1/1	0.96	0.72	-	62,62,62,62	0
59	MG	AA	3582	1/1	0.69	0.59	-	76,76,76,76	0
59	MG	CA	3143	1/1	0.92	0.58	-	41,41,41,41	0
59	MG	CA	3623	1/1	0.90	0.15	-	64,64,64,64	0
59	MG	AA	3804	1/1	0.95	0.19	-	50,50,50,50	0
59	MG	BA	1810	1/1	0.81	0.13	-	82,82,82,82	0
59	MG	AA	3348	1/1	0.95	0.06	-	53,53,53,53	0
59	MG	BA	1799	1/1	0.95	0.13	-	64,64,64,64	0
59	MG	AA	3687	1/1	0.94	0.30	-	52,52,52,52	0
59	MG	BA	1722	1/1	0.98	0.30	-	51,51,51,51	0
59	MG	AA	3281	1/1	0.79	0.29	-	75,75,75,75	0
59	MG	BA	1643	1/1	0.69	0.36	-	66,66,66,66	0
59	MG	AA	3400	1/1	0.95	0.17	-	13,13,13,13	0
59	MG	CA	3585	1/1	0.92	0.16	-	36,36,36,36	1
59	MG	AA	3333	1/1	0.95	0.20	-	11,11,11,11	0
59	MG	AA	3167	1/1	0.78	0.19	-	45,45,45,45	0
59	MG	BA	1682	1/1	0.84	0.84	-	70,70,70,70	0
59	MG	BA	1753	1/1	0.91	0.12	-	48,48,48,48	0
59	MG	BA	1689	1/1	0.81	0.51	-	71,71,71,71	0
59	MG	CA	3072	1/1	0.80	0.36	-	66,66,66,66	0
59	MG	CA	3156	1/1	0.93	0.37	-	52,52,52,52	0
59	MG	CA	3613	1/1	0.98	0.22	-	57,57,57,57	0
59	MG	BA	1651	1/1	0.94	0.34	-	55,55,55,55	0
59	MG	BA	1601	1/1	0.73	0.33	-	95,95,95,95	0
59	MG	DA	1679	1/1	0.87	0.12	-	70,70,70,70	0
59	MG	CA	3001	1/1	0.83	0.25	-	64,64,64,64	0
59	MG	DA	1763	1/1	0.95	0.31	-	76,76,76,76	0
59	MG	AA	3554	1/1	0.97	0.20	-	40,40,40,40	0
59	MG	AA	3707	1/1	0.92	0.09	-	59,59,59,59	0
59	MG	CA	3578	1/1	0.94	0.09	-	38,38,38,38	0
59	MG	AA	3220	1/1	0.98	0.15	-	62,62,62,62	0
59	MG	BA	1658	1/1	0.87	0.62	-	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3122	1/1	0.53	0.70	-	99,99,99,99	0
59	MG	CA	3536	1/1	0.72	0.26	-	84,84,84,84	0
59	MG	BA	1778	1/1	0.79	0.16	-	54,54,54,54	0
59	MG	AA	3601	1/1	0.82	0.11	-	61,61,61,61	0
59	MG	AA	3567	1/1	0.96	0.12	-	26,26,26,26	0
59	MG	CA	3538	1/1	0.70	0.15	-	72,72,72,72	0
59	MG	AA	3750	1/1	0.96	0.34	-	51,51,51,51	0
59	MG	CA	3180	1/1	0.79	0.36	-	62,62,62,62	0
59	MG	AW	3002	1/1	0.81	0.26	-	47,47,47,47	0
59	MG	AA	3087	1/1	0.82	0.47	-	55,55,55,55	0
59	MG	CA	3582	1/1	0.90	0.08	-	99,99,99,99	0
59	MG	BA	1775	1/1	0.57	0.35	-	90,90,90,90	0
59	MG	AA	3728	1/1	0.96	0.26	-	29,29,29,29	0
59	MG	AA	3650	1/1	0.97	0.12	-	49,49,49,49	0
59	MG	AA	3219	1/1	0.80	0.23	-	61,61,61,61	0
59	MG	AA	3116	1/1	0.96	0.63	-	35,35,35,35	0
59	MG	AA	3263	1/1	0.96	0.42	-	24,24,24,24	1
59	MG	CA	3185	1/1	0.95	0.30	-	48,48,48,48	0
59	MG	CA	3286	1/1	0.96	0.20	-	58,58,58,58	0
59	MG	BA	1664	1/1	0.94	0.14	-	56,56,56,56	0
59	MG	BD	502	1/1	0.86	0.55	-	64,64,64,64	0
59	MG	CA	3336	1/1	0.88	0.09	-	64,64,64,64	0
59	MG	DA	1748	1/1	0.92	0.18	-	70,70,70,70	0
59	MG	AA	3472	1/1	0.91	0.23	-	42,42,42,42	0
59	MG	CA	3400	1/1	0.98	0.14	-	57,57,57,57	0
59	MG	AA	3572	1/1	0.94	0.20	-	17,17,17,17	0
59	MG	CA	3602	1/1	0.75	0.10	-	84,84,84,84	0
59	MG	BA	1678	1/1	0.96	0.21	-	54,54,54,54	0
59	MG	AA	3581	1/1	0.96	0.17	-	52,52,52,52	0
59	MG	AA	3645	1/1	0.92	0.21	-	58,58,58,58	0
59	MG	CA	3493	1/1	0.94	0.54	-	65,65,65,65	0
59	MG	AA	3268	1/1	0.92	0.07	-	66,66,66,66	0
59	MG	CA	3495	1/1	0.88	0.22	-	70,70,70,70	0
59	MG	CP	201	1/1	0.65	0.17	-	62,62,62,62	1
59	MG	AA	3356	1/1	0.93	0.15	-	80,80,80,80	0
59	MG	AA	3637	1/1	0.95	0.32	-	17,17,17,17	1
59	MG	AA	3322	1/1	0.96	0.20	-	61,61,61,61	0
59	MG	AA	3724	1/1	0.88	0.24	-	47,47,47,47	0
59	MG	CA	3607	1/1	0.94	0.09	-	64,64,64,64	0
59	MG	CA	3533	1/1	0.94	0.18	-	45,45,45,45	0
59	MG	AA	3108	1/1	0.40	0.64	-	101,101,101,101	0
59	MG	CA	3511	1/1	0.87	0.20	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1718	1/1	0.91	0.09	-	63,63,63,63	0
59	MG	AN	3001	1/1	0.92	0.32	-	58,58,58,58	0
59	MG	DA	1620	1/1	0.91	0.22	-	57,57,57,57	0
59	MG	AA	3153	1/1	0.88	0.33	-	59,59,59,59	0
59	MG	AA	3784	1/1	0.94	0.21	-	59,59,59,59	0
59	MG	BA	1784	1/1	0.86	0.27	-	68,68,68,68	0
59	MG	AA	3015	1/1	0.87	0.36	-	57,57,57,57	0
59	MG	AA	3726	1/1	0.99	0.17	-	12,12,12,12	0
59	MG	AA	3693	1/1	0.82	0.14	-	69,69,69,69	0
59	MG	AA	3550	1/1	0.96	0.20	-	38,38,38,38	0
59	MG	CA	3622	1/1	0.94	0.18	-	50,50,50,50	0
59	MG	AA	3808	1/1	0.84	0.41	-	72,72,72,72	0
59	MG	AA	3148	1/1	0.94	0.44	-	29,29,29,29	1
59	MG	AA	3270	1/1	0.91	0.57	-	55,55,55,55	0
59	MG	AB	3015	1/1	0.97	0.14	-	28,28,28,28	0
59	MG	DA	1739	1/1	0.88	0.13	-	73,73,73,73	0
59	MG	CA	3363	1/1	0.84	0.17	-	88,88,88,88	0
59	MG	BA	1716	1/1	0.73	0.24	-	86,86,86,86	0
59	MG	CA	3435	1/1	0.98	0.11	-	55,55,55,55	0
59	MG	AA	3716	1/1	0.92	0.25	-	66,66,66,66	0
59	MG	CA	3408	1/1	0.85	0.12	-	58,58,58,58	0
59	MG	A2	3001	1/1	0.87	0.25	-	53,53,53,53	0
59	MG	DA	1662	1/1	0.86	0.23	-	75,75,75,75	0
59	MG	AA	3499	1/1	0.89	0.14	-	48,48,48,48	0
59	MG	CA	3341	1/1	0.85	0.35	-	73,73,73,73	0
59	MG	AA	3026	1/1	0.84	0.23	-	47,47,47,47	0
59	MG	CA	3034	1/1	0.79	0.30	-	77,77,77,77	0
59	MG	AA	3040	1/1	0.41	0.17	-	113,113,113,113	0
59	MG	CA	3219	1/1	0.97	0.25	-	42,42,42,42	0
59	MG	AA	3468	1/1	0.96	0.06	-	55,55,55,55	0
59	MG	CA	3290	1/1	0.96	0.34	-	34,34,34,34	0
59	MG	CA	3014	1/1	0.85	0.25	-	50,50,50,50	0
59	MG	AA	3788	1/1	0.88	0.29	-	61,61,61,61	0
59	MG	BA	1703	1/1	0.88	0.30	-	51,51,51,51	0
59	MG	AA	3247	1/1	0.96	0.16	-	55,55,55,55	0
59	MG	AA	3756	1/1	0.89	0.15	-	49,49,49,49	0
59	MG	AA	3162	1/1	0.89	0.26	-	67,67,67,67	0
59	MG	AA	3615	1/1	0.94	0.26	-	43,43,43,43	0
59	MG	CA	3377	1/1	0.83	0.10	-	52,52,52,52	0
59	MG	AA	3181	1/1	0.78	0.34	-	79,79,79,79	0
59	MG	DA	1660	1/1	0.86	0.14	-	80,80,80,80	0
59	MG	AA	3451	1/1	0.94	0.07	-	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3341	1/1	0.97	0.19	-	25,25,25,25	0
59	MG	CA	3649	1/1	0.88	0.25	-	51,51,51,51	0
59	MG	AB	3017	1/1	0.58	0.17	-	59,59,59,59	0
59	MG	CA	3316	1/1	0.95	0.17	-	43,43,43,43	0
59	MG	AA	3786	1/1	0.84	0.17	-	53,53,53,53	0
59	MG	AA	3258	1/1	0.82	0.44	-	68,68,68,68	0
59	MG	CA	3575	1/1	0.82	0.21	-	71,71,71,71	0
59	MG	BL	201	1/1	0.66	0.37	-	84,84,84,84	0
59	MG	AA	3778	1/1	0.98	0.14	-	43,43,43,43	0
59	MG	CA	3347	1/1	0.96	0.15	-	45,45,45,45	0
59	MG	DA	1631	1/1	0.76	0.09	-	74,74,74,74	0
59	MG	AA	3365	1/1	0.94	0.40	-	77,77,77,77	0
59	MG	DA	1684	1/1	0.90	0.18	-	69,69,69,69	0
59	MG	DA	1725	1/1	0.95	0.17	-	58,58,58,58	0
59	MG	AA	3173	1/1	0.94	0.29	-	46,46,46,46	0
59	MG	AA	3430	1/1	0.97	0.16	-	39,39,39,39	0
59	MG	CA	3411	1/1	0.87	0.25	-	57,57,57,57	0
59	MG	AA	3298	1/1	0.97	0.16	-	58,58,58,58	0
59	MG	DA	1770	1/1	0.84	0.15	-	63,63,63,63	0
59	MG	CA	3202	1/1	0.81	0.73	-	73,73,73,73	0
59	MG	BA	1719	1/1	0.84	0.16	-	62,62,62,62	0
59	MG	CA	3631	1/1	0.81	0.11	-	65,65,65,65	0
59	MG	AA	3025	1/1	0.87	0.43	-	68,68,68,68	0
59	MG	AA	3470	1/1	0.98	0.08	-	39,39,39,39	0
59	MG	AA	3336	1/1	0.96	0.14	-	51,51,51,51	0
59	MG	AA	3734	1/1	0.98	0.25	-	26,26,26,26	0
59	MG	CA	3551	1/1	0.87	0.07	-	63,63,63,63	0
59	MG	AA	3455	1/1	0.94	0.19	-	32,32,32,32	1
59	MG	BA	1699	1/1	0.90	0.19	-	72,72,72,72	0
59	MG	CA	3088	1/1	0.85	0.32	-	67,67,67,67	0
59	MG	CA	3148	1/1	0.91	0.34	-	62,62,62,62	0
59	MG	DA	1707	1/1	0.95	0.07	-	61,61,61,61	0
59	MG	CA	3305	1/1	0.95	0.28	-	48,48,48,48	0
59	MG	AA	3231	1/1	0.93	0.21	-	64,64,64,64	0
59	MG	CA	3356	1/1	0.95	0.19	-	44,44,44,44	0
59	MG	CA	3196	1/1	0.94	0.68	-	68,68,68,68	0
59	MG	CA	3633	1/1	0.84	0.27	-	68,68,68,68	0
59	MG	AA	3114	1/1	0.95	0.21	-	26,26,26,26	0
59	MG	CA	3593	1/1	0.89	0.61	-	61,61,61,61	0
59	MG	CA	3546	1/1	0.56	0.15	-	88,88,88,88	0
59	MG	DA	1751	1/1	0.92	0.17	-	64,64,64,64	0
59	MG	AA	3046	1/1	0.93	0.34	-	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3697	1/1	0.95	0.24	-	40,40,40,40	0
59	MG	AA	3586	1/1	0.80	0.36	-	74,74,74,74	0
59	MG	CA	3475	1/1	0.97	0.26	-	50,50,50,50	0
59	MG	AA	3056	1/1	0.83	1.09	-	96,96,96,96	0
59	MG	BA	1650	1/1	0.92	0.15	-	55,55,55,55	0
59	MG	DA	1645	1/1	0.96	0.10	-	58,58,58,58	0
59	MG	AA	3061	1/1	0.84	0.59	-	59,59,59,59	0
59	MG	BA	1708	1/1	0.91	0.23	-	64,64,64,64	0
59	MG	BA	1773	1/1	0.97	0.14	-	40,40,40,40	0
59	MG	AB	3019	1/1	0.97	0.12	-	70,70,70,70	0
59	MG	CA	3393	1/1	0.94	0.07	-	68,68,68,68	0
59	MG	AA	3761	1/1	0.80	0.39	-	92,92,92,92	0
59	MG	CA	3580	1/1	0.91	0.24	-	76,76,76,76	0
59	MG	AA	3525	1/1	0.97	0.18	-	35,35,35,35	0
59	MG	AA	3210	1/1	0.96	0.31	-	59,59,59,59	1
59	MG	CA	3260	1/1	0.87	0.15	-	35,35,35,35	0
59	MG	BA	1637	1/1	0.91	0.47	-	72,72,72,72	0
59	MG	AA	3595	1/1	0.98	0.15	-	42,42,42,42	0
59	MG	AA	3135	1/1	0.91	0.55	-	55,55,55,55	0
59	MG	BA	1770	1/1	0.96	0.13	-	54,54,54,54	0
59	MG	AA	3516	1/1	0.91	0.24	-	65,65,65,65	0
59	MG	AA	3564	1/1	0.96	0.21	-	44,44,44,44	0
59	MG	CA	3654	1/1	0.66	0.40	-	90,90,90,90	0
59	MG	AA	3196	1/1	0.88	0.20	-	55,55,55,55	0
59	MG	CA	3092	1/1	0.78	0.82	-	79,79,79,79	0
59	MG	CA	3042	1/1	0.90	0.31	-	65,65,65,65	0
59	MG	DA	1623	1/1	0.64	0.25	-	72,72,72,72	0
59	MG	CA	3246	1/1	0.87	0.51	-	57,57,57,57	0
59	MG	AA	3618	1/1	0.90	0.16	-	72,72,72,72	0
59	MG	AQ	201	1/1	0.97	0.44	-	48,48,48,48	0
59	MG	AP	203	1/1	0.84	0.19	-	59,59,59,59	0
59	MG	CA	3102	1/1	0.96	0.50	-	62,62,62,62	0
59	MG	CA	3130	1/1	0.85	0.17	-	55,55,55,55	0
59	MG	AA	3802	1/1	0.95	0.15	-	86,86,86,86	0
59	MG	AA	3478	1/1	0.95	0.24	-	33,33,33,33	0
59	MG	AA	3605	1/1	0.96	0.33	-	45,45,45,45	0
59	MG	CA	3430	1/1	0.93	0.36	-	41,41,41,41	0
59	MG	DA	1758	1/1	0.93	0.18	-	75,75,75,75	0
59	MG	AA	3580	1/1	0.94	0.22	-	54,54,54,54	0
59	MG	DA	1675	1/1	0.91	0.42	-	70,70,70,70	0
59	MG	AA	3797	1/1	0.92	0.18	-	52,52,52,52	0
59	MG	AA	3132	1/1	0.95	0.22	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CQ	203	1/1	0.88	0.35	-	54,54,54,54	0
59	MG	CA	3496	1/1	0.88	0.13	-	56,56,56,56	0
59	MG	CA	3165	1/1	0.85	0.25	-	57,57,57,57	0
59	MG	AA	3755	1/1	0.97	0.65	-	78,78,78,78	0
59	MG	AA	3662	1/1	0.94	0.07	-	60,60,60,60	0
59	MG	AA	3358	1/1	0.91	0.12	-	45,45,45,45	0
59	MG	AA	3248	1/1	0.99	0.14	-	22,22,22,22	0
59	MG	CA	3567	1/1	0.98	0.23	-	26,26,26,26	0
59	MG	CA	3244	1/1	0.53	0.31	-	89,89,89,89	0
59	MG	AA	3664	1/1	0.88	0.21	-	62,62,62,62	0
59	MG	AA	3078	1/1	0.91	0.33	-	70,70,70,70	0
59	MG	CA	3295	1/1	0.96	0.25	-	66,66,66,66	0
59	MG	CA	3080	1/1	0.57	0.24	-	75,75,75,75	0
59	MG	BW	503	1/1	0.88	0.21	-	60,60,60,60	0
59	MG	CD	303	1/1	0.92	0.08	-	70,70,70,70	0
59	MG	CA	3656	1/1	0.86	0.57	-	63,63,63,63	0
59	MG	AA	3433	1/1	0.98	0.14	-	37,37,37,37	0
59	MG	CA	3335	1/1	0.96	0.20	-	66,66,66,66	0
59	MG	CA	3011	1/1	0.97	0.39	-	63,63,63,63	0
59	MG	AA	3435	1/1	0.96	0.18	-	52,52,52,52	0
59	MG	BA	1798	1/1	0.96	0.43	-	73,73,73,73	0
59	MG	CA	3135	1/1	0.72	0.32	-	59,59,59,59	0
59	MG	AA	3119	1/1	0.96	0.32	-	47,47,47,47	0
59	MG	AA	3385	1/1	0.89	0.21	-	49,49,49,49	0
59	MG	BA	1608	1/1	0.90	0.55	-	57,57,57,57	0
59	MG	AA	3609	1/1	0.93	0.11	-	58,58,58,58	0
59	MG	BA	1622	1/1	0.87	0.53	-	65,65,65,65	0
59	MG	DA	1656	1/1	0.83	0.13	-	63,63,63,63	0
59	MG	AA	3229	1/1	0.87	0.36	-	67,67,67,67	0
59	MG	AA	3256	1/1	0.90	0.35	-	49,49,49,49	0
59	MG	CA	3350	1/1	0.74	0.09	-	82,82,82,82	0
59	MG	BA	1752	1/1	0.97	0.28	-	59,59,59,59	0
59	MG	BA	1729	1/1	0.84	0.16	-	53,53,53,53	0
59	MG	CA	3591	1/1	0.79	0.12	-	60,60,60,60	0
59	MG	CA	3050	1/1	0.81	0.46	-	75,75,75,75	0
59	MG	CA	3186	1/1	0.58	0.61	-	77,77,77,77	0
59	MG	AA	3154	1/1	0.98	0.19	-	57,57,57,57	0
59	MG	AA	3194	1/1	0.88	0.25	-	82,82,82,82	0
59	MG	BS	101	1/1	0.80	0.16	-	79,79,79,79	0
59	MG	CA	3271	1/1	0.91	0.18	-	48,48,48,48	0
59	MG	CA	3548	1/1	0.70	0.09	-	90,90,90,90	0
59	MG	CA	3251	1/1	0.85	0.18	-	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3610	1/1	0.94	0.23	-	59,59,59,59	0
59	MG	CA	3541	1/1	0.77	0.28	-	63,63,63,63	0
59	MG	AA	3807	1/1	0.50	0.32	-	77,77,77,77	0
59	MG	AA	3719	1/1	0.94	0.10	-	59,59,59,59	0
59	MG	AA	3668	1/1	0.96	0.17	-	54,54,54,54	0
59	MG	AA	3285	1/1	0.88	0.30	-	51,51,51,51	0
59	MG	CA	3149	1/1	0.60	0.17	-	100,100,100,100	0
59	MG	DA	1720	1/1	0.96	0.10	-	60,60,60,60	0
59	MG	CA	3354	1/1	0.95	0.26	-	49,49,49,49	0
59	MG	DA	1709	1/1	0.94	0.16	-	70,70,70,70	0
59	MG	A5	502	1/1	0.94	0.16	-	51,51,51,51	0
59	MG	CA	3456	1/1	0.84	0.09	-	54,54,54,54	0
59	MG	CB	3002	1/1	0.90	0.10	-	63,63,63,63	0
59	MG	AA	3790	1/1	0.95	0.46	-	57,57,57,57	0
59	MG	DA	1746	1/1	0.66	0.10	-	81,81,81,81	0
59	MG	CA	3422	1/1	0.97	0.24	-	43,43,43,43	0
59	MG	CA	3109	1/1	0.97	0.22	-	35,35,35,35	0
59	MG	AA	3202	1/1	0.87	0.11	-	61,61,61,61	0
59	MG	BA	1806	1/1	0.90	0.34	-	55,55,55,55	0
59	MG	BA	1657	1/1	0.47	0.25	-	78,78,78,78	0
59	MG	BA	1710	1/1	0.93	0.24	-	81,81,81,81	0
59	MG	AA	3346	1/1	0.99	0.14	-	59,59,59,59	0
59	MG	AA	3665	1/1	0.97	0.31	-	40,40,40,40	0
59	MG	BA	1624	1/1	0.84	0.18	-	58,58,58,58	0
59	MG	AA	3063	1/1	0.93	0.27	-	54,54,54,54	0
59	MG	CA	3395	1/1	0.86	0.42	-	50,50,50,50	0
59	MG	AA	3692	1/1	0.96	0.15	-	36,36,36,36	1
59	MG	AA	3686	1/1	0.95	0.21	-	61,61,61,61	0
59	MG	AA	3703	1/1	0.96	0.23	-	56,56,56,56	0
59	MG	CA	3176	1/1	0.83	0.43	-	60,60,60,60	0
59	MG	DA	1740	1/1	0.96	0.58	-	68,68,68,68	0
59	MG	DA	1695	1/1	0.94	0.18	-	63,63,63,63	0
59	MG	CA	3142	1/1	0.94	0.45	-	61,61,61,61	0
59	MG	CA	3639	1/1	0.95	0.61	-	61,61,61,61	0
59	MG	CA	3329	1/1	0.98	0.14	-	21,21,21,21	0
59	MG	CA	3470	1/1	0.94	0.20	-	74,74,74,74	0
59	MG	CA	3520	1/1	0.92	0.16	-	73,73,73,73	0
59	MG	AA	3699	1/1	0.88	0.28	-	71,71,71,71	0
59	MG	AZ	301	1/1	0.93	0.15	-	55,55,55,55	0
59	MG	DA	1619	1/1	0.95	0.60	-	59,59,59,59	0
59	MG	AA	3500	1/1	0.96	0.12	-	59,59,59,59	0
59	MG	AA	3309	1/1	0.97	0.25	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3295	1/1	0.89	0.14	-	57,57,57,57	0
59	MG	BA	1683	1/1	0.87	0.22	-	71,71,71,71	0
59	MG	AA	3354	1/1	0.99	0.12	-	27,27,27,27	0
59	MG	AA	3796	1/1	0.88	0.51	-	78,78,78,78	0
59	MG	BA	1724	1/1	0.92	0.20	-	67,67,67,67	0
59	MG	CA	3586	1/1	0.90	0.17	-	93,93,93,93	0
59	MG	CA	3057	1/1	0.88	0.30	-	60,60,60,60	0
59	MG	AA	3395	1/1	0.97	0.17	-	54,54,54,54	0
59	MG	AA	3791	1/1	0.96	0.18	-	51,51,51,51	0
59	MG	AA	3748	1/1	0.93	0.20	-	45,45,45,45	0
59	MG	BA	1781	1/1	0.94	0.15	-	63,63,63,63	0
59	MG	AA	3573	1/1	0.94	0.16	-	12,12,12,12	0
59	MG	CB	3009	1/1	0.97	0.19	-	67,67,67,67	0
59	MG	CD	302	1/1	0.83	0.54	-	56,56,56,56	0
59	MG	AA	3091	1/1	0.99	0.76	-	47,47,47,47	1
59	MG	CA	3078	1/1	0.81	0.49	-	57,57,57,57	0
59	MG	CA	3338	1/1	0.96	0.14	-	64,64,64,64	0
59	MG	CA	3016	1/1	0.85	0.26	-	52,52,52,52	0
59	MG	CA	3512	1/1	0.91	0.15	-	53,53,53,53	0
59	MG	CA	3394	1/1	0.96	0.13	-	69,69,69,69	0
59	MG	AA	3197	1/1	0.87	0.20	-	45,45,45,45	0
59	MG	CA	3507	1/1	0.85	0.27	-	83,83,83,83	0
59	MG	BA	1733	1/1	0.91	0.21	-	78,78,78,78	0
59	MG	CA	3414	1/1	0.93	0.19	-	34,34,34,34	1
59	MG	DA	1658	1/1	0.89	0.33	-	51,51,51,51	0
59	MG	AA	3331	1/1	0.86	0.17	-	15,15,15,15	0
59	MG	AB	3005	1/1	0.97	0.20	-	44,44,44,44	0
59	MG	DZ	702	1/1	0.96	0.22	-	57,57,57,57	0
59	MG	BA	1673	1/1	0.61	0.21	-	80,80,80,80	0
59	MG	AA	3491	1/1	0.96	0.09	-	46,46,46,46	0
59	MG	CA	3374	1/1	0.91	0.31	-	60,60,60,60	0
59	MG	CA	3128	1/1	0.92	0.40	-	50,50,50,50	0
59	MG	A7	101	1/1	0.82	0.16	-	55,55,55,55	0
59	MG	BA	1661	1/1	0.89	0.33	-	63,63,63,63	0
59	MG	AA	3677	1/1	0.87	0.10	-	69,69,69,69	0
59	MG	AA	3089	1/1	0.94	0.30	-	49,49,49,49	0
59	MG	CA	3073	1/1	0.93	0.28	-	49,49,49,49	0
59	MG	DA	1705	1/1	0.91	0.10	-	68,68,68,68	0
59	MG	CA	3471	1/1	0.96	0.19	-	33,33,33,33	0
59	MG	CA	3098	1/1	0.87	0.14	-	70,70,70,70	0
59	MG	AA	3717	1/1	0.70	0.56	-	68,68,68,68	0
59	MG	BA	1644	1/1	0.78	0.18	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3410	1/1	0.99	0.15	-	57,57,57,57	0
59	MG	DF	3001	1/1	0.90	0.20	-	54,54,54,54	0
59	MG	DA	1694	1/1	0.91	0.35	-	106,106,106,106	0
59	MG	CA	3402	1/1	0.94	0.09	-	66,66,66,66	0
59	MG	CA	3188	1/1	0.94	0.83	-	94,94,94,94	0
59	MG	AA	3251	1/1	0.94	0.36	-	56,56,56,56	0
59	MG	DA	1729	1/1	0.85	0.17	-	49,49,49,49	0
59	MG	DA	1728	1/1	0.92	0.08	-	71,71,71,71	0
59	MG	AA	3273	1/1	0.79	0.76	-	90,90,90,90	0
59	MG	AA	3383	1/1	0.96	0.16	-	20,20,20,20	0
59	MG	AA	3126	1/1	0.86	0.37	-	79,79,79,79	0
59	MG	AA	3484	1/1	0.98	0.11	-	53,53,53,53	0
59	MG	CA	3443	1/1	0.98	0.18	-	28,28,28,28	0
59	MG	AW	3001	1/1	0.89	0.29	-	54,54,54,54	0
59	MG	DA	1674	1/1	0.77	0.28	-	77,77,77,77	0
59	MG	CA	3003	1/1	0.94	0.31	-	62,62,62,62	0
59	MG	CA	3134	1/1	0.90	0.69	-	71,71,71,71	0
59	MG	AA	3638	1/1	0.91	0.36	-	71,71,71,71	0
59	MG	AA	3681	1/1	0.97	0.13	-	42,42,42,42	0
59	MG	CA	3587	1/1	0.67	0.33	-	70,70,70,70	0
59	MG	CA	3477	1/1	0.90	0.15	-	69,69,69,69	0
59	MG	AA	3524	1/1	0.97	0.19	-	41,41,41,41	0
59	MG	AA	3088	1/1	0.90	0.43	-	39,39,39,39	0
59	MG	BA	1785	1/1	0.97	0.18	-	62,62,62,62	0
59	MG	CB	3011	1/1	0.88	0.23	-	56,56,56,56	0
59	MG	DA	1701	1/1	0.90	0.24	-	68,68,68,68	0
59	MG	DA	1760	1/1	0.95	0.14	-	61,61,61,61	0
59	MG	BA	1666	1/1	0.92	0.38	-	61,61,61,61	0
59	MG	AA	3329	1/1	0.96	0.08	-	40,40,40,40	1
59	MG	AA	3591	1/1	0.90	0.27	-	52,52,52,52	0
59	MG	AA	3507	1/1	0.96	0.15	-	50,50,50,50	0
59	MG	AA	3394	1/1	0.92	0.17	-	39,39,39,39	0
59	MG	AA	3293	1/1	0.88	0.15	-	27,27,27,27	0
59	MG	AA	3557	1/1	0.89	0.20	-	37,37,37,37	0
59	MG	AA	3098	1/1	0.97	0.28	-	51,51,51,51	0
59	MG	DA	1677	1/1	0.91	0.42	-	78,78,78,78	0
59	MG	DA	1738	1/1	0.29	0.47	-	95,95,95,95	0
59	MG	BA	1802	1/1	0.71	0.24	-	76,76,76,76	0
59	MG	AA	3206	1/1	0.81	0.55	-	106,106,106,106	0
59	MG	CA	3379	1/1	0.85	0.23	-	83,83,83,83	0
59	MG	AA	3661	1/1	0.92	0.24	-	41,41,41,41	1
59	MG	AA	3574	1/1	0.96	0.17	-	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3678	1/1	0.92	0.15	-	77,77,77,77	0
59	MG	AA	3138	1/1	0.89	0.13	-	38,38,38,38	0
59	MG	AA	3212	1/1	0.45	0.85	-	81,81,81,81	0
59	MG	AA	3211	1/1	0.91	0.28	-	56,56,56,56	0
59	MG	DA	1698	1/1	0.94	0.33	-	97,97,97,97	0
59	MG	CA	3074	1/1	0.96	0.34	-	49,49,49,49	0
59	MG	CA	3307	1/1	0.80	0.31	-	60,60,60,60	0
59	MG	AA	3700	1/1	0.90	0.22	-	70,70,70,70	0
59	MG	CA	3577	1/1	0.85	0.16	-	51,51,51,51	1
59	MG	CA	3465	1/1	0.90	0.31	-	70,70,70,70	0
59	MG	BA	1772	1/1	0.84	0.12	-	66,66,66,66	0
59	MG	AA	3751	1/1	0.86	0.34	-	61,61,61,61	0
59	MG	AA	3450	1/1	0.83	0.10	-	58,58,58,58	0
59	MG	DA	1691	1/1	0.92	0.18	-	63,63,63,63	0
59	MG	AA	3290	1/1	0.95	0.13	-	64,64,64,64	0
59	MG	AA	3227	1/1	0.81	0.19	-	22,22,22,22	0
59	MG	AA	3096	1/1	0.93	0.20	-	59,59,59,59	0
59	MG	CA	3494	1/1	0.78	0.23	-	97,97,97,97	0
59	MG	DA	1654	1/1	0.70	0.36	-	63,63,63,63	0
59	MG	DA	1732	1/1	0.84	0.15	-	85,85,85,85	0
59	MG	DA	1767	1/1	0.89	0.13	-	74,74,74,74	0
59	MG	BA	1685	1/1	0.85	0.14	-	50,50,50,50	0
59	MG	AA	3243	1/1	0.98	0.23	-	43,43,43,43	0
59	MG	CA	3111	1/1	0.85	0.25	-	79,79,79,79	0
59	MG	AA	3149	1/1	0.81	0.32	-	51,51,51,51	0
59	MG	BA	1734	1/1	0.93	0.14	-	61,61,61,61	0
59	MG	BA	1674	1/1	0.95	0.59	-	48,48,48,48	0
59	MG	DA	1613	1/1	0.92	0.25	-	48,48,48,48	0
59	MG	DA	1765	1/1	0.96	0.13	-	64,64,64,64	0
59	MG	AA	3679	1/1	0.90	0.08	-	36,36,36,36	0
59	MG	AA	3680	1/1	0.69	0.33	-	79,79,79,79	0
59	MG	A8	5001	1/1	0.94	0.28	-	30,30,30,30	0
59	MG	AA	3644	1/1	0.77	0.33	-	56,56,56,56	0
59	MG	BA	1654	1/1	0.67	0.23	-	76,76,76,76	0
59	MG	CA	3340	1/1	0.86	0.17	-	66,66,66,66	0
59	MG	AO	5001	1/1	0.95	0.10	-	34,34,34,34	0
59	MG	CA	3173	1/1	0.88	0.38	-	61,61,61,61	0
59	MG	AA	3559	1/1	0.97	0.24	-	46,46,46,46	0
59	MG	AA	3545	1/1	0.98	0.19	-	43,43,43,43	0
59	MG	AA	3366	1/1	0.97	0.24	-	35,35,35,35	1
59	MG	CA	3625	1/1	0.89	0.27	-	64,64,64,64	0
59	MG	AA	3759	1/1	0.94	0.11	-	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3160	1/1	0.95	0.16	-	30,30,30,30	0
59	MG	AA	3492	1/1	0.90	0.19	-	26,26,26,26	0
59	MG	CA	3327	1/1	0.96	0.16	-	38,38,38,38	0
59	MG	CA	3431	1/1	0.92	0.21	-	75,75,75,75	0
59	MG	BA	1796	1/1	0.89	0.27	-	57,57,57,57	0
59	MG	AA	3810	1/1	0.90	0.26	-	67,67,67,67	0
59	MG	CA	3053	1/1	0.97	0.47	-	32,32,32,32	0
59	MG	BA	1738	1/1	0.90	0.08	-	66,66,66,66	0
59	MG	CA	3153	1/1	0.84	0.23	-	73,73,73,73	0
59	MG	BA	1790	1/1	0.61	0.15	-	96,96,96,96	0
59	MG	BA	1606	1/1	0.96	0.29	-	126,126,126,126	0
59	MG	AA	3092	1/1	0.95	0.17	-	39,39,39,39	0
59	MG	BA	1646	1/1	0.85	0.97	-	66,66,66,66	0
59	MG	CA	3485	1/1	0.56	0.31	-	85,85,85,85	0
59	MG	CA	3418	1/1	0.96	0.29	-	34,34,34,34	0
59	MG	CA	3579	1/1	0.70	0.23	-	65,65,65,65	0
59	MG	CA	3289	1/1	0.80	0.28	-	65,65,65,65	0
59	MG	CA	3114	1/1	0.88	0.19	-	66,66,66,66	0
59	MG	CA	3501	1/1	0.70	0.46	-	74,74,74,74	0
59	MG	CA	3424	1/1	0.97	0.19	-	66,66,66,66	0
59	MG	DA	1636	1/1	0.86	0.51	-	62,62,62,62	0
59	MG	BA	1797	1/1	0.90	0.18	-	59,59,59,59	0
59	MG	AA	3296	1/1	0.72	0.25	-	67,67,67,67	0
59	MG	AA	3617	1/1	0.54	0.15	-	77,77,77,77	0
59	MG	AA	3787	1/1	0.90	0.20	-	82,82,82,82	0
59	MG	BA	1779	1/1	0.89	0.19	-	85,85,85,85	0
59	MG	DA	1643	1/1	0.85	0.24	-	79,79,79,79	0
59	MG	AB	3002	1/1	0.93	0.17	-	52,52,52,52	0
59	MG	AA	3419	1/1	0.97	0.17	-	20,20,20,20	0
59	MG	CA	3629	1/1	0.84	0.08	-	55,55,55,55	0
59	MG	CA	3193	1/1	0.83	0.45	-	89,89,89,89	0
59	MG	CB	3012	1/1	0.87	0.27	-	62,62,62,62	0
59	MG	CB	3010	1/1	0.96	0.13	-	51,51,51,51	0
59	MG	AA	3340	1/1	0.96	0.23	-	3,3,3,3	0
59	MG	CA	3119	1/1	0.97	0.55	-	55,55,55,55	0
59	MG	AA	3431	1/1	0.95	0.16	-	25,25,25,25	0
59	MG	AA	3533	1/1	0.95	0.17	-	22,22,22,22	0
59	MG	DA	1624	1/1	0.84	0.12	-	82,82,82,82	0
59	MG	AA	3646	1/1	0.93	0.23	-	53,53,53,53	0
59	MG	AA	3635	1/1	0.89	0.32	-	49,49,49,49	0
59	MG	DA	1754	1/1	0.48	0.40	-	120,120,120,120	0
59	MG	AA	3271	1/1	0.95	0.34	-	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	1741	1/1	0.62	0.19	-	88,88,88,88	0
59	MG	CA	3152	1/1	0.72	0.35	-	64,64,64,64	0
59	MG	CA	3234	1/1	0.91	0.36	-	50,50,50,50	0
59	MG	BA	1791	1/1	0.85	0.18	-	72,72,72,72	0
59	MG	CA	3023	1/1	0.83	0.44	-	68,68,68,68	0
59	MG	DA	1606	1/1	0.91	0.31	-	85,85,85,85	0
59	MG	AA	3260	1/1	0.95	0.17	-	21,21,21,21	0
59	MG	AA	3639	1/1	0.97	0.13	-	18,18,18,18	0
59	MG	CA	3648	1/1	0.98	0.35	-	52,52,52,52	0
59	MG	DA	1659	1/1	0.68	0.29	-	78,78,78,78	0
59	MG	BA	1639	1/1	0.93	0.47	-	61,61,61,61	0
59	MG	BA	1715	1/1	0.96	0.12	-	60,60,60,60	0
59	MG	CA	3482	1/1	0.97	0.17	-	61,61,61,61	0
59	MG	AA	3754	1/1	0.57	0.26	-	64,64,64,64	0
59	MG	CA	3099	1/1	0.96	0.26	-	58,58,58,58	0
59	MG	BA	1707	1/1	0.76	0.11	-	72,72,72,72	0
59	MG	AA	3801	1/1	0.99	0.15	-	27,27,27,27	0
59	MG	DA	1611	1/1	0.72	0.39	-	89,89,89,89	0
59	MG	CA	3183	1/1	0.93	0.21	-	49,49,49,49	0
59	MG	CA	3044	1/1	0.78	0.21	-	89,89,89,89	0
59	MG	CA	3249	1/1	0.91	0.16	-	61,61,61,61	0
59	MG	AA	3076	1/1	0.99	0.14	-	0,0,0,0	0
59	MG	AA	3660	1/1	0.82	0.23	-	61,61,61,61	0
59	MG	CA	3167	1/1	0.93	0.08	-	50,50,50,50	0
59	MG	AA	3720	1/1	0.96	0.16	-	55,55,55,55	0
59	MG	CA	3117	1/1	0.69	0.29	-	67,67,67,67	0
59	MG	BA	1728	1/1	0.90	0.20	-	47,47,47,47	0
59	MG	CA	3497	1/1	0.97	0.09	-	45,45,45,45	0
59	MG	AA	3115	1/1	0.92	0.34	-	44,44,44,44	0
59	MG	AA	3596	1/1	0.83	0.32	-	65,65,65,65	0
59	MG	CA	3179	1/1	0.98	0.33	-	60,60,60,60	0
59	MG	CA	3560	1/1	0.85	0.23	-	79,79,79,79	0
59	MG	CA	3030	1/1	0.79	0.52	-	59,59,59,59	0
59	MG	AA	3310	1/1	0.91	0.15	-	56,56,56,56	0
59	MG	DA	1693	1/1	0.96	0.15	-	67,67,67,67	0
59	MG	AA	3760	1/1	0.98	0.38	-	55,55,55,55	0
59	MG	DA	1653	1/1	0.98	0.30	-	55,55,55,55	0
59	MG	AA	3178	1/1	0.93	0.38	-	48,48,48,48	0
59	MG	AA	3287	1/1	0.92	0.40	-	43,43,43,43	0
59	MG	AA	3316	1/1	0.97	0.23	-	36,36,36,36	0
59	MG	DA	1663	1/1	0.88	0.42	-	91,91,91,91	0
59	MG	CA	3454	1/1	0.85	0.16	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3505	1/1	0.73	0.10	-	67,67,67,67	0
59	MG	AA	3583	1/1	0.84	0.14	-	63,63,63,63	0
59	MG	AA	3685	1/1	0.95	0.20	-	72,72,72,72	0
59	MG	AA	3375	1/1	0.96	0.30	-	48,48,48,48	0
59	MG	AA	3542	1/1	0.85	0.23	-	58,58,58,58	0
59	MG	BA	1610	1/1	0.85	0.08	-	78,78,78,78	0
59	MG	AA	3085	1/1	0.91	0.20	-	46,46,46,46	0
59	MG	AA	3641	1/1	0.92	0.29	-	51,51,51,51	0
59	MG	AA	3071	1/1	0.94	0.62	-	40,40,40,40	0
59	MG	CA	3545	1/1	0.87	0.48	-	86,86,86,86	0
59	MG	AA	3611	1/1	0.85	0.18	-	47,47,47,47	0
59	MG	DA	1629	1/1	0.93	0.43	-	59,59,59,59	0
59	MG	CA	3643	1/1	0.94	0.18	-	79,79,79,79	0
59	MG	AA	3323	1/1	0.77	0.22	-	64,64,64,64	0
59	MG	AA	3517	1/1	0.97	0.08	-	23,23,23,23	0
59	MG	AA	3180	1/1	0.84	0.26	-	69,69,69,69	0
59	MG	AA	3266	1/1	0.50	0.78	-	90,90,90,90	0
59	MG	AA	3612	1/1	0.91	0.14	-	68,68,68,68	0
59	MG	CA	3597	1/1	0.91	0.21	-	58,58,58,58	0
59	MG	CA	3110	1/1	0.91	0.27	-	56,56,56,56	0
59	MG	AA	3758	1/1	0.96	0.28	-	43,43,43,43	1
59	MG	CA	3404	1/1	0.97	0.16	-	65,65,65,65	0
59	MG	AA	3363	1/1	0.75	0.21	-	82,82,82,82	0
59	MG	AA	3457	1/1	0.98	0.14	-	30,30,30,30	0
59	MG	AA	3330	1/1	0.95	0.07	-	66,66,66,66	0
59	MG	BA	1675	1/1	0.92	0.07	-	100,100,100,100	0
59	MG	BA	1706	1/1	0.90	0.21	-	63,63,63,63	0
59	MG	AA	3723	1/1	0.88	0.09	-	49,49,49,49	0
59	MG	CA	3293	1/1	0.93	0.17	-	60,60,60,60	0
59	MG	CA	3472	1/1	0.90	0.48	-	62,62,62,62	0
59	MG	DA	1644	1/1	0.84	0.36	-	94,94,94,94	0
59	MG	AA	3405	1/1	0.99	0.27	-	44,44,44,44	0
59	MG	CA	3423	1/1	0.99	0.23	-	46,46,46,46	0
59	MG	AA	3111	1/1	0.97	0.24	-	24,24,24,24	0
59	MG	AA	3482	1/1	0.99	0.12	-	41,41,41,41	0
59	MG	AA	3378	1/1	0.94	0.17	-	56,56,56,56	0
59	MG	BA	1807	1/1	0.91	0.13	-	61,61,61,61	0
59	MG	AA	3711	1/1	0.94	0.35	-	43,43,43,43	1
59	MG	CA	3384	1/1	0.98	0.12	-	55,55,55,55	0
59	MG	CA	3521	1/1	0.84	0.22	-	74,74,74,74	0
59	MG	AB	3013	1/1	0.95	0.15	-	53,53,53,53	0
59	MG	AA	3005	1/1	0.88	0.16	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3107	1/1	0.96	0.13	-	49,49,49,49	0
59	MG	CA	3646	1/1	0.36	0.17	-	91,91,91,91	0
59	MG	CA	3107	1/1	0.95	0.27	-	77,77,77,77	0
59	MG	AA	3434	1/1	0.98	0.06	-	17,17,17,17	0
59	MG	CA	3248	1/1	0.94	0.44	-	53,53,53,53	0
59	MG	AA	3531	1/1	0.96	0.13	-	24,24,24,24	0
59	MG	DA	1632	1/1	0.82	0.29	-	57,57,57,57	0
59	MG	AA	3643	1/1	0.81	0.24	-	84,84,84,84	0
59	MG	CA	3284	1/1	0.83	0.17	-	75,75,75,75	0
59	MG	CA	3049	1/1	0.98	0.37	-	46,46,46,46	0
59	MG	CA	3351	1/1	0.97	0.14	-	46,46,46,46	0
59	MG	CA	3063	1/1	0.94	0.10	-	34,34,34,34	0
59	MG	BA	1693	1/1	0.81	0.47	-	76,76,76,76	0
59	MG	AA	3314	1/1	0.93	0.27	-	57,57,57,57	0
59	MG	CA	3147	1/1	0.96	0.28	-	55,55,55,55	0
59	MG	BA	1694	1/1	0.85	0.25	-	83,83,83,83	0
59	MG	CA	3297	1/1	0.97	0.35	-	36,36,36,36	0
59	MG	DA	1716	1/1	0.96	0.10	-	57,57,57,57	0
59	MG	CA	3032	1/1	0.91	0.56	-	100,100,100,100	0
59	MG	CA	3120	1/1	0.84	0.21	-	42,42,42,42	0
59	MG	CA	3301	1/1	0.91	0.20	-	60,60,60,60	0
59	MG	AA	3016	1/1	0.65	0.46	-	64,64,64,64	0
59	MG	BA	1712	1/1	0.87	0.41	-	57,57,57,57	0
59	MG	CA	3474	1/1	0.88	0.22	-	59,59,59,59	0
59	MG	BA	1811	1/1	0.78	0.20	-	77,77,77,77	0
59	MG	AE	301	1/1	0.76	0.58	-	69,69,69,69	0
59	MG	CA	3583	1/1	0.80	0.17	-	80,80,80,80	0
59	MG	AA	3376	1/1	0.93	0.22	-	35,35,35,35	0
59	MG	DW	501	1/1	0.98	0.17	-	44,44,44,44	0
59	MG	DA	1741	1/1	0.92	0.36	-	67,67,67,67	0
59	MG	DA	1757	1/1	0.25	1.15	-	111,111,111,111	0
59	MG	AN	3002	1/1	0.96	0.44	-	69,69,69,69	0
59	MG	AA	3562	1/1	0.97	0.09	-	56,56,56,56	0
59	MG	DA	1743	1/1	0.94	0.13	-	59,59,59,59	0
59	MG	CA	3175	1/1	0.97	0.19	-	31,31,31,31	0
59	MG	BA	1769	1/1	0.97	0.10	-	58,58,58,58	0
59	MG	CA	3240	1/1	0.77	0.49	-	71,71,71,71	0
59	MG	CA	3479	1/1	0.99	0.18	-	50,50,50,50	0
59	MG	BA	1645	1/1	0.89	0.19	-	74,74,74,74	0
59	MG	CA	3624	1/1	0.66	0.17	-	118,118,118,118	0
59	MG	CA	3250	1/1	0.90	0.15	-	38,38,38,38	0
59	MG	CA	3237	1/1	0.69	0.48	-	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3288	1/1	0.85	0.17	-	49,49,49,49	0
59	MG	CA	3136	1/1	0.97	0.10	-	63,63,63,63	0
59	MG	AA	3105	1/1	0.90	0.15	-	52,52,52,52	0
59	MG	BA	1647	1/1	0.91	0.52	-	57,57,57,57	0
59	MG	AA	3141	1/1	0.92	0.10	-	68,68,68,68	0
59	MG	AA	3054	1/1	0.97	0.17	-	21,21,21,21	0
59	MG	BA	1764	1/1	0.60	0.09	-	71,71,71,71	0
59	MG	AA	3792	1/1	0.83	0.13	-	48,48,48,48	0
59	MG	AA	3374	1/1	0.94	0.32	-	49,49,49,49	0
59	MG	AA	3368	1/1	0.98	0.25	-	49,49,49,49	0
59	MG	CA	3662	1/1	0.96	0.32	-	33,33,33,33	0
59	MG	DA	1610	1/1	0.82	0.73	-	71,71,71,71	0
59	MG	CA	3238	1/1	0.92	0.25	-	69,69,69,69	0
59	MG	AA	3487	1/1	0.92	0.03	-	49,49,49,49	0
59	MG	CA	3197	1/1	0.97	0.41	-	45,45,45,45	0
59	MG	AA	3349	1/1	0.96	0.17	-	47,47,47,47	0
59	MG	BA	1771	1/1	0.95	0.20	-	65,65,65,65	0
59	MG	AA	3474	1/1	0.94	0.15	-	18,18,18,18	1
59	MG	AA	3014	1/1	0.91	0.13	-	31,31,31,31	0
59	MG	DA	1612	1/1	0.94	0.14	-	57,57,57,57	0
59	MG	AA	3275	1/1	0.86	0.34	-	89,89,89,89	0
59	MG	BA	1737	1/1	0.87	0.20	-	79,79,79,79	0
59	MG	AA	3614	1/1	0.84	0.29	-	50,50,50,50	1
59	MG	AA	3669	1/1	0.93	0.18	-	81,81,81,81	0
59	MG	AA	3683	1/1	0.90	0.28	-	62,62,62,62	0
59	MG	BA	1756	1/1	0.84	0.07	-	85,85,85,85	0
59	MG	AA	3736	1/1	0.86	0.30	-	59,59,59,59	0
59	MG	DA	1704	1/1	0.81	0.18	-	49,49,49,49	0
59	MG	CA	3263	1/1	0.95	0.15	-	64,64,64,64	0
59	MG	CA	3150	1/1	0.78	0.20	-	57,57,57,57	0
59	MG	CA	3436	1/1	0.93	0.11	-	64,64,64,64	0
59	MG	AA	3124	1/1	0.93	0.71	-	62,62,62,62	0
59	MG	DA	1753	1/1	0.90	0.30	-	79,79,79,79	0
59	MG	BA	1623	1/1	0.92	0.64	-	67,67,67,67	0
59	MG	DA	1651	1/1	0.98	0.11	-	63,63,63,63	0
59	MG	CA	3645	1/1	0.95	0.12	-	69,69,69,69	0
59	MG	AA	3696	1/1	0.92	0.18	-	66,66,66,66	0
59	MG	AA	3175	1/1	0.88	0.57	-	63,63,63,63	0
59	MG	AA	3252	1/1	0.90	0.20	-	44,44,44,44	0
59	MG	AA	3715	1/1	0.90	0.53	-	33,33,33,33	1
59	MG	AA	3027	1/1	0.89	0.51	-	75,75,75,75	0
59	MG	CA	3588	1/1	0.93	0.12	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3471	1/1	0.96	0.08	-	56,56,56,56	0
59	MG	CA	3094	1/1	0.93	0.22	-	59,59,59,59	0
59	MG	CA	3061	1/1	0.68	0.36	-	68,68,68,68	0
59	MG	CA	3371	1/1	0.89	0.19	-	52,52,52,52	0
59	MG	BA	1721	1/1	0.75	0.20	-	66,66,66,66	0
59	MG	AA	3288	1/1	0.91	0.27	-	39,39,39,39	0
59	MG	BA	1767	1/1	0.44	0.41	-	96,96,96,96	0
59	MG	BA	1619	1/1	0.80	0.22	-	59,59,59,59	0
59	MG	BA	1713	1/1	0.81	0.60	-	68,68,68,68	0
59	MG	BA	1626	1/1	0.95	0.13	-	41,41,41,41	0
59	MG	DA	1708	1/1	0.87	0.26	-	77,77,77,77	0
59	MG	CA	3236	1/1	0.77	0.70	-	81,81,81,81	0
59	MG	DA	1735	1/1	0.87	0.12	-	73,73,73,73	0
59	MG	AA	3302	1/1	0.98	0.06	-	51,51,51,51	0
59	MG	BA	1670	1/1	0.75	0.24	-	69,69,69,69	0
59	MG	CA	3272	1/1	0.97	0.33	-	49,49,49,49	0
59	MG	CA	3369	1/1	0.98	0.14	-	48,48,48,48	0
59	MG	CA	3242	1/1	0.70	0.40	-	82,82,82,82	0
59	MG	CA	3621	1/1	0.94	0.21	-	61,61,61,61	0
59	MG	AA	3462	1/1	0.96	0.09	-	54,54,54,54	0
59	MG	CA	3367	1/1	0.83	0.22	-	63,63,63,63	0
59	MG	AA	3440	1/1	0.88	0.24	-	63,63,63,63	0
59	MG	AA	3672	1/1	0.94	0.15	-	48,48,48,48	0
59	MG	AA	3192	1/1	0.98	0.24	-	30,30,30,30	0
59	MG	CN	5001	1/1	0.93	0.17	-	65,65,65,65	0
59	MG	CB	3005	1/1	0.93	0.39	-	63,63,63,63	0
59	MG	BA	1709	1/1	0.87	0.29	-	50,50,50,50	0
59	MG	AA	3701	1/1	0.91	0.15	-	81,81,81,81	0
59	MG	BA	1609	1/1	0.87	0.13	-	62,62,62,62	0
59	MG	AA	3577	1/1	0.93	0.08	-	42,42,42,42	0
59	MG	CA	3651	1/1	0.93	0.56	-	76,76,76,76	0
59	MG	BA	1809	1/1	0.95	0.23	-	61,61,61,61	0
59	MG	AA	3816	1/1	0.80	0.72	-	66,66,66,66	0
59	MG	AA	3142	1/1	0.88	0.26	-	64,64,64,64	0
59	MG	AA	3300	1/1	0.84	0.16	-	22,22,22,22	0
59	MG	AA	3062	1/1	0.93	0.18	-	47,47,47,47	0
59	MG	AA	3364	1/1	0.99	0.18	-	23,23,23,23	0
59	MG	AA	3123	1/1	0.90	0.34	-	54,54,54,54	0
59	MG	AA	3019	1/1	0.83	0.30	-	70,70,70,70	0
59	MG	BA	1762	1/1	0.97	0.06	-	74,74,74,74	0
59	MG	CA	3390	1/1	0.76	0.23	-	80,80,80,80	0
59	MG	AA	3165	1/1	0.98	0.17	-	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3705	1/1	0.86	0.56	-	53,53,53,53	1
59	MG	CA	3031	1/1	0.90	0.50	-	68,68,68,68	0
59	MG	AA	3805	1/1	0.97	0.22	-	58,58,58,58	0
59	MG	AQ	203	1/1	0.91	0.29	-	32,32,32,32	0
59	MG	AB	3021	1/1	0.87	0.26	-	65,65,65,65	0
59	MG	AA	3013	1/1	0.95	0.18	-	28,28,28,28	0
59	MG	AA	3357	1/1	0.89	0.16	-	55,55,55,55	0
59	MG	CA	3302	1/1	0.98	0.29	-	37,37,37,37	0
59	MG	CA	3412	1/1	0.93	0.18	-	59,59,59,59	0
59	MG	AA	3579	1/1	0.91	0.18	-	54,54,54,54	0
59	MG	CA	3401	1/1	0.98	0.23	-	28,28,28,28	0
59	MG	CA	3224	1/1	0.88	0.54	-	59,59,59,59	0
59	MG	CA	3052	1/1	0.92	0.18	-	44,44,44,44	0
59	MG	CA	3568	1/1	0.94	0.11	-	39,39,39,39	0
59	MG	AA	3100	1/1	0.96	0.24	-	29,29,29,29	0
59	MG	CA	3184	1/1	0.85	0.33	-	77,77,77,77	0
59	MG	CA	3516	1/1	0.85	0.36	-	79,79,79,79	0
59	MG	AA	3481	1/1	0.86	0.13	-	78,78,78,78	0
59	MG	AA	3067	1/1	0.75	0.43	-	61,61,61,61	0
59	MG	CA	3270	1/1	0.89	0.29	-	76,76,76,76	0
59	MG	AA	3458	1/1	0.99	0.10	-	40,40,40,40	0
59	MG	CQ	204	1/1	0.75	0.32	-	74,74,74,74	0
59	MG	AA	3292	1/1	0.98	0.20	-	24,24,24,24	0
59	MG	AA	3321	1/1	0.99	0.10	-	61,61,61,61	0
59	MG	CA	3205	1/1	0.73	0.51	-	81,81,81,81	0
59	MG	CF	302	1/1	0.90	0.54	-	69,69,69,69	0
59	MG	AA	3636	1/1	0.88	0.34	-	86,86,86,86	0
59	MG	CA	3556	1/1	0.97	0.19	-	62,62,62,62	0
59	MG	AA	3649	1/1	0.85	0.34	-	62,62,62,62	0
59	MG	AA	3051	1/1	0.81	0.48	-	48,48,48,48	0
59	MG	AA	3189	1/1	0.91	0.20	-	62,62,62,62	0
59	MG	CA	3527	1/1	0.92	0.14	-	76,76,76,76	0
59	MG	CA	3220	1/1	0.97	0.07	-	59,59,59,59	0
59	MG	CA	3231	1/1	0.97	0.73	-	60,60,60,60	0
59	MG	AF	305	1/1	0.56	0.54	-	76,76,76,76	0
59	MG	CA	3382	1/1	0.98	0.22	-	38,38,38,38	0
59	MG	CA	3076	1/1	0.93	0.35	-	64,64,64,64	0
59	MG	AA	3230	1/1	0.88	0.29	-	69,69,69,69	0
59	MG	AA	3461	1/1	0.84	0.19	-	62,62,62,62	0
59	MG	AA	3570	1/1	0.96	0.15	-	14,14,14,14	0
59	MG	DA	1756	1/1	0.71	0.57	-	86,86,86,86	0
59	MG	AA	3631	1/1	0.98	0.18	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AB	3001	1/1	0.84	0.38	-	74,74,74,74	0
59	MG	DA	1764	1/1	0.96	0.08	-	71,71,71,71	0
59	MG	CA	3487	1/1	0.97	0.20	-	60,60,60,60	0
59	MG	BA	1633	1/1	0.83	0.25	-	63,63,63,63	0
59	MG	DA	1670	1/1	0.92	0.13	-	49,49,49,49	0
59	MG	CA	3570	1/1	0.99	0.12	-	36,36,36,36	0
59	MG	AB	3009	1/1	0.91	0.09	-	50,50,50,50	0
59	MG	CE	304	1/1	0.89	0.36	-	75,75,75,75	0
59	MG	DA	1731	1/1	0.96	0.09	-	49,49,49,49	0
59	MG	AE	302	1/1	0.70	0.24	-	57,57,57,57	0
59	MG	AA	3598	1/1	0.97	0.25	-	51,51,51,51	0
59	MG	CA	3634	1/1	0.83	0.23	-	82,82,82,82	0
59	MG	AA	3361	1/1	0.94	0.17	-	53,53,53,53	0
59	MG	BA	1720	1/1	0.93	0.21	-	61,61,61,61	0
59	MG	AA	3731	1/1	0.93	0.14	-	51,51,51,51	0
59	MG	AA	3237	1/1	0.85	0.40	-	76,76,76,76	0
59	MG	DW	502	1/1	0.92	0.08	-	58,58,58,58	0
59	MG	AA	3552	1/1	0.97	0.18	-	63,63,63,63	0
59	MG	CA	3439	1/1	0.96	0.24	-	32,32,32,32	0
59	MG	AA	3207	1/1	0.94	0.19	-	60,60,60,60	0
59	MG	AA	3441	1/1	0.95	0.30	-	58,58,58,58	0
59	MG	DA	1605	1/1	0.83	0.32	-	105,105,105,105	0
59	MG	AA	3074	1/1	0.97	0.30	-	14,14,14,14	0
59	MG	AA	3094	1/1	0.96	0.25	-	80,80,80,80	0
59	MG	CA	3543	1/1	0.95	0.19	-	71,71,71,71	0
59	MG	CA	3097	1/1	0.77	0.30	-	66,66,66,66	0
59	MG	AA	3150	1/1	0.86	0.28	-	45,45,45,45	0
59	MG	DJ	5001	1/1	0.93	0.32	-	82,82,82,82	0
59	MG	CA	3398	1/1	0.88	0.16	-	67,67,67,67	0
59	MG	DZ	701	1/1	0.87	0.25	-	72,72,72,72	0
59	MG	CA	3481	1/1	0.86	0.22	-	64,64,64,64	0
59	MG	CA	3365	1/1	0.97	0.20	-	55,55,55,55	0
59	MG	CA	3015	1/1	0.99	0.29	-	51,51,51,51	0
59	MG	CA	3233	1/1	0.93	0.12	-	59,59,59,59	0
59	MG	AA	3480	1/1	0.84	0.31	-	88,88,88,88	0
59	MG	AA	3299	1/1	0.95	0.27	-	47,47,47,47	0
59	MG	CA	3067	1/1	0.90	0.19	-	63,63,63,63	0
59	MG	CA	3641	1/1	0.97	0.22	-	46,46,46,46	0
59	MG	DA	1668	1/1	0.93	0.38	-	65,65,65,65	0
59	MG	CA	3537	1/1	0.97	0.30	-	59,59,59,59	0
59	MG	CA	3467	1/1	0.88	0.64	-	77,77,77,77	0
59	MG	AA	3648	1/1	0.93	0.17	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3473	1/1	0.91	0.16	-	51,51,51,51	0
59	MG	CA	3055	1/1	0.78	0.13	-	77,77,77,77	0
59	MG	AA	3339	1/1	0.91	0.17	-	49,49,49,49	0
59	MG	AA	3640	1/1	0.82	0.21	-	68,68,68,68	0
59	MG	DA	1608	1/1	0.90	0.17	-	57,57,57,57	0
59	MG	AA	3520	1/1	0.95	0.14	-	17,17,17,17	0
59	MG	CA	3659	1/1	0.96	0.11	-	55,55,55,55	0
59	MG	AB	3011	1/1	0.97	0.16	-	29,29,29,29	0
59	MG	AA	3763	1/1	0.90	0.27	-	47,47,47,47	0
59	MG	CA	3091	1/1	0.84	0.28	-	69,69,69,69	0
59	MG	AA	3351	1/1	0.94	0.21	-	29,29,29,29	0
59	MG	AA	3476	1/1	0.92	0.17	-	28,28,28,28	0
59	MG	DA	1664	1/1	0.90	0.13	-	66,66,66,66	0
59	MG	AA	3447	1/1	0.91	0.34	-	56,56,56,56	0
59	MG	CA	3200	1/1	0.84	0.31	-	51,51,51,51	0
59	MG	BA	1783	1/1	0.95	0.19	-	57,57,57,57	0
59	MG	BA	1711	1/1	0.89	0.14	-	61,61,61,61	0
59	MG	CA	3638	1/1	0.91	0.36	-	76,76,76,76	0
59	MG	AA	3527	1/1	0.97	0.16	-	27,27,27,27	0
59	MG	CA	3519	1/1	0.96	0.23	-	48,48,48,48	0
59	MG	AA	3008	1/1	0.96	0.21	-	26,26,26,26	0
59	MG	AA	3633	1/1	0.91	0.16	-	48,48,48,48	0
59	MG	DA	1762	1/1	0.94	0.21	-	61,61,61,61	0
59	MG	BA	1776	1/1	0.64	0.21	-	97,97,97,97	0
59	MG	DA	1682	1/1	0.93	0.33	-	52,52,52,52	0
59	MG	AA	3555	1/1	0.94	0.15	-	45,45,45,45	0
59	MG	AA	3780	1/1	0.79	0.41	-	72,72,72,72	0
59	MG	DA	1699	1/1	0.90	0.19	-	74,74,74,74	0
59	MG	AA	3698	1/1	0.92	0.16	-	41,41,41,41	0
59	MG	BA	1789	1/1	0.94	0.16	-	72,72,72,72	0
59	MG	BA	1602	1/1	0.71	0.18	-	79,79,79,79	0
59	MG	CA	3084	1/1	0.77	0.43	-	56,56,56,56	0
59	MG	CA	3258	1/1	0.98	0.36	-	51,51,51,51	0
59	MG	CA	3483	1/1	0.94	0.33	-	64,64,64,64	0
59	MG	AA	3278	1/1	0.94	0.21	-	60,60,60,60	0
59	MG	AA	3454	1/1	0.94	0.24	-	61,61,61,61	0
59	MG	A0	104	1/1	0.89	0.35	-	51,51,51,51	0
59	MG	DA	1727	1/1	0.80	0.13	-	61,61,61,61	0
59	MG	BN	502	1/1	0.91	0.18	-	87,87,87,87	0
59	MG	DA	1618	1/1	0.84	0.66	-	91,91,91,91	0
59	MG	DA	1604	1/1	0.89	0.13	-	80,80,80,80	0
59	MG	CA	3007	1/1	0.77	0.39	-	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3534	1/1	0.89	0.12	-	73,73,73,73	0
59	MG	DA	1766	1/1	0.95	0.12	-	74,74,74,74	0
59	MG	CA	3029	1/1	0.93	0.10	-	56,56,56,56	0
59	MG	AA	3498	1/1	0.98	0.24	-	47,47,47,47	0
59	MG	AA	3742	1/1	0.96	0.13	-	68,68,68,68	0
59	MG	BA	1744	1/1	0.88	0.17	-	57,57,57,57	0
59	MG	CA	3334	1/1	0.97	0.22	-	47,47,47,47	0
59	MG	CA	3460	1/1	0.09	0.96	-	104,104,104,104	0
59	MG	CA	3294	1/1	0.72	0.09	-	72,72,72,72	0
59	MG	CA	3616	1/1	0.91	0.66	-	74,74,74,74	0
59	MG	CA	3484	1/1	0.93	0.26	-	78,78,78,78	0
59	MG	CA	3478	1/1	0.86	0.32	-	65,65,65,65	0
59	MG	CA	3437	1/1	0.97	0.18	-	64,64,64,64	0
59	MG	AA	3239	1/1	0.96	0.27	-	25,25,25,25	1
59	MG	CA	3434	1/1	0.93	0.16	-	32,32,32,32	0
59	MG	CA	3141	1/1	0.89	0.46	-	68,68,68,68	0
59	MG	AA	3785	1/1	0.95	0.16	-	61,61,61,61	0
59	MG	BA	1660	1/1	0.10	0.39	-	82,82,82,82	0
59	MG	AB	3010	1/1	0.92	0.11	-	62,62,62,62	0
59	MG	CA	3555	1/1	0.80	0.13	-	71,71,71,71	0
59	MG	CA	3373	1/1	0.85	0.30	-	58,58,58,58	0
59	MG	AA	3503	1/1	0.95	0.06	-	54,54,54,54	0
59	MG	CA	3191	1/1	0.88	0.22	-	46,46,46,46	0
59	MG	DA	1706	1/1	0.94	0.34	-	66,66,66,66	0
59	MG	BA	1808	1/1	0.96	0.16	-	54,54,54,54	0
59	MG	AA	3651	1/1	0.93	0.22	-	77,77,77,77	0
59	MG	BA	1793	1/1	0.93	0.09	-	65,65,65,65	0
59	MG	AA	3504	1/1	0.95	0.09	-	29,29,29,29	0
59	MG	CA	3426	1/1	0.89	0.20	-	38,38,38,38	0
59	MG	BA	1814	1/1	0.85	0.22	-	69,69,69,69	0
59	MG	CA	3606	1/1	0.94	0.49	-	73,73,73,73	0
59	MG	CA	3164	1/1	0.93	0.57	-	64,64,64,64	0
59	MG	CA	3126	1/1	0.90	0.32	-	62,62,62,62	0
59	MG	BA	1698	1/1	0.78	0.43	-	63,63,63,63	0
59	MG	DA	1602	1/1	0.94	0.10	-	45,45,45,45	0
59	MG	AA	3424	1/1	0.97	0.18	-	14,14,14,14	0
59	MG	CA	3255	1/1	0.96	0.25	-	28,28,28,28	0
59	MG	AA	3332	1/1	0.98	0.18	-	17,17,17,17	0
59	MG	AA	3594	1/1	0.94	0.25	-	56,56,56,56	0
59	MG	CA	3466	1/1	0.98	0.41	-	56,56,56,56	0
59	MG	CA	3610	1/1	0.91	0.13	-	69,69,69,69	0
59	MG	CA	3620	1/1	0.49	0.65	-	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3031	1/1	0.88	0.48	-	63,63,63,63	0
59	MG	AA	3414	1/1	0.88	0.17	-	37,37,37,37	0
59	MG	CA	3461	1/1	0.97	0.16	-	34,34,34,34	0
59	MG	BA	1659	1/1	0.86	0.35	-	67,67,67,67	0
59	MG	CA	3022	1/1	0.93	0.53	-	69,69,69,69	0
59	MG	AA	3588	1/1	0.96	0.15	-	47,47,47,47	0
59	MG	AA	3590	1/1	0.95	0.18	-	60,60,60,60	0
59	MG	AA	3658	1/1	0.95	0.22	-	42,42,42,42	0
59	MG	AA	3752	1/1	0.97	0.12	-	42,42,42,42	0
59	MG	AA	3106	1/1	0.91	0.18	-	33,33,33,33	0
59	MG	AA	3352	1/1	0.80	0.38	-	47,47,47,47	0
59	MG	CA	3574	1/1	0.96	0.15	-	37,37,37,37	0
59	MG	BA	1692	1/1	0.95	0.29	-	55,55,55,55	0
59	MG	DA	1749	1/1	0.85	0.34	-	77,77,77,77	0
59	MG	CB	3003	1/1	0.90	0.09	-	65,65,65,65	0
59	MG	DA	1755	1/1	0.93	0.53	-	88,88,88,88	0
59	MG	AA	3408	1/1	0.94	0.35	-	41,41,41,41	0
59	MG	AA	3028	1/1	0.90	0.29	-	39,39,39,39	0
59	MG	AA	3798	1/1	0.96	0.22	-	25,25,25,25	0
59	MG	CA	3576	1/1	0.92	0.11	-	71,71,71,71	0
59	MG	AA	3446	1/1	0.91	0.09	-	59,59,59,59	0
59	MG	AA	3269	1/1	0.54	0.34	-	63,63,63,63	0
59	MG	CA	3215	1/1	0.89	0.07	-	54,54,54,54	0
59	MG	DA	1692	1/1	0.87	0.16	-	53,53,53,53	0
59	MG	DK	5001	1/1	0.65	0.15	-	76,76,76,76	0
59	MG	AA	3657	1/1	0.85	0.17	-	63,63,63,63	0
59	MG	AA	3616	1/1	0.88	0.18	-	57,57,57,57	0
59	MG	BA	1774	1/1	0.91	0.28	-	50,50,50,50	0
59	MG	AA	3238	1/1	0.70	0.45	-	76,76,76,76	0
59	MG	AF	306	1/1	0.95	0.25	-	57,57,57,57	0
59	MG	AA	3002	1/1	0.77	0.21	-	57,57,57,57	0
59	MG	CA	3518	1/1	0.83	0.12	-	65,65,65,65	0
59	MG	AA	3151	1/1	0.99	0.23	-	62,62,62,62	0
59	MG	AA	3629	1/1	0.82	0.17	-	77,77,77,77	0
59	MG	CA	3261	1/1	0.99	0.16	-	47,47,47,47	0
59	MG	CA	3366	1/1	0.96	0.17	-	49,49,49,49	0
59	MG	CA	3199	1/1	0.91	0.22	-	55,55,55,55	0
59	MG	DA	1742	1/1	0.75	0.21	-	72,72,72,72	0
59	MG	BA	1804	1/1	0.97	0.10	-	45,45,45,45	0
59	MG	AA	3427	1/1	0.92	0.12	-	61,61,61,61	0
59	MG	AA	3483	1/1	0.92	0.21	-	46,46,46,46	0
59	MG	CA	3151	1/1	0.94	0.16	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3344	1/1	0.96	0.06	-	68,68,68,68	0
59	MG	AA	3279	1/1	0.94	0.23	-	34,34,34,34	0
59	MG	CA	3530	1/1	0.84	0.51	-	71,71,71,71	0
59	MG	AA	3272	1/1	0.96	0.16	-	55,55,55,55	0
59	MG	BA	1704	1/1	0.79	0.31	-	71,71,71,71	0
59	MG	AA	3666	1/1	0.97	0.14	-	41,41,41,41	0
59	MG	AA	3371	1/1	0.89	0.24	-	53,53,53,53	0
59	MG	AA	3622	1/1	0.82	0.22	-	60,60,60,60	0
59	MG	AA	3283	1/1	0.97	0.34	-	43,43,43,43	0
59	MG	AA	3246	1/1	0.90	0.14	-	52,52,52,52	0
59	MG	CA	3181	1/1	0.99	0.16	-	40,40,40,40	0
59	MG	AA	3652	1/1	0.94	0.15	-	53,53,53,53	0
59	MG	CA	3133	1/1	0.97	0.21	-	85,85,85,85	0
59	MG	CA	3124	1/1	0.85	0.27	-	65,65,65,65	0
59	MG	CA	3323	1/1	0.83	0.40	-	87,87,87,87	0
59	MG	AA	3064	1/1	0.95	0.13	-	32,32,32,32	0
59	MG	AA	3789	1/1	0.98	0.21	-	44,44,44,44	0
59	MG	CA	3325	1/1	0.72	0.13	-	38,38,38,38	0
59	MG	AA	3544	1/1	0.84	0.22	-	26,26,26,26	0
59	MG	AA	3075	1/1	0.97	0.30	-	49,49,49,49	0
59	MG	AA	3811	1/1	0.97	0.16	-	56,56,56,56	0
59	MG	CA	3385	1/1	0.89	0.38	-	61,61,61,61	0
59	MG	BA	1717	1/1	0.95	0.18	-	78,78,78,78	0
59	MG	AA	3670	1/1	0.96	0.08	-	54,54,54,54	0
59	MG	AA	3259	1/1	0.96	0.33	-	41,41,41,41	1
59	MG	AA	3536	1/1	0.74	0.25	-	66,66,66,66	0
59	MG	CA	3198	1/1	0.95	0.24	-	34,34,34,34	0
59	MG	CA	3144	1/1	0.95	0.23	-	40,40,40,40	0
59	MG	DA	1615	1/1	0.95	0.25	-	58,58,58,58	0
59	MG	DA	1690	1/1	0.93	0.19	-	73,73,73,73	0
59	MG	A6	103	1/1	0.92	0.36	-	72,72,72,72	0
59	MG	CA	3059	1/1	0.87	0.44	-	58,58,58,58	0
59	MG	CA	3115	1/1	0.86	0.42	-	67,67,67,67	0
59	MG	AA	3592	1/1	0.86	0.15	-	26,26,26,26	0
59	MG	CA	3331	1/1	0.98	0.27	-	52,52,52,52	0
59	MG	CA	3407	1/1	0.97	0.19	-	36,36,36,36	0
59	MG	A6	101	1/1	0.87	0.23	-	60,60,60,60	0
59	MG	AA	3747	1/1	0.47	0.33	-	85,85,85,85	0
59	MG	CA	3280	1/1	0.90	0.16	-	48,48,48,48	0
59	MG	CA	3612	1/1	0.85	0.37	-	83,83,83,83	0
59	MG	AA	3694	1/1	0.87	0.15	-	53,53,53,53	0
59	MG	BA	1765	1/1	0.98	0.23	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3200	1/1	0.95	0.23	-	30,30,30,30	0
59	MG	AA	3274	1/1	0.86	0.37	-	75,75,75,75	0
59	MG	AA	3198	1/1	0.93	0.15	-	63,63,63,63	0
59	MG	AA	3086	1/1	0.93	0.40	-	55,55,55,55	0
59	MG	AA	3632	1/1	0.95	0.20	-	54,54,54,54	0
59	MG	AA	3530	1/1	0.96	0.19	-	20,20,20,20	1
59	MG	AA	3513	1/1	0.95	0.10	-	41,41,41,41	0
59	MG	AA	3464	1/1	0.87	0.40	-	66,66,66,66	0
59	MG	AA	3599	1/1	0.96	0.17	-	59,59,59,59	0
59	MG	CA	3506	1/1	0.90	0.12	-	63,63,63,63	0
59	MG	AA	3297	1/1	0.99	0.23	-	27,27,27,27	0
59	MG	BA	1605	1/1	0.86	0.13	-	73,73,73,73	0
59	MG	CB	3006	1/1	0.96	0.06	-	71,71,71,71	0
59	MG	CA	3513	1/1	0.81	0.17	-	70,70,70,70	0
59	MG	BA	1792	1/1	0.83	0.19	-	80,80,80,80	0
59	MG	BA	1634	1/1	0.79	0.39	-	64,64,64,64	0
59	MG	DA	1686	1/1	0.87	0.20	-	56,56,56,56	0
59	MG	AA	3425	1/1	0.94	0.06	-	77,77,77,77	0
59	MG	CA	3203	1/1	0.84	0.20	-	73,73,73,73	0
59	MG	AA	3127	1/1	0.97	0.35	-	57,57,57,57	0
59	MG	AA	3501	1/1	0.95	0.06	-	49,49,49,49	0
59	MG	BW	502	1/1	0.90	0.10	-	59,59,59,59	0
59	MG	AA	3145	1/1	0.97	0.30	-	44,44,44,44	0
59	MG	AA	3448	1/1	0.94	0.12	-	62,62,62,62	0
59	MG	CA	3378	1/1	0.71	0.23	-	97,97,97,97	0
59	MG	AA	3549	1/1	0.94	0.05	-	66,66,66,66	0
59	MG	AA	3773	1/1	0.76	0.44	-	35,35,35,35	1
59	MG	BA	1697	1/1	0.71	1.10	-	99,99,99,99	0
59	MG	AA	3118	1/1	0.90	0.41	-	76,76,76,76	0
59	MG	DA	1712	1/1	0.99	0.33	-	53,53,53,53	0
59	MG	CA	3131	1/1	0.92	0.23	-	26,26,26,26	0
59	MG	BA	1800	1/1	0.92	0.46	-	77,77,77,77	0
59	MG	CA	3510	1/1	0.85	0.11	-	95,95,95,95	0
59	MG	AA	3372	1/1	0.98	0.23	-	37,37,37,37	0
59	MG	BA	1759	1/1	0.93	0.33	-	63,63,63,63	0
59	MG	CA	3630	1/1	0.78	0.10	-	65,65,65,65	0
59	MG	CA	3547	1/1	0.93	0.13	-	69,69,69,69	0
59	MG	CB	3001	1/1	0.89	0.29	-	72,72,72,72	0
59	MG	AA	3417	1/1	0.95	0.18	-	25,25,25,25	0
59	MG	CA	3208	1/1	0.79	0.66	-	74,74,74,74	0
59	MG	AA	3642	1/1	0.87	0.34	-	71,71,71,71	0
59	MG	AA	3195	1/1	0.65	0.38	-	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3467	1/1	0.84	0.32	-	49,49,49,49	0
59	MG	CA	3071	1/1	0.91	0.28	-	45,45,45,45	0
59	MG	CA	3112	1/1	0.72	0.38	-	69,69,69,69	0
59	MG	AA	3265	1/1	0.93	0.18	-	43,43,43,43	0
59	MG	CA	3445	1/1	0.95	0.21	-	22,22,22,22	0
59	MG	AA	3355	1/1	0.97	0.17	-	57,57,57,57	0
59	MG	AA	3733	1/1	0.92	0.15	-	49,49,49,49	0
59	MG	CA	3287	1/1	0.98	0.22	-	45,45,45,45	0
59	MG	CA	3349	1/1	0.95	0.21	-	23,23,23,23	0
59	MG	CA	3158	1/1	0.78	0.38	-	54,54,54,54	0
59	MG	CA	3535	1/1	0.88	0.22	-	77,77,77,77	0
59	MG	CA	3254	1/1	0.94	0.16	-	85,85,85,85	0
59	MG	CB	3008	1/1	0.73	0.20	-	66,66,66,66	0
59	MG	CA	3083	1/1	0.92	0.41	-	61,61,61,61	0
59	MG	AA	3121	1/1	0.96	0.16	-	53,53,53,53	0
59	MG	BA	1701	1/1	0.90	0.09	-	54,54,54,54	0
59	MG	AA	3412	1/1	0.98	0.21	-	39,39,39,39	0
59	MG	CA	3559	1/1	0.83	0.12	-	75,75,75,75	0
59	MG	CA	3590	1/1	0.94	0.10	-	59,59,59,59	0
59	MG	AA	3233	1/1	0.88	0.18	-	46,46,46,46	0
59	MG	AA	3746	1/1	0.92	0.17	-	73,73,73,73	0
59	MG	BF	3001	1/1	0.96	0.18	-	49,49,49,49	0
59	MG	AA	3613	1/1	0.97	0.17	-	48,48,48,48	0
59	MG	AA	3324	1/1	0.94	0.14	-	15,15,15,15	0
59	MG	AA	3465	1/1	0.98	0.21	-	42,42,42,42	0
59	MG	CA	3596	1/1	0.92	0.13	-	51,51,51,51	0
59	MG	CA	3628	1/1	0.89	0.19	-	54,54,54,54	0
59	MG	AA	3695	1/1	0.86	0.08	-	67,67,67,67	0
59	MG	CA	3204	1/1	0.87	0.19	-	54,54,54,54	0
59	MG	CA	3005	1/1	0.80	0.20	-	48,48,48,48	0
59	MG	AA	3767	1/1	0.75	0.36	-	67,67,67,67	0
59	MG	CA	3387	1/1	0.92	0.34	-	50,50,50,50	0
59	MG	AA	3428	1/1	0.97	0.19	-	18,18,18,18	0
59	MG	CA	3313	1/1	0.94	0.27	-	38,38,38,38	0
59	MG	AA	3765	1/1	0.98	0.39	-	60,60,60,60	0
59	MG	AA	3073	1/1	0.97	0.14	-	31,31,31,31	0
59	MG	CA	3038	1/1	0.81	0.50	-	97,97,97,97	0
59	MG	CA	3008	1/1	0.94	0.39	-	46,46,46,46	0
59	MG	AV	202	1/1	0.96	0.24	-	33,33,33,33	0
59	MG	CA	3399	1/1	0.94	0.07	-	57,57,57,57	0
59	MG	DA	1633	1/1	0.80	0.27	-	55,55,55,55	0
59	MG	CA	3267	1/1	0.98	0.13	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	CA	3195	1/1	0.98	0.32	-	47,47,47,47	0
59	MG	CA	3118	1/1	0.87	0.65	-	65,65,65,65	0
59	MG	AA	3422	1/1	0.97	0.18	-	23,23,23,23	0
59	MG	BA	1732	1/1	0.93	0.25	-	70,70,70,70	0
59	MG	AB	3004	1/1	0.72	0.32	-	69,69,69,69	0
59	MG	AA	3343	1/1	0.96	0.10	-	46,46,46,46	0
59	MG	CA	3389	1/1	0.78	0.35	-	59,59,59,59	0
59	MG	CA	3563	1/1	0.80	0.09	-	75,75,75,75	0
59	MG	CA	3406	1/1	0.82	0.13	-	77,77,77,77	0
59	MG	AA	3155	1/1	0.90	0.21	-	93,93,93,93	0
59	MG	CA	3447	1/1	0.97	0.26	-	73,73,73,73	0
59	MG	AA	3774	1/1	0.98	0.34	-	25,25,25,25	1
59	MG	DA	1627	1/1	0.89	0.08	-	77,77,77,77	0
59	MG	CA	3540	1/1	0.86	0.08	-	54,54,54,54	0
59	MG	CA	3381	1/1	0.96	0.15	-	50,50,50,50	0
59	MG	AA	3764	1/1	0.93	0.16	-	73,73,73,73	0
59	MG	BA	1667	1/1	0.92	0.25	-	74,74,74,74	0
59	MG	AA	3709	1/1	0.99	0.42	-	23,23,23,23	1
59	MG	AA	3782	1/1	0.89	0.20	-	44,44,44,44	0
59	MG	AA	3548	1/1	0.95	0.12	-	7,7,7,7	0
59	MG	CA	3047	1/1	0.96	0.16	-	84,84,84,84	0
59	MG	CA	3405	1/1	0.98	0.10	-	55,55,55,55	0
59	MG	C8	5001	1/1	0.97	0.34	-	37,37,37,37	0
59	MG	DA	1626	1/1	0.46	0.30	-	71,71,71,71	0
59	MG	AA	3208	1/1	0.84	0.43	-	54,54,54,54	0
59	MG	BA	1731	1/1	0.92	0.17	-	45,45,45,45	0
59	MG	CA	3216	1/1	0.75	0.47	-	79,79,79,79	0
59	MG	AA	3291	1/1	0.96	0.28	-	45,45,45,45	0
59	MG	CA	3558	1/1	0.92	0.09	-	64,64,64,64	0
59	MG	AA	3459	1/1	0.98	0.20	-	53,53,53,53	0
59	MG	CA	3139	1/1	0.32	0.71	-	126,126,126,126	0
59	MG	BA	1763	1/1	0.93	0.17	-	76,76,76,76	0
59	MG	BA	1736	1/1	0.91	0.17	-	67,67,67,67	0
59	MG	CA	3542	1/1	0.75	0.41	-	87,87,87,87	0
59	MG	DA	1724	1/1	0.73	0.42	-	70,70,70,70	0
59	MG	DA	1736	1/1	0.89	0.13	-	78,78,78,78	0
59	MG	CA	3359	1/1	0.94	0.08	-	33,33,33,33	0
59	MG	CA	3522	1/1	0.94	0.13	-	54,54,54,54	0
59	MG	CA	3241	1/1	0.89	0.18	-	72,72,72,72	0
59	MG	BA	1636	1/1	0.94	0.18	-	57,57,57,57	0
59	MG	AA	3604	1/1	0.86	0.45	-	81,81,81,81	0
59	MG	AA	3079	1/1	0.87	0.12	-	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	3768	1/1	0.79	0.20	-	58,58,58,58	0
59	MG	CA	3222	1/1	0.92	0.35	-	57,57,57,57	0
59	MG	CA	3093	1/1	0.74	0.69	-	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.