



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:12 PM GMT

PDB ID : 4V9A
Title : Crystal Structure of the 70S ribosome with tetracycline.
Authors : Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2012-07-18
Resolution : 3.30 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

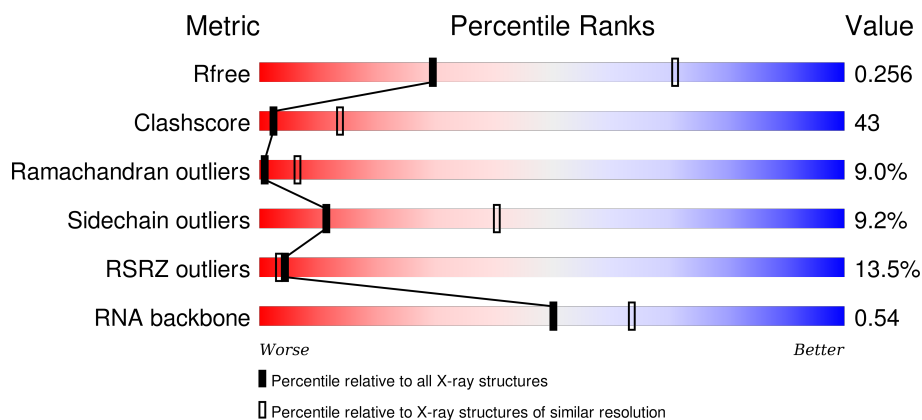
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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	1506	<div> <div>25%</div> <div>58%</div> <div>17%</div> </div>
1	CA	1506	<div> <div>25%</div> <div>59%</div> <div>16%</div> </div>
2	AE	256	<div> <div>18%</div> <div>22%</div> <div>56%</div> <div>14%</div> <div>7%</div> </div>
2	CE	256	<div> <div>36%</div> <div>20%</div> <div>54%</div> <div>18%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	128	
12	CO	128	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	

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Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AC	77	
22	CC	77	
23	A1	4	
23	C1	4	
24	BA	2912	
24	DA	2912	
25	BB	122	
25	DB	122	
26	BD	276	
26	DD	276	
27	BE	206	
27	DE	206	

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Mol	Chain	Length	Quality of chain
28	BF	210	
28	DF	210	
29	BG	182	
29	DG	182	
30	BH	180	
30	DH	180	
31	BK	148	
31	DK	148	
32	BM	140	
32	DM	140	
33	BN	122	
33	DN	122	
34	BO	150	
34	DO	150	
35	BP	141	
35	DP	141	
36	B0	118	
36	D0	118	
37	BQ	112	
37	DQ	112	
38	BR	146	
38	DR	146	
39	B1	118	
39	D1	118	
40	B2	101	

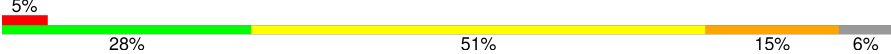
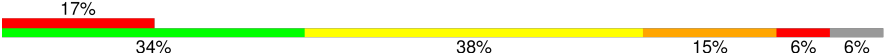
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Mol	Chain	Length	Quality of chain
40	D2	101	
41	BS	113	
41	DS	113	
42	BT	96	
42	DT	96	
43	BU	110	
43	DU	110	
44	BV	206	
44	DV	206	
45	B3	85	
45	D3	85	
46	BZ	98	
46	DZ	98	
47	BW	72	
47	DW	72	
48	BX	60	
48	DX	60	
49	B4	71	
49	D4	71	
50	B5	60	
50	D5	60	
51	B6	54	
51	D6	54	
52	B7	49	
52	D7	49	

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Mol	Chain	Length	Quality of chain
53	B8	65	
53	D8	65	

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
54	MG	AA	1601	-	-	-	X
54	MG	AA	1610	-	-	-	X
54	MG	AA	1620	-	-	-	X
54	MG	AA	1625	-	-	-	X
54	MG	AA	1631	-	-	-	X
54	MG	AA	1634	-	-	-	X
54	MG	AA	1644	-	-	-	X
54	MG	AA	1650	-	-	-	X
54	MG	AA	1657	-	-	-	X
54	MG	AA	1662	-	-	-	X
54	MG	AA	1677	-	-	-	X
54	MG	AA	1678	-	-	-	X
54	MG	AA	1712	-	-	-	X
54	MG	AA	1715	-	-	-	X
54	MG	AA	1743	-	-	-	X
54	MG	AA	1745	-	-	-	X
54	MG	AA	1750	-	-	-	X
54	MG	AA	1778	-	-	-	X
54	MG	AA	1788	-	-	-	X
54	MG	AA	1817	-	-	-	X
54	MG	AA	1826	-	-	-	X
54	MG	AC	107	-	-	-	X
54	MG	AQ	101	-	-	-	X
54	MG	AR	101	-	-	-	X
54	MG	B6	101	-	-	-	X
54	MG	B7	101	-	-	-	X
54	MG	BA	3002	-	-	-	X
54	MG	BA	3008	-	-	-	X
54	MG	BA	3009	-	-	-	X
54	MG	BA	3010	-	-	-	X
54	MG	BA	3013	-	-	-	X
54	MG	BA	3015	-	-	-	X
54	MG	BA	3018	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3021	-	-	-	X
54	MG	BA	3023	-	-	-	X
54	MG	BA	3025	-	-	-	X
54	MG	BA	3028	-	-	-	X
54	MG	BA	3029	-	-	-	X
54	MG	BA	3031	-	-	-	X
54	MG	BA	3038	-	-	-	X
54	MG	BA	3040	-	-	-	X
54	MG	BA	3043	-	-	-	X
54	MG	BA	3049	-	-	-	X
54	MG	BA	3050	-	-	-	X
54	MG	BA	3052	-	-	-	X
54	MG	BA	3054	-	-	-	X
54	MG	BA	3057	-	-	-	X
54	MG	BA	3060	-	-	-	X
54	MG	BA	3061	-	-	-	X
54	MG	BA	3063	-	-	-	X
54	MG	BA	3069	-	-	-	X
54	MG	BA	3070	-	-	-	X
54	MG	BA	3072	-	-	-	X
54	MG	BA	3073	-	-	-	X
54	MG	BA	3089	-	-	-	X
54	MG	BA	3097	-	-	-	X
54	MG	BA	3098	-	-	-	X
54	MG	BA	3099	-	-	-	X
54	MG	BA	3118	-	-	-	X
54	MG	BA	3125	-	-	-	X
54	MG	BA	3128	-	-	-	X
54	MG	BA	3136	-	-	-	X
54	MG	BA	3137	-	-	-	X
54	MG	BA	3138	-	-	-	X
54	MG	BA	3142	-	-	-	X
54	MG	BA	3143	-	-	-	X
54	MG	BA	3144	-	-	-	X
54	MG	BA	3147	-	-	-	X
54	MG	BA	3151	-	-	-	X
54	MG	BA	3155	-	-	-	X
54	MG	BA	3157	-	-	-	X
54	MG	BA	3158	-	-	-	X
54	MG	BA	3163	-	-	-	X
54	MG	BA	3174	-	-	-	X
54	MG	BA	3179	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3180	-	-	-	X
54	MG	BA	3187	-	-	-	X
54	MG	BA	3193	-	-	-	X
54	MG	BA	3198	-	-	-	X
54	MG	BA	3204	-	-	-	X
54	MG	BA	3206	-	-	-	X
54	MG	BA	3209	-	-	-	X
54	MG	BA	3218	-	-	-	X
54	MG	BA	3220	-	-	-	X
54	MG	BA	3221	-	-	-	X
54	MG	BA	3222	-	-	-	X
54	MG	BA	3223	-	-	-	X
54	MG	BA	3224	-	-	-	X
54	MG	BA	3225	-	-	-	X
54	MG	BA	3232	-	-	-	X
54	MG	BA	3243	-	-	-	X
54	MG	BA	3246	-	-	-	X
54	MG	BA	3264	-	-	-	X
54	MG	BA	3273	-	-	-	X
54	MG	BA	3279	-	-	-	X
54	MG	BA	3280	-	-	-	X
54	MG	BA	3285	-	-	-	X
54	MG	BA	3288	-	-	-	X
54	MG	BA	3297	-	-	-	X
54	MG	BA	3299	-	-	-	X
54	MG	BA	3302	-	-	-	X
54	MG	BA	3305	-	-	-	X
54	MG	BA	3310	-	-	-	X
54	MG	BA	3311	-	-	-	X
54	MG	BA	3314	-	-	-	X
54	MG	BA	3349	-	-	-	X
54	MG	BA	3350	-	-	-	X
54	MG	BA	3363	-	-	-	X
54	MG	BA	3367	-	-	-	X
54	MG	BA	3378	-	-	-	X
54	MG	BA	3385	-	-	-	X
54	MG	BA	3393	-	-	-	X
54	MG	BA	3405	-	-	-	X
54	MG	BA	3418	-	-	-	X
54	MG	BA	3434	-	-	-	X
54	MG	BA	3438	-	-	-	X
54	MG	BA	3463	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3491	-	-	-	X
54	MG	BA	3498	-	-	-	X
54	MG	BA	3501	-	-	-	X
54	MG	BA	3526	-	-	-	X
54	MG	BA	3528	-	-	-	X
54	MG	BA	3544	-	-	-	X
54	MG	BA	3553	-	-	-	X
54	MG	BA	3570	-	-	-	X
54	MG	BA	3573	-	-	-	X
54	MG	BA	3577	-	-	-	X
54	MG	BA	3579	-	-	-	X
54	MG	BA	3580	-	-	-	X
54	MG	BA	3581	-	-	-	X
54	MG	BA	3582	-	-	-	X
54	MG	BA	3583	-	-	-	X
54	MG	BA	3589	-	-	-	X
54	MG	BA	3592	-	-	-	X
54	MG	BA	3593	-	-	-	X
54	MG	BA	3596	-	-	-	X
54	MG	BA	3601	-	-	-	X
54	MG	BA	3606	-	-	-	X
54	MG	BA	3624	-	-	-	X
54	MG	BB	202	-	-	-	X
54	MG	BB	212	-	-	-	X
54	MG	BE	302	-	-	-	X
54	MG	CA	1604	-	-	-	X
54	MG	CA	1606	-	-	-	X
54	MG	CA	1617	-	-	-	X
54	MG	CA	1622	-	-	-	X
54	MG	CA	1625	-	-	-	X
54	MG	CA	1640	-	-	-	X
54	MG	CA	1646	-	-	-	X
54	MG	CA	1647	-	-	-	X
54	MG	CA	1650	-	-	-	X
54	MG	CA	1654	-	-	-	X
54	MG	CA	1656	-	-	-	X
54	MG	CA	1657	-	-	-	X
54	MG	CA	1658	-	-	-	X
54	MG	CA	1668	-	-	-	X
54	MG	CA	1674	-	-	-	X
54	MG	CA	1676	-	-	-	X
54	MG	CA	1686	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	CA	1690	-	-	-	X
54	MG	CA	1691	-	-	-	X
54	MG	CA	1699	-	-	-	X
54	MG	CA	1740	-	-	-	X
54	MG	CA	1751	-	-	-	X
54	MG	CA	1781	-	-	-	X
54	MG	CA	1794	-	-	-	X
54	MG	CA	1798	-	-	-	X
54	MG	CA	1799	-	-	-	X
54	MG	CC	108	-	-	-	X
54	MG	CG	302	-	-	-	X
54	MG	CH	201	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3023	-	-	-	X
54	MG	DA	3031	-	-	-	X
54	MG	DA	3033	-	-	-	X
54	MG	DA	3037	-	-	-	X
54	MG	DA	3039	-	-	-	X
54	MG	DA	3055	-	-	-	X
54	MG	DA	3068	-	-	-	X
54	MG	DA	3072	-	-	-	X
54	MG	DA	3085	-	-	-	X
54	MG	DA	3092	-	-	-	X
54	MG	DA	3106	-	-	-	X
54	MG	DA	3114	-	-	-	X
54	MG	DA	3116	-	-	-	X
54	MG	DA	3119	-	-	-	X
54	MG	DA	3127	-	-	-	X
54	MG	DA	3141	-	-	-	X
54	MG	DA	3147	-	-	-	X
54	MG	DA	3150	-	-	-	X
54	MG	DA	3151	-	-	-	X
54	MG	DA	3154	-	-	-	X
54	MG	DA	3156	-	-	-	X
54	MG	DA	3164	-	-	-	X
54	MG	DA	3169	-	-	-	X
54	MG	DA	3170	-	-	-	X
54	MG	DA	3171	-	-	-	X
54	MG	DA	3177	-	-	-	X
54	MG	DA	3182	-	-	-	X
54	MG	DA	3184	-	-	-	X
54	MG	DA	3190	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3201	-	-	-	X
54	MG	DA	3205	-	-	-	X
54	MG	DA	3207	-	-	-	X
54	MG	DA	3211	-	-	-	X
54	MG	DA	3212	-	-	-	X
54	MG	DA	3214	-	-	-	X
54	MG	DA	3221	-	-	-	X
54	MG	DA	3222	-	-	-	X
54	MG	DA	3230	-	-	-	X
54	MG	DA	3233	-	-	-	X
54	MG	DA	3239	-	-	-	X
54	MG	DA	3242	-	-	-	X
54	MG	DA	3244	-	-	-	X
54	MG	DA	3248	-	-	-	X
54	MG	DA	3254	-	-	-	X
54	MG	DA	3271	-	-	-	X
54	MG	DA	3281	-	-	-	X
54	MG	DA	3286	-	-	-	X
54	MG	DA	3290	-	-	-	X
54	MG	DA	3295	-	-	-	X
54	MG	DA	3299	-	-	-	X
54	MG	DA	3316	-	-	-	X
54	MG	DA	3317	-	-	-	X
54	MG	DA	3326	-	-	-	X
54	MG	DA	3332	-	-	-	X
54	MG	DA	3351	-	-	-	X
54	MG	DA	3356	-	-	-	X
54	MG	DA	3357	-	-	-	X
54	MG	DA	3361	-	-	-	X
54	MG	DA	3367	-	-	-	X
54	MG	DA	3368	-	-	-	X
54	MG	DA	3369	-	-	-	X
54	MG	DA	3389	-	-	-	X
54	MG	DA	3390	-	-	-	X
54	MG	DA	3395	-	-	-	X
54	MG	DA	3399	-	-	-	X
54	MG	DA	3418	-	-	-	X
54	MG	DA	3455	-	-	-	X
54	MG	DA	3491	-	-	-	X
54	MG	DA	3495	-	-	-	X
54	MG	DA	3501	-	-	-	X
54	MG	DA	3503	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3504	-	-	-	X
54	MG	DA	3506	-	-	-	X
54	MG	DA	3516	-	-	-	X
54	MG	DA	3517	-	-	-	X
54	MG	DB	206	-	-	-	X
54	MG	DB	211	-	-	-	X
54	MG	DD	301	-	-	-	X
56	ZN	CG	303	-	-	X	-

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 292440 atoms, of which 1 is hydrogen and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
1	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
2	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
13	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AU	72	Total	C	N	O	0	0	0
			591	376	117	98			
18	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AX	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			
22	CC	77	Total	C	N	O	P	0	0	0
			1640	732	298	534	76			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	17A	C	U	CONFLICT	GB AP008226.1
AC	50	U	C	CONFLICT	GB AP008226.1
AC	51	C	G	CONFLICT	GB AP008226.1
AC	63	G	C	CONFLICT	GB AP008226.1
CC	17A	C	U	CONFLICT	GB AP008226.1
CC	50	U	C	CONFLICT	GB AP008226.1
CC	51	C	G	CONFLICT	GB AP008226.1
CC	63	G	C	CONFLICT	GB AP008226.1

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			
23	C1	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
24	DA	2909	Total	C	N	O	P	0	0	0
			62647	27884	11716	20139	2908			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	161	U	-	INSERTION	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	158	U	-	INSERTION	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

- Molecule 25 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
25	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
26	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
27	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
28	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
30	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 31 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
31	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 32 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
32	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	DN	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
34	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
35	DP	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
36	D0	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
37	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
38	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
40	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
41	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
42	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
43	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
44	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
45	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
46	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
47	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			
48	DX	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
51	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
52	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
53	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	627	Total	Mg	0	0
			627	627		
54	CA	204	Total	Mg	0	0
			204	204		

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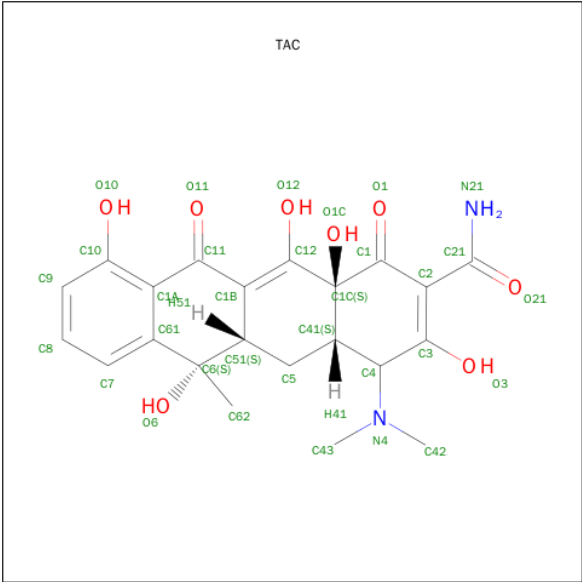
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CH	1	Total 1	Mg 1	0	0
54	DZ	2	Total 2	Mg 2	0	0
54	B8	1	Total 1	Mg 1	0	0
54	BE	5	Total 5	Mg 5	0	0
54	DU	1	Total 1	Mg 1	0	0
54	B1	2	Total 2	Mg 2	0	0
54	BP	1	Total 1	Mg 1	0	0
54	AS	1	Total 1	Mg 1	0	0
54	B5	2	Total 2	Mg 2	0	0
54	BB	17	Total 17	Mg 17	0	0
54	AJ	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	DR	1	Total 1	Mg 1	0	0
54	B2	1	Total 1	Mg 1	0	0
54	AA	232	Total 232	Mg 232	0	0
54	AR	1	Total 1	Mg 1	0	0
54	B6	1	Total 1	Mg 1	0	0
54	CG	2	Total 2	Mg 2	0	0
54	BU	2	Total 2	Mg 2	0	0
54	A1	1	Total 1	Mg 1	0	0
54	DD	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	CC	8	Total 8	Mg 8	0	0
54	DE	3	Total 3	Mg 3	0	0
54	B3	2	Total 2	Mg 2	0	0
54	DA	525	Total 525	Mg 525	0	0
54	B7	3	Total 3	Mg 3	0	0
54	AG	2	Total 2	Mg 2	0	0
54	BO	3	Total 3	Mg 3	0	0
54	AQ	2	Total 2	Mg 2	0	0
54	D1	1	Total 1	Mg 1	0	0
54	AH	2	Total 2	Mg 2	0	0
54	BZ	1	Total 1	Mg 1	0	0
54	AC	9	Total 9	Mg 9	0	0
54	D5	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	CS	1	Total 1	Mg 1	0	0
54	DB	14	Total 14	Mg 14	0	0

- Molecule 55 is TETRACYCLINE (three-letter code: TAC) (formula: $C_{22}H_{24}N_2O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	AA	1	Total	C	H	N	O	0	0
			33	22	1	2	8		
55	CA	1	Total	C		N	O	0	0
			32	22		2	8		

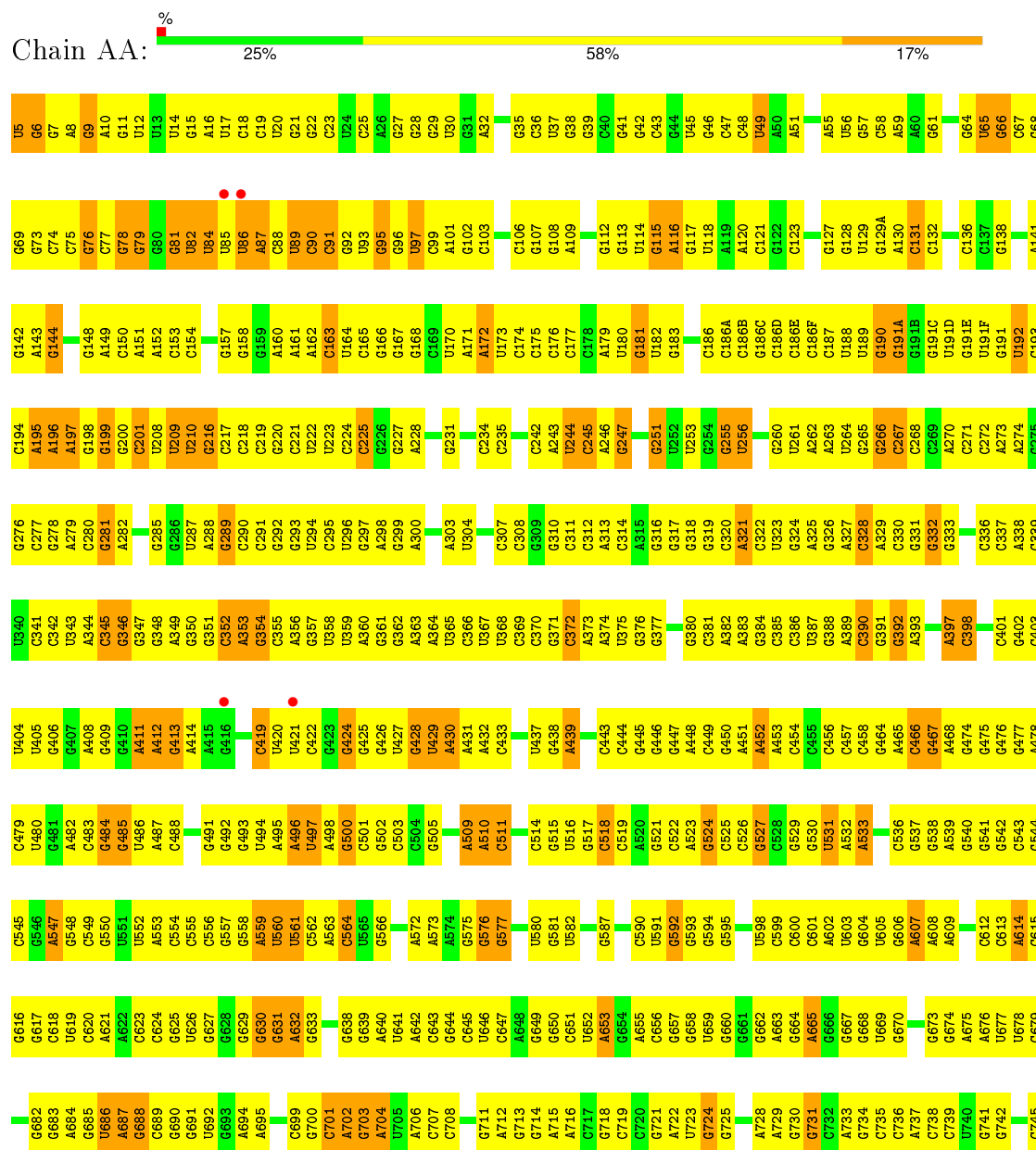
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total	Zn	0	0
			1	1		
56	AQ	1	Total	Zn	0	0
			1	1		
56	CQ	1	Total	Zn	0	0
			1	1		
56	CG	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

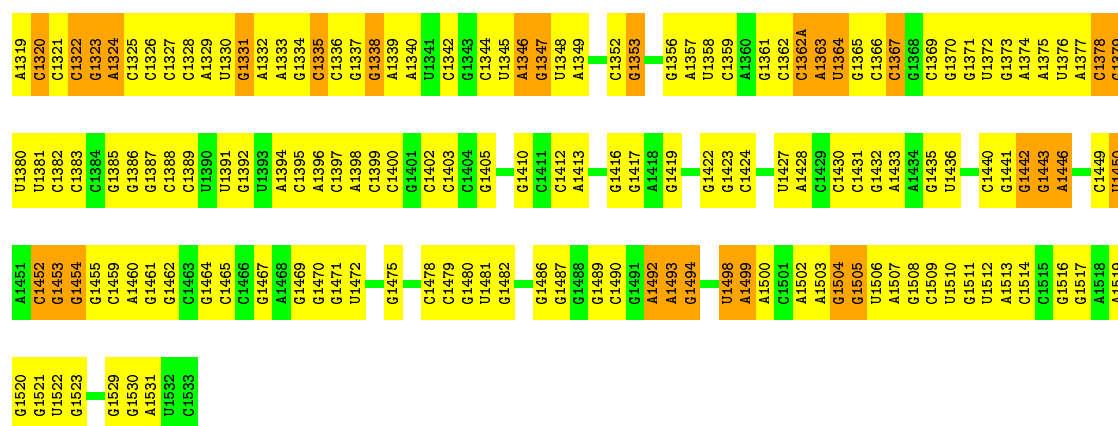
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

- Molecule 1: 16S ribosomal RNA

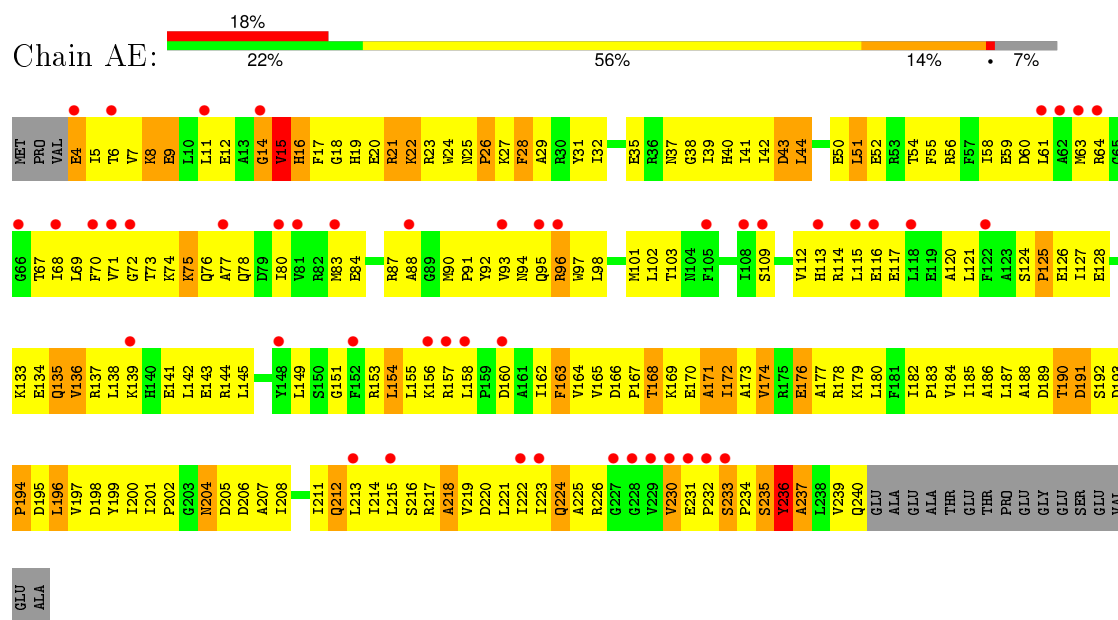




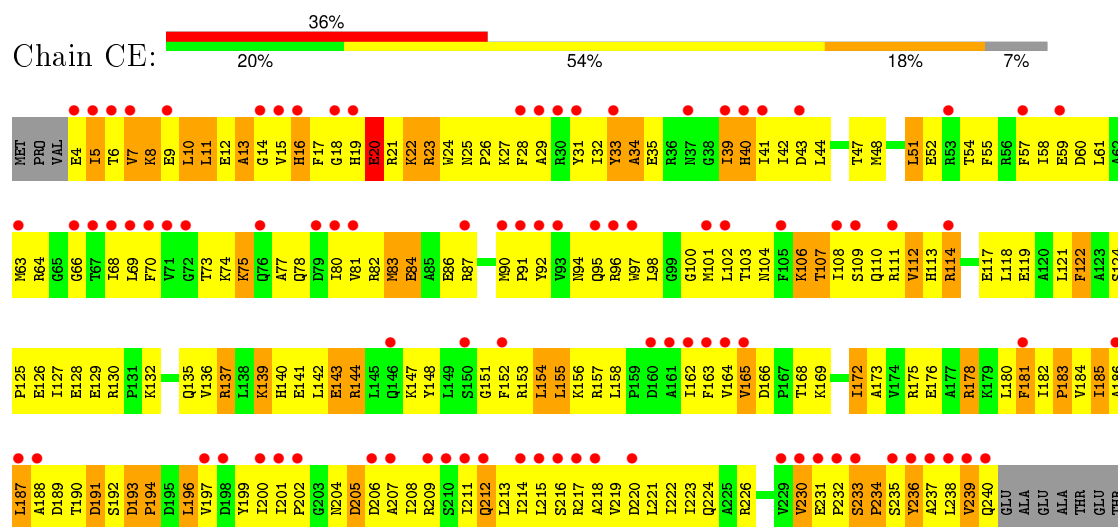
G1255	C1128	G1067	G1009	U950	G880	U801	G730	G661	G594	C528	A452	C386	G316	C225
A1256	C1129	G1068	G1010	G951	G881	A802	G731	G662	G595	G529	A453	U387	G317	G226
G1257	G1130	G1069	G1011	G952	C882	G803	G732	A663	C596	U531	C454	G388	A321	U229
G1258	G1131	U1070	U1012	G953	C883	G804	G733	G664	G597	U532	C455	A389	G230	G230
G1259	G1132	G1071	G1013	G954	U884	C811	G734	A665	U598	A533	C456	C390	U322	G231
G1260	G1133	G1072	A1014	G955	G885	C812	G735	A666	C599	A534	C457	G391	U323	
	A1201	U1073	A1015	U956		U813	G736	G666	C600	U535	C458	G392	U324	C241
C1263	G1134	G1074	A1016	U957	A889	A814	A737		C601	C536	C459	G393	G324	C242
C1264	U1136	G1075	G1017	A958	G890	A815	C738	G671	A602	C537	C460	G394	A325	C243
G1265	G1137	C1076		A959	U891	A816	C739	G672		C538	C461	G395	A326	A243
G1266	G1138	G1077	U1020	U960	A892	C817	U740	G673	U605	G538	C462	G396	C327	C244
C1267	G1139	U1078	G1021	U961	C893	G818	G741	G674	G606	A539	C463	G397	C328	C245
G1268	G1140	G1079	G1022	G962	G894	A819	G742	A675	A607	G540	C464	A397	A329	A246
A1269	C1141	A1080	G1023	G963	G895	U820	G743	G676	A608	G541	C465	C398	G247	
C1270	G1142	G1081	U1024	A964	C896	U821	G744	U677		G542	C466	G402	G332	A250
	G1143	G1082	U1025	A965	C897		G745	U678	A611	G543	C467	C403	G333	G251
A1275	G1144	U1083	G1026	G966		C826	C746	G682	C612	G544	C468	U404	C337	U252
G1276	C1145	G1084	G1027	G967	A900	U827	G747	G683	C613	G545	U405	U405	A338	U253
C1277	A1146	A901	A902	A968	A901	A828	U751	A684	A614	G546	C469	G406	C339	G254
U1278	A1147	U1086	G903	A969	G902	G829	G752	G685	C615	A547	C470	U407	U340	G255
A1279	U1148	G1087	G1028A		G903		G753	G686	G616		C471	A408	C341	U256
A1280	C1149	U1088	G1029	G971	G906	U833	A754	A687	G617	G550	C472	G409		
U1281	U1150	G1089	G1030	C972	A907	C834	G755	G688	C618	U551	C473	G410	A344	U261
C1282	A1151	U1090	G1031	G973		G835	G756	G689	U619	U552	C474	A411	C345	A262
G1283	A1152	U1091	A1032	A974		G836	U757	G690	C620	U553	C475	A412	G346	A263
G1284	C1153	A1092	G1032A	A975	G912	G837		G691	A621	C554	C476	G413	G347	U264
A1285	G1154	A1093	G1032B	G976	A913	G838	G763	G692	A622	C555	C477	A414	A348	G265
A1286	G1155	G1094	G1033	A977	A914	U841	G764	G693	C623		C478	G415	A349	G266
A1287	G1156	U1095	G1034	A978	A915	C842	G765	A694	C624	G558	C479	A417	G350	C267
C1288	G1157	U1096	A1035	C979	A916	U843	A766	A695	G625	G559	C480	C418	G351	C268
A1289	C1158	C1097	G1036	G980	G917	C848	A767	A696	U626	U560	C481	G422	C352	C269
C1290	U1159	C1098	C1037	U981	A918	C849	A768	U697	G627	U561	C482	U421	C353	A270
G1291	G1160	G1099	G1038	U982	A919	U850	G769	G698	G628	G562	C483	G423	G354	C271
U1292	C1161	C1100	G1039	A983	U920	G851	C770	G699	C629	A563	C484	G424	C355	C272
G1293	C1162	A1101	U1040	C984	U921	G852	G771	G708	G630	C564	C485	G425	A356	A273
G1294		A1102	A1041	C985	G922	G853	U772	G709	G631	U565	C486	G426	G357	A274
G1295	A1167	C1103	G1042	A986	A923	G854	G773	A704	A632	G566	C487	U427	U358	G275
C1296	A1169	G1104	C1043	G987	G926	G855		U705	G633	G505	C488	U428	U359	G276
C1297		A1105	A1044	G988	G927	C856	A777	A706	C634	G506	C489	U429	A360	C277
C1298	C1172	G1106	C1045	C989		C857	G778	C707	G635	A572	C490	G430	G361	G278
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G1300		G1108	G1047	U991	C930	A860	A782	G709	G637	A574	C492	A432	U366	G281
C1301	A1176	C1109	U1048	U992	C931	G861	C783	G710	G638	G575	C493	G433	C367	A282
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C1303	G1178	A1111	G1050	A994	G933	C863	G785	A712		G577	C495	U435	C370	
G1304	A1179	C1112	U1051	C995	C934	U863	G786	G713	C643	U580	C496	C436	G371	G286
G1305	A1180	U1052	U1052	A996	A935	A864	A787	G714	G644	G581	C497	U437	C372	U287
A1306	C1181	G1053	U997	G997	C936	A865	U788	A715	C645	U582	C498	U438	A373	A288
G1307	G1182	C1114		G998	A937	G866	U789	A716		U583	C499	U439	A374	G289
U1308	A1183	G1117	G1054	C998A	A938	G867	A790	C717	A648	G584	C500	A440	U375	
G1309	G1184	C1118	G1057	U999	G939	C868	G791	G718	G649	G585	C501	C442	G376	C295
G1310	G1185	C1119	G1058	A1000	C940	C869	A792	C719	G650	C586	C502	C443	U377	U296
G1311	G1186	G1120	G1059	G1001	G941	U870	U793	C720	C651	C587	C503	C444	G378	G297
G1312	G1187	U1121	C1060	G1002	U871	U871	A794	G721	G652	G588	C504	G445	C379	A298
U1313	A1188	U1122	G1061	G1003	G944	A872	C795	A722	A653	G589	C505	G446	A382	G299
C1314	C1189	A1123	U1062	A1004	G945	A873	C796	U723		C590	C506	G447	A383	A300
U1315	G1190	G1124	C1063	A1005	A946	G874	C797	G724	G657	G591	C507	G448	A384	G301
G1316	A1191	U1125	G1064	A1006	G947		C798	G725	G658	G592	C508	G449	G385	
C1317		U1126	U1065	C1007	C948	G878	G799	C726	U659	G593	C509	G450		
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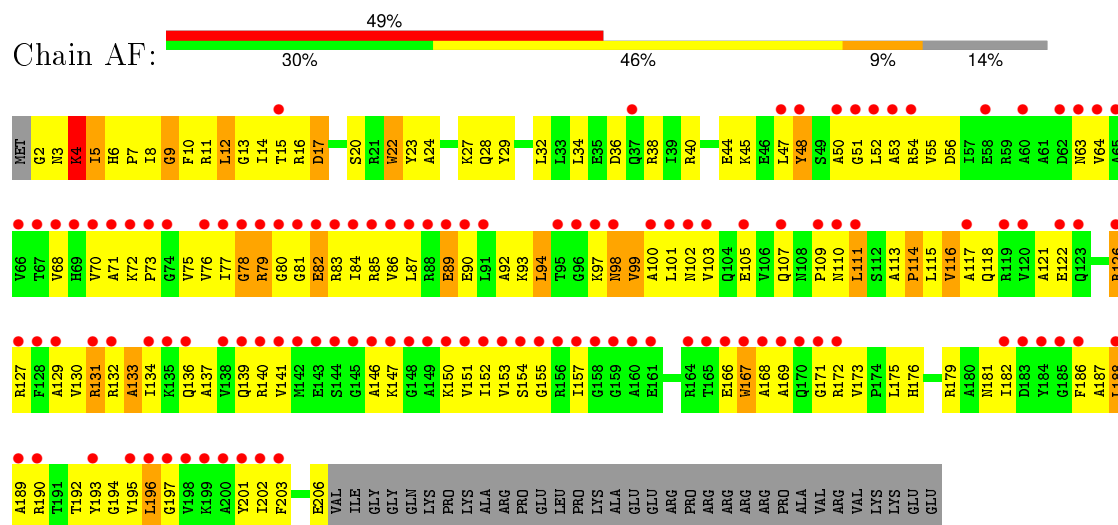


• Molecule 2: 30S RIBOSOMAL PROTEIN S2

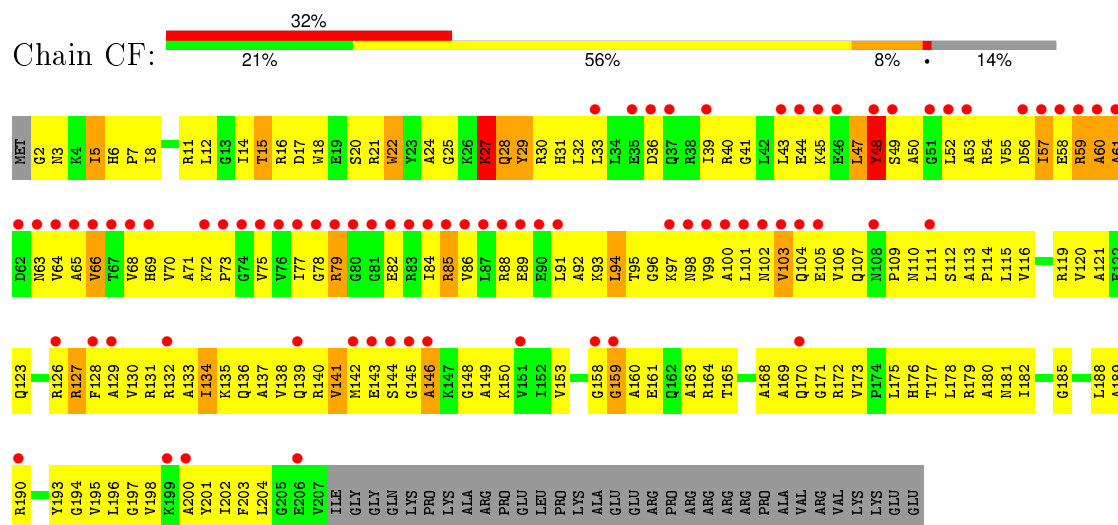


PRO
GLU
GLY
GLY
SER
GLU
VAL
GLU
ALA

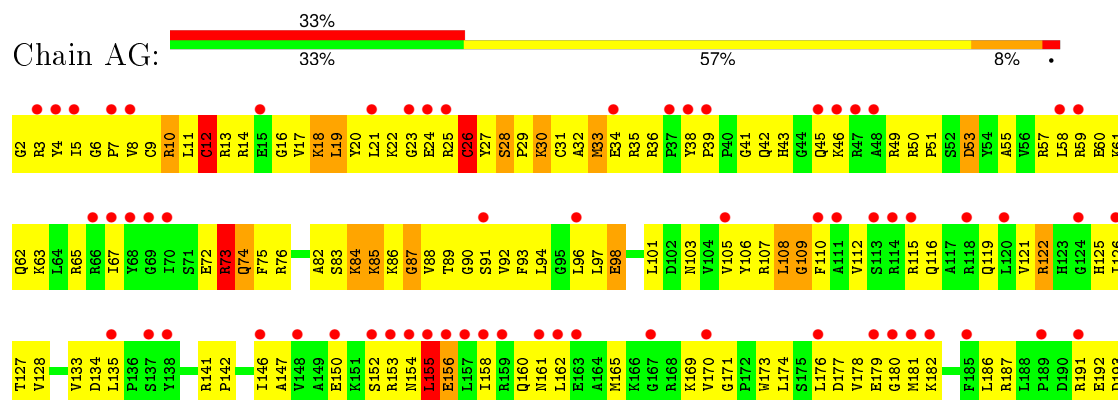
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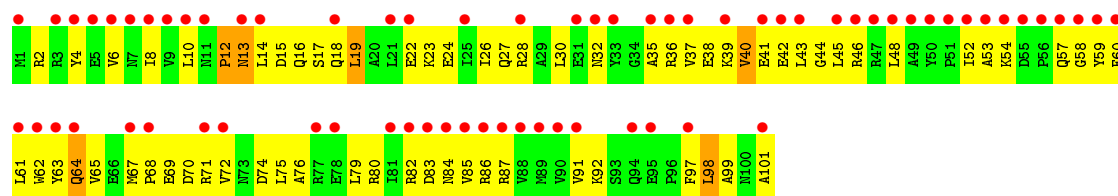
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



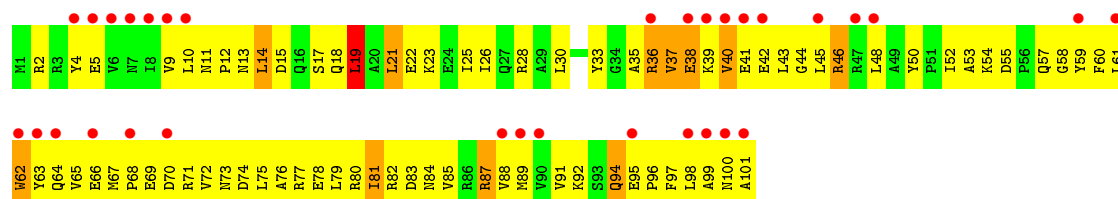
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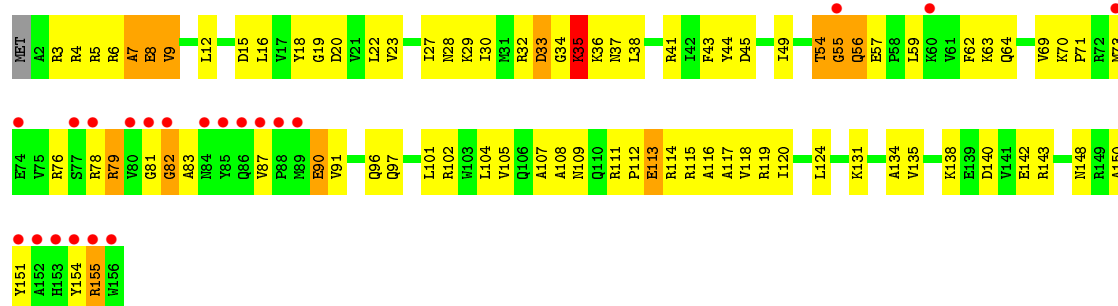




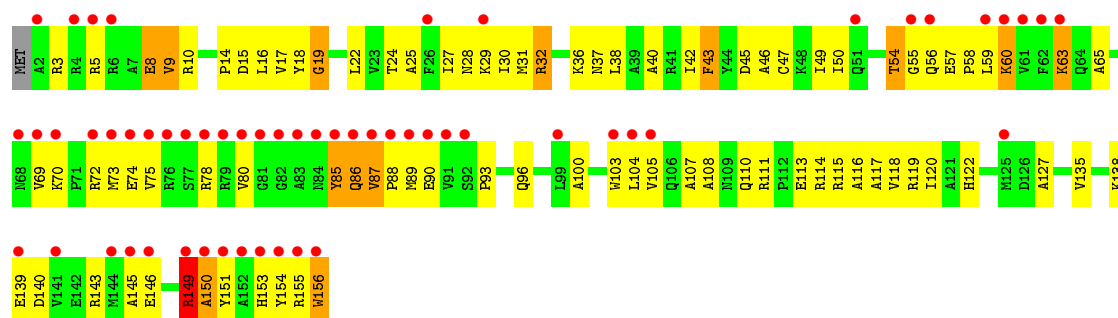
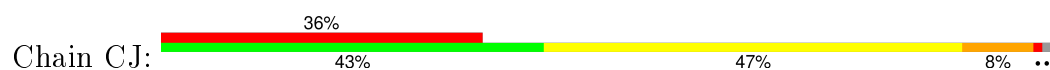
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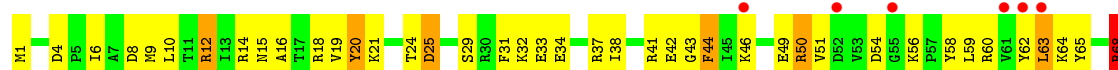
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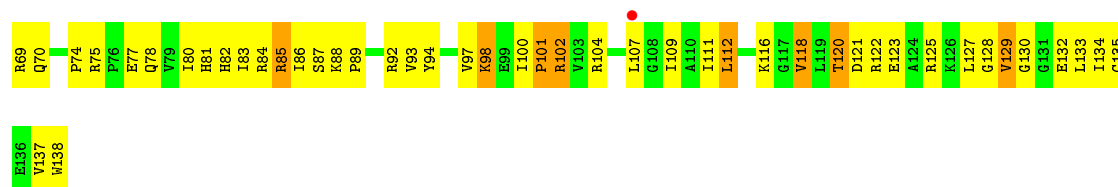


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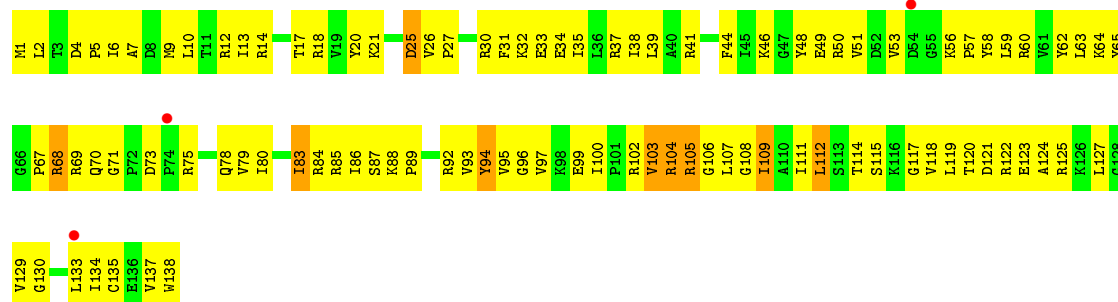


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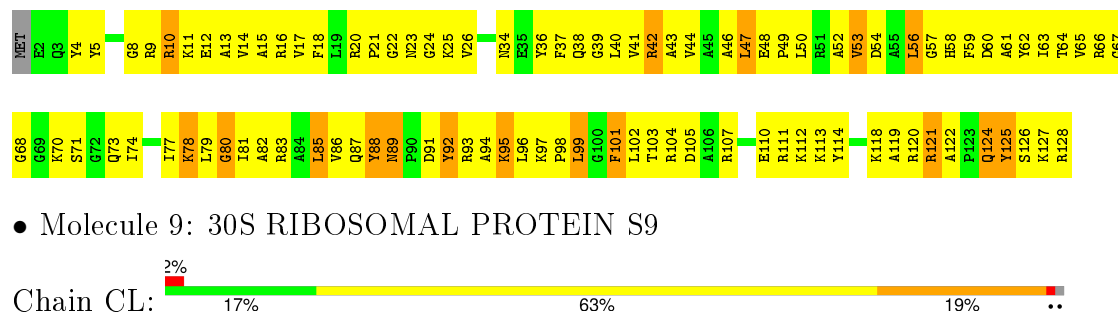




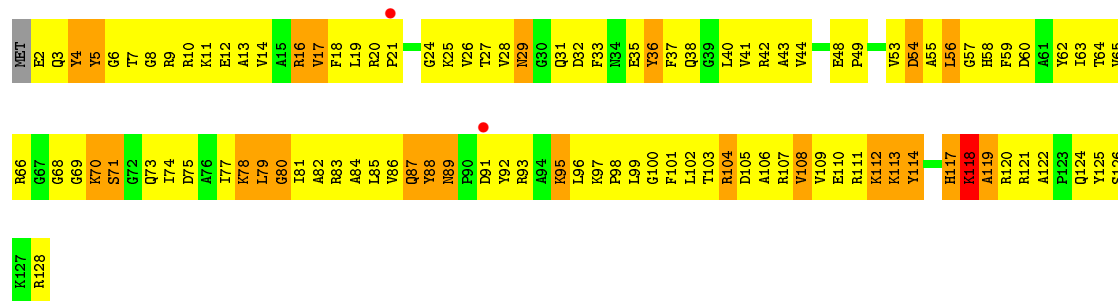
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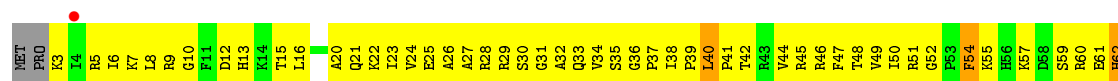
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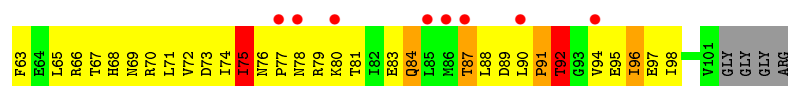


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

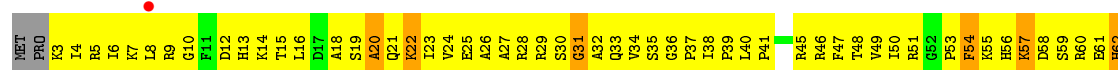


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

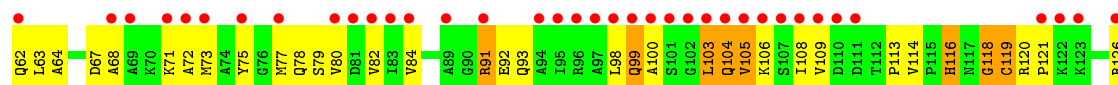
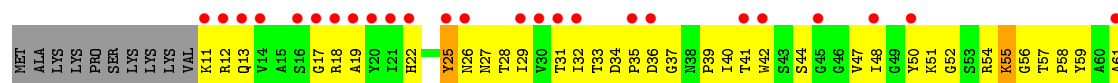




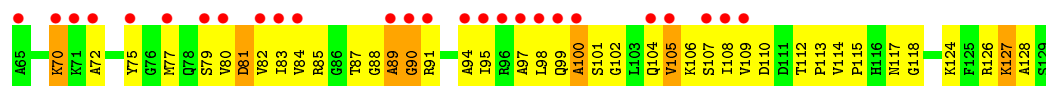
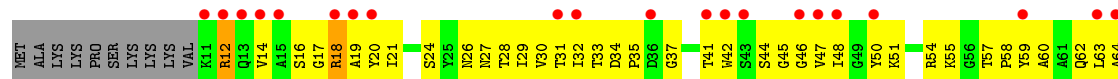
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



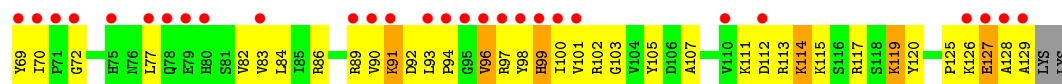
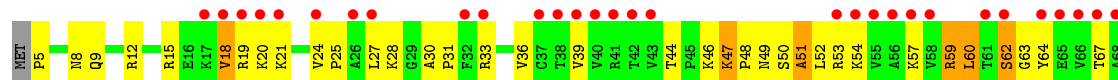
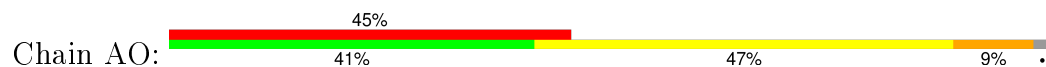
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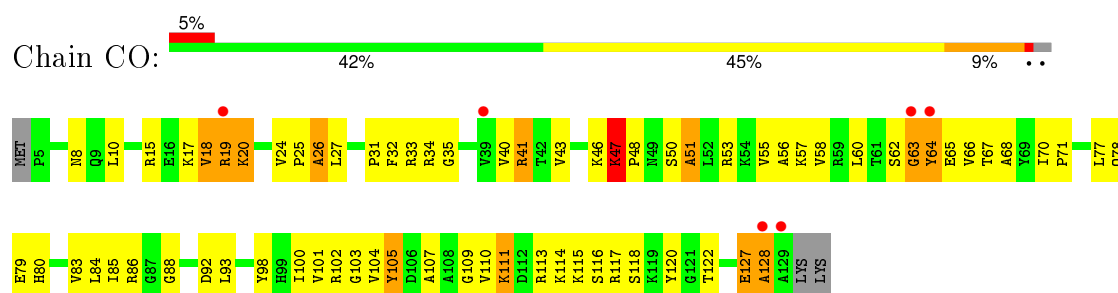
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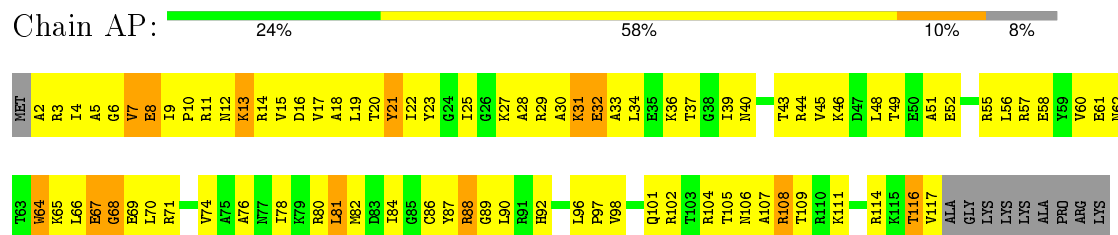
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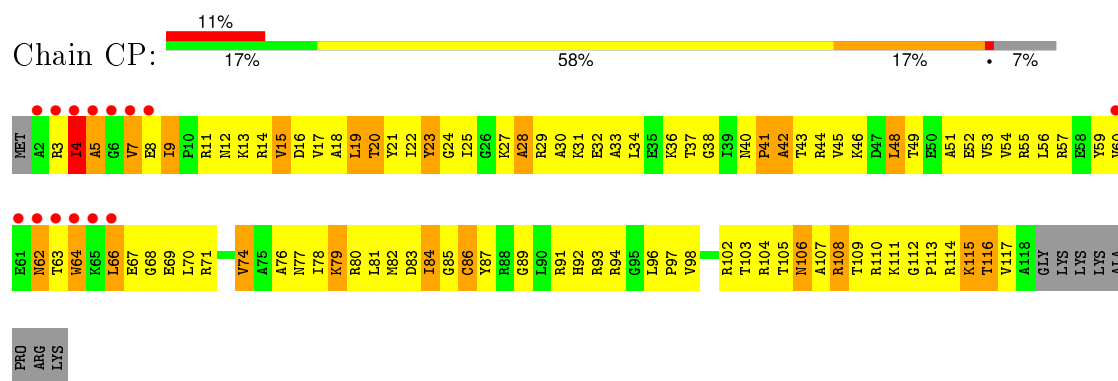
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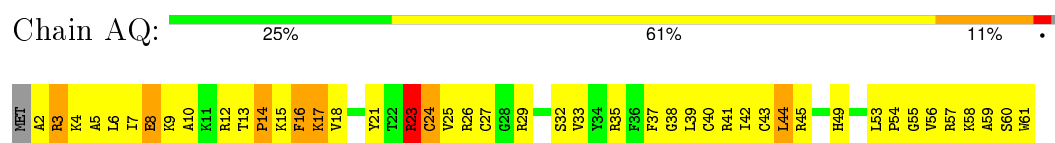
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



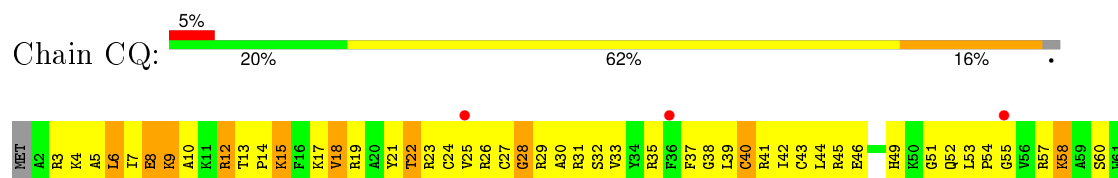
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



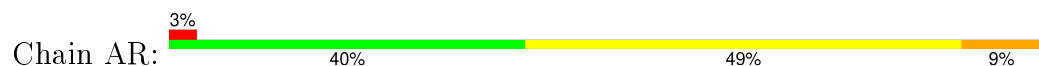
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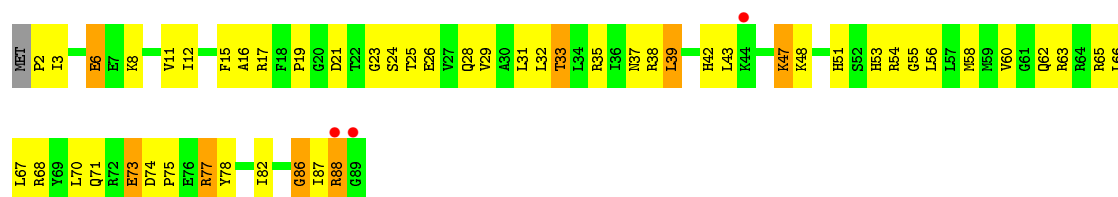


• Molecule 14: 30S RIBOSOMAL PROTEIN S14

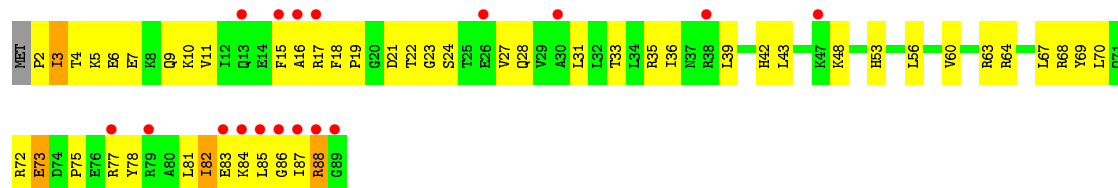
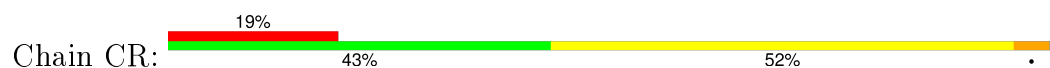


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

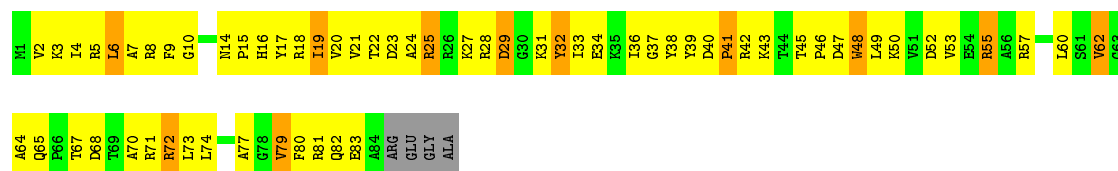




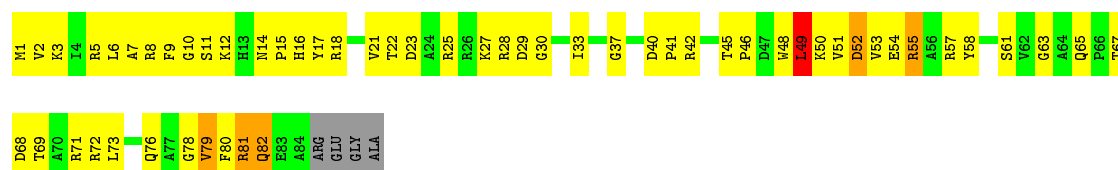
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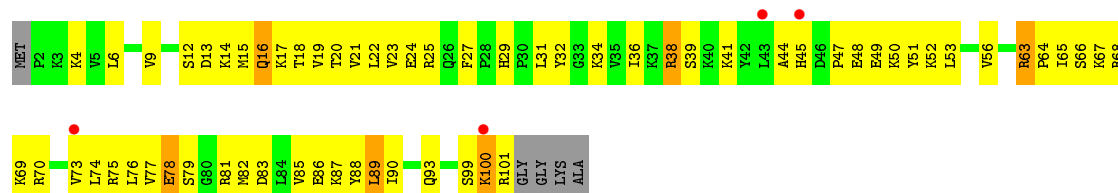
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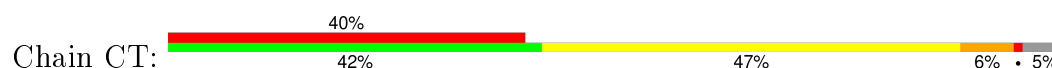
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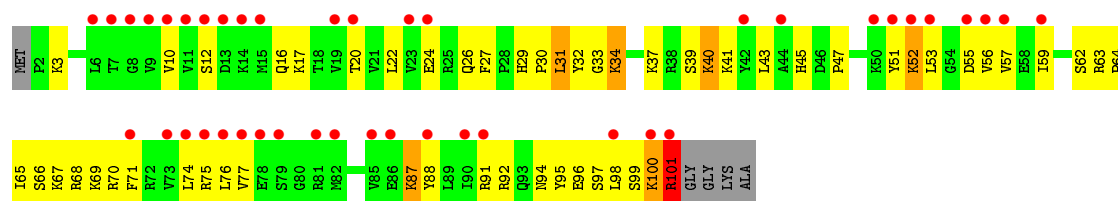


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

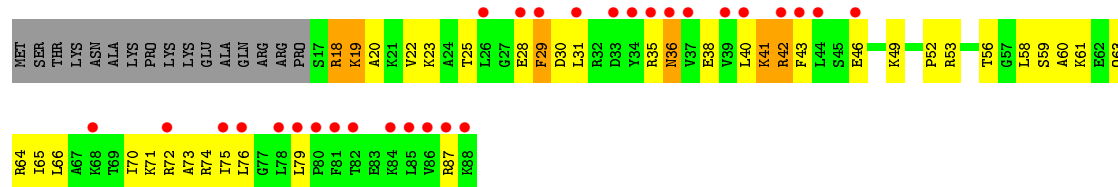


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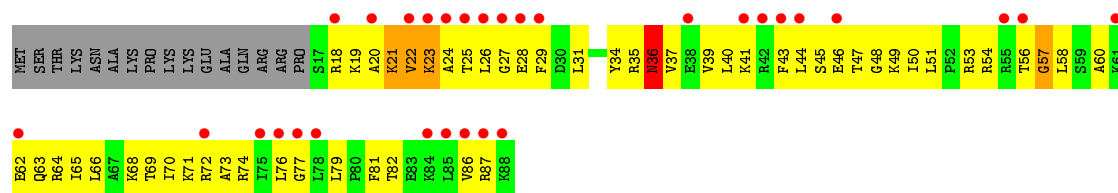




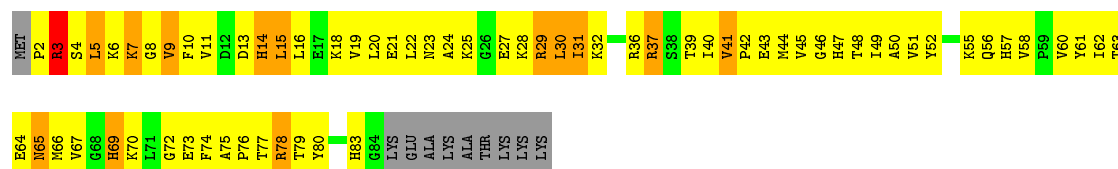
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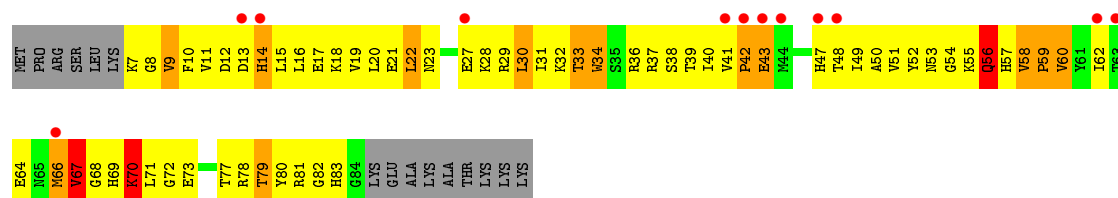
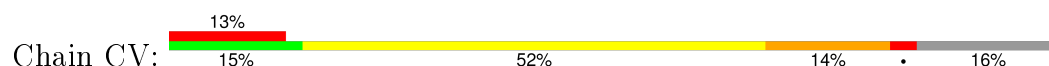
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



A16
U17
G18
U19

• Molecule 23: MRNA

Chain C1: 50% 50%

A16
U17
G18
U19

• Molecule 24: 23S ribosomal RNA

Chain BA: 3% 33% 52% 15%

G1 G2 G3 G4 A5 A6 A7 A8 A9 G10 G11 G12 A13 A14 A15 G16 G17 C18 U25 U26 U27 A28 U29 G30 G31 G32 G33 G34 G35 G36 G39 G40 G46 A49 U50 U51 G55 A56 A57 C57 G58 U63 A64 U67 G68 G69 G70 U71 U72 U73 A74 G75 A78

G79 G85 G86 G92 G93 G94 G95 U99 G101 G102 A103 A104 C105 G106 G107 U108 U109 G110 A111 U112 G113 G116 G117 A118 A119 U120 G125 A126 G136 C137 G139 A140 A141 C141A G142 C143 C144 C150 C151 G152 G153 G154 C155 U161 U162 U163 U164 U165 G171 G172 G173 C174

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G248 C249 G250 A251 C252 C253 G254 G259 G260 G261 A265 G266 U270F U270G U270H U270I U270J U270K U270L U270M U270N U270O U270P U270Q U270R U270S U270T U270U G271A G271B U271C G272 G273 G273A U273E C273F G274 A275 A276 C277 A278 C285 C286 C287 C288 A289 G290

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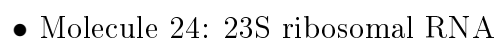
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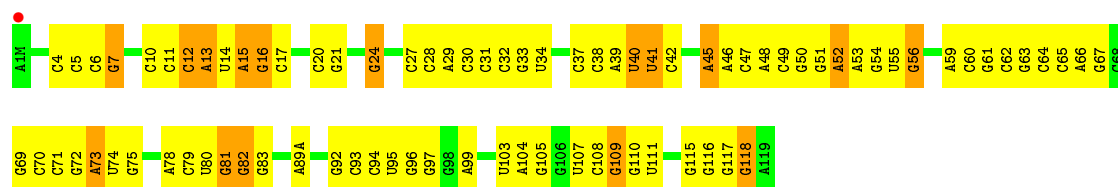
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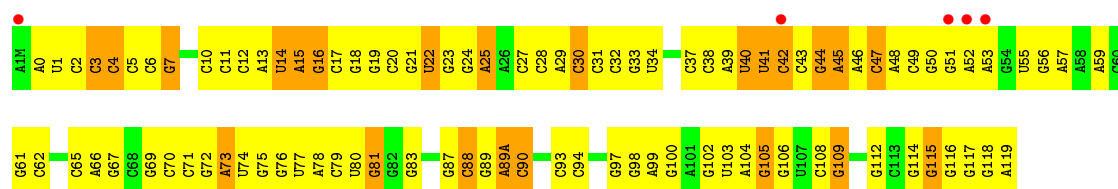
WORLDWIDE
PDB
PROTEIN DATA BANK

- Molecule 25: 5S RIBOSOMAL RNA

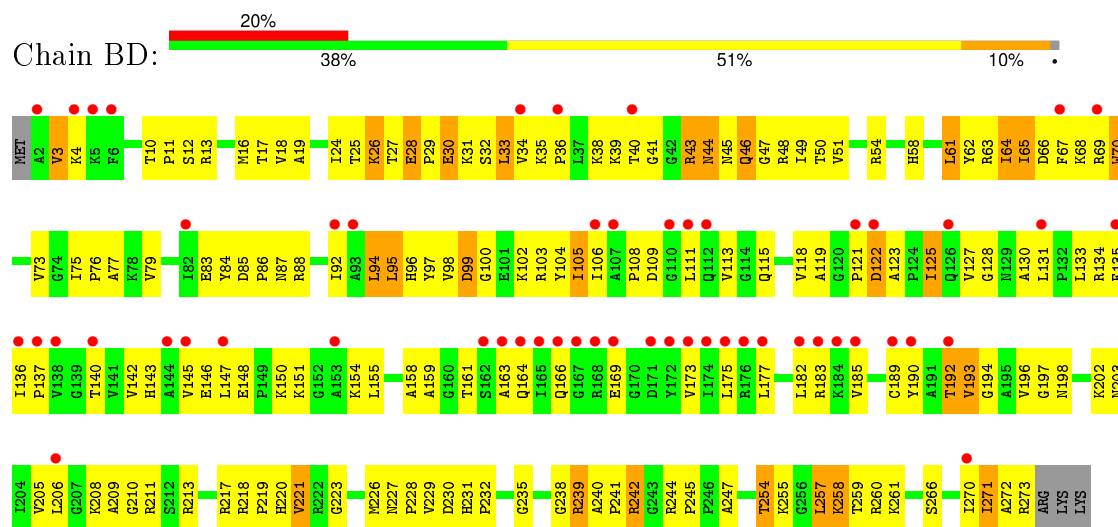


- Molecule 25: 5S RIBOSOMAL RNA

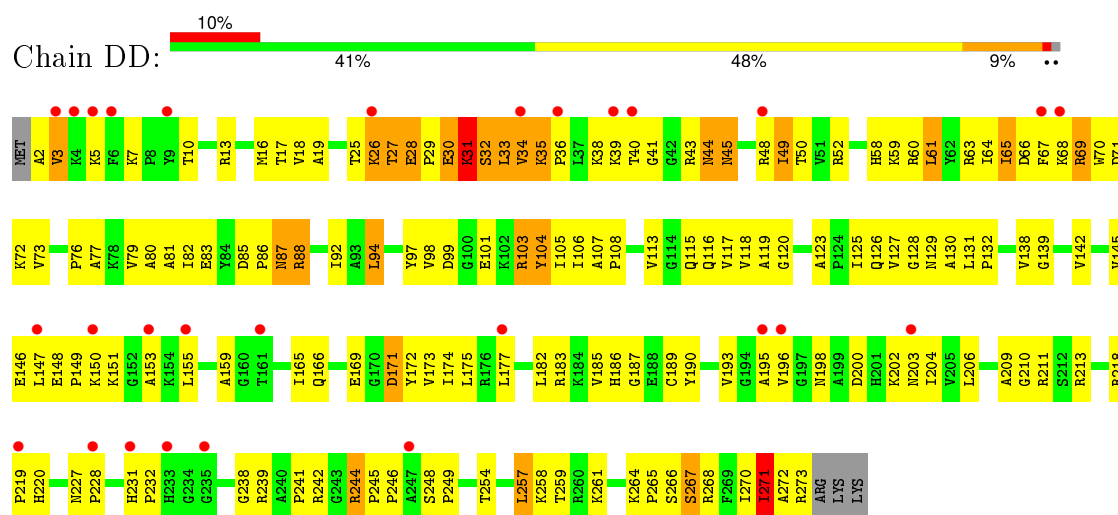




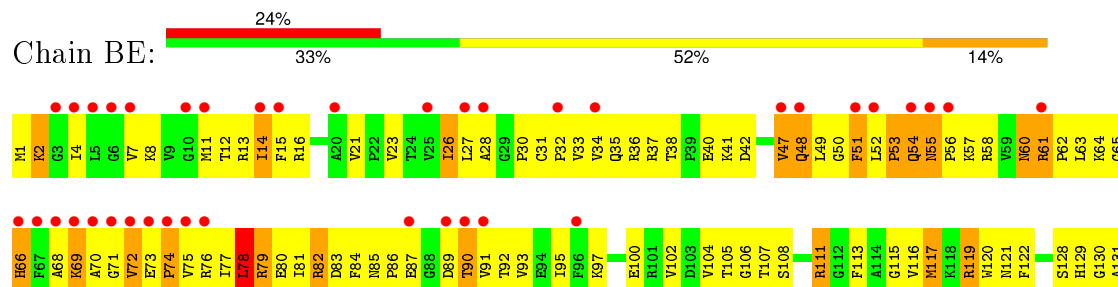
• Molecule 26: 50S ribosomal protein L2



• Molecule 26: 50S ribosomal protein L2

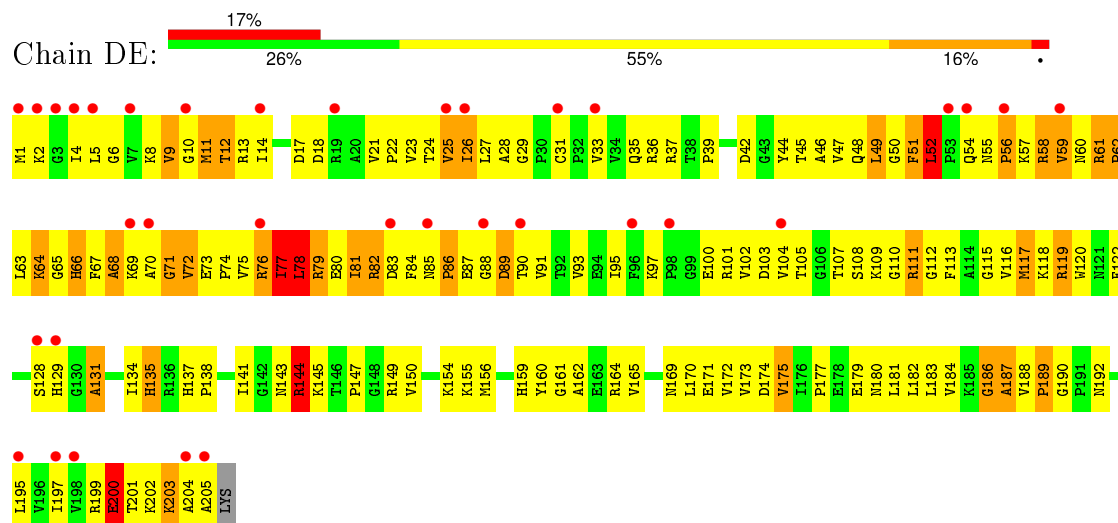


• Molecule 27: 50S ribosomal protein L3

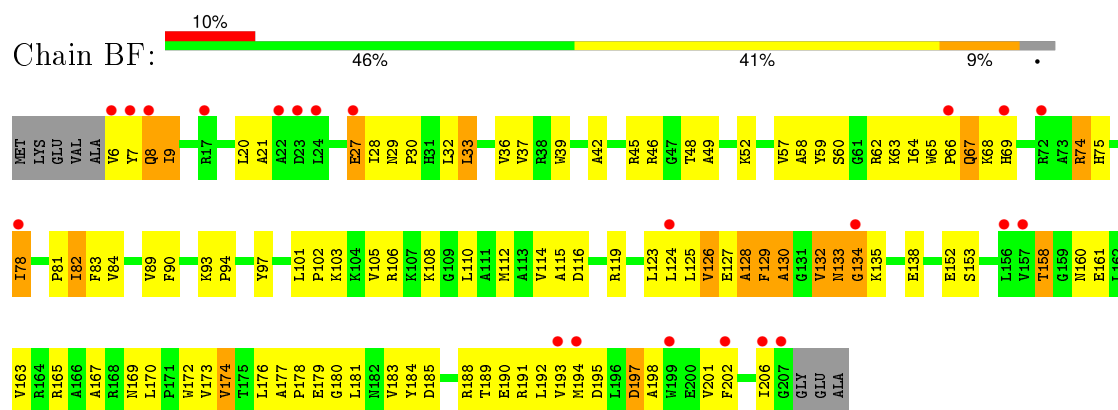




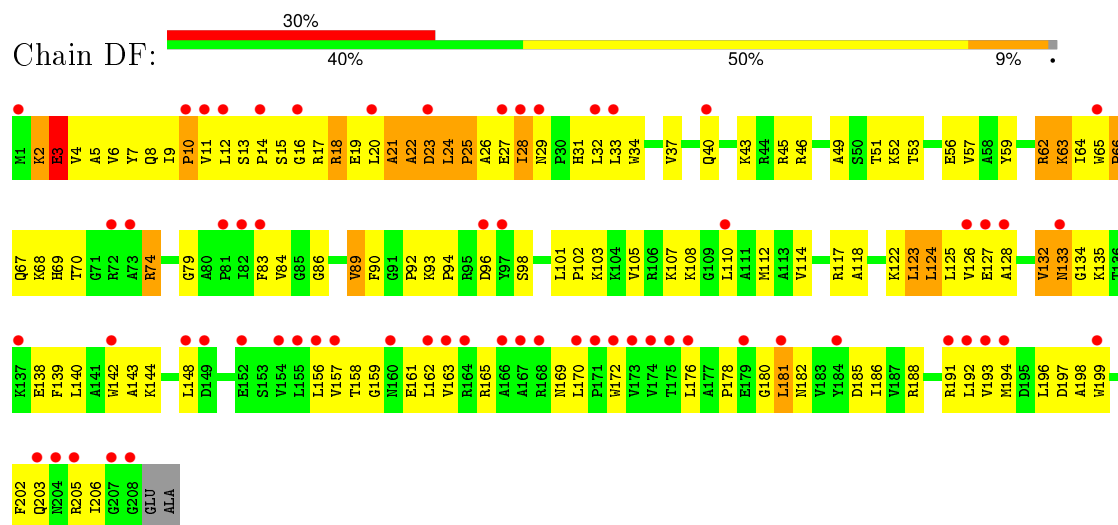
• Molecule 27: 50S ribosomal protein L3



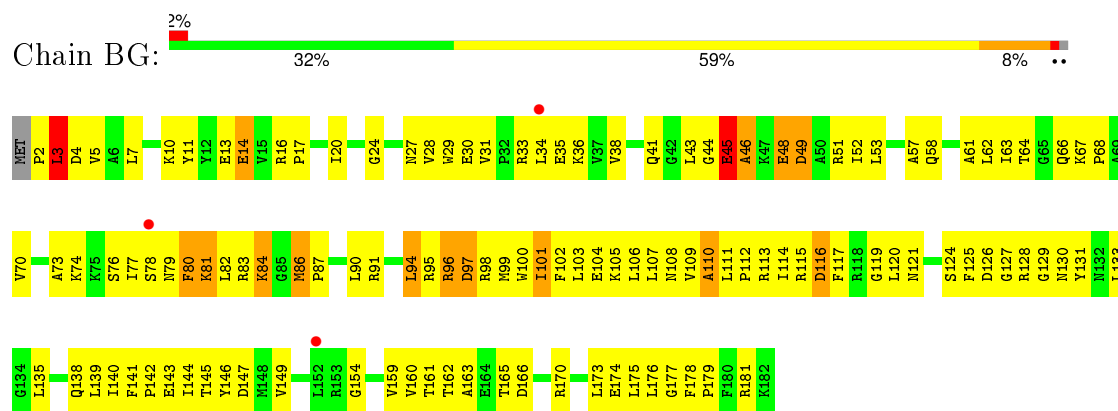
• Molecule 28: 50S ribosomal protein L4



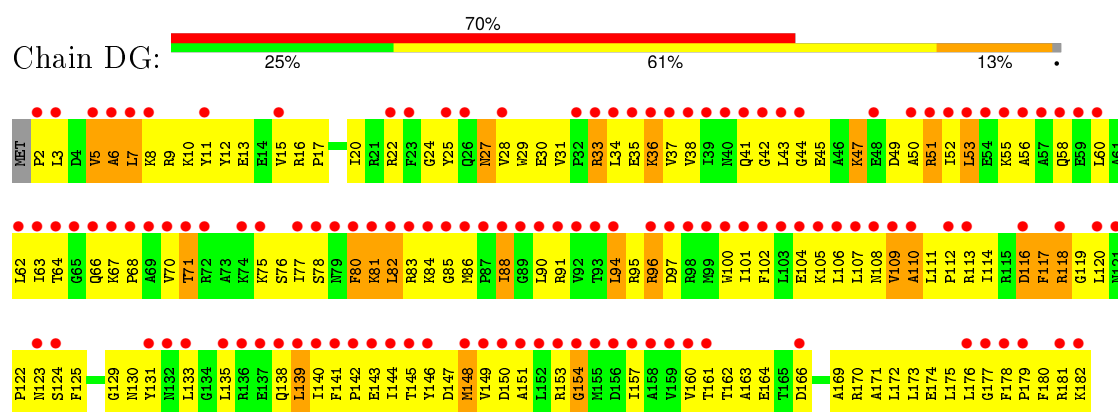
• Molecule 28: 50S ribosomal protein L4



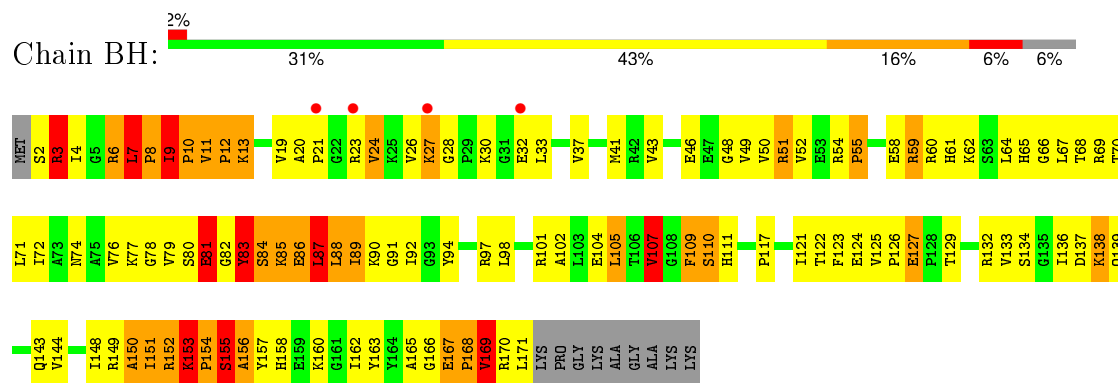
- Molecule 29: 50S ribosomal protein L5



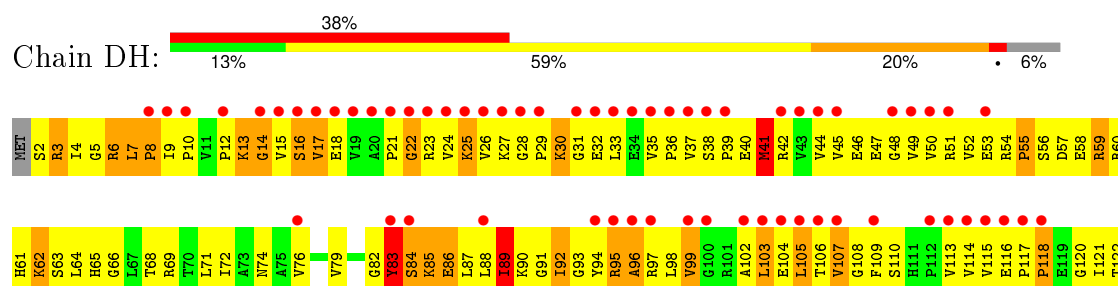
- Molecule 29: 50S ribosomal protein L5

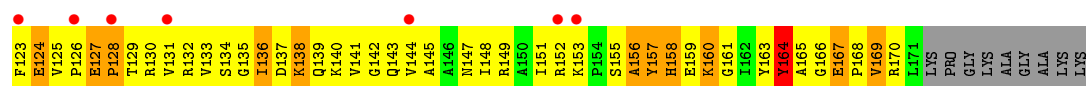


- Molecule 30: 50S ribosomal protein L6

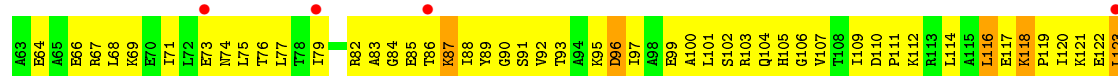


- Molecule 30: 50S ribosomal protein L6

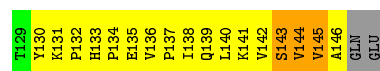
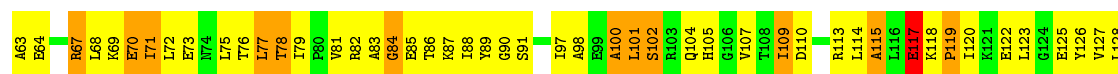
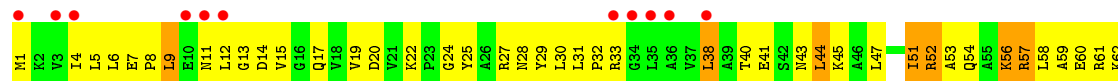




• Molecule 31: 50S ribosomal protein L9



• Molecule 31: 50S ribosomal protein L9



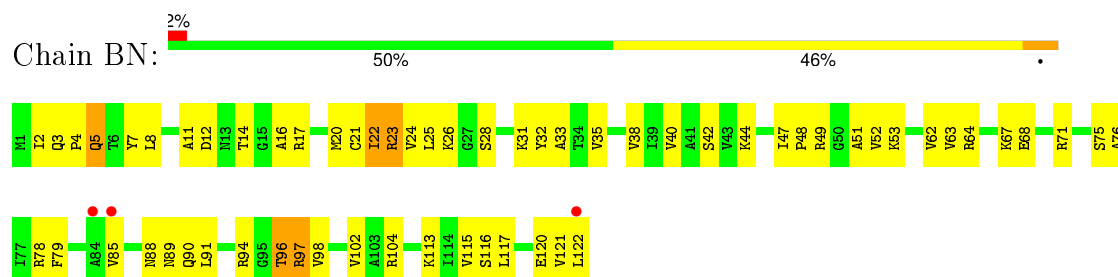
• Molecule 32: 50S ribosomal protein L13



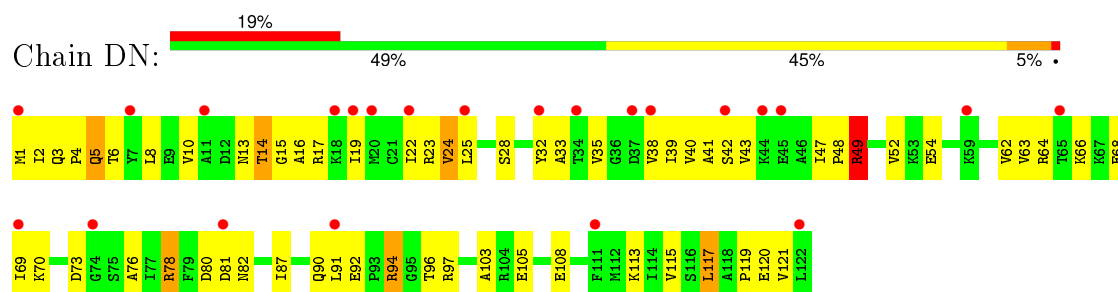
• Molecule 32: 50S ribosomal protein L13



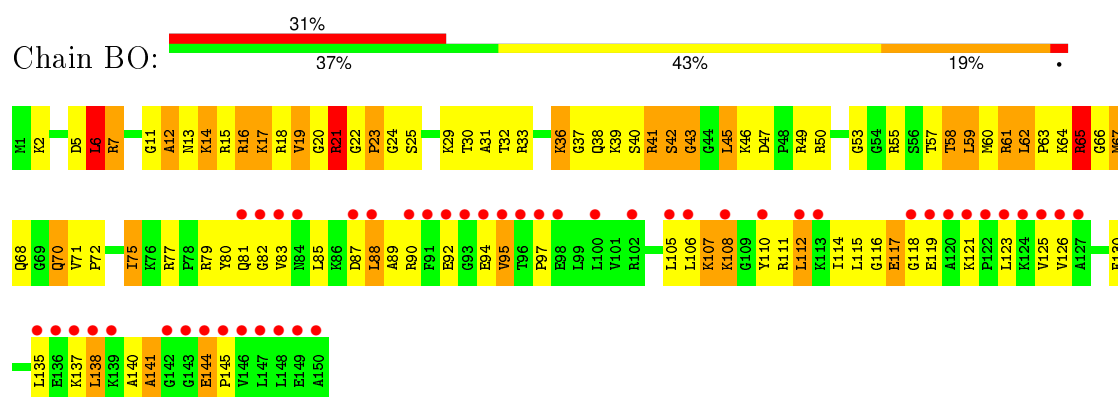
- Molecule 33: 50S ribosomal protein L14



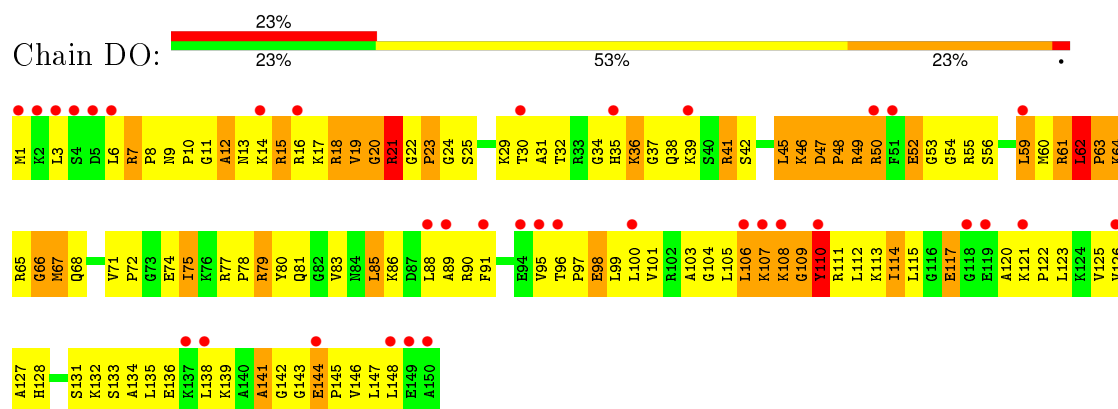
- Molecule 33: 50S ribosomal protein L14



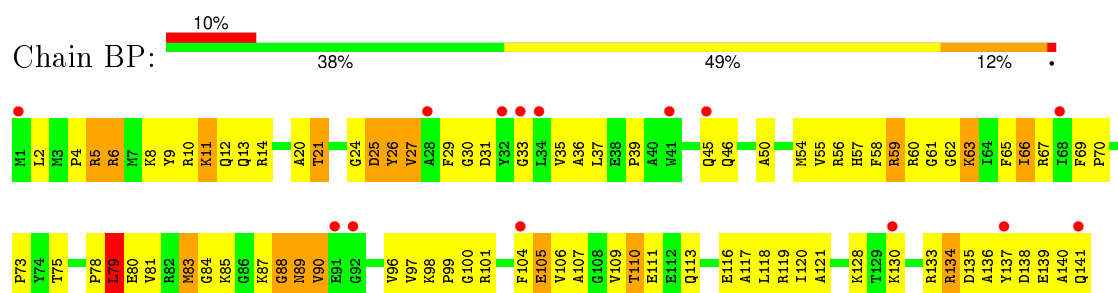
- Molecule 34: 50S ribosomal protein L15



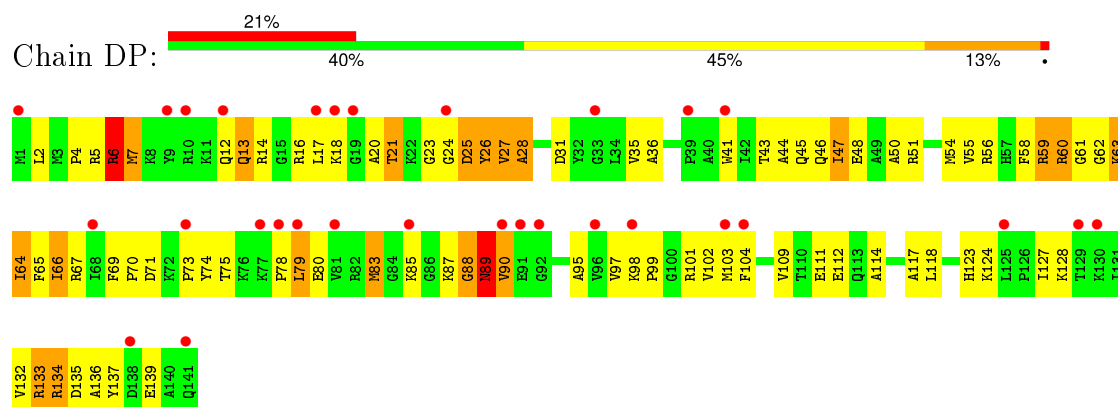
- Molecule 34: 50S ribosomal protein L15



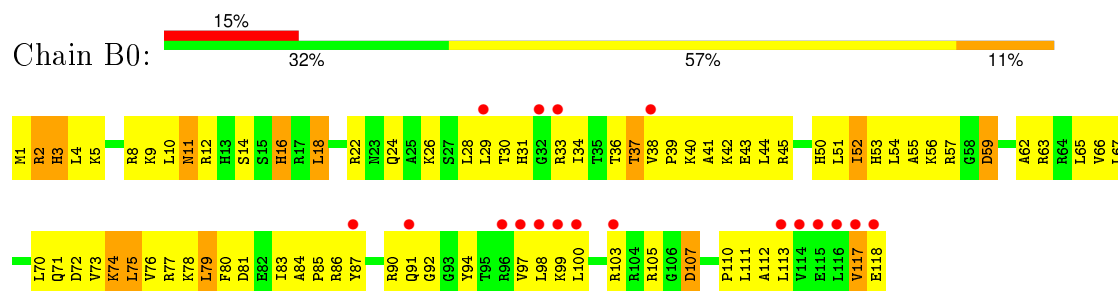
- Molecule 35: 50S ribosomal protein L16



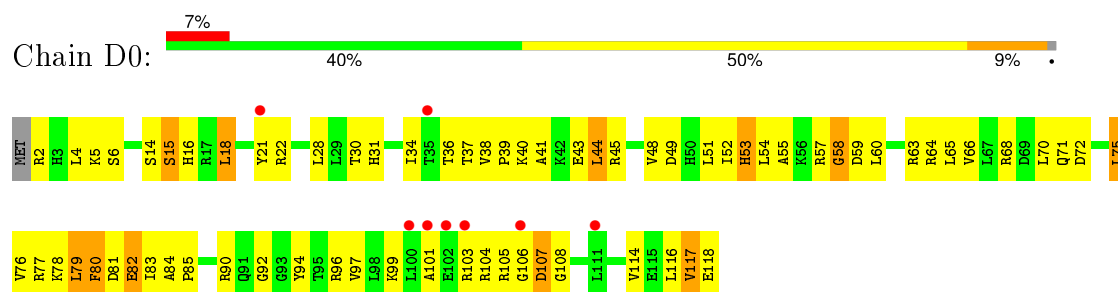
• Molecule 35: 50S ribosomal protein L16



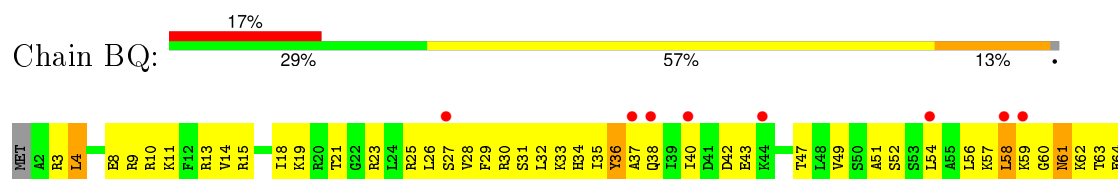
• Molecule 36: 50S ribosomal protein L17

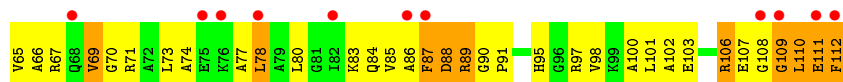


• Molecule 36: 50S ribosomal protein L17

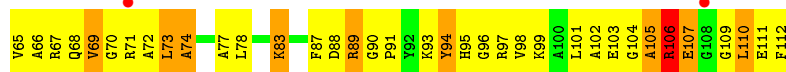
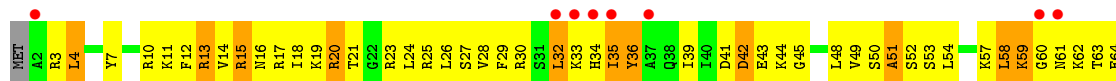


• Molecule 37: 50S ribosomal protein L18

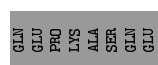
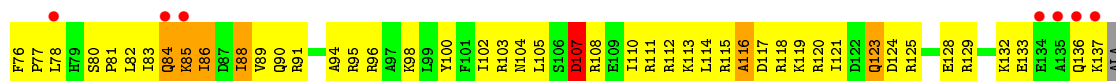
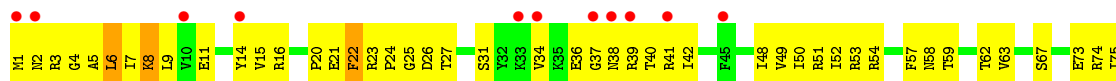




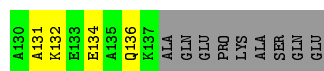
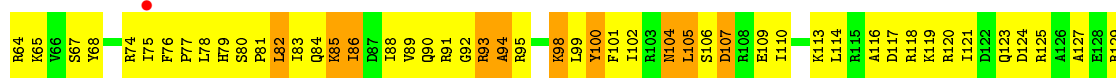
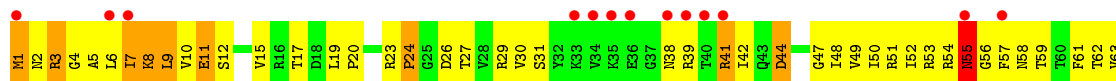
- Molecule 37: 50S ribosomal protein L18



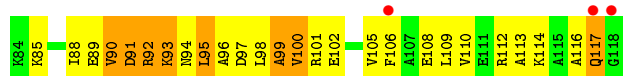
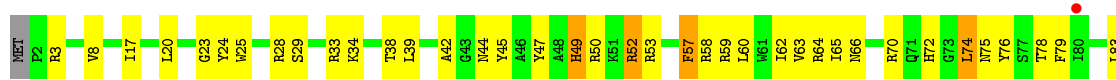
- Molecule 38: 50S ribosomal protein L19



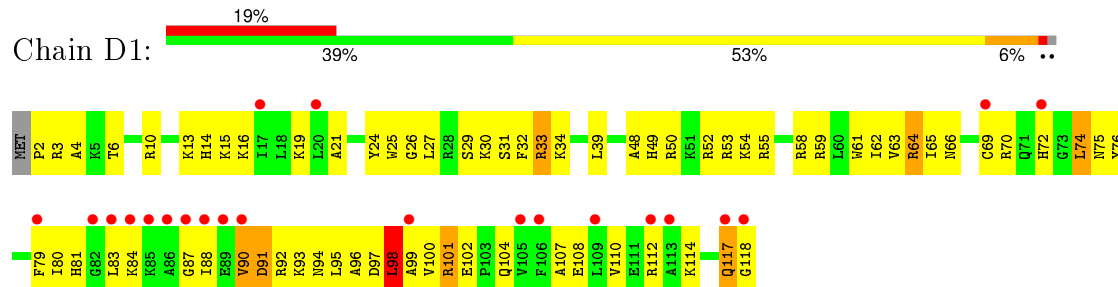
- Molecule 38: 50S ribosomal protein L19



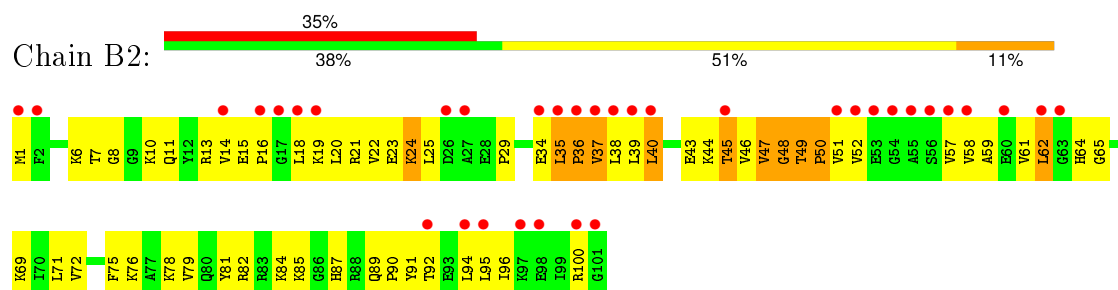
- Molecule 39: 50S ribosomal protein L20



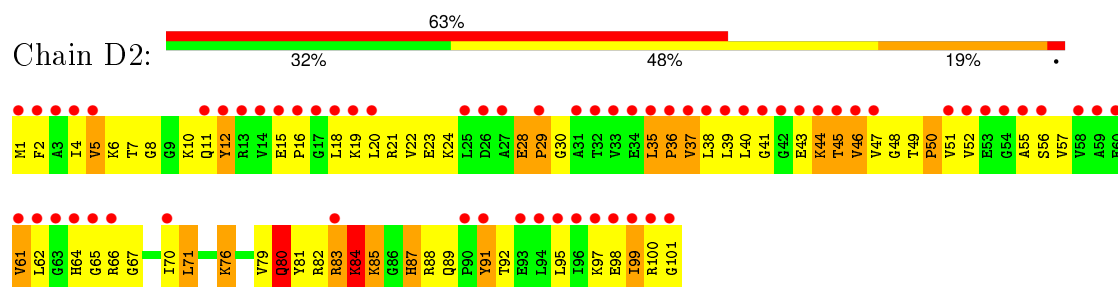
- Molecule 39: 50S ribosomal protein L20



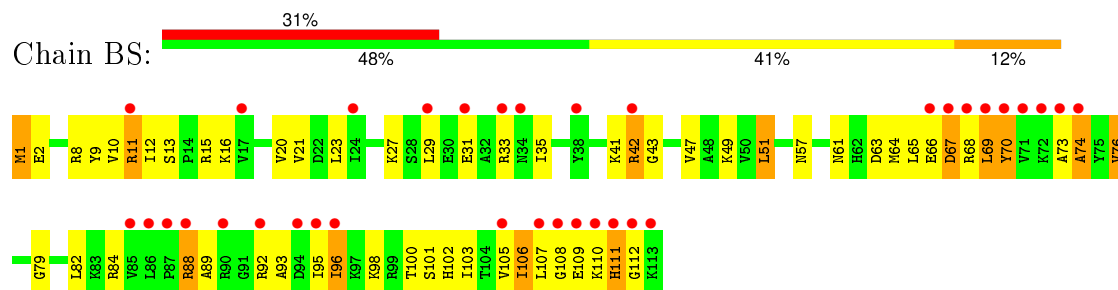
- Molecule 40: 50S ribosomal protein L21



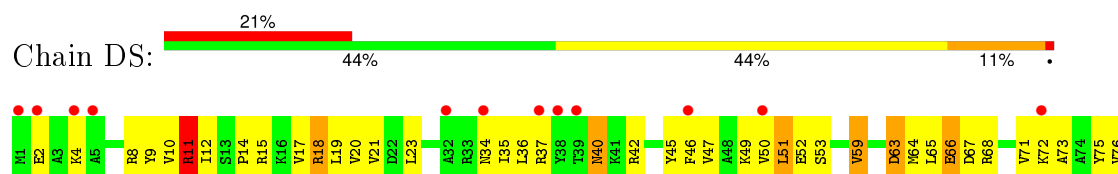
- Molecule 40: 50S ribosomal protein L21

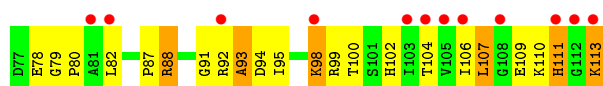


- Molecule 41: 50S ribosomal protein L22

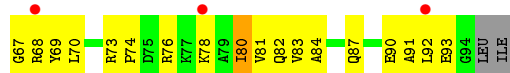


- Molecule 41: 50S ribosomal protein L22

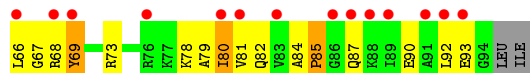
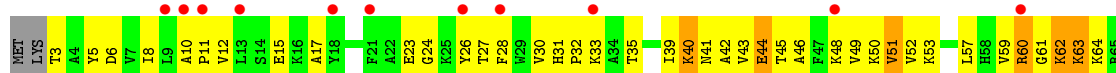
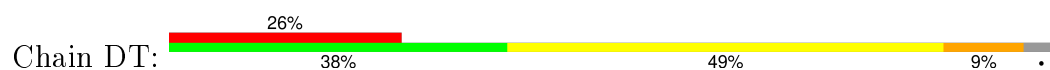




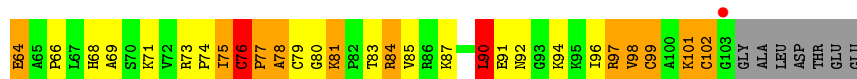
- Molecule 42: 50S ribosomal protein L23



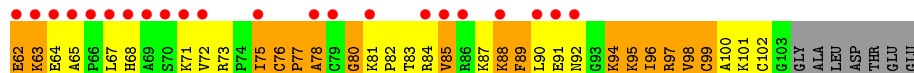
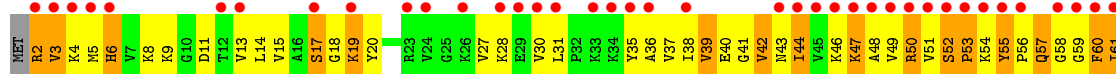
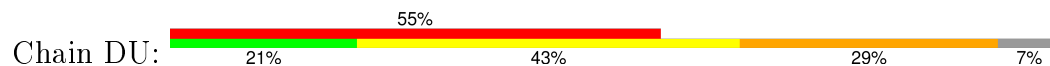
- Molecule 42: 50S ribosomal protein L23



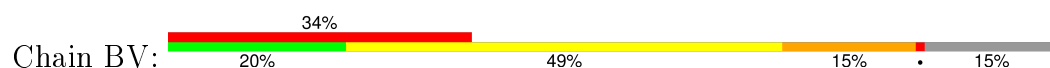
- Molecule 43: 50S ribosomal protein L24

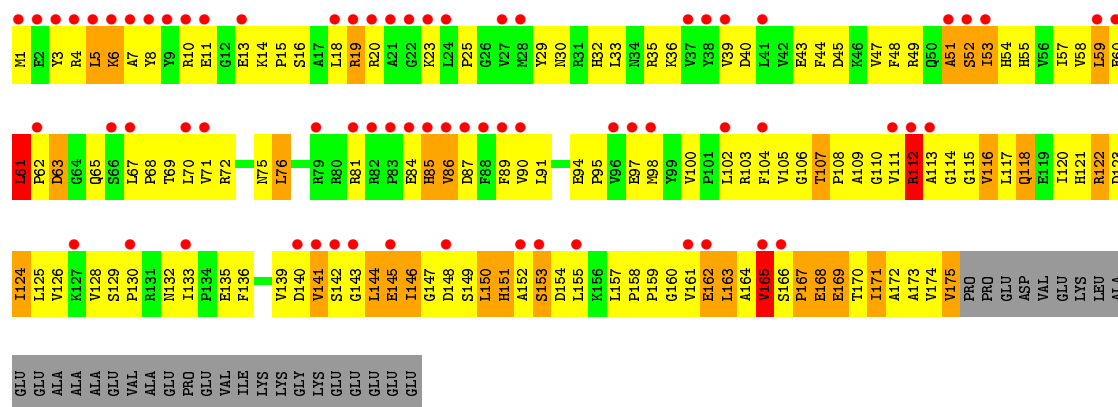


- Molecule 43: 50S ribosomal protein L24

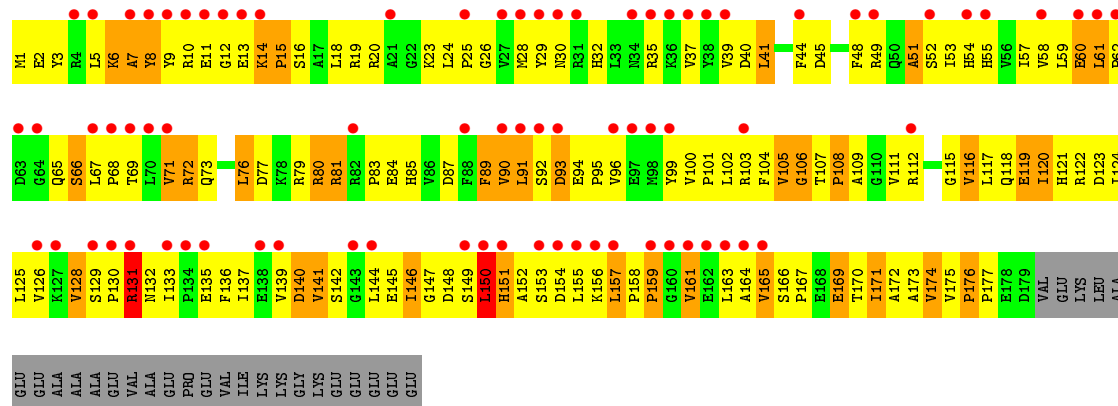
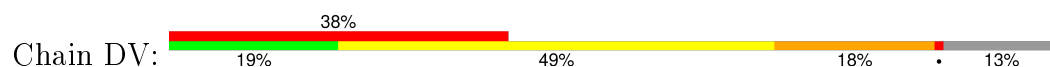


- Molecule 44: 50S ribosomal protein L25

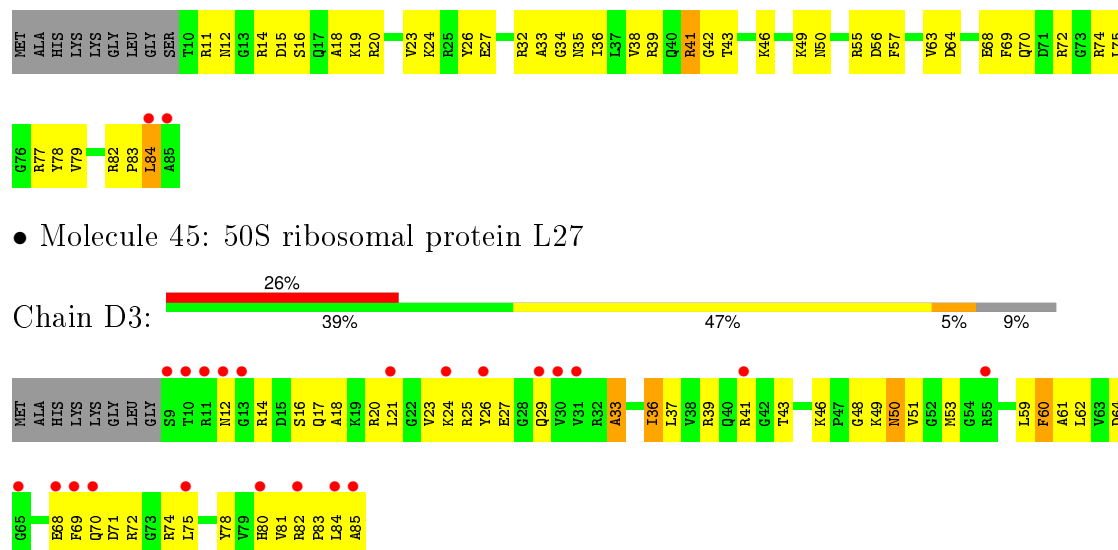
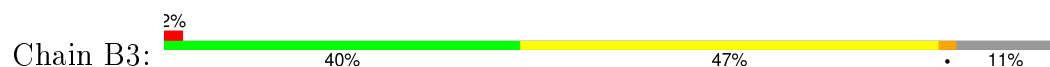




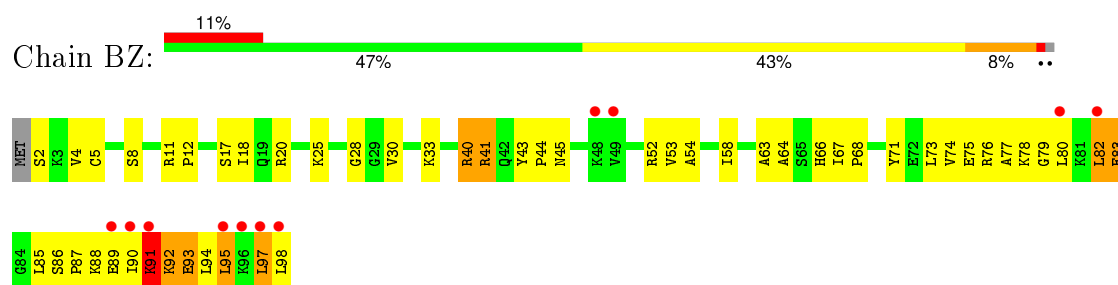
• Molecule 44: 50S ribosomal protein L25



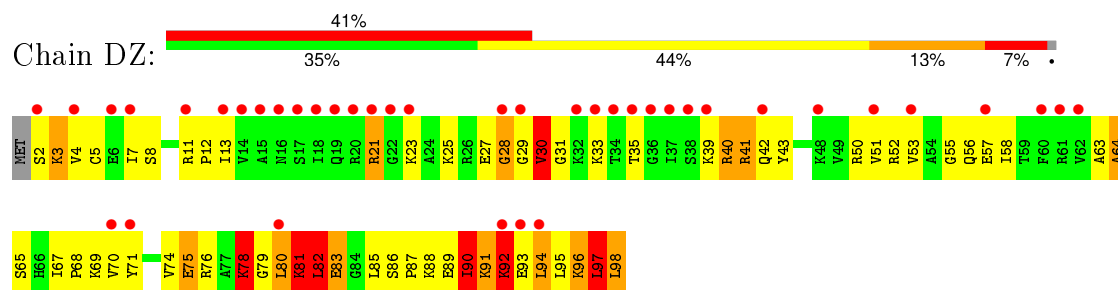
• Molecule 45: 50S ribosomal protein L27



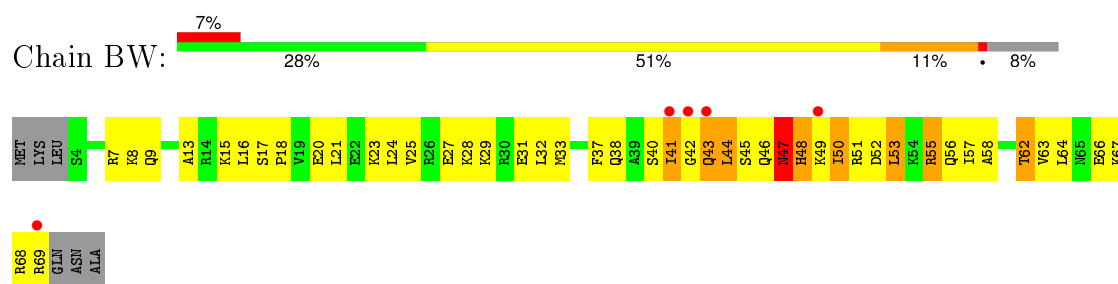
• Molecule 46: 50S ribosomal protein L28



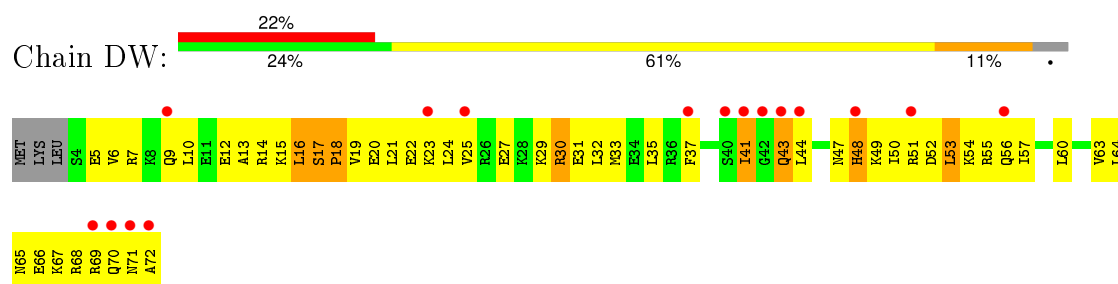
- Molecule 46: 50S ribosomal protein L28



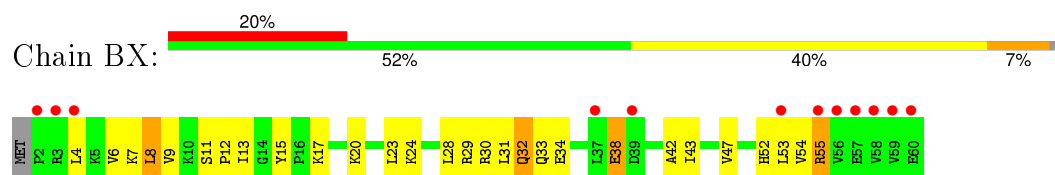
- Molecule 47: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L29

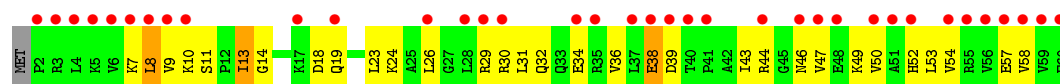


- Molecule 48: 50S ribosomal protein L30

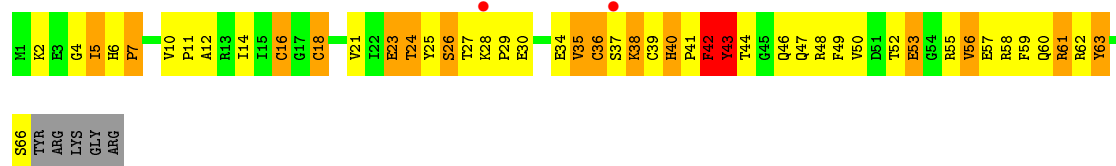


- Molecule 48: 50S ribosomal protein L30

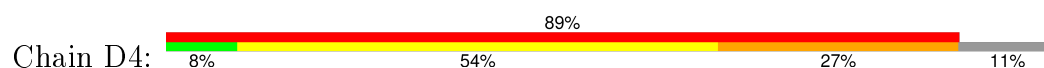




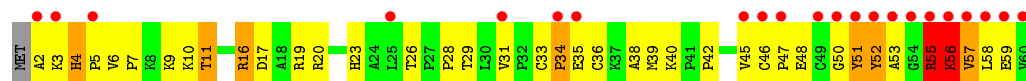
- Molecule 49: 50S ribosomal protein L31



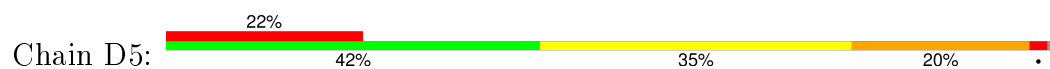
- Molecule 49: 50S ribosomal protein L31



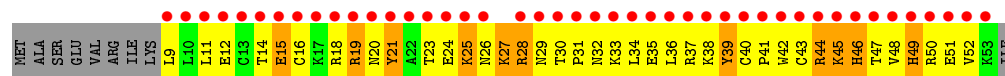
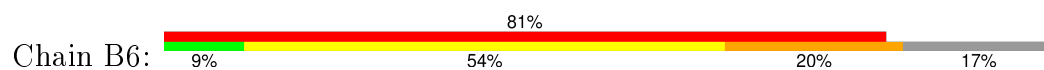
- Molecule 50: 50S ribosomal protein L32



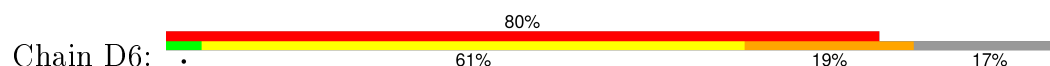
- Molecule 50: 50S ribosomal protein L32

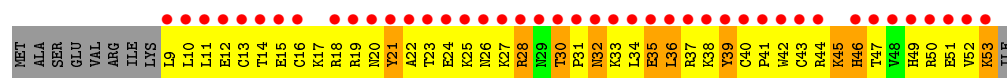


- Molecule 51: 50S ribosomal protein L33



- Molecule 51: 50S ribosomal protein L33





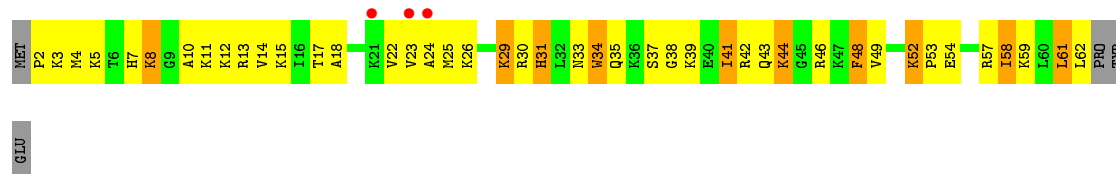
- Molecule 52: 50S ribosomal protein L34



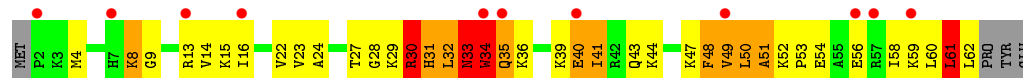
- Molecule 52: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L35



- Molecule 53: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.27Å 448.54Å 615.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	173.07 – 3.30 224.27 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (173.07-3.30) 93.5 (224.27-3.30)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_987)	Depositor
R, R_{free}	0.202 , 0.254 0.197 , 0.256	Depositor DCC
R_{free} test set	1850 reflections (0.23%)	DCC
Wilson B-factor (Å ²)	101.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 83.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 859965 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	292440	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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: ZN, MG, TAC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.31	2/36234 (0.0%)	0.62	7/56554 (0.0%)
1	CA	0.30	0/36237	0.60	4/56558 (0.0%)
2	AE	0.28	0/1959	0.47	0/2642
2	CE	0.25	0/1959	0.43	0/2642
3	AF	0.25	0/1629	0.41	0/2195
3	CF	0.26	0/1636	0.42	0/2205
4	AG	0.40	2/1733 (0.1%)	0.49	0/2318
4	CG	0.36	1/1733 (0.1%)	0.50	1/2318 (0.0%)
5	AH	0.29	0/1171	0.46	0/1576
5	CH	0.28	0/1171	0.47	0/1576
6	AI	0.28	0/856	0.43	0/1154
6	CI	0.27	0/856	0.43	0/1154
7	AJ	0.28	0/1276	0.42	0/1709
7	CJ	0.32	0/1276	0.45	0/1709
8	AK	0.28	0/1136	0.46	0/1527
8	CK	0.68	4/1136 (0.4%)	0.57	1/1527 (0.1%)
9	AL	0.39	1/1029 (0.1%)	0.49	0/1379
9	CL	0.31	0/1029	0.46	0/1379
10	AM	0.25	0/814	0.44	0/1095
10	CM	0.28	0/814	0.47	0/1095
11	AN	0.27	0/900	0.46	0/1213
11	CN	0.25	0/900	0.43	0/1213
12	AO	0.29	0/991	0.47	0/1327
12	CO	0.31	0/991	0.47	0/1327
13	AP	0.30	0/938	0.47	0/1258
13	CP	0.26	0/943	0.44	0/1265
14	AQ	0.31	0/501	0.45	0/664
14	CQ	0.31	0/501	0.54	1/664 (0.2%)
15	AR	0.27	0/745	0.42	0/992
15	CR	0.26	0/745	0.38	0/992
16	AS	0.32	0/721	0.47	0/970
16	CS	0.27	0/721	0.44	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.30	0/847	0.44	0/1131
17	CT	0.33	0/847	0.53	1/1131 (0.1%)
18	AU	0.26	0/596	0.44	0/790
18	CU	0.28	0/596	0.45	0/790
19	AV	0.34	0/680	0.58	0/915
19	CV	0.35	0/638	0.58	0/860
20	AW	0.41	0/765	0.54	0/1007
20	CW	0.27	0/765	0.44	0/1007
21	AX	0.28	0/221	0.43	0/288
21	CX	0.41	0/221	0.61	0/288
22	AC	0.47	2/1832 (0.1%)	0.82	5/2855 (0.2%)
22	CC	0.45	2/1832 (0.1%)	0.80	5/2855 (0.2%)
23	A1	0.33	0/94	0.62	0/144
23	C1	0.40	0/94	0.67	0/144
24	BA	0.43	1/70233 (0.0%)	0.77	36/109643 (0.0%)
24	DA	0.39	4/70167 (0.0%)	0.73	38/109541 (0.0%)
25	BB	0.37	0/2928	0.73	1/4568 (0.0%)
25	DB	0.34	0/2928	0.62	0/4568
26	BD	0.39	0/2165	0.57	0/2919
26	DD	0.59	5/2165 (0.2%)	0.55	0/2919
27	BE	0.32	0/1601	0.52	0/2160
27	DE	0.32	0/1601	0.55	0/2160
28	BF	0.32	0/1620	0.49	0/2194
28	DF	0.29	0/1662	0.49	0/2249
29	BG	0.30	0/1499	0.48	0/2016
29	DG	0.27	0/1499	0.46	0/2016
30	BH	0.38	0/1332	0.63	2/1802 (0.1%)
30	DH	0.25	0/1332	0.52	2/1802 (0.1%)
31	BK	0.28	0/1151	0.47	0/1558
31	DK	0.27	0/1151	0.48	0/1558
32	BM	0.28	0/1131	0.50	0/1525
32	DM	0.28	0/1131	0.46	0/1525
33	BN	0.30	0/943	0.48	0/1269
33	DN	0.30	0/943	0.47	0/1269
34	BO	0.39	0/1162	0.64	0/1544
34	DO	0.38	0/1162	0.57	0/1544
35	BP	0.35	0/1143	0.53	0/1527
35	DP	0.41	2/1143 (0.2%)	0.82	3/1527 (0.2%)
36	B0	0.35	0/982	0.53	1/1312 (0.1%)
36	D0	0.30	0/974	0.50	0/1302
37	BQ	0.32	0/892	0.54	0/1187
37	DQ	0.39	0/892	0.51	0/1187
38	BR	0.31	0/1155	0.47	0/1542

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.34	0/1155	0.51	0/1542
39	B1	0.36	0/982	0.52	0/1306
39	D1	0.31	0/982	0.46	0/1306
40	B2	0.32	0/790	0.52	0/1057
40	D2	0.35	0/790	0.53	0/1057
41	BS	0.31	0/911	0.50	0/1220
41	DS	0.30	0/911	0.50	0/1220
42	BT	0.42	0/739	0.52	0/993
42	DT	0.36	0/739	0.50	0/993
43	BU	0.37	0/798	0.51	0/1064
43	DU	0.33	0/798	0.50	0/1064
44	BV	0.32	0/1427	0.50	0/1935
44	DV	0.27	0/1460	0.45	0/1982
45	B3	0.33	0/615	0.50	0/819
45	D3	0.32	0/621	0.48	0/827
46	BZ	0.37	0/770	0.56	0/1022
46	DZ	0.33	0/770	0.55	0/1022
47	BW	0.39	0/560	0.55	0/741
47	DW	0.29	0/583	0.48	0/771
48	BX	0.31	0/474	0.48	0/635
48	DX	0.26	0/474	0.45	0/635
49	B4	0.81	3/545 (0.6%)	0.65	2/733 (0.3%)
49	D4	0.44	1/527 (0.2%)	0.55	0/709
50	B5	0.33	0/473	0.54	0/639
50	D5	0.29	0/473	0.47	0/639
51	B6	0.44	0/396	0.70	2/529 (0.4%)
51	D6	0.44	0/396	0.62	0/529
52	B7	0.43	0/438	0.68	0/575
52	D7	0.31	0/438	0.53	0/575
53	B8	0.40	0/494	0.58	0/649
53	D8	0.49	0/494	0.84	3/649 (0.5%)
All	All	0.37	30/316019 (0.0%)	0.66	115/472742 (0.0%)

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	DA	2377	A	N9-C4	20.50	1.50	1.37
26	DD	104	TYR	CD1-CE1	13.75	1.59	1.39
8	CK	94	TYR	CD2-CE2	-13.18	1.19	1.39
49	B4	16	CYS	CB-SG	-12.84	1.60	1.82
26	DD	104	TYR	CD2-CE2	12.77	1.58	1.39

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	DA	2377	A	C2-N3-C4	28.76	124.98	110.60
24	BA	2751	G	N1-C6-O6	20.94	132.47	119.90
24	DA	2377	A	C8-N9-C4	-20.26	97.69	105.80
35	DP	6	ARG	NE-CZ-NH1	19.44	130.02	120.30
22	CC	17(A)	C	N3-C4-C5	-18.15	114.64	121.90

There are no chirality outliers.

There are no planarity outliers.

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	32369	0	16335	1780	1
1	CA	32372	0	16338	2038	3
2	AE	1924	0	1975	321	0
2	CE	1924	0	1975	349	0
3	AF	1605	0	1668	210	0
3	CF	1612	0	1677	235	0
4	AG	1703	0	1764	273	0
4	CG	1703	0	1763	334	0
5	AH	1155	0	1213	125	0
5	CH	1155	0	1212	196	0
6	AI	843	0	857	100	0
6	CI	843	0	857	107	0
7	AJ	1257	0	1296	153	0
7	CJ	1257	0	1296	176	0
8	AK	1116	0	1177	120	0
8	CK	1116	0	1176	177	0
9	AL	1010	0	1037	267	0
9	CL	1010	0	1037	291	0
10	AM	801	0	849	149	0
10	CM	801	0	849	238	1
11	AN	885	0	904	79	0
11	CN	885	0	904	87	0
12	AO	975	0	1062	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CO	975	0	1062	91	0
13	AP	928	0	987	157	0
13	CP	933	0	992	195	0
14	AQ	492	0	529	74	0
14	CQ	492	0	530	133	0
15	AR	734	0	771	54	0
15	CR	734	0	771	76	0
16	AS	705	0	725	116	0
16	CS	705	0	725	94	0
17	AT	834	0	904	96	0
17	CT	834	0	904	88	0
18	AU	591	0	662	60	0
18	CU	591	0	662	69	0
19	AV	665	0	686	181	0
19	CV	624	0	636	250	0
20	AW	763	0	861	140	0
20	CW	763	0	861	87	0
21	AX	217	0	234	26	0
21	CX	217	0	234	60	0
22	AC	1640	0	836	47	0
22	CC	1640	0	836	67	0
23	A1	85	0	43	1	0
23	C1	85	0	43	5	0
24	BA	62707	0	31611	2736	0
24	DA	62647	0	31583	2861	2
25	BB	2617	0	1328	127	0
25	DB	2617	0	1328	167	0
26	BD	2115	0	2195	286	0
26	DD	2115	0	2192	237	0
27	BE	1568	0	1634	180	0
27	DE	1568	0	1634	297	0
28	BF	1585	0	1632	147	0
28	DF	1627	0	1680	173	0
29	BG	1474	0	1535	213	0
29	DG	1474	0	1535	220	0
30	BH	1307	0	1382	220	0
30	DH	1307	0	1382	277	0
31	BK	1136	0	1223	174	1
31	DK	1136	0	1223	158	0
32	BM	1104	0	1180	105	0
32	DM	1104	0	1180	132	0
33	BN	933	0	996	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DN	933	0	996	84	0
34	BO	1145	0	1228	187	0
34	DO	1145	0	1228	239	0
35	BP	1122	0	1179	127	0
35	DP	1122	0	1178	151	0
36	B0	968	0	1033	102	0
36	D0	960	0	1021	95	0
37	BQ	882	0	943	149	0
37	DQ	882	0	943	207	0
38	BR	1141	0	1202	135	0
38	DR	1141	0	1202	123	0
39	B1	964	0	1022	114	0
39	D1	964	0	1021	140	0
40	B2	779	0	852	103	0
40	D2	779	0	851	175	0
41	BS	900	0	964	66	0
41	DS	900	0	964	75	0
42	BT	725	0	778	72	0
42	DT	725	0	778	86	0
43	BU	785	0	878	136	0
43	DU	785	0	878	153	0
44	BV	1397	0	1430	209	0
44	DV	1428	0	1454	255	0
45	B3	607	0	628	43	0
45	D3	613	0	633	59	0
46	BZ	763	0	848	91	0
46	DZ	763	0	848	93	0
47	BW	558	0	610	62	0
47	DW	581	0	629	71	0
48	BX	469	0	518	31	0
48	DX	469	0	518	39	0
49	B4	533	0	522	132	0
49	D4	515	0	510	157	0
50	B5	459	0	480	67	0
50	D5	459	0	476	46	0
51	B6	389	0	404	142	0
51	D6	389	0	404	166	0
52	B7	430	0	480	55	0
52	D7	430	0	479	73	0
53	B8	488	0	560	110	0
53	D8	488	0	559	138	0
54	A1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AA	232	0	0	0	0
54	AC	9	0	0	0	0
54	AG	2	0	0	0	0
54	AH	2	0	0	0	0
54	AJ	1	0	0	0	0
54	AQ	2	0	0	0	0
54	AR	1	0	0	0	0
54	AS	1	0	0	0	0
54	B1	2	0	0	0	0
54	B2	1	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B6	1	0	0	0	0
54	B7	3	0	0	0	0
54	B8	1	0	0	0	0
54	BA	627	0	0	0	0
54	BB	17	0	0	0	0
54	BE	5	0	0	0	0
54	BF	2	0	0	0	0
54	BO	3	0	0	0	0
54	BP	1	0	0	0	0
54	BU	2	0	0	0	0
54	BZ	1	0	0	0	0
54	CA	204	0	0	0	0
54	CC	8	0	0	0	0
54	CG	2	0	0	0	0
54	CH	1	0	0	0	0
54	CS	1	0	0	0	0
54	D1	1	0	0	0	0
54	D5	1	0	0	0	0
54	DA	525	0	0	0	0
54	DB	14	0	0	0	0
54	DD	1	0	0	0	0
54	DE	3	0	0	0	0
54	DP	1	0	0	0	0
54	DR	1	0	0	0	0
54	DU	1	0	0	0	0
54	DZ	2	0	0	0	0
55	AA	32	1	21	4	0
55	CA	32	0	22	3	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CG	1	0	0	2	0
56	CQ	1	0	0	0	0
All	All	292439	1	197340	20528	4

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 43.

The worst 5 of 20528 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)
24:DA:1600:C:C2'	52:D7:49:ARG:HE	0.98	1.56
4:CG:31:CYS:SG	4:CG:33:MET:HE2	1.43	1.53
1:CA:598:U:O3'	8:CK:94:TYR:CE2	1.65	1.48
19:CV:70:LYS:CE	19:CV:73:GLU:HG3	1.44	1.48
24:DA:1600:C:H2'	52:D7:49:ARG:NE	1.12	1.43

All (4) 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)
31:BK:89:TYR:O	1:CA:357:G:O2'[4_555]	2.01	0.19
1:CA:86:U:O2'	24:DA:276:A:OP2[3_545]	2.09	0.11
1:AA:1175:G:O2'	10:CM:80:LYS:NZ[4_555]	2.18	0.02
1:CA:84:U:O2'	24:DA:273:G:OP1[3_545]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AE	235/256 (92%)	162 (69%)	47 (20%)	26 (11%)	0 3
2	CE	235/256 (92%)	166 (71%)	44 (19%)	25 (11%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AF	203/239 (85%)	150 (74%)	36 (18%)	17 (8%)	1	7
3	CF	204/239 (85%)	138 (68%)	51 (25%)	15 (7%)	1	10
4	AG	206/208 (99%)	157 (76%)	35 (17%)	14 (7%)	1	12
4	CG	206/208 (99%)	140 (68%)	44 (21%)	22 (11%)	0	4
5	AH	149/162 (92%)	127 (85%)	17 (11%)	5 (3%)	5	29
5	CH	149/162 (92%)	112 (75%)	31 (21%)	6 (4%)	4	24
6	AI	99/101 (98%)	81 (82%)	14 (14%)	4 (4%)	4	24
6	CI	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	14
7	AJ	153/156 (98%)	126 (82%)	17 (11%)	10 (6%)	1	13
7	CJ	153/156 (98%)	112 (73%)	33 (22%)	8 (5%)	2	18
8	AK	136/138 (99%)	103 (76%)	27 (20%)	6 (4%)	3	22
8	CK	136/138 (99%)	114 (84%)	15 (11%)	7 (5%)	2	19
9	AL	125/128 (98%)	93 (74%)	26 (21%)	6 (5%)	3	20
9	CL	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1	7
10	AM	97/105 (92%)	75 (77%)	17 (18%)	5 (5%)	2	18
10	CM	97/105 (92%)	69 (71%)	23 (24%)	5 (5%)	2	18
11	AN	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	9
11	CN	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	2	19
12	AO	123/128 (96%)	96 (78%)	17 (14%)	10 (8%)	1	8
12	CO	123/128 (96%)	91 (74%)	23 (19%)	9 (7%)	1	10
13	AP	114/126 (90%)	87 (76%)	15 (13%)	12 (10%)	1	4
13	CP	115/126 (91%)	82 (71%)	19 (16%)	14 (12%)	0	2
14	AQ	58/61 (95%)	43 (74%)	11 (19%)	4 (7%)	1	11
14	CQ	58/61 (95%)	40 (69%)	12 (21%)	6 (10%)	1	4
15	AR	86/89 (97%)	71 (83%)	9 (10%)	6 (7%)	1	11
15	CR	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	16	54
16	AS	82/88 (93%)	61 (74%)	18 (22%)	3 (4%)	4	27
16	CS	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	1	10
17	AT	98/105 (93%)	78 (80%)	16 (16%)	4 (4%)	3	24
17	CT	98/105 (93%)	76 (78%)	15 (15%)	7 (7%)	1	11
18	AU	70/88 (80%)	58 (83%)	7 (10%)	5 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	2	16
19	AV	81/93 (87%)	53 (65%)	19 (24%)	9 (11%)	0	3
19	CV	76/93 (82%)	48 (63%)	19 (25%)	9 (12%)	0	3
20	AW	97/106 (92%)	67 (69%)	17 (18%)	13 (13%)	0	2
20	CW	97/106 (92%)	64 (66%)	22 (23%)	11 (11%)	0	3
21	AX	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	7
21	CX	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	1
26	BD	270/276 (98%)	227 (84%)	31 (12%)	12 (4%)	3	22
26	DD	270/276 (98%)	223 (83%)	35 (13%)	12 (4%)	3	22
27	BE	203/206 (98%)	151 (74%)	35 (17%)	17 (8%)	1	7
27	DE	203/206 (98%)	133 (66%)	40 (20%)	30 (15%)	0	1
28	BF	200/210 (95%)	171 (86%)	21 (10%)	8 (4%)	4	24
28	DF	206/210 (98%)	155 (75%)	33 (16%)	18 (9%)	1	7
29	BG	179/182 (98%)	132 (74%)	32 (18%)	15 (8%)	1	7
29	DG	179/182 (98%)	128 (72%)	35 (20%)	16 (9%)	1	6
30	BH	168/180 (93%)	107 (64%)	30 (18%)	31 (18%)	0	1
30	DH	168/180 (93%)	103 (61%)	30 (18%)	35 (21%)	0	1
31	BK	144/148 (97%)	102 (71%)	28 (19%)	14 (10%)	1	5
31	DK	144/148 (97%)	98 (68%)	31 (22%)	15 (10%)	1	4
32	BM	136/140 (97%)	101 (74%)	24 (18%)	11 (8%)	1	8
32	DM	136/140 (97%)	103 (76%)	22 (16%)	11 (8%)	1	8
33	BN	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	11	47
33	DN	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	7	37
34	BO	148/150 (99%)	99 (67%)	27 (18%)	22 (15%)	0	1
34	DO	148/150 (99%)	85 (57%)	31 (21%)	32 (22%)	0	0
35	BP	139/141 (99%)	104 (75%)	21 (15%)	14 (10%)	1	5
35	DP	139/141 (99%)	100 (72%)	24 (17%)	15 (11%)	0	4
36	B0	116/118 (98%)	91 (78%)	14 (12%)	11 (10%)	1	6
36	D0	115/118 (98%)	85 (74%)	21 (18%)	9 (8%)	1	9
37	BQ	109/112 (97%)	82 (75%)	15 (14%)	12 (11%)	0	4
37	DQ	109/112 (97%)	74 (68%)	22 (20%)	13 (12%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BR	135/146 (92%)	101 (75%)	25 (18%)	9 (7%)	1	12
38	DR	135/146 (92%)	105 (78%)	19 (14%)	11 (8%)	1	8
39	B1	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	2	18
39	D1	115/118 (98%)	89 (77%)	20 (17%)	6 (5%)	2	18
40	B2	99/101 (98%)	74 (75%)	17 (17%)	8 (8%)	1	8
40	D2	99/101 (98%)	68 (69%)	16 (16%)	15 (15%)	0	1
41	BS	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	2	17
41	DS	111/113 (98%)	86 (78%)	17 (15%)	8 (7%)	1	11
42	BT	90/96 (94%)	75 (83%)	13 (14%)	2 (2%)	8	41
42	DT	90/96 (94%)	67 (74%)	13 (14%)	10 (11%)	0	3
43	BU	100/110 (91%)	64 (64%)	18 (18%)	18 (18%)	0	1
43	DU	100/110 (91%)	57 (57%)	18 (18%)	25 (25%)	0	0
44	BV	173/206 (84%)	105 (61%)	47 (27%)	21 (12%)	0	3
44	DV	177/206 (86%)	110 (62%)	37 (21%)	30 (17%)	0	1
45	B3	74/85 (87%)	57 (77%)	15 (20%)	2 (3%)	6	35
45	D3	75/85 (88%)	63 (84%)	9 (12%)	3 (4%)	4	24
46	BZ	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	13
46	DZ	95/98 (97%)	69 (73%)	12 (13%)	14 (15%)	0	1
47	BW	64/72 (89%)	54 (84%)	5 (8%)	5 (8%)	1	9
47	DW	67/72 (93%)	51 (76%)	9 (13%)	7 (10%)	1	4
48	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	11	46
48	DX	57/60 (95%)	46 (81%)	9 (16%)	2 (4%)	4	29
49	B4	64/71 (90%)	33 (52%)	21 (33%)	10 (16%)	0	1
49	D4	61/71 (86%)	22 (36%)	23 (38%)	16 (26%)	0	0
50	B5	57/60 (95%)	42 (74%)	10 (18%)	5 (9%)	1	7
50	D5	57/60 (95%)	41 (72%)	6 (10%)	10 (18%)	0	1
51	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
51	D6	43/54 (80%)	24 (56%)	13 (30%)	6 (14%)	0	2
52	B7	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	9	42
52	D7	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
53	B8	59/65 (91%)	44 (75%)	10 (17%)	5 (8%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	D8	59/65 (91%)	38 (64%)	8 (14%)	13 (22%)	0	0
All	All	11341/12044 (94%)	8378 (74%)	1945 (17%)	1018 (9%)	1	6

5 of 1018 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	135	GLN
2	AE	136	VAL
2	AE	194	PRO
2	AE	195	ASP
2	AE	214	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	182 (89%)	23 (11%)	7	30
2	CE	205/220 (93%)	176 (86%)	29 (14%)	4	20
3	AF	159/188 (85%)	147 (92%)	12 (8%)	17	52
3	CF	160/188 (85%)	146 (91%)	14 (9%)	12	44
4	AG	180/180 (100%)	166 (92%)	14 (8%)	16	50
4	CG	180/180 (100%)	161 (89%)	19 (11%)	8	33
5	AH	116/123 (94%)	105 (90%)	11 (10%)	11	38
5	CH	116/123 (94%)	104 (90%)	12 (10%)	9	34
6	AI	90/90 (100%)	85 (94%)	5 (6%)	26	65
6	CI	90/90 (100%)	81 (90%)	9 (10%)	9	36
7	AJ	126/127 (99%)	118 (94%)	8 (6%)	22	60
7	CJ	126/127 (99%)	116 (92%)	10 (8%)	15	49
8	AK	119/119 (100%)	108 (91%)	11 (9%)	11	40
8	CK	119/119 (100%)	108 (91%)	11 (9%)	11	40
9	AL	98/99 (99%)	86 (88%)	12 (12%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CL	98/99 (99%)	79 (81%)	19 (19%)	2	7
10	AM	89/92 (97%)	82 (92%)	7 (8%)	15	49
10	CM	89/92 (97%)	82 (92%)	7 (8%)	15	49
11	AN	90/99 (91%)	86 (96%)	4 (4%)	35	72
11	CN	90/99 (91%)	85 (94%)	5 (6%)	26	65
12	AO	104/107 (97%)	97 (93%)	7 (7%)	20	58
12	CO	104/107 (97%)	97 (93%)	7 (7%)	20	58
13	AP	94/101 (93%)	89 (95%)	5 (5%)	28	66
13	CP	94/101 (93%)	78 (83%)	16 (17%)	2	12
14	AQ	49/50 (98%)	44 (90%)	5 (10%)	9	35
14	CQ	49/50 (98%)	45 (92%)	4 (8%)	14	48
15	AR	79/80 (99%)	73 (92%)	6 (8%)	16	51
15	CR	79/80 (99%)	76 (96%)	3 (4%)	40	75
16	AS	72/74 (97%)	62 (86%)	10 (14%)	4	20
16	CS	72/74 (97%)	68 (94%)	4 (6%)	26	65
17	AT	95/97 (98%)	90 (95%)	5 (5%)	28	66
17	CT	95/97 (98%)	92 (97%)	3 (3%)	46	79
18	AU	63/77 (82%)	60 (95%)	3 (5%)	31	70
18	CU	63/77 (82%)	59 (94%)	4 (6%)	22	60
19	AV	72/80 (90%)	63 (88%)	9 (12%)	6	24
19	CV	67/80 (84%)	56 (84%)	11 (16%)	3	14
20	AW	76/82 (93%)	70 (92%)	6 (8%)	15	49
20	CW	76/82 (93%)	69 (91%)	7 (9%)	11	40
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	18 (90%)	2 (10%)	9	36
26	BD	214/218 (98%)	192 (90%)	22 (10%)	9	34
26	DD	214/218 (98%)	197 (92%)	17 (8%)	15	49
27	BE	165/166 (99%)	149 (90%)	16 (10%)	10	38
27	DE	165/166 (99%)	150 (91%)	15 (9%)	12	41
28	BF	161/166 (97%)	150 (93%)	11 (7%)	20	57
28	DF	165/166 (99%)	156 (94%)	9 (6%)	27	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BG	155/156 (99%)	145 (94%)	10 (6%)	21	59
29	DG	155/156 (99%)	141 (91%)	14 (9%)	12	42
30	BH	142/148 (96%)	119 (84%)	23 (16%)	3	14
30	DH	142/148 (96%)	128 (90%)	14 (10%)	10	37
31	BK	122/124 (98%)	110 (90%)	12 (10%)	10	37
31	DK	122/124 (98%)	109 (89%)	13 (11%)	8	32
32	BM	117/119 (98%)	113 (97%)	4 (3%)	44	77
32	DM	117/119 (98%)	109 (93%)	8 (7%)	20	57
33	BN	100/100 (100%)	95 (95%)	5 (5%)	30	68
33	DN	100/100 (100%)	95 (95%)	5 (5%)	30	68
34	BO	116/116 (100%)	101 (87%)	15 (13%)	5	23
34	DO	116/116 (100%)	102 (88%)	14 (12%)	6	26
35	BP	111/111 (100%)	102 (92%)	9 (8%)	15	48
35	DP	111/111 (100%)	102 (92%)	9 (8%)	15	48
36	B0	101/101 (100%)	94 (93%)	7 (7%)	19	57
36	D0	100/101 (99%)	95 (95%)	5 (5%)	30	68
37	BQ	87/88 (99%)	82 (94%)	5 (6%)	25	65
37	DQ	87/88 (99%)	78 (90%)	9 (10%)	9	34
38	BR	120/127 (94%)	111 (92%)	9 (8%)	17	52
38	DR	120/127 (94%)	107 (89%)	13 (11%)	8	32
39	B1	93/94 (99%)	87 (94%)	6 (6%)	21	59
39	D1	93/94 (99%)	88 (95%)	5 (5%)	27	66
40	B2	82/82 (100%)	75 (92%)	7 (8%)	13	46
40	D2	82/82 (100%)	71 (87%)	11 (13%)	5	21
41	BS	92/92 (100%)	82 (89%)	10 (11%)	8	32
41	DS	92/92 (100%)	82 (89%)	10 (11%)	8	32
42	BT	74/78 (95%)	69 (93%)	5 (7%)	20	57
42	DT	74/78 (95%)	69 (93%)	5 (7%)	20	57
43	BU	85/91 (93%)	70 (82%)	15 (18%)	2	10
43	DU	85/91 (93%)	73 (86%)	12 (14%)	4	20
44	BV	154/179 (86%)	135 (88%)	19 (12%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DV	158/179 (88%)	144 (91%)	14 (9%)	12	43
45	B3	61/67 (91%)	58 (95%)	3 (5%)	31	69
45	D3	62/67 (92%)	57 (92%)	5 (8%)	15	48
46	BZ	82/83 (99%)	77 (94%)	5 (6%)	23	62
46	DZ	82/83 (99%)	65 (79%)	17 (21%)	1	6
47	BW	62/67 (92%)	55 (89%)	7 (11%)	7	30
47	DW	64/67 (96%)	62 (97%)	2 (3%)	47	79
48	BX	51/52 (98%)	47 (92%)	4 (8%)	16	50
48	DX	51/52 (98%)	48 (94%)	3 (6%)	24	63
49	B4	59/63 (94%)	51 (86%)	8 (14%)	5	21
49	D4	57/63 (90%)	51 (90%)	6 (10%)	8	33
50	B5	51/52 (98%)	44 (86%)	7 (14%)	4	20
50	D5	51/52 (98%)	44 (86%)	7 (14%)	4	20
51	B6	44/52 (85%)	40 (91%)	4 (9%)	12	41
51	D6	44/52 (85%)	38 (86%)	6 (14%)	5	21
52	B7	42/42 (100%)	38 (90%)	4 (10%)	11	38
52	D7	42/42 (100%)	36 (86%)	6 (14%)	4	19
53	B8	51/55 (93%)	43 (84%)	8 (16%)	3	15
53	D8	51/55 (93%)	45 (88%)	6 (12%)	6	27
All	All	9584/9992 (96%)	8705 (91%)	879 (9%)	11	40

5 of 879 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B4	53	GLU
5	CH	78	HIS
44	DV	72	ARG
51	B6	44	ARG
2	CE	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
2	CE	25	ASN

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Mol	Chain	Res	Type
8	CK	82	HIS
43	DU	6	HIS
2	CE	94	ASN
4	CG	43	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1506/1506 (100%)	279 (18%)	29 (1%)
1	CA	1505/1506 (99%)	284 (18%)	32 (2%)
22	AC	76/77 (98%)	5 (6%)	1 (1%)
22	CC	77/77 (100%)	9 (11%)	2 (2%)
23	A1	3/4 (75%)	1 (33%)	0
23	C1	3/4 (75%)	0	0
24	BA	2911/2912 (99%)	552 (18%)	37 (1%)
24	DA	2908/2912 (99%)	571 (19%)	43 (1%)
25	BB	121/122 (99%)	21 (17%)	0
25	DB	121/122 (99%)	25 (20%)	0
All	All	9231/9242 (99%)	1747 (18%)	144 (1%)

5 of 1747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 144 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2689	U
1	CA	560	U
24	DA	2439	A
1	CA	89	U
1	CA	328	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1693 ligands modelled in this entry, 1691 are monoatomic - leaving 2 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	$\# Z > 2$
55	TAC	AA	1833	54	33,35,35	1.38	4 (12%)	44,58,58	1.68	6 (13%)
55	TAC	CA	1805	54	33,35,35	1.35	4 (12%)	44,58,58	1.64	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	TAC	AA	1833	54	-	0/8/74/74	0/4/4/4
55	TAC	CA	1805	54	-	0/8/74/74	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1805	TAC	C6-C61	-3.72	1.50	1.53
55	AA	1833	TAC	C6-C61	-3.13	1.50	1.53
55	AA	1833	TAC	C1C-C1	-2.91	1.50	1.55
55	CA	1805	TAC	C1C-C1	-2.61	1.51	1.55
55	CA	1805	TAC	C1A-C61	3.39	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
55	AA	1833	TAC	O12-C12-C1B	-5.71	118.37	123.84
55	CA	1805	TAC	O12-C12-C1B	-5.42	118.66	123.84
55	AA	1833	TAC	C41-C1C-C1	-5.20	105.24	111.17
55	CA	1805	TAC	C41-C1C-C1	-4.98	105.49	111.17
55	AA	1833	TAC	C61-C1A-C11	-2.44	118.01	121.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	AA	1833	TAC	4	0
55	CA	1805	TAC	3	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	1506/1506 (100%)	-0.52	9 (0%) 90 88	89, 141, 216, 277	0
1	CA	1506/1506 (100%)	-0.65	10 (0%) 89 86	103, 152, 218, 275	0
2	AE	237/256 (92%)	0.79	47 (19%) 1 1	139, 172, 204, 216	0
2	CE	237/256 (92%)	1.68	91 (38%) 0 1	160, 191, 219, 228	0
3	AF	205/239 (85%)	2.33	118 (57%) 0 0	116, 151, 183, 201	0
3	CF	206/239 (86%)	1.82	77 (37%) 0 1	148, 179, 201, 211	0
4	AG	208/208 (100%)	1.45	68 (32%) 1 1	112, 149, 172, 183	0
4	CG	208/208 (100%)	0.39	20 (9%) 10 9	128, 153, 171, 180	0
5	AH	151/162 (93%)	1.75	57 (37%) 0 1	111, 139, 161, 195	0
5	CH	151/162 (93%)	0.84	27 (17%) 2 1	129, 154, 177, 196	0
6	AI	101/101 (100%)	3.05	68 (67%) 0 0	116, 141, 162, 167	0
6	CI	101/101 (100%)	1.33	32 (31%) 1 1	128, 149, 163, 178	0
7	AJ	155/156 (99%)	0.25	21 (13%) 4 3	129, 151, 187, 211	0
7	CJ	155/156 (99%)	1.76	56 (36%) 0 1	146, 167, 195, 204	0
8	AK	138/138 (100%)	0.18	7 (5%) 32 25	118, 148, 162, 170	0
8	CK	138/138 (100%)	0.15	3 (2%) 65 59	131, 159, 174, 180	0
9	AL	127/128 (99%)	-0.71	0 100 100	119, 169, 186, 192	0
9	CL	127/128 (99%)	-0.43	2 (1%) 74 69	133, 185, 199, 208	0
10	AM	99/105 (94%)	0.36	9 (9%) 11 9	119, 170, 197, 210	0
10	CM	99/105 (94%)	-0.20	4 (4%) 42 34	149, 191, 204, 209	0
11	AN	119/129 (92%)	2.68	65 (54%) 0 0	115, 137, 170, 198	0
11	CN	119/129 (92%)	1.75	47 (39%) 0 1	124, 149, 178, 196	0
12	AO	125/128 (97%)	2.15	58 (46%) 0 0	106, 128, 150, 192	0
12	CO	125/128 (97%)	0.30	6 (4%) 34 28	111, 134, 159, 205	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	-0.69	0 100 100	103, 153, 174, 184	0
13	CP	117/126 (92%)	0.06	14 (11%) 6 5	143, 179, 196, 205	0
14	AQ	60/61 (98%)	-0.17	0 100 100	123, 143, 159, 161	0
14	CQ	60/61 (98%)	-0.35	3 (5%) 32 26	148, 176, 188, 191	0
15	AR	88/89 (98%)	0.05	3 (3%) 49 42	109, 136, 155, 162	0
15	CR	88/89 (98%)	1.02	17 (19%) 2 1	121, 151, 168, 172	0
16	AS	84/88 (95%)	-0.95	0 100 100	135, 156, 179, 198	0
16	CS	84/88 (95%)	-0.63	0 100 100	121, 143, 167, 203	0
17	AT	100/105 (95%)	0.15	4 (4%) 42 34	123, 147, 162, 173	0
17	CT	100/105 (95%)	1.59	42 (42%) 0 0	122, 145, 159, 182	0
18	AU	72/88 (81%)	1.66	29 (40%) 0 0	118, 142, 168, 195	0
18	CU	72/88 (81%)	1.84	30 (41%) 0 0	134, 157, 181, 199	0
19	AV	83/93 (89%)	-0.36	0 100 100	133, 158, 180, 191	0
19	CV	78/93 (83%)	0.53	12 (15%) 3 2	169, 195, 210, 221	0
20	AW	99/106 (93%)	-0.41	2 (2%) 68 62	137, 159, 187, 196	0
20	CW	99/106 (93%)	-0.18	1 (1%) 84 80	112, 142, 177, 194	0
21	AX	25/27 (92%)	-0.64	0 100 100	120, 150, 170, 187	0
21	CX	25/27 (92%)	-1.02	0 100 100	144, 171, 192, 209	0
22	AC	77/77 (100%)	-0.24	1 (1%) 79 74	102, 125, 153, 175	0
22	CC	77/77 (100%)	0.56	12 (15%) 3 2	106, 145, 175, 205	0
23	A1	4/4 (100%)	-0.34	0 100 100	106, 109, 114, 165	0
23	C1	4/4 (100%)	-0.25	0 100 100	127, 131, 143, 184	0
24	BA	2912/2912 (100%)	-0.13	77 (2%) 59 53	68, 102, 240, 278	0
24	DA	2909/2912 (99%)	-0.22	100 (3%) 49 42	79, 114, 258, 279	0
25	BB	122/122 (100%)	-0.55	1 (0%) 87 84	92, 122, 145, 211	0
25	DB	122/122 (100%)	-0.36	5 (4%) 41 34	115, 152, 178, 226	0
26	BD	272/276 (98%)	0.98	54 (19%) 1 1	69, 96, 117, 140	0
26	DD	272/276 (98%)	0.77	28 (10%) 9 7	72, 106, 130, 155	0
27	BE	205/206 (99%)	1.16	49 (23%) 1 1	73, 117, 163, 177	0
27	DE	205/206 (99%)	0.89	34 (16%) 2 2	79, 122, 168, 196	0
28	BF	202/210 (96%)	0.41	22 (10%) 7 6	74, 108, 149, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DF	208/210 (99%)	1.56	63 (30%) 1 1	82, 125, 187, 213	0
29	BG	181/182 (99%)	-0.20	3 (1%) 73 67	105, 127, 167, 186	0
29	DG	181/182 (99%)	3.32	128 (70%) 0 0	136, 166, 194, 204	0
30	BH	170/180 (94%)	-0.16	4 (2%) 62 55	103, 135, 159, 175	0
30	DH	170/180 (94%)	2.08	69 (40%) 0 0	154, 222, 249, 262	0
31	BK	146/148 (98%)	-0.09	8 (5%) 29 23	103, 151, 170, 179	0
31	DK	146/148 (98%)	-0.10	11 (7%) 17 14	111, 159, 178, 185	0
32	BM	138/140 (98%)	0.67	12 (8%) 13 10	90, 115, 153, 183	0
32	DM	138/140 (98%)	0.84	24 (17%) 2 2	93, 129, 168, 189	0
33	BN	122/122 (100%)	0.12	3 (2%) 61 54	83, 111, 132, 139	0
33	DN	122/122 (100%)	1.09	23 (18%) 2 1	86, 116, 130, 140	0
34	BO	150/150 (100%)	1.18	47 (31%) 1 1	70, 113, 143, 207	0
34	DO	150/150 (100%)	1.27	35 (23%) 1 1	85, 129, 167, 206	0
35	BP	141/141 (100%)	0.52	14 (9%) 9 8	85, 107, 132, 163	0
35	DP	141/141 (100%)	1.00	30 (21%) 1 1	95, 126, 152, 177	0
36	B0	118/118 (100%)	0.93	18 (15%) 3 2	90, 110, 131, 148	0
36	D0	117/118 (99%)	0.31	8 (6%) 20 17	88, 111, 135, 146	0
37	BQ	111/112 (99%)	0.74	19 (17%) 2 2	90, 119, 148, 164	0
37	DQ	111/112 (99%)	0.49	10 (9%) 12 9	114, 146, 168, 190	0
38	BR	137/146 (93%)	0.55	18 (13%) 5 3	104, 125, 173, 202	0
38	DR	137/146 (93%)	0.62	14 (10%) 9 7	103, 121, 177, 212	0
39	B1	117/118 (99%)	0.06	4 (3%) 49 42	77, 106, 141, 168	0
39	D1	117/118 (99%)	0.92	22 (18%) 2 1	90, 122, 155, 178	0
40	B2	101/101 (100%)	1.33	35 (34%) 0 1	79, 122, 154, 181	0
40	D2	101/101 (100%)	3.01	64 (63%) 0 0	95, 149, 165, 181	0
41	BS	113/113 (100%)	1.57	35 (30%) 1 1	81, 102, 141, 191	0
41	DS	113/113 (100%)	1.19	24 (21%) 1 1	83, 107, 140, 194	0
42	BT	92/96 (95%)	0.66	8 (8%) 13 10	81, 98, 126, 145	0
42	DT	92/96 (95%)	1.23	25 (27%) 1 1	96, 117, 140, 159	0
43	BU	102/110 (92%)	0.08	5 (4%) 33 27	95, 123, 171, 190	0
43	DU	102/110 (92%)	2.86	61 (59%) 0 0	104, 142, 195, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	175/206 (84%)	1.92	70 (40%) 0 0	104, 142, 218, 229	0
44	DV	179/206 (86%)	1.85	79 (44%) 0 0	132, 174, 237, 251	0
45	B3	76/85 (89%)	0.16	2 (2%) 59 53	85, 101, 121, 163	0
45	D3	77/85 (90%)	1.82	22 (28%) 1 1	98, 117, 141, 175	0
46	BZ	97/98 (98%)	0.54	11 (11%) 7 5	83, 106, 149, 195	0
46	DZ	97/98 (98%)	1.90	40 (41%) 0 0	87, 116, 159, 191	0
47	BW	66/72 (91%)	0.66	5 (7%) 17 14	80, 108, 133, 171	0
47	DW	69/72 (95%)	1.16	16 (23%) 1 1	106, 138, 163, 196	0
48	BX	59/60 (98%)	1.24	12 (20%) 1 1	85, 106, 148, 160	0
48	DX	59/60 (98%)	2.64	36 (61%) 0 0	97, 126, 159, 194	0
49	B4	66/71 (92%)	-0.04	2 (3%) 54 47	127, 176, 209, 219	0
49	D4	63/71 (88%)	7.66	63 (100%) 0 0	181, 212, 226, 235	0
50	B5	59/60 (98%)	2.53	22 (37%) 0 1	78, 115, 194, 210	0
50	D5	59/60 (98%)	1.44	13 (22%) 1 1	87, 114, 191, 218	0
51	B6	45/54 (83%)	8.45	44 (97%) 0 0	149, 184, 197, 201	0
51	D6	45/54 (83%)	11.36	43 (95%) 0 0	158, 195, 212, 215	0
52	B7	49/49 (100%)	0.76	8 (16%) 2 2	73, 83, 124, 154	0
52	D7	49/49 (100%)	2.38	22 (44%) 0 0	78, 91, 134, 156	0
53	B8	61/65 (93%)	0.19	3 (4%) 33 27	81, 96, 116, 145	0
53	D8	61/65 (93%)	1.22	11 (18%) 2 1	94, 109, 131, 161	0
All	All	20772/21286 (97%)	0.44	2810 (13%) 4 3	68, 133, 207, 279	0

The worst 5 of 2810 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	D6	13	CYS	26.3
50	D5	59	GLU	23.6
51	D6	22	ALA	23.3
24	BA	654(K)	C	23.2
24	BA	1	G	22.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
54	MG	BA	3434	1/1	0.96	0.61	70.64	107,107,107,107	0
54	MG	BA	3350	1/1	0.93	1.45	57.11	115,115,115,115	0
54	MG	AA	1662	1/1	0.79	1.51	56.73	111,111,111,111	0
54	MG	DA	3299	1/1	0.82	2.18	54.81	105,105,105,105	0
54	MG	DA	3156	1/1	0.93	0.78	50.73	113,113,113,113	0
54	MG	DA	3316	1/1	0.92	0.70	46.41	124,124,124,124	0
54	MG	CA	1668	1/1	0.92	0.36	44.67	145,145,145,145	0
54	MG	DA	3367	1/1	0.47	1.34	43.50	125,125,125,125	0
54	MG	BA	3073	1/1	0.87	1.03	39.86	108,108,108,108	0
54	MG	BA	3179	1/1	0.95	0.78	35.75	108,108,108,108	0
54	MG	CA	1794	1/1	0.72	0.43	31.77	109,109,109,109	0
54	MG	DA	3239	1/1	0.72	0.62	30.08	105,105,105,105	0
54	MG	BA	3142	1/1	0.95	0.47	29.61	48,48,48,48	0
54	MG	CA	1674	1/1	0.94	0.80	29.34	117,117,117,117	0
54	MG	BA	3050	1/1	0.92	0.47	29.07	75,75,75,75	0
54	MG	DA	3368	1/1	0.82	1.09	27.80	95,95,95,95	0
54	MG	BA	3498	1/1	0.87	0.56	27.41	107,107,107,107	0
54	MG	BA	3002	1/1	0.98	0.38	25.84	63,63,63,63	0
54	MG	AR	101	1/1	0.86	0.39	24.01	98,98,98,98	0
54	MG	DA	3169	1/1	0.98	0.36	23.71	76,76,76,76	0
54	MG	DA	3119	1/1	0.96	0.31	22.98	65,65,65,65	0
54	MG	BA	3305	1/1	0.96	0.31	22.61	80,80,80,80	0
54	MG	BA	3302	1/1	0.84	0.33	22.18	101,101,101,101	0
54	MG	BA	3285	1/1	0.52	0.51	22.14	114,114,114,114	0
54	MG	DA	3164	1/1	0.61	0.37	22.10	136,136,136,136	0
54	MG	BA	3243	1/1	0.98	0.48	21.94	122,122,122,122	0
54	MG	DA	3068	1/1	0.90	0.48	21.89	122,122,122,122	0
54	MG	BA	3097	1/1	0.85	0.39	21.32	83,83,83,83	0
54	MG	CA	1691	1/1	0.92	0.34	21.30	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3052	1/1	0.43	0.26	21.10	107,107,107,107	0
54	MG	BA	3180	1/1	0.98	0.50	20.99	73,73,73,73	0
54	MG	BA	3528	1/1	0.84	0.54	20.66	104,104,104,104	0
54	MG	CA	1686	1/1	0.95	0.40	20.03	79,79,79,79	0
54	MG	AA	1625	1/1	0.56	0.35	19.37	110,110,110,110	0
54	MG	BA	3526	1/1	0.79	0.49	19.35	115,115,115,115	0
54	MG	DA	3190	1/1	0.95	0.39	19.18	80,80,80,80	0
54	MG	BA	3624	1/1	0.88	0.53	19.16	92,92,92,92	0
54	MG	DA	3212	1/1	0.90	0.31	18.86	59,59,59,59	0
54	MG	BA	3021	1/1	0.95	0.43	18.75	72,72,72,72	0
54	MG	BA	3223	1/1	0.96	0.45	18.68	84,84,84,84	0
54	MG	CA	1604	1/1	0.71	0.47	17.99	105,105,105,105	0
54	MG	CA	1676	1/1	0.86	0.32	17.96	102,102,102,102	0
54	MG	BA	3288	1/1	0.92	0.61	17.80	100,100,100,100	0
54	MG	BA	3089	1/1	0.99	0.52	17.63	77,77,77,77	0
54	MG	DA	3003	1/1	0.98	0.36	17.56	130,130,130,130	0
54	MG	BA	3098	1/1	0.97	0.40	17.28	75,75,75,75	0
54	MG	BA	3363	1/1	0.92	0.41	16.80	73,73,73,73	0
54	MG	BA	3596	1/1	0.95	0.46	16.67	88,88,88,88	0
54	MG	DA	3351	1/1	0.84	0.38	16.66	90,90,90,90	0
54	MG	DA	3286	1/1	0.95	0.49	16.63	115,115,115,115	0
54	MG	CA	1781	1/1	0.79	0.25	16.50	126,126,126,126	0
54	MG	CA	1622	1/1	0.69	0.49	16.49	122,122,122,122	0
54	MG	BA	3501	1/1	0.98	0.39	16.37	99,99,99,99	0
54	MG	AA	1631	1/1	0.91	0.43	16.10	96,96,96,96	0
54	MG	CA	1658	1/1	0.87	0.46	16.02	120,120,120,120	0
54	MG	BA	3606	1/1	0.84	0.38	15.95	84,84,84,84	0
54	MG	DA	3039	1/1	0.98	0.56	15.83	116,116,116,116	0
54	MG	BA	3279	1/1	0.85	0.45	15.69	74,74,74,74	0
54	MG	DA	3418	1/1	0.96	0.35	15.67	61,61,61,61	0
54	MG	DA	3455	1/1	0.63	0.25	15.25	147,147,147,147	0
54	MG	BA	3057	1/1	0.97	0.34	15.23	93,93,93,93	0
54	MG	DA	3150	1/1	0.94	0.41	15.13	96,96,96,96	0
54	MG	BA	3553	1/1	0.89	0.38	15.07	99,99,99,99	0
54	MG	BA	3264	1/1	0.92	0.43	15.04	75,75,75,75	0
54	MG	AA	1678	1/1	0.87	0.40	14.95	108,108,108,108	0
54	MG	BA	3072	1/1	0.95	0.42	14.94	87,87,87,87	0
54	MG	DA	3504	1/1	0.99	0.45	14.94	67,67,67,67	0
54	MG	AA	1745	1/1	0.68	0.26	14.64	128,128,128,128	0
54	MG	CA	1647	1/1	0.82	0.29	14.62	83,83,83,83	0
54	MG	BA	3143	1/1	0.98	0.42	14.59	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3128	1/1	0.94	0.58	14.54	99,99,99,99	0
54	MG	BA	3273	1/1	0.93	0.36	14.25	70,70,70,70	0
54	MG	DA	3361	1/1	0.98	0.30	14.04	93,93,93,93	0
54	MG	BA	3299	1/1	0.89	0.47	13.96	78,78,78,78	0
54	MG	DA	3242	1/1	0.98	0.34	13.89	64,64,64,64	0
54	MG	BA	3544	1/1	0.90	0.37	13.68	77,77,77,77	0
54	MG	DA	3023	1/1	0.95	0.26	13.66	86,86,86,86	0
54	MG	BA	3061	1/1	0.96	0.42	13.63	64,64,64,64	0
54	MG	CA	1751	1/1	0.67	0.60	13.60	118,118,118,118	0
54	MG	BA	3054	1/1	0.97	0.41	13.47	91,91,91,91	0
54	MG	DA	3201	1/1	0.96	0.28	13.35	73,73,73,73	0
54	MG	DA	3085	1/1	0.72	0.41	13.10	113,113,113,113	0
54	MG	BA	3349	1/1	0.96	0.46	13.03	69,69,69,69	0
54	MG	BA	3246	1/1	0.86	0.35	12.72	78,78,78,78	0
54	MG	BA	3206	1/1	0.87	0.29	12.53	99,99,99,99	0
54	MG	DA	3369	1/1	0.90	0.36	12.43	76,76,76,76	0
54	MG	DA	3254	1/1	0.94	0.40	12.36	74,74,74,74	0
54	MG	BA	3438	1/1	0.96	0.43	12.19	62,62,62,62	0
54	MG	DA	3147	1/1	0.99	0.33	12.08	82,82,82,82	0
54	MG	BA	3010	1/1	0.89	0.34	11.97	128,128,128,128	0
54	MG	DB	206	1/1	0.42	0.39	11.72	142,142,142,142	0
54	MG	DA	3092	1/1	0.83	0.30	11.55	80,80,80,80	0
54	MG	BA	3144	1/1	0.98	0.42	11.48	73,73,73,73	0
54	MG	BA	3418	1/1	0.87	0.29	11.23	98,98,98,98	0
54	MG	BA	3193	1/1	0.96	0.44	11.16	76,76,76,76	0
54	MG	BA	3118	1/1	0.99	0.42	11.15	90,90,90,90	0
54	MG	BA	3221	1/1	0.98	0.44	11.08	89,89,89,89	0
54	MG	BA	3491	1/1	0.94	0.39	10.89	84,84,84,84	0
54	MG	BB	212	1/1	0.83	0.39	10.87	103,103,103,103	0
54	MG	BA	3049	1/1	1.00	0.29	10.86	88,88,88,88	0
54	MG	BA	3157	1/1	0.98	0.36	10.84	74,74,74,74	0
54	MG	BA	3070	1/1	0.84	0.37	10.78	119,119,119,119	0
54	MG	BA	3013	1/1	0.96	0.24	10.73	63,63,63,63	0
54	MG	BA	3136	1/1	0.93	0.31	10.55	62,62,62,62	0
54	MG	BA	3601	1/1	0.98	0.48	10.36	52,52,52,52	0
54	MG	BA	3099	1/1	0.99	0.38	10.28	74,74,74,74	0
54	MG	BA	3008	1/1	0.99	0.49	10.18	58,58,58,58	0
54	MG	BA	3209	1/1	0.92	0.36	10.13	79,79,79,79	0
54	MG	DA	3517	1/1	0.64	0.41	10.03	106,106,106,106	0
54	MG	CA	1699	1/1	0.79	0.25	9.85	81,81,81,81	0
54	MG	DA	3295	1/1	0.59	0.50	9.84	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3577	1/1	0.97	0.30	9.80	61,61,61,61	0
54	MG	AA	1657	1/1	0.99	0.40	9.74	63,63,63,63	0
54	MG	BA	3137	1/1	0.72	0.25	9.32	105,105,105,105	0
54	MG	AA	1634	1/1	0.81	0.29	9.18	97,97,97,97	0
54	MG	DA	3141	1/1	0.91	0.24	9.11	85,85,85,85	0
54	MG	DA	3230	1/1	0.96	0.31	9.10	65,65,65,65	0
54	MG	CA	1640	1/1	0.96	0.30	9.09	92,92,92,92	0
54	MG	DA	3154	1/1	0.92	0.22	9.01	111,111,111,111	0
54	MG	DA	3182	1/1	0.98	0.25	8.94	62,62,62,62	0
54	MG	AA	1650	1/1	0.96	0.25	8.86	85,85,85,85	0
54	MG	DA	3233	1/1	0.82	0.28	8.53	79,79,79,79	0
54	MG	DA	3491	1/1	0.97	0.32	8.48	65,65,65,65	0
54	MG	DA	3395	1/1	0.87	0.28	8.32	87,87,87,87	0
54	MG	BA	3583	1/1	0.96	0.27	8.31	59,59,59,59	0
54	MG	BA	3580	1/1	0.95	0.34	8.30	64,64,64,64	0
54	MG	BA	3063	1/1	0.90	0.21	8.28	121,121,121,121	0
54	MG	BA	3222	1/1	0.98	0.36	8.19	57,57,57,57	0
54	MG	BA	3155	1/1	0.87	0.27	8.04	113,113,113,113	0
54	MG	CA	1606	1/1	0.94	0.38	8.02	100,100,100,100	0
54	MG	DA	3177	1/1	0.66	0.28	7.99	99,99,99,99	0
54	MG	CA	1740	1/1	0.89	0.20	7.98	109,109,109,109	0
54	MG	BA	3043	1/1	0.86	0.29	7.97	83,83,83,83	0
54	MG	BA	3204	1/1	0.76	0.61	7.80	98,98,98,98	0
54	MG	AA	1712	1/1	0.88	0.31	7.72	97,97,97,97	0
54	MG	BA	3589	1/1	0.98	0.31	7.58	77,77,77,77	0
54	MG	B7	101	1/1	0.83	0.36	7.53	67,67,67,67	0
54	MG	BA	3378	1/1	0.87	0.28	7.49	129,129,129,129	0
54	MG	BA	3198	1/1	0.99	0.32	7.47	70,70,70,70	0
54	MG	BA	3573	1/1	0.91	0.38	7.46	96,96,96,96	0
54	MG	DA	3317	1/1	0.96	0.54	7.43	131,131,131,131	0
54	MG	CA	1617	1/1	0.97	0.23	7.34	140,140,140,140	0
54	MG	BA	3069	1/1	0.71	0.48	7.32	115,115,115,115	0
54	MG	DA	3072	1/1	0.97	0.29	7.30	94,94,94,94	0
54	MG	BA	3038	1/1	0.97	0.28	7.29	67,67,67,67	0
54	MG	BA	3158	1/1	0.97	0.52	7.26	67,67,67,67	0
54	MG	BA	3579	1/1	0.96	0.42	7.18	85,85,85,85	0
54	MG	AA	1715	1/1	0.82	0.31	7.18	115,115,115,115	0
54	MG	DA	3106	1/1	0.82	1.42	7.14	122,122,122,122	0
54	MG	DA	3170	1/1	0.97	0.29	7.12	80,80,80,80	0
54	MG	AC	107	1/1	0.82	0.19	6.93	111,111,111,111	0
54	MG	BA	3311	1/1	0.86	0.24	6.91	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1656	1/1	0.93	0.18	6.90	129,129,129,129	0
54	MG	BA	3463	1/1	0.93	0.28	6.82	77,77,77,77	0
54	MG	BA	3225	1/1	0.97	0.54	6.76	92,92,92,92	0
54	MG	BA	3147	1/1	0.99	0.37	6.75	64,64,64,64	0
54	MG	AA	1778	1/1	0.70	0.20	6.71	136,136,136,136	0
54	MG	DA	3399	1/1	0.84	0.27	6.61	126,126,126,126	0
54	MG	DA	3171	1/1	0.97	0.36	6.54	87,87,87,87	0
54	MG	BA	3385	1/1	0.86	0.42	6.53	72,72,72,72	0
54	MG	CA	1798	1/1	0.88	0.35	6.46	84,84,84,84	0
54	MG	BA	3029	1/1	0.98	0.27	6.43	74,74,74,74	0
54	MG	BA	3218	1/1	0.97	0.36	6.42	75,75,75,75	0
54	MG	BA	3581	1/1	0.97	0.32	6.41	82,82,82,82	0
54	MG	BA	3187	1/1	0.97	0.32	6.41	56,56,56,56	0
54	MG	BA	3593	1/1	0.97	0.34	6.39	57,57,57,57	0
54	MG	DA	3503	1/1	0.93	0.80	6.36	105,105,105,105	0
54	MG	BA	3224	1/1	0.98	0.32	6.20	101,101,101,101	0
54	MG	BA	3125	1/1	0.98	0.34	6.16	88,88,88,88	0
54	MG	DA	3281	1/1	0.98	0.24	6.14	74,74,74,74	0
54	MG	BA	3310	1/1	0.84	0.28	6.13	103,103,103,103	0
54	MG	AA	1610	1/1	0.94	0.30	6.06	71,71,71,71	0
54	MG	BA	3031	1/1	0.91	0.31	6.00	63,63,63,63	0
54	MG	DA	3151	1/1	0.87	0.28	5.92	113,113,113,113	0
54	MG	DA	3248	1/1	0.88	0.39	5.88	112,112,112,112	0
54	MG	BB	202	1/1	0.97	0.27	5.85	92,92,92,92	0
54	MG	BA	3297	1/1	0.97	0.39	5.84	78,78,78,78	0
54	MG	DA	3207	1/1	0.79	0.21	5.70	86,86,86,86	0
54	MG	DA	3332	1/1	0.82	0.25	5.53	120,120,120,120	0
54	MG	BA	3280	1/1	0.94	0.28	5.27	106,106,106,106	0
54	MG	DA	3214	1/1	0.97	0.20	5.26	63,63,63,63	0
54	MG	DA	3055	1/1	0.99	0.26	5.18	59,59,59,59	0
54	MG	AA	1817	1/1	0.92	0.51	5.12	101,101,101,101	0
54	MG	BE	302	1/1	0.86	0.80	5.08	104,104,104,104	0
54	MG	BA	3009	1/1	0.98	0.23	5.04	53,53,53,53	0
54	MG	CA	1650	1/1	0.23	0.73	5.03	151,151,151,151	0
54	MG	BA	3151	1/1	0.95	0.28	4.97	103,103,103,103	0
54	MG	BA	3028	1/1	0.97	0.33	4.96	57,57,57,57	0
54	MG	DA	3506	1/1	0.97	0.27	4.92	61,61,61,61	0
54	MG	CA	1690	1/1	0.97	0.22	4.92	102,102,102,102	0
54	MG	AA	1620	1/1	0.96	0.24	4.76	105,105,105,105	0
54	MG	CA	1646	1/1	0.98	0.22	4.74	101,101,101,101	0
54	MG	DA	3326	1/1	0.92	0.29	4.60	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3040	1/1	0.96	0.26	4.48	88,88,88,88	0
54	MG	DA	3222	1/1	0.98	0.26	4.44	62,62,62,62	0
54	MG	DA	3037	1/1	0.76	1.08	4.40	117,117,117,117	0
54	MG	AA	1601	1/1	0.99	0.26	4.35	80,80,80,80	0
54	MG	BA	3138	1/1	0.95	0.27	4.23	81,81,81,81	0
54	MG	DA	3221	1/1	0.97	0.26	4.21	61,61,61,61	0
54	MG	BA	3393	1/1	0.78	0.18	4.17	108,108,108,108	0
54	MG	BA	3163	1/1	0.93	0.22	4.15	104,104,104,104	0
54	MG	AA	1644	1/1	0.96	0.25	4.14	72,72,72,72	0
54	MG	DA	3290	1/1	0.94	0.21	4.14	107,107,107,107	0
54	MG	AQ	101	1/1	0.83	0.33	4.03	84,84,84,84	0
54	MG	DA	3501	1/1	0.98	0.24	4.01	73,73,73,73	0
54	MG	BA	3405	1/1	0.87	0.23	4.01	73,73,73,73	0
54	MG	BA	3025	1/1	0.95	0.36	3.99	65,65,65,65	0
54	MG	AA	1677	1/1	0.96	0.31	3.92	125,125,125,125	0
54	MG	BA	3582	1/1	0.98	0.24	3.85	68,68,68,68	0
54	MG	DA	3211	1/1	0.96	0.22	3.77	71,71,71,71	0
54	MG	DA	3356	1/1	0.93	0.28	3.75	64,64,64,64	0
54	MG	BA	3570	1/1	0.90	0.24	3.66	82,82,82,82	0
54	MG	BA	3220	1/1	0.97	0.22	3.66	76,76,76,76	0
54	MG	AA	1788	1/1	0.92	0.30	3.60	124,124,124,124	0
54	MG	BA	3023	1/1	0.94	0.21	3.57	66,66,66,66	0
54	MG	DA	3495	1/1	0.99	0.28	3.56	78,78,78,78	0
54	MG	BA	3592	1/1	0.93	0.23	3.51	112,112,112,112	0
54	MG	AA	1743	1/1	0.85	0.21	3.42	136,136,136,136	0
54	MG	DA	3390	1/1	0.86	0.19	3.40	144,144,144,144	0
54	MG	CG	302	1/1	0.95	0.36	3.29	180,180,180,180	0
54	MG	DA	3205	1/1	0.86	0.19	3.29	106,106,106,106	0
54	MG	DA	3516	1/1	0.88	0.25	3.23	92,92,92,92	0
54	MG	DA	3389	1/1	0.95	0.19	3.22	94,94,94,94	0
54	MG	DB	211	1/1	0.84	0.22	3.13	107,107,107,107	0
54	MG	DA	3031	1/1	0.87	0.58	2.93	70,70,70,70	0
54	MG	CA	1654	1/1	0.96	0.18	2.86	128,128,128,128	0
54	MG	CA	1657	1/1	0.93	0.16	2.86	142,142,142,142	0
54	MG	DA	3116	1/1	0.94	0.25	2.75	77,77,77,77	0
54	MG	AA	1826	1/1	0.91	0.17	2.73	94,94,94,94	0
54	MG	BA	3232	1/1	0.92	0.19	2.71	93,93,93,93	0
54	MG	CA	1799	1/1	0.58	0.21	2.70	150,150,150,150	0
54	MG	BA	3018	1/1	0.94	0.29	2.69	53,53,53,53	0
54	MG	DA	3357	1/1	0.92	0.17	2.65	105,105,105,105	0
54	MG	DA	3114	1/1	0.99	0.20	2.59	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3271	1/1	0.95	0.26	2.47	62,62,62,62	0
54	MG	BA	3174	1/1	0.98	0.18	2.45	61,61,61,61	0
54	MG	DA	3244	1/1	0.96	0.20	2.45	84,84,84,84	0
54	MG	BA	3314	1/1	0.67	0.17	2.36	104,104,104,104	0
54	MG	BA	3367	1/1	0.56	0.20	2.36	124,124,124,124	0
54	MG	BA	3060	1/1	0.91	0.27	2.34	105,105,105,105	0
54	MG	BA	3015	1/1	0.97	0.24	2.30	61,61,61,61	0
54	MG	DA	3184	1/1	0.99	0.21	2.28	68,68,68,68	0
54	MG	DA	3033	1/1	0.81	0.19	2.12	89,89,89,89	0
54	MG	DA	3127	1/1	0.98	0.21	2.11	66,66,66,66	0
54	MG	CA	1625	1/1	0.95	0.38	2.10	142,142,142,142	0
54	MG	CH	201	1/1	0.89	0.29	2.04	114,114,114,114	0
54	MG	DZ	101	1/1	0.78	0.25	1.97	113,113,113,113	0
54	MG	DA	3117	1/1	0.96	0.27	1.96	72,72,72,72	0
54	MG	DA	3362	1/1	0.79	0.16	1.95	120,120,120,120	0
54	MG	DA	3236	1/1	0.97	0.26	1.93	60,60,60,60	0
54	MG	DA	3327	1/1	0.99	0.30	1.91	70,70,70,70	0
54	MG	DD	301	1/1	0.73	0.47	1.90	119,119,119,119	0
54	MG	DA	3061	1/1	0.94	0.23	1.88	64,64,64,64	0
54	MG	DA	3223	1/1	0.96	0.24	1.84	54,54,54,54	0
54	MG	BA	3105	1/1	0.96	0.23	1.83	68,68,68,68	0
54	MG	DA	3132	1/1	0.97	0.22	1.70	78,78,78,78	0
54	MG	DA	3499	1/1	0.99	0.17	1.70	103,103,103,103	0
54	MG	DA	3089	1/1	0.86	0.20	1.69	117,117,117,117	0
54	MG	BB	215	1/1	0.94	0.13	1.61	129,129,129,129	0
54	MG	DA	3304	1/1	0.66	0.24	1.57	83,83,83,83	0
54	MG	BA	3186	1/1	0.95	0.27	1.54	62,62,62,62	0
54	MG	AA	1750	1/1	0.69	0.72	1.45	110,110,110,110	0
54	MG	DA	3057	1/1	0.82	0.20	1.41	104,104,104,104	0
54	MG	AA	1816	1/1	0.53	0.33	1.36	115,115,115,115	0
54	MG	DA	3469	1/1	0.90	0.19	1.30	107,107,107,107	0
55	TAC	AA	1833	32/32	0.91	0.20	1.29	99,129,142,143	0
54	MG	DA	3319	1/1	0.95	0.16	1.18	77,77,77,77	0
54	MG	BA	3313	1/1	0.96	0.25	1.09	61,61,61,61	0
54	MG	DA	3173	1/1	0.85	0.14	1.07	92,92,92,92	0
54	MG	CA	1634	1/1	0.91	0.14	1.02	110,110,110,110	0
54	MG	AA	1672	1/1	0.65	0.24	1.00	112,112,112,112	0
54	MG	BA	3605	1/1	0.94	0.17	0.95	82,82,82,82	0
54	MG	DA	3062	1/1	0.94	0.38	0.89	112,112,112,112	0
54	MG	DA	3227	1/1	0.95	0.25	0.76	83,83,83,83	0
54	MG	BE	305	1/1	0.82	0.39	0.76	111,111,111,111	0
54	MG	BE	301	1/1	0.96	0.27	0.73	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3006	1/1	0.98	0.21	0.72	50,50,50,50	0
54	MG	DA	3189	1/1	0.98	0.25	0.70	65,65,65,65	0
54	MG	DA	3091	1/1	0.95	0.13	0.54	87,87,87,87	0
54	MG	CA	1753	1/1	0.76	0.19	0.53	95,95,95,95	0
54	MG	B6	101	1/1	0.47	0.57	0.52	128,128,128,128	0
54	MG	DA	3231	1/1	0.97	0.23	0.51	74,74,74,74	0
54	MG	AA	1605	1/1	0.93	0.20	0.47	108,108,108,108	0
54	MG	CC	108	1/1	0.74	0.46	0.44	129,129,129,129	0
54	MG	BA	3270	1/1	0.94	0.20	0.44	87,87,87,87	0
54	MG	DE	302	1/1	0.69	0.28	0.36	97,97,97,97	0
54	MG	DA	3507	1/1	0.97	0.18	0.34	79,79,79,79	0
54	MG	BA	3027	1/1	0.93	0.23	0.20	69,69,69,69	0
54	MG	DA	3269	1/1	0.90	0.20	0.14	78,78,78,78	0
54	MG	BA	3036	1/1	0.97	0.22	-0.08	63,63,63,63	0
54	MG	DA	3311	1/1	0.91	0.16	-0.09	92,92,92,92	0
54	MG	DA	3019	1/1	0.94	0.23	-0.12	84,84,84,84	0
54	MG	DA	3497	1/1	0.99	0.19	-0.13	50,50,50,50	0
54	MG	D1	201	1/1	0.91	0.19	-0.13	87,87,87,87	0
54	MG	AA	1619	1/1	0.94	0.18	-0.14	96,96,96,96	0
54	MG	DA	3510	1/1	0.91	0.19	-0.14	77,77,77,77	0
54	MG	BA	3165	1/1	0.96	0.18	-0.17	119,119,119,119	0
54	MG	BA	3005	1/1	0.94	0.21	-0.20	61,61,61,61	0
54	MG	BA	3161	1/1	0.90	0.16	-0.22	101,101,101,101	0
54	MG	AA	1774	1/1	0.97	0.18	-0.22	72,72,72,72	0
54	MG	BA	3181	1/1	0.97	0.23	-0.23	79,79,79,79	0
54	MG	DA	3079	1/1	0.92	0.21	-0.25	97,97,97,97	0
54	MG	CA	1660	1/1	0.96	0.14	-0.26	118,118,118,118	0
54	MG	DA	3193	1/1	0.92	0.16	-0.28	69,69,69,69	0
54	MG	DA	3109	1/1	0.97	0.24	-0.31	63,63,63,63	0
56	ZN	AG	303	1/1	0.96	0.25	-0.33	153,153,153,153	0
56	ZN	CG	303	1/1	0.95	0.19	-0.50	161,161,161,161	0
54	MG	DA	3263	1/1	0.99	0.14	-0.57	129,129,129,129	0
54	MG	DB	202	1/1	0.97	0.13	-0.57	113,113,113,113	0
54	MG	B7	103	1/1	0.93	0.15	-0.63	88,88,88,88	0
54	MG	CC	102	1/1	0.98	0.15	-0.77	83,83,83,83	0
54	MG	AA	1608	1/1	0.95	0.13	-0.81	111,111,111,111	0
54	MG	DA	3015	1/1	0.94	0.20	-0.83	98,98,98,98	0
54	MG	DE	303	1/1	0.95	0.16	-0.85	70,70,70,70	0
54	MG	BA	3197	1/1	0.98	0.17	-0.88	66,66,66,66	0
54	MG	AA	1700	1/1	0.94	0.13	-0.90	123,123,123,123	0
54	MG	DA	3120	1/1	0.97	0.15	-0.92	75,75,75,75	0
56	ZN	CQ	101	1/1	0.95	0.07	-0.95	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	ZN	AQ	103	1/1	0.98	0.09	-0.95	186,186,186,186	0
54	MG	DA	3267	1/1	0.99	0.15	-1.06	79,79,79,79	0
54	MG	DA	3185	1/1	0.95	0.19	-1.08	66,66,66,66	0
54	MG	DA	3262	1/1	0.99	0.13	-1.08	112,112,112,112	0
54	MG	BA	3111	1/1	0.93	0.18	-1.10	68,68,68,68	0
54	MG	CA	1648	1/1	0.96	0.12	-1.11	96,96,96,96	0
54	MG	DA	3493	1/1	0.95	0.14	-1.11	64,64,64,64	0
54	MG	DA	3323	1/1	0.91	0.12	-1.14	79,79,79,79	0
54	MG	DA	3268	1/1	0.96	0.14	-1.15	63,63,63,63	0
54	MG	BA	3184	1/1	0.98	0.20	-1.15	70,70,70,70	0
54	MG	BB	217	1/1	0.98	0.10	-1.16	132,132,132,132	0
54	MG	DA	3473	1/1	0.96	0.11	-1.17	157,157,157,157	0
54	MG	AA	1755	1/1	0.96	0.20	-1.24	143,143,143,143	0
54	MG	CA	1623	1/1	0.93	0.08	-1.29	180,180,180,180	0
54	MG	DA	3364	1/1	0.95	0.16	-1.29	112,112,112,112	0
54	MG	DA	3143	1/1	0.97	0.10	-1.30	117,117,117,117	0
54	MG	DA	3082	1/1	0.95	0.11	-1.36	99,99,99,99	0
54	MG	AA	1666	1/1	0.97	0.08	-1.39	123,123,123,123	0
54	MG	CA	1685	1/1	0.83	0.10	-1.40	121,121,121,121	0
54	MG	DA	3297	1/1	0.98	0.13	-1.52	71,71,71,71	0
54	MG	DA	3181	1/1	0.98	0.15	-1.55	74,74,74,74	0
54	MG	DA	3153	1/1	0.96	0.11	-1.59	145,145,145,145	0
54	MG	DA	3505	1/1	0.97	0.12	-1.61	72,72,72,72	0
54	MG	AA	1707	1/1	0.90	0.10	-1.65	94,94,94,94	0
55	TAC	CA	1805	32/32	0.89	0.11	-1.66	126,153,170,174	0
54	MG	DA	3046	1/1	0.85	0.12	-1.79	82,82,82,82	0
54	MG	AA	1681	1/1	0.94	0.12	-1.86	146,146,146,146	0
54	MG	DA	3186	1/1	0.95	0.12	-1.86	60,60,60,60	0
54	MG	AC	101	1/1	0.96	0.13	-2.02	78,78,78,78	0
54	MG	AA	1753	1/1	0.88	0.08	-2.29	143,143,143,143	0
54	MG	AA	1709	1/1	0.85	0.07	-2.37	155,155,155,155	0
54	MG	CA	1675	1/1	0.94	0.07	-2.48	111,111,111,111	0
54	MG	B5	101	1/1	0.97	0.13	-2.56	61,61,61,61	0
54	MG	BA	3377	1/1	0.86	0.11	-2.58	109,109,109,109	0
54	MG	DA	3225	1/1	0.98	0.12	-2.59	89,89,89,89	0
54	MG	AA	1706	1/1	0.98	0.06	-2.69	134,134,134,134	0
54	MG	BA	3610	1/1	0.96	0.13	-2.72	85,85,85,85	0
54	MG	BA	3373	1/1	0.90	0.10	-2.75	131,131,131,131	0
54	MG	BA	3557	1/1	0.89	0.15	-3.01	92,92,92,92	0
54	MG	DA	3331	1/1	0.99	0.09	-3.01	116,116,116,116	0
54	MG	BA	3387	1/1	0.93	0.08	-3.04	135,135,135,135	0
54	MG	BA	3175	1/1	0.99	0.10	-3.21	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3244	1/1	0.96	0.10	-3.28	112,112,112,112	0
54	MG	CA	1721	1/1	0.99	0.11	-3.79	128,128,128,128	0
54	MG	D5	101	1/1	0.97	0.11	-3.91	63,63,63,63	0
54	MG	DA	3047	1/1	0.88	0.08	-4.19	124,124,124,124	0
54	MG	DA	3298	1/1	0.98	0.09	-4.41	96,96,96,96	0
54	MG	CA	1643	1/1	0.96	0.07	-4.79	148,148,148,148	0
54	MG	BA	3475	1/1	0.84	0.06	-4.81	270,270,270,270	0
54	MG	BA	3176	1/1	0.99	0.08	-5.19	89,89,89,89	0
54	MG	BA	3087	1/1	0.98	0.05	-5.31	142,142,142,142	0
54	MG	DA	3049	1/1	0.95	0.08	-5.52	105,105,105,105	0
54	MG	CA	1678	1/1	0.97	0.07	-6.34	140,140,140,140	0
54	MG	DA	3237	1/1	0.99	0.10	-6.65	63,63,63,63	0
54	MG	BA	3202	1/1	0.95	0.24	-	65,65,65,65	0
54	MG	CA	1706	1/1	0.82	0.34	-	126,126,126,126	0
54	MG	BA	3566	1/1	0.69	0.40	-	100,100,100,100	0
54	MG	DA	3058	1/1	0.90	0.56	-	109,109,109,109	0
54	MG	BA	3413	1/1	0.83	0.40	-	120,120,120,120	0
54	MG	BA	3338	1/1	0.96	0.25	-	103,103,103,103	0
54	MG	BA	3256	1/1	0.91	0.28	-	68,68,68,68	0
54	MG	BA	3421	1/1	0.79	0.97	-	106,106,106,106	0
54	MG	CA	1763	1/1	0.85	0.27	-	94,94,94,94	0
54	MG	DA	3040	1/1	0.81	0.14	-	98,98,98,98	0
54	MG	BB	209	1/1	0.91	0.33	-	116,116,116,116	0
54	MG	BA	3384	1/1	0.59	0.20	-	107,107,107,107	0
54	MG	BA	3319	1/1	0.64	0.56	-	129,129,129,129	0
54	MG	BA	3032	1/1	0.95	0.30	-	69,69,69,69	0
54	MG	DA	3232	1/1	0.97	0.23	-	78,78,78,78	0
54	MG	BA	3426	1/1	0.92	0.35	-	77,77,77,77	0
54	MG	BA	3485	1/1	0.75	0.27	-	90,90,90,90	0
54	MG	BA	3332	1/1	0.84	0.32	-	83,83,83,83	0
54	MG	DA	3192	1/1	0.95	0.23	-	64,64,64,64	0
54	MG	DA	3352	1/1	0.73	0.36	-	81,81,81,81	0
54	MG	BA	3119	1/1	0.62	0.39	-	78,78,78,78	0
54	MG	AA	1768	1/1	0.98	0.14	-	126,126,126,126	0
54	MG	BA	3394	1/1	0.95	0.45	-	85,85,85,85	0
54	MG	AC	102	1/1	0.04	0.30	-	123,123,123,123	0
54	MG	BA	3201	1/1	0.97	0.31	-	122,122,122,122	0
54	MG	BA	3308	1/1	0.94	0.40	-	110,110,110,110	0
54	MG	DA	3525	1/1	0.82	0.33	-	103,103,103,103	0
54	MG	BA	3156	1/1	0.86	0.98	-	108,108,108,108	0
54	MG	AA	1744	1/1	0.91	0.21	-	180,180,180,180	0
54	MG	DA	3404	1/1	0.91	0.13	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3574	1/1	0.93	0.36	-	60,60,60,60	0
54	MG	DA	3429	1/1	0.92	0.23	-	97,97,97,97	0
54	MG	AA	1669	1/1	0.81	0.22	-	79,79,79,79	0
54	MG	CA	1723	1/1	0.73	0.46	-	111,111,111,111	0
54	MG	CA	1692	1/1	0.93	0.22	-	104,104,104,104	0
54	MG	BA	3196	1/1	0.74	0.28	-	109,109,109,109	0
54	MG	DA	3440	1/1	0.97	0.43	-	83,83,83,83	0
54	MG	AA	1630	1/1	0.92	0.23	-	105,105,105,105	0
54	MG	BA	3608	1/1	0.89	0.21	-	108,108,108,108	0
54	MG	AA	1782	1/1	0.75	0.15	-	168,168,168,168	0
54	MG	BA	3219	1/1	0.99	0.12	-	123,123,123,123	0
54	MG	BA	3357	1/1	0.69	0.93	-	119,119,119,119	0
54	MG	CA	1683	1/1	0.87	0.23	-	113,113,113,113	0
54	MG	CA	1661	1/1	0.92	0.36	-	98,98,98,98	0
54	MG	BA	3567	1/1	0.87	0.54	-	114,114,114,114	0
54	MG	DA	3359	1/1	0.68	0.30	-	102,102,102,102	0
54	MG	DA	3021	1/1	0.85	0.15	-	77,77,77,77	0
54	MG	CA	1611	1/1	0.81	0.39	-	114,114,114,114	0
54	MG	BA	3545	1/1	0.89	0.21	-	108,108,108,108	0
54	MG	BA	3334	1/1	0.84	0.32	-	115,115,115,115	0
54	MG	BP	201	1/1	0.87	1.40	-	115,115,115,115	0
54	MG	CA	1754	1/1	0.82	0.43	-	97,97,97,97	0
54	MG	CA	1739	1/1	0.94	0.23	-	112,112,112,112	0
54	MG	BA	3237	1/1	0.24	0.38	-	117,117,117,117	0
54	MG	DA	3274	1/1	0.94	0.23	-	83,83,83,83	0
54	MG	BA	3262	1/1	0.98	0.34	-	63,63,63,63	0
54	MG	BA	3051	1/1	0.95	0.21	-	72,72,72,72	0
54	MG	AA	1767	1/1	0.93	0.39	-	100,100,100,100	0
54	MG	DA	3112	1/1	0.95	0.24	-	71,71,71,71	0
54	MG	CA	1701	1/1	0.84	0.56	-	92,92,92,92	0
54	MG	AA	1626	1/1	0.95	0.19	-	80,80,80,80	0
54	MG	DA	3235	1/1	0.82	0.25	-	89,89,89,89	0
54	MG	BA	3022	1/1	0.98	0.41	-	65,65,65,65	0
54	MG	BA	3182	1/1	0.91	0.20	-	101,101,101,101	0
54	MG	BA	3322	1/1	0.90	0.26	-	78,78,78,78	0
54	MG	CA	1714	1/1	0.92	0.32	-	94,94,94,94	0
54	MG	BA	3150	1/1	0.83	0.17	-	90,90,90,90	0
54	MG	DA	3305	1/1	0.82	0.34	-	91,91,91,91	0
54	MG	DA	3266	1/1	0.99	0.12	-	110,110,110,110	0
54	MG	AA	1757	1/1	0.84	0.10	-	118,118,118,118	0
54	MG	BA	3110	1/1	0.77	0.34	-	92,92,92,92	0
54	MG	DA	3466	1/1	0.90	0.20	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1801	1/1	0.96	0.24	-	139,139,139,139	0
54	MG	CS	101	1/1	0.86	0.44	-	115,115,115,115	0
54	MG	BA	3154	1/1	0.63	0.37	-	104,104,104,104	0
54	MG	BA	3364	1/1	0.95	0.23	-	137,137,137,137	0
54	MG	CC	104	1/1	0.82	0.36	-	95,95,95,95	0
54	MG	DA	3134	1/1	0.93	0.11	-	105,105,105,105	0
54	MG	BA	3091	1/1	0.81	0.29	-	103,103,103,103	0
54	MG	CA	1633	1/1	0.81	0.38	-	107,107,107,107	0
54	MG	BA	3431	1/1	0.77	0.39	-	96,96,96,96	0
54	MG	DA	3409	1/1	0.93	0.36	-	132,132,132,132	0
54	MG	CA	1745	1/1	0.67	0.23	-	132,132,132,132	0
54	MG	BA	3011	1/1	0.79	0.35	-	72,72,72,72	0
54	MG	DA	3083	1/1	0.89	0.48	-	117,117,117,117	0
54	MG	CC	101	1/1	0.83	0.43	-	130,130,130,130	0
54	MG	BA	3269	1/1	0.74	0.23	-	85,85,85,85	0
54	MG	BA	3330	1/1	0.97	0.26	-	102,102,102,102	0
54	MG	AA	1614	1/1	0.86	0.38	-	114,114,114,114	0
54	MG	BA	3131	1/1	0.91	0.22	-	101,101,101,101	0
54	MG	BA	3216	1/1	0.91	0.20	-	95,95,95,95	0
54	MG	BA	3127	1/1	0.75	0.25	-	109,109,109,109	0
54	MG	BA	3164	1/1	0.91	0.44	-	80,80,80,80	0
54	MG	DA	3521	1/1	0.91	0.08	-	111,111,111,111	0
54	MG	AA	1639	1/1	0.87	0.40	-	91,91,91,91	0
54	MG	BA	3442	1/1	0.69	0.53	-	112,112,112,112	0
54	MG	DA	3020	1/1	0.92	0.10	-	62,62,62,62	0
54	MG	BA	3484	1/1	0.74	0.32	-	116,116,116,116	0
54	MG	BA	3166	1/1	0.89	0.27	-	86,86,86,86	0
54	MG	DA	3102	1/1	0.96	0.10	-	150,150,150,150	0
54	MG	DA	3241	1/1	0.96	0.24	-	69,69,69,69	0
54	MG	BA	3391	1/1	0.95	0.31	-	103,103,103,103	0
54	MG	DA	3370	1/1	0.77	0.16	-	96,96,96,96	0
54	MG	DA	3099	1/1	0.92	0.30	-	74,74,74,74	0
54	MG	BA	3547	1/1	0.88	0.33	-	108,108,108,108	0
54	MG	BA	3509	1/1	0.52	0.43	-	104,104,104,104	0
54	MG	AA	1628	1/1	0.57	0.36	-	142,142,142,142	0
54	MG	BA	3607	1/1	0.85	0.49	-	94,94,94,94	0
54	MG	DA	3464	1/1	0.77	0.17	-	101,101,101,101	0
54	MG	AA	1618	1/1	0.80	0.20	-	98,98,98,98	0
54	MG	BE	304	1/1	0.41	0.73	-	112,112,112,112	0
54	MG	CA	1635	1/1	0.96	0.27	-	78,78,78,78	0
54	MG	BA	3409	1/1	0.95	0.46	-	86,86,86,86	0
54	MG	CA	1614	1/1	0.94	0.17	-	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3001	1/1	0.93	0.22	-	83,83,83,83	0
54	MG	CA	1663	1/1	0.69	0.14	-	105,105,105,105	0
54	MG	DA	3407	1/1	0.68	0.20	-	114,114,114,114	0
54	MG	BA	3271	1/1	0.87	0.37	-	96,96,96,96	0
54	MG	BA	3153	1/1	0.88	0.29	-	89,89,89,89	0
54	MG	DA	3438	1/1	0.90	0.19	-	134,134,134,134	0
54	MG	CA	1791	1/1	0.98	0.30	-	78,78,78,78	0
54	MG	BA	3134	1/1	0.88	0.45	-	130,130,130,130	0
54	MG	DA	3179	1/1	0.96	0.18	-	85,85,85,85	0
54	MG	DA	3306	1/1	0.92	0.20	-	92,92,92,92	0
54	MG	BA	3295	1/1	0.97	0.45	-	70,70,70,70	0
54	MG	AG	301	1/1	0.69	0.12	-	114,114,114,114	0
54	MG	BA	3088	1/1	0.82	0.41	-	97,97,97,97	0
54	MG	BA	3627	1/1	0.91	0.47	-	89,89,89,89	0
54	MG	CA	1728	1/1	0.76	0.29	-	144,144,144,144	0
54	MG	DA	3524	1/1	0.92	0.57	-	86,86,86,86	0
54	MG	BA	3214	1/1	0.72	0.75	-	93,93,93,93	0
54	MG	DA	3096	1/1	0.80	0.24	-	125,125,125,125	0
54	MG	DA	3435	1/1	0.81	0.23	-	99,99,99,99	0
54	MG	CA	1803	1/1	0.76	0.37	-	123,123,123,123	0
54	MG	DA	3341	1/1	0.62	0.57	-	107,107,107,107	0
54	MG	AA	1758	1/1	0.60	0.25	-	111,111,111,111	0
54	MG	CA	1787	1/1	0.59	0.26	-	129,129,129,129	0
54	MG	BA	3274	1/1	0.94	0.52	-	93,93,93,93	0
54	MG	CA	1671	1/1	0.89	0.36	-	75,75,75,75	0
54	MG	DA	3512	1/1	0.75	0.38	-	81,81,81,81	0
54	MG	DA	3228	1/1	0.97	0.07	-	80,80,80,80	0
54	MG	BB	214	1/1	0.61	0.47	-	108,108,108,108	0
54	MG	CA	1608	1/1	0.78	0.20	-	103,103,103,103	0
54	MG	BO	203	1/1	0.94	0.17	-	70,70,70,70	0
54	MG	B3	102	1/1	0.87	0.44	-	93,93,93,93	0
54	MG	CA	1789	1/1	0.85	0.29	-	121,121,121,121	0
54	MG	DA	3258	1/1	0.89	0.23	-	98,98,98,98	0
54	MG	BU	202	1/1	0.94	0.20	-	80,80,80,80	0
54	MG	DA	3041	1/1	0.25	0.23	-	142,142,142,142	0
54	MG	AA	1632	1/1	0.93	0.30	-	116,116,116,116	0
54	MG	DA	3140	1/1	0.95	0.12	-	74,74,74,74	0
54	MG	BA	3587	1/1	0.93	0.34	-	102,102,102,102	0
54	MG	BA	3539	1/1	0.59	0.46	-	99,99,99,99	0
54	MG	DA	3103	1/1	0.78	0.12	-	117,117,117,117	0
54	MG	DA	3482	1/1	0.74	0.14	-	120,120,120,120	0
54	MG	BA	3041	1/1	0.97	0.07	-	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3415	1/1	0.85	0.53	-	90,90,90,90	0
54	MG	BA	3172	1/1	0.96	0.18	-	93,93,93,93	0
54	MG	CA	1779	1/1	0.88	0.21	-	112,112,112,112	0
54	MG	BA	3312	1/1	0.82	0.45	-	98,98,98,98	0
54	MG	BA	3588	1/1	0.93	0.41	-	109,109,109,109	0
54	MG	AA	1823	1/1	0.96	0.10	-	138,138,138,138	0
54	MG	CA	1602	1/1	0.45	0.55	-	115,115,115,115	0
54	MG	DA	3030	1/1	0.97	0.27	-	89,89,89,89	0
54	MG	BA	3345	1/1	0.82	0.15	-	95,95,95,95	0
54	MG	BA	3289	1/1	0.82	0.25	-	83,83,83,83	0
54	MG	BA	3382	1/1	0.96	0.45	-	78,78,78,78	0
54	MG	DA	3325	1/1	0.90	0.37	-	74,74,74,74	0
54	MG	DA	3400	1/1	0.80	0.27	-	105,105,105,105	0
54	MG	BA	3230	1/1	0.63	0.34	-	97,97,97,97	0
54	MG	BA	3615	1/1	0.72	0.21	-	92,92,92,92	0
54	MG	BA	3375	1/1	0.96	0.50	-	80,80,80,80	0
54	MG	AA	1716	1/1	0.85	0.43	-	107,107,107,107	0
54	MG	DA	3200	1/1	0.90	0.16	-	112,112,112,112	0
54	MG	BA	3527	1/1	0.43	0.42	-	109,109,109,109	0
54	MG	DA	3216	1/1	0.94	0.18	-	77,77,77,77	0
54	MG	DA	3218	1/1	0.97	0.34	-	77,77,77,77	0
54	MG	BA	3591	1/1	0.99	0.45	-	57,57,57,57	0
54	MG	BA	3424	1/1	0.62	0.61	-	111,111,111,111	0
54	MG	DA	3421	1/1	0.72	0.23	-	141,141,141,141	0
54	MG	BA	3626	1/1	0.80	0.50	-	103,103,103,103	0
54	MG	DA	3461	1/1	0.74	0.18	-	102,102,102,102	0
54	MG	BA	3185	1/1	0.81	1.06	-	112,112,112,112	0
54	MG	DA	3479	1/1	0.88	0.28	-	106,106,106,106	0
54	MG	AA	1609	1/1	0.97	0.39	-	87,87,87,87	0
54	MG	BA	3465	1/1	0.73	0.64	-	107,107,107,107	0
54	MG	BA	3352	1/1	0.96	0.33	-	87,87,87,87	0
54	MG	DA	3081	1/1	0.38	0.42	-	116,116,116,116	0
54	MG	CA	1749	1/1	0.68	0.22	-	120,120,120,120	0
54	MG	B8	101	1/1	0.87	0.26	-	101,101,101,101	0
54	MG	CA	1716	1/1	0.70	0.46	-	126,126,126,126	0
54	MG	BA	3211	1/1	0.91	0.41	-	77,77,77,77	0
54	MG	DA	3439	1/1	0.96	0.07	-	84,84,84,84	0
54	MG	BA	3602	1/1	0.96	0.49	-	66,66,66,66	0
54	MG	AA	1785	1/1	0.92	0.18	-	131,131,131,131	0
54	MG	DA	3260	1/1	0.76	0.36	-	128,128,128,128	0
54	MG	BA	3247	1/1	0.84	0.41	-	80,80,80,80	0
54	MG	CA	1659	1/1	0.89	0.14	-	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3012	1/1	0.81	0.82	-	129,129,129,129	0
54	MG	DA	3377	1/1	0.65	0.34	-	102,102,102,102	0
54	MG	DA	3346	1/1	0.80	0.24	-	93,93,93,93	0
54	MG	DA	3398	1/1	0.68	0.35	-	130,130,130,130	0
54	MG	DA	3468	1/1	0.71	0.29	-	126,126,126,126	0
54	MG	DA	3408	1/1	0.93	0.31	-	107,107,107,107	0
54	MG	BA	3556	1/1	0.92	0.14	-	91,91,91,91	0
54	MG	DA	3075	1/1	0.99	0.30	-	105,105,105,105	0
54	MG	CA	1624	1/1	0.94	0.33	-	129,129,129,129	0
54	MG	BA	3325	1/1	0.90	0.14	-	89,89,89,89	0
54	MG	CA	1790	1/1	0.81	0.41	-	118,118,118,118	0
54	MG	AA	1623	1/1	0.85	0.30	-	81,81,81,81	0
54	MG	BA	3599	1/1	0.91	0.32	-	115,115,115,115	0
54	MG	BA	3569	1/1	0.94	0.45	-	79,79,79,79	0
54	MG	BA	3124	1/1	0.63	0.29	-	110,110,110,110	0
54	MG	BA	3077	1/1	0.86	0.34	-	77,77,77,77	0
54	MG	BO	202	1/1	0.57	0.29	-	98,98,98,98	0
54	MG	BA	3292	1/1	0.72	0.50	-	113,113,113,113	0
54	MG	DA	3276	1/1	0.94	0.17	-	97,97,97,97	0
54	MG	AA	1718	1/1	0.87	0.34	-	124,124,124,124	0
54	MG	AA	1799	1/1	0.94	0.41	-	79,79,79,79	0
54	MG	BA	3548	1/1	0.74	0.35	-	96,96,96,96	0
54	MG	AA	1676	1/1	0.65	0.46	-	132,132,132,132	0
54	MG	DA	3445	1/1	0.90	0.30	-	89,89,89,89	0
54	MG	DA	3487	1/1	0.62	0.32	-	108,108,108,108	0
54	MG	BA	3603	1/1	0.94	1.36	-	113,113,113,113	0
54	MG	AA	1731	1/1	0.97	0.54	-	90,90,90,90	0
54	MG	BA	3117	1/1	0.92	0.23	-	102,102,102,102	0
54	MG	DA	3340	1/1	0.92	0.13	-	89,89,89,89	0
54	MG	CA	1639	1/1	0.98	0.36	-	129,129,129,129	0
54	MG	DA	3310	1/1	0.68	0.62	-	111,111,111,111	0
54	MG	DA	3010	1/1	0.88	0.23	-	103,103,103,103	0
54	MG	BA	3093	1/1	0.29	0.33	-	154,154,154,154	0
54	MG	CA	1631	1/1	0.42	0.26	-	134,134,134,134	0
54	MG	BA	3429	1/1	0.30	0.55	-	129,129,129,129	0
54	MG	B1	201	1/1	0.95	0.28	-	61,61,61,61	0
54	MG	AA	1802	1/1	0.56	0.31	-	136,136,136,136	0
54	MG	AA	1720	1/1	0.97	0.16	-	101,101,101,101	0
54	MG	BA	3026	1/1	0.98	0.19	-	66,66,66,66	0
54	MG	BA	3278	1/1	0.68	0.30	-	101,101,101,101	0
54	MG	DA	3363	1/1	0.98	0.06	-	125,125,125,125	0
54	MG	AA	1727	1/1	0.82	0.12	-	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3060	1/1	0.90	0.15	-	101,101,101,101	0
54	MG	BA	3257	1/1	0.97	0.28	-	70,70,70,70	0
54	MG	BA	3552	1/1	0.87	0.17	-	98,98,98,98	0
54	MG	DA	3322	1/1	0.87	0.28	-	110,110,110,110	0
54	MG	BB	207	1/1	0.77	0.40	-	131,131,131,131	0
54	MG	DA	3131	1/1	0.91	0.16	-	94,94,94,94	0
54	MG	BA	3600	1/1	0.84	0.57	-	97,97,97,97	0
54	MG	CA	1681	1/1	0.81	0.29	-	96,96,96,96	0
54	MG	AA	1796	1/1	0.75	0.28	-	109,109,109,109	0
54	MG	AA	1769	1/1	0.45	0.24	-	124,124,124,124	0
54	MG	DA	3476	1/1	0.94	0.43	-	99,99,99,99	0
54	MG	DA	3090	1/1	0.95	0.22	-	90,90,90,90	0
54	MG	BA	3422	1/1	0.90	0.18	-	120,120,120,120	0
54	MG	DB	213	1/1	0.82	0.13	-	91,91,91,91	0
54	MG	BB	206	1/1	0.68	0.28	-	97,97,97,97	0
54	MG	BA	3039	1/1	0.96	0.34	-	98,98,98,98	0
54	MG	BA	3411	1/1	0.24	0.49	-	110,110,110,110	0
54	MG	AC	109	1/1	0.84	0.30	-	105,105,105,105	0
54	MG	BA	3275	1/1	0.74	0.51	-	111,111,111,111	0
54	MG	BA	3480	1/1	0.62	0.17	-	187,187,187,187	0
54	MG	AA	1770	1/1	0.78	0.50	-	98,98,98,98	0
54	MG	BA	3543	1/1	0.61	0.30	-	90,90,90,90	0
54	MG	CA	1742	1/1	0.97	0.34	-	98,98,98,98	0
54	MG	BA	3067	1/1	0.93	1.01	-	108,108,108,108	0
54	MG	BA	3205	1/1	0.72	0.26	-	88,88,88,88	0
54	MG	DA	3463	1/1	0.63	0.38	-	109,109,109,109	0
54	MG	BA	3252	1/1	0.97	0.26	-	70,70,70,70	0
54	MG	DA	3056	1/1	0.94	0.17	-	86,86,86,86	0
54	MG	CA	1687	1/1	0.83	0.38	-	106,106,106,106	0
54	MG	BA	3561	1/1	0.81	0.24	-	86,86,86,86	0
54	MG	BF	302	1/1	0.98	0.43	-	127,127,127,127	0
54	MG	CA	1784	1/1	0.73	0.16	-	94,94,94,94	0
54	MG	CA	1705	1/1	0.78	0.49	-	114,114,114,114	0
54	MG	AA	1756	1/1	0.93	0.27	-	86,86,86,86	0
54	MG	CA	1694	1/1	0.82	0.22	-	108,108,108,108	0
54	MG	BA	3208	1/1	0.88	0.30	-	91,91,91,91	0
54	MG	DA	3220	1/1	0.98	0.23	-	70,70,70,70	0
54	MG	AA	1713	1/1	0.97	0.15	-	107,107,107,107	0
54	MG	DA	3292	1/1	0.85	0.16	-	129,129,129,129	0
54	MG	AA	1717	1/1	0.97	0.08	-	137,137,137,137	0
54	MG	BA	3443	1/1	0.67	0.48	-	124,124,124,124	0
54	MG	DA	3133	1/1	0.94	0.18	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3067	1/1	0.81	0.16	-	97,97,97,97	0
54	MG	CA	1760	1/1	0.90	0.22	-	135,135,135,135	0
54	MG	DA	3393	1/1	0.93	0.25	-	76,76,76,76	0
54	MG	AA	1654	1/1	0.92	0.40	-	113,113,113,113	0
54	MG	DB	207	1/1	0.32	0.19	-	114,114,114,114	0
54	MG	DA	3515	1/1	0.95	0.08	-	94,94,94,94	0
54	MG	DA	3115	1/1	0.96	0.21	-	75,75,75,75	0
54	MG	DA	3366	1/1	0.79	0.36	-	103,103,103,103	0
54	MG	AA	1690	1/1	0.55	0.28	-	128,128,128,128	0
54	MG	BA	3200	1/1	0.97	0.23	-	149,149,149,149	0
54	MG	BA	3152	1/1	0.90	0.54	-	90,90,90,90	0
54	MG	BA	3495	1/1	0.99	0.33	-	73,73,73,73	0
54	MG	DA	3044	1/1	0.83	0.10	-	96,96,96,96	0
54	MG	DA	3383	1/1	0.97	0.36	-	84,84,84,84	0
54	MG	BA	3343	1/1	0.91	0.21	-	86,86,86,86	0
54	MG	DA	3064	1/1	0.96	0.25	-	79,79,79,79	0
54	MG	CA	1776	1/1	0.85	0.42	-	125,125,125,125	0
54	MG	BA	3096	1/1	0.58	0.55	-	129,129,129,129	0
54	MG	CA	1724	1/1	0.89	0.12	-	98,98,98,98	0
54	MG	AA	1723	1/1	0.83	0.26	-	92,92,92,92	0
54	MG	BA	3369	1/1	0.67	0.44	-	94,94,94,94	0
54	MG	DA	3007	1/1	0.88	0.23	-	116,116,116,116	0
54	MG	BA	3272	1/1	0.94	0.29	-	52,52,52,52	0
54	MG	BA	3267	1/1	0.99	0.07	-	126,126,126,126	0
54	MG	AA	1822	1/1	0.93	0.10	-	144,144,144,144	0
54	MG	BA	3562	1/1	0.74	0.32	-	97,97,97,97	0
54	MG	DA	3180	1/1	0.91	0.31	-	82,82,82,82	0
54	MG	DA	3086	1/1	0.89	0.11	-	84,84,84,84	0
54	MG	CA	1758	1/1	0.80	0.48	-	110,110,110,110	0
54	MG	CA	1616	1/1	0.71	0.27	-	108,108,108,108	0
54	MG	CA	1679	1/1	0.75	0.14	-	94,94,94,94	0
54	MG	BA	3260	1/1	0.96	0.24	-	126,126,126,126	0
54	MG	AA	1749	1/1	0.63	0.22	-	112,112,112,112	0
54	MG	DA	3330	1/1	0.87	0.32	-	82,82,82,82	0
54	MG	AA	1791	1/1	0.88	0.23	-	104,104,104,104	0
54	MG	DA	3051	1/1	0.66	0.28	-	81,81,81,81	0
54	MG	CA	1712	1/1	0.76	0.23	-	105,105,105,105	0
54	MG	BA	3276	1/1	0.98	0.26	-	90,90,90,90	0
54	MG	DA	3467	1/1	0.94	0.10	-	159,159,159,159	0
54	MG	BA	3417	1/1	0.96	0.23	-	78,78,78,78	0
54	MG	BA	3358	1/1	0.87	0.39	-	108,108,108,108	0
54	MG	BA	3380	1/1	0.81	0.26	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3020	1/1	0.93	0.16	-	109,109,109,109	0
54	MG	BA	3471	1/1	0.97	0.45	-	91,91,91,91	0
54	MG	AA	1705	1/1	0.91	0.27	-	98,98,98,98	0
54	MG	AS	101	1/1	0.61	0.30	-	106,106,106,106	0
54	MG	AA	1621	1/1	0.91	0.47	-	147,147,147,147	0
54	MG	DA	3296	1/1	0.03	0.34	-	114,114,114,114	0
54	MG	DA	3011	1/1	0.48	0.25	-	128,128,128,128	0
54	MG	DA	3477	1/1	0.97	0.20	-	93,93,93,93	0
54	MG	BA	3403	1/1	0.59	0.36	-	114,114,114,114	0
54	MG	BA	3167	1/1	0.90	0.39	-	95,95,95,95	0
54	MG	BA	3507	1/1	0.87	0.53	-	127,127,127,127	0
54	MG	AA	1819	1/1	0.92	0.20	-	81,81,81,81	0
54	MG	BA	3139	1/1	0.90	0.28	-	66,66,66,66	0
54	MG	CC	103	1/1	0.84	0.20	-	150,150,150,150	0
54	MG	DA	3344	1/1	0.99	0.15	-	124,124,124,124	0
54	MG	BA	3344	1/1	0.84	0.22	-	93,93,93,93	0
54	MG	DA	3433	1/1	0.94	0.20	-	66,66,66,66	0
54	MG	DA	3204	1/1	0.93	0.17	-	126,126,126,126	0
54	MG	DA	3078	1/1	0.94	0.12	-	97,97,97,97	0
54	MG	BA	3300	1/1	0.74	0.33	-	102,102,102,102	0
54	MG	DA	3338	1/1	0.89	0.35	-	95,95,95,95	0
54	MG	DA	3199	1/1	0.96	0.14	-	77,77,77,77	0
54	MG	BA	3282	1/1	0.87	0.51	-	107,107,107,107	0
54	MG	DA	3402	1/1	0.64	0.35	-	105,105,105,105	0
54	MG	DA	3382	1/1	0.89	0.37	-	80,80,80,80	0
54	MG	DA	3110	1/1	0.94	0.27	-	75,75,75,75	0
54	MG	BA	3353	1/1	0.89	0.36	-	93,93,93,93	0
54	MG	BA	3456	1/1	0.90	0.27	-	108,108,108,108	0
54	MG	CA	1652	1/1	0.96	0.42	-	120,120,120,120	0
54	MG	DA	3394	1/1	0.87	1.09	-	106,106,106,106	0
54	MG	DA	3423	1/1	0.88	0.13	-	123,123,123,123	0
54	MG	CA	1621	1/1	0.90	0.30	-	84,84,84,84	0
54	MG	BE	303	1/1	0.81	0.27	-	72,72,72,72	0
54	MG	DA	3208	1/1	0.92	0.28	-	94,94,94,94	0
54	MG	AA	1808	1/1	0.96	0.15	-	139,139,139,139	0
54	MG	DA	3139	1/1	0.97	0.25	-	67,67,67,67	0
54	MG	B1	202	1/1	0.89	0.28	-	100,100,100,100	0
54	MG	BA	3149	1/1	0.61	0.25	-	110,110,110,110	0
54	MG	DA	3373	1/1	0.92	0.19	-	112,112,112,112	0
54	MG	DA	3336	1/1	0.91	0.15	-	115,115,115,115	0
54	MG	AA	1780	1/1	0.95	0.07	-	154,154,154,154	0
54	MG	DA	3277	1/1	0.97	0.34	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3346	1/1	0.97	0.26	-	112,112,112,112	0
54	MG	AA	1735	1/1	0.82	0.46	-	91,91,91,91	0
54	MG	DA	3252	1/1	0.66	0.27	-	108,108,108,108	0
54	MG	CA	1704	1/1	0.86	0.57	-	95,95,95,95	0
54	MG	DA	3270	1/1	0.99	0.20	-	63,63,63,63	0
54	MG	DA	3247	1/1	0.86	0.20	-	89,89,89,89	0
54	MG	DA	3105	1/1	0.95	0.12	-	110,110,110,110	0
54	MG	BB	208	1/1	0.85	0.44	-	90,90,90,90	0
54	MG	AA	1738	1/1	0.62	0.27	-	117,117,117,117	0
54	MG	BA	3076	1/1	0.98	0.09	-	74,74,74,74	0
54	MG	DA	3443	1/1	0.88	0.15	-	103,103,103,103	0
54	MG	DA	3413	1/1	0.93	0.60	-	115,115,115,115	0
54	MG	BA	3467	1/1	0.83	0.16	-	102,102,102,102	0
54	MG	DA	3335	1/1	0.87	0.19	-	78,78,78,78	0
54	MG	BA	3130	1/1	0.98	0.06	-	92,92,92,92	0
54	MG	BA	3178	1/1	0.90	0.46	-	78,78,78,78	0
54	MG	AA	1667	1/1	0.94	0.35	-	88,88,88,88	0
54	MG	BA	3541	1/1	0.73	0.50	-	120,120,120,120	0
54	MG	DA	3384	1/1	0.95	0.09	-	77,77,77,77	0
54	MG	CA	1734	1/1	0.98	0.07	-	93,93,93,93	0
54	MG	BA	3095	1/1	0.35	0.41	-	92,92,92,92	0
54	MG	BA	3537	1/1	0.71	0.36	-	124,124,124,124	0
54	MG	AA	1763	1/1	0.50	0.41	-	110,110,110,110	0
54	MG	CA	1670	1/1	0.95	0.21	-	91,91,91,91	0
54	MG	AA	1642	1/1	0.88	0.15	-	103,103,103,103	0
54	MG	AA	1665	1/1	0.92	0.24	-	84,84,84,84	0
54	MG	BA	3493	1/1	0.59	0.39	-	116,116,116,116	0
54	MG	BA	3245	1/1	0.64	0.45	-	120,120,120,120	0
54	MG	CA	1649	1/1	0.98	0.22	-	113,113,113,113	0
54	MG	BA	3094	1/1	0.86	0.45	-	97,97,97,97	0
54	MG	AA	1825	1/1	0.81	0.34	-	93,93,93,93	0
54	MG	DA	3416	1/1	0.78	0.31	-	100,100,100,100	0
54	MG	BA	3428	1/1	0.82	0.36	-	80,80,80,80	0
54	MG	DA	3162	1/1	0.65	0.48	-	108,108,108,108	0
54	MG	B2	201	1/1	0.85	0.12	-	90,90,90,90	0
54	MG	DB	201	1/1	0.92	0.18	-	88,88,88,88	0
54	MG	DA	3095	1/1	0.85	0.09	-	121,121,121,121	0
54	MG	BA	3337	1/1	0.87	0.14	-	75,75,75,75	0
54	MG	AA	1673	1/1	0.95	0.14	-	133,133,133,133	0
54	MG	CA	1601	1/1	0.75	0.19	-	108,108,108,108	0
54	MG	BA	3469	1/1	0.90	0.53	-	125,125,125,125	0
54	MG	BA	3290	1/1	0.93	0.23	-	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3053	1/1	0.97	0.33	-	100,100,100,100	0
54	MG	DA	3118	1/1	0.96	0.20	-	61,61,61,61	0
54	MG	BA	3400	1/1	0.78	0.25	-	101,101,101,101	0
54	MG	DA	3294	1/1	0.95	0.31	-	64,64,64,64	0
54	MG	DA	3172	1/1	0.77	0.80	-	110,110,110,110	0
54	MG	BA	3034	1/1	0.85	0.37	-	69,69,69,69	0
54	MG	CA	1665	1/1	0.95	0.46	-	103,103,103,103	0
54	MG	AA	1629	1/1	0.88	0.08	-	186,186,186,186	0
54	MG	DA	3436	1/1	0.83	0.11	-	120,120,120,120	0
54	MG	DA	3183	1/1	0.83	0.37	-	92,92,92,92	0
54	MG	DB	204	1/1	0.75	0.11	-	111,111,111,111	0
54	MG	AA	1754	1/1	0.81	0.14	-	85,85,85,85	0
54	MG	CA	1672	1/1	0.89	0.19	-	101,101,101,101	0
54	MG	DA	3496	1/1	0.97	0.12	-	72,72,72,72	0
54	MG	CA	1793	1/1	0.42	0.38	-	115,115,115,115	0
54	MG	BA	3168	1/1	0.96	0.31	-	52,52,52,52	0
54	MG	DA	3071	1/1	0.82	0.68	-	123,123,123,123	0
54	MG	BA	3177	1/1	0.83	1.70	-	101,101,101,101	0
54	MG	BA	3622	1/1	0.87	0.22	-	120,120,120,120	0
54	MG	DA	3520	1/1	0.84	0.17	-	100,100,100,100	0
54	MG	AA	1794	1/1	0.87	0.17	-	116,116,116,116	0
54	MG	AA	1622	1/1	0.87	0.39	-	96,96,96,96	0
54	MG	AA	1671	1/1	0.55	0.26	-	110,110,110,110	0
54	MG	AA	1776	1/1	0.35	0.22	-	116,116,116,116	0
54	MG	AA	1818	1/1	0.95	0.22	-	156,156,156,156	0
54	MG	CA	1736	1/1	0.88	0.54	-	85,85,85,85	0
54	MG	DA	3122	1/1	0.96	0.27	-	67,67,67,67	0
54	MG	CA	1629	1/1	0.93	0.07	-	164,164,164,164	0
54	MG	AA	1740	1/1	0.79	0.37	-	75,75,75,75	0
54	MG	AC	103	1/1	0.94	0.38	-	75,75,75,75	0
54	MG	BA	3194	1/1	0.87	0.28	-	113,113,113,113	0
54	MG	CA	1628	1/1	0.87	0.04	-	149,149,149,149	0
54	MG	BA	3530	1/1	0.61	0.40	-	110,110,110,110	0
54	MG	DA	3005	1/1	0.92	0.21	-	86,86,86,86	0
54	MG	BA	3250	1/1	0.84	0.49	-	87,87,87,87	0
54	MG	DA	3428	1/1	0.81	0.11	-	89,89,89,89	0
54	MG	DB	210	1/1	0.74	0.20	-	73,73,73,73	0
54	MG	DA	3045	1/1	0.79	0.16	-	67,67,67,67	0
54	MG	DA	3149	1/1	0.71	0.14	-	112,112,112,112	0
54	MG	BA	3210	1/1	0.97	0.51	-	78,78,78,78	0
54	MG	BA	3207	1/1	0.83	0.97	-	116,116,116,116	0
54	MG	BA	3441	1/1	0.81	0.25	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1772	1/1	0.70	0.33	-	155,155,155,155	0
54	MG	BA	3473	1/1	0.97	0.41	-	82,82,82,82	0
54	MG	BA	3496	1/1	0.74	0.47	-	108,108,108,108	0
54	MG	BA	3045	1/1	0.96	0.42	-	66,66,66,66	0
54	MG	DA	3446	1/1	0.90	0.25	-	92,92,92,92	0
54	MG	BA	3115	1/1	0.95	0.37	-	68,68,68,68	0
54	MG	BA	3614	1/1	0.88	1.64	-	109,109,109,109	0
54	MG	AA	1685	1/1	0.57	0.39	-	95,95,95,95	0
54	MG	DA	3283	1/1	0.83	0.26	-	114,114,114,114	0
54	MG	BA	3229	1/1	0.97	0.33	-	89,89,89,89	0
54	MG	BA	3033	1/1	0.94	0.27	-	75,75,75,75	0
54	MG	DA	3437	1/1	0.79	0.21	-	96,96,96,96	0
54	MG	AA	1827	1/1	0.94	0.15	-	82,82,82,82	0
54	MG	BA	3162	1/1	0.97	0.28	-	72,72,72,72	0
54	MG	AA	1611	1/1	0.67	0.17	-	138,138,138,138	0
54	MG	CA	1632	1/1	0.87	0.41	-	111,111,111,111	0
54	MG	BA	3120	1/1	0.95	0.52	-	97,97,97,97	0
54	MG	DA	3321	1/1	0.68	0.21	-	89,89,89,89	0
54	MG	BA	3251	1/1	0.76	0.66	-	109,109,109,109	0
54	MG	BA	3047	1/1	0.95	0.19	-	64,64,64,64	0
54	MG	BA	3430	1/1	0.92	0.13	-	87,87,87,87	0
54	MG	DA	3427	1/1	0.70	0.26	-	114,114,114,114	0
54	MG	BF	301	1/1	0.80	0.66	-	100,100,100,100	0
54	MG	CA	1770	1/1	0.86	0.09	-	106,106,106,106	0
54	MG	BA	3109	1/1	0.98	0.46	-	94,94,94,94	0
54	MG	AA	1687	1/1	0.63	0.40	-	99,99,99,99	0
54	MG	BA	3504	1/1	0.85	0.56	-	88,88,88,88	0
54	MG	AA	1655	1/1	0.95	0.46	-	106,106,106,106	0
54	MG	BA	3259	1/1	0.98	0.28	-	53,53,53,53	0
54	MG	DA	3375	1/1	0.93	0.21	-	127,127,127,127	0
54	MG	CA	1693	1/1	0.83	0.42	-	117,117,117,117	0
54	MG	AA	1764	1/1	0.84	0.13	-	118,118,118,118	0
54	MG	BA	3012	1/1	0.97	0.21	-	70,70,70,70	0
54	MG	BB	213	1/1	0.90	0.40	-	72,72,72,72	0
54	MG	DA	3038	1/1	0.36	0.25	-	122,122,122,122	0
54	MG	BA	3510	1/1	0.89	0.44	-	118,118,118,118	0
54	MG	AA	1701	1/1	0.84	0.40	-	115,115,115,115	0
54	MG	AA	1781	1/1	0.94	0.46	-	120,120,120,120	0
54	MG	DA	3449	1/1	0.60	0.38	-	106,106,106,106	0
54	MG	CA	1677	1/1	0.92	0.16	-	114,114,114,114	0
54	MG	DA	3475	1/1	0.72	0.47	-	121,121,121,121	0
54	MG	BA	3619	1/1	0.82	0.23	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3086	1/1	0.85	0.28	-	88,88,88,88	0
54	MG	BA	3399	1/1	0.86	0.28	-	90,90,90,90	0
54	MG	DA	3018	1/1	0.68	0.51	-	83,83,83,83	0
54	MG	BA	3454	1/1	0.88	0.27	-	103,103,103,103	0
54	MG	BA	3286	1/1	0.82	0.21	-	98,98,98,98	0
54	MG	DA	3365	1/1	0.89	0.20	-	100,100,100,100	0
54	MG	AA	1674	1/1	0.75	0.46	-	119,119,119,119	0
54	MG	CA	1797	1/1	0.89	0.14	-	127,127,127,127	0
54	MG	AA	1722	1/1	0.78	0.12	-	109,109,109,109	0
54	MG	DA	3009	1/1	0.95	0.31	-	74,74,74,74	0
54	MG	DA	3318	1/1	0.76	0.40	-	91,91,91,91	0
54	MG	DA	3234	1/1	0.91	0.29	-	92,92,92,92	0
54	MG	CA	1644	1/1	-0.06	0.46	-	133,133,133,133	0
54	MG	CA	1773	1/1	0.60	0.20	-	114,114,114,114	0
54	MG	BA	3381	1/1	0.95	0.53	-	65,65,65,65	0
54	MG	AA	1682	1/1	0.98	0.13	-	113,113,113,113	0
54	MG	BA	3502	1/1	0.97	0.52	-	90,90,90,90	0
54	MG	BA	3116	1/1	0.57	0.26	-	137,137,137,137	0
54	MG	CA	1767	1/1	0.94	0.37	-	90,90,90,90	0
54	MG	AA	1747	1/1	0.91	0.12	-	159,159,159,159	0
54	MG	DA	3471	1/1	0.90	0.13	-	102,102,102,102	0
54	MG	BA	3487	1/1	0.96	0.06	-	116,116,116,116	0
54	MG	CA	1765	1/1	0.66	0.23	-	126,126,126,126	0
54	MG	BA	3003	1/1	0.98	0.28	-	78,78,78,78	0
54	MG	DA	3420	1/1	0.92	0.09	-	108,108,108,108	0
54	MG	BA	3560	1/1	0.83	0.72	-	91,91,91,91	0
54	MG	DA	3459	1/1	0.92	0.24	-	108,108,108,108	0
54	MG	BA	3440	1/1	0.73	0.33	-	79,79,79,79	0
54	MG	BA	3512	1/1	0.95	0.23	-	97,97,97,97	0
54	MG	AA	1787	1/1	0.67	0.19	-	115,115,115,115	0
54	MG	BA	3048	1/1	0.92	0.11	-	70,70,70,70	0
54	MG	DA	3441	1/1	0.81	0.20	-	116,116,116,116	0
54	MG	DA	3349	1/1	0.87	0.18	-	88,88,88,88	0
54	MG	BA	3114	1/1	0.93	0.45	-	83,83,83,83	0
54	MG	AA	1606	1/1	0.96	0.08	-	155,155,155,155	0
54	MG	BA	3336	1/1	0.85	0.27	-	109,109,109,109	0
54	MG	BA	3351	1/1	0.82	0.56	-	84,84,84,84	0
54	MG	DA	3300	1/1	0.81	0.60	-	107,107,107,107	0
54	MG	CA	1735	1/1	0.90	0.13	-	103,103,103,103	0
54	MG	AA	1670	1/1	0.69	0.29	-	83,83,83,83	0
54	MG	BA	3241	1/1	0.87	0.38	-	91,91,91,91	0
54	MG	DU	201	1/1	0.81	0.18	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3617	1/1	0.65	0.45	-	134,134,134,134	0
54	MG	DA	3194	1/1	0.89	0.22	-	91,91,91,91	0
54	MG	DA	3486	1/1	0.65	1.21	-	112,112,112,112	0
54	MG	AA	1724	1/1	0.64	0.41	-	115,115,115,115	0
54	MG	BA	3460	1/1	0.81	0.28	-	90,90,90,90	0
54	MG	BB	203	1/1	0.98	0.41	-	73,73,73,73	0
54	MG	DA	3360	1/1	0.90	0.24	-	85,85,85,85	0
54	MG	BA	3046	1/1	0.85	0.39	-	86,86,86,86	0
54	MG	AC	108	1/1	0.59	2.28	-	112,112,112,112	0
54	MG	BA	3324	1/1	0.59	0.31	-	101,101,101,101	0
54	MG	AA	1803	1/1	0.84	0.17	-	133,133,133,133	0
54	MG	BB	205	1/1	0.90	0.48	-	93,93,93,93	0
54	MG	AA	1635	1/1	0.93	0.34	-	122,122,122,122	0
54	MG	DA	3163	1/1	0.40	0.14	-	120,120,120,120	0
54	MG	DB	208	1/1	0.73	0.10	-	105,105,105,105	0
54	MG	CA	1804	1/1	0.88	0.24	-	119,119,119,119	0
54	MG	DA	3087	1/1	0.61	0.15	-	111,111,111,111	0
54	MG	DA	3217	1/1	0.96	0.21	-	89,89,89,89	0
54	MG	AA	1815	1/1	0.82	0.70	-	88,88,88,88	0
54	MG	BA	3056	1/1	0.66	0.51	-	101,101,101,101	0
54	MG	DA	3014	1/1	0.97	0.38	-	69,69,69,69	0
54	MG	AC	104	1/1	0.89	0.27	-	107,107,107,107	0
54	MG	BA	3625	1/1	0.83	0.35	-	99,99,99,99	0
54	MG	BA	3445	1/1	0.91	0.18	-	156,156,156,156	0
54	MG	BA	3595	1/1	0.80	0.34	-	105,105,105,105	0
54	MG	CA	1717	1/1	0.82	0.24	-	135,135,135,135	0
54	MG	AA	1792	1/1	0.82	0.47	-	93,93,93,93	0
54	MG	DA	3353	1/1	0.95	0.43	-	108,108,108,108	0
54	MG	CG	301	1/1	0.70	0.38	-	115,115,115,115	0
54	MG	BA	3597	1/1	0.91	0.24	-	69,69,69,69	0
54	MG	BA	3398	1/1	0.68	0.59	-	105,105,105,105	0
54	MG	CA	1700	1/1	0.68	0.32	-	92,92,92,92	0
54	MG	AA	1664	1/1	0.79	0.28	-	96,96,96,96	0
54	MG	BA	3554	1/1	0.80	0.33	-	99,99,99,99	0
54	MG	DA	3481	1/1	0.73	0.40	-	101,101,101,101	0
54	MG	BA	3433	1/1	0.93	0.18	-	107,107,107,107	0
54	MG	BA	3410	1/1	0.88	0.27	-	120,120,120,120	0
54	MG	CA	1626	1/1	0.59	0.19	-	117,117,117,117	0
54	MG	CA	1768	1/1	0.90	0.11	-	106,106,106,106	0
54	MG	AA	1734	1/1	0.03	0.35	-	146,146,146,146	0
54	MG	DA	3255	1/1	0.90	0.15	-	87,87,87,87	0
54	MG	DA	3176	1/1	0.90	0.27	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3249	1/1	0.84	0.32	-	84,84,84,84	0
54	MG	AA	1721	1/1	0.85	0.24	-	115,115,115,115	0
54	MG	CA	1744	1/1	0.96	0.33	-	97,97,97,97	0
54	MG	AA	1680	1/1	0.79	0.40	-	104,104,104,104	0
54	MG	BA	3386	1/1	0.96	0.15	-	117,117,117,117	0
54	MG	AA	1668	1/1	0.82	0.21	-	105,105,105,105	0
54	MG	AA	1696	1/1	0.54	0.26	-	104,104,104,104	0
54	MG	BA	3140	1/1	0.89	0.28	-	84,84,84,84	0
54	MG	BA	3065	1/1	0.92	0.17	-	135,135,135,135	0
54	MG	BA	3258	1/1	0.97	0.45	-	74,74,74,74	0
54	MG	AA	1633	1/1	0.95	0.40	-	80,80,80,80	0
54	MG	BA	3517	1/1	0.89	0.20	-	121,121,121,121	0
54	MG	CA	1641	1/1	0.86	0.17	-	135,135,135,135	0
54	MG	DA	3513	1/1	0.83	0.26	-	95,95,95,95	0
54	MG	AA	1663	1/1	0.98	0.13	-	76,76,76,76	0
54	MG	BA	3106	1/1	0.95	0.26	-	52,52,52,52	0
54	MG	BA	3549	1/1	0.99	0.12	-	140,140,140,140	0
54	MG	AA	1805	1/1	0.75	1.00	-	108,108,108,108	0
54	MG	DA	3337	1/1	0.94	0.15	-	88,88,88,88	0
54	MG	AA	1773	1/1	0.69	0.56	-	137,137,137,137	0
54	MG	BA	3141	1/1	0.97	0.23	-	63,63,63,63	0
54	MG	BA	3212	1/1	0.68	0.44	-	124,124,124,124	0
54	MG	DA	3123	1/1	0.79	0.19	-	106,106,106,106	0
54	MG	BA	3240	1/1	0.95	0.58	-	93,93,93,93	0
54	MG	BA	3291	1/1	0.63	0.39	-	99,99,99,99	0
54	MG	DA	3238	1/1	0.97	0.12	-	117,117,117,117	0
54	MG	BA	3080	1/1	0.96	0.19	-	125,125,125,125	0
54	MG	BA	3014	1/1	0.89	0.35	-	68,68,68,68	0
54	MG	DA	3155	1/1	0.91	0.17	-	80,80,80,80	0
54	MG	BA	3486	1/1	0.82	0.19	-	108,108,108,108	0
54	MG	DA	3339	1/1	0.80	0.39	-	152,152,152,152	0
54	MG	BA	3303	1/1	0.82	0.12	-	119,119,119,119	0
54	MG	AA	1759	1/1	0.80	0.35	-	87,87,87,87	0
54	MG	AA	1806	1/1	0.93	0.44	-	100,100,100,100	0
54	MG	CA	1610	1/1	0.90	0.19	-	147,147,147,147	0
54	MG	BA	3406	1/1	0.80	0.51	-	86,86,86,86	0
54	MG	AA	1658	1/1	0.81	0.19	-	79,79,79,79	0
54	MG	BA	3004	1/1	0.98	0.30	-	79,79,79,79	0
54	MG	DA	3104	1/1	0.56	0.42	-	107,107,107,107	0
54	MG	AA	1766	1/1	0.82	0.12	-	94,94,94,94	0
54	MG	CA	1696	1/1	0.89	0.35	-	98,98,98,98	0
54	MG	BA	3342	1/1	0.86	0.50	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3287	1/1	0.83	0.27	-	95,95,95,95	0
54	MG	DA	3265	1/1	0.80	0.35	-	115,115,115,115	0
54	MG	CA	1636	1/1	0.81	0.21	-	91,91,91,91	0
54	MG	AA	1820	1/1	0.61	1.53	-	130,130,130,130	0
54	MG	BA	3420	1/1	0.94	0.40	-	70,70,70,70	0
54	MG	AA	1719	1/1	0.67	0.24	-	110,110,110,110	0
54	MG	BA	3090	1/1	0.76	0.18	-	78,78,78,78	0
54	MG	BA	3078	1/1	0.94	0.33	-	106,106,106,106	0
54	MG	BA	3455	1/1	0.53	0.54	-	107,107,107,107	0
54	MG	BA	3476	1/1	0.94	0.44	-	59,59,59,59	0
54	MG	BA	3215	1/1	0.93	0.24	-	119,119,119,119	0
54	MG	A1	101	1/1	0.93	0.28	-	72,72,72,72	0
54	MG	BA	3075	1/1	0.60	0.50	-	97,97,97,97	0
54	MG	CA	1800	1/1	0.96	0.12	-	145,145,145,145	0
54	MG	DA	3198	1/1	0.89	0.26	-	95,95,95,95	0
54	MG	CA	1662	1/1	0.60	0.36	-	120,120,120,120	0
54	MG	BA	3594	1/1	0.89	0.68	-	94,94,94,94	0
54	MG	BA	3542	1/1	0.93	0.49	-	100,100,100,100	0
54	MG	CA	1609	1/1	0.80	0.33	-	119,119,119,119	0
54	MG	CA	1780	1/1	0.86	0.11	-	137,137,137,137	0
54	MG	AA	1613	1/1	0.96	0.19	-	144,144,144,144	0
54	MG	BA	3462	1/1	0.95	0.36	-	113,113,113,113	0
54	MG	BA	3016	1/1	0.97	0.06	-	143,143,143,143	0
54	MG	AA	1831	1/1	0.85	0.16	-	124,124,124,124	0
54	MG	DA	3048	1/1	0.81	0.17	-	84,84,84,84	0
54	MG	DA	3376	1/1	0.91	0.28	-	87,87,87,87	0
54	MG	AA	1746	1/1	0.94	0.15	-	92,92,92,92	0
54	MG	DA	3250	1/1	0.80	1.13	-	105,105,105,105	0
54	MG	BA	3598	1/1	0.77	0.38	-	84,84,84,84	0
54	MG	AA	1821	1/1	0.90	0.15	-	110,110,110,110	0
54	MG	BA	3505	1/1	0.54	0.46	-	108,108,108,108	0
54	MG	DA	3522	1/1	0.80	0.31	-	113,113,113,113	0
54	MG	DA	3034	1/1	0.89	0.17	-	91,91,91,91	0
54	MG	BA	3062	1/1	0.98	0.28	-	70,70,70,70	0
54	MG	BA	3122	1/1	0.69	0.23	-	114,114,114,114	0
54	MG	DA	3424	1/1	0.57	0.58	-	115,115,115,115	0
54	MG	DA	3029	1/1	0.82	0.25	-	87,87,87,87	0
54	MG	AA	1649	1/1	0.80	0.15	-	90,90,90,90	0
54	MG	BA	3309	1/1	0.92	0.38	-	84,84,84,84	0
54	MG	BA	3479	1/1	0.99	0.39	-	72,72,72,72	0
54	MG	DA	3069	1/1	0.90	0.31	-	101,101,101,101	0
54	MG	BA	3425	1/1	0.90	0.10	-	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3169	1/1	0.81	0.41	-	104,104,104,104	0
54	MG	BA	3317	1/1	0.87	0.38	-	99,99,99,99	0
54	MG	DA	3498	1/1	0.94	0.09	-	106,106,106,106	0
54	MG	BA	3540	1/1	0.80	0.48	-	122,122,122,122	0
54	MG	BA	3239	1/1	0.97	0.40	-	82,82,82,82	0
54	MG	BA	3242	1/1	0.81	0.53	-	115,115,115,115	0
54	MG	BB	210	1/1	0.92	0.40	-	78,78,78,78	0
54	MG	BA	3449	1/1	0.79	0.46	-	118,118,118,118	0
54	MG	DA	3452	1/1	0.87	0.94	-	91,91,91,91	0
54	MG	BA	3515	1/1	0.90	0.50	-	112,112,112,112	0
54	MG	DA	3308	1/1	0.94	0.25	-	94,94,94,94	0
54	MG	BA	3123	1/1	0.93	0.34	-	73,73,73,73	0
54	MG	DA	3158	1/1	0.37	0.66	-	113,113,113,113	0
54	MG	DA	3431	1/1	0.91	0.43	-	101,101,101,101	0
54	MG	BA	3103	1/1	0.96	0.16	-	93,93,93,93	0
54	MG	DA	3215	1/1	0.84	0.19	-	80,80,80,80	0
54	MG	BA	3171	1/1	0.96	0.25	-	87,87,87,87	0
54	MG	DA	3209	1/1	0.85	0.24	-	100,100,100,100	0
54	MG	AQ	102	1/1	0.63	0.30	-	118,118,118,118	0
54	MG	BA	3189	1/1	0.85	0.22	-	88,88,88,88	0
54	MG	BA	3265	1/1	0.76	0.29	-	96,96,96,96	0
54	MG	DA	3470	1/1	0.91	0.25	-	124,124,124,124	0
54	MG	CA	1747	1/1	0.52	0.52	-	122,122,122,122	0
54	MG	BA	3524	1/1	0.94	0.43	-	90,90,90,90	0
54	MG	CA	1703	1/1	0.95	0.11	-	93,93,93,93	0
54	MG	DA	3165	1/1	0.96	0.16	-	59,59,59,59	0
54	MG	BZ	101	1/1	0.95	0.20	-	69,69,69,69	0
54	MG	BA	3416	1/1	0.94	0.13	-	70,70,70,70	0
54	MG	BA	3499	1/1	0.92	0.14	-	103,103,103,103	0
54	MG	CA	1802	1/1	0.98	0.40	-	136,136,136,136	0
54	MG	DA	3450	1/1	0.64	0.28	-	130,130,130,130	0
54	MG	CA	1605	1/1	0.28	0.34	-	131,131,131,131	0
54	MG	AA	1603	1/1	0.99	0.23	-	109,109,109,109	0
54	MG	CA	1689	1/1	0.93	0.42	-	122,122,122,122	0
54	MG	DA	3004	1/1	0.71	0.34	-	120,120,120,120	0
54	MG	CA	1769	1/1	0.88	0.16	-	136,136,136,136	0
54	MG	CA	1638	1/1	0.75	0.30	-	128,128,128,128	0
54	MG	BA	3315	1/1	0.98	0.34	-	91,91,91,91	0
54	MG	BA	3432	1/1	0.85	0.20	-	126,126,126,126	0
54	MG	B7	102	1/1	0.89	0.29	-	75,75,75,75	0
54	MG	BA	3461	1/1	0.89	0.29	-	79,79,79,79	0
54	MG	DA	3084	1/1	0.94	0.11	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1669	1/1	0.97	0.15	-	130,130,130,130	0
54	MG	DA	3465	1/1	0.82	0.64	-	111,111,111,111	0
54	MG	DA	3016	1/1	0.49	0.36	-	123,123,123,123	0
54	MG	BA	3079	1/1	0.88	0.51	-	99,99,99,99	0
54	MG	DA	3462	1/1	0.89	0.09	-	102,102,102,102	0
54	MG	BA	3402	1/1	0.95	0.19	-	81,81,81,81	0
54	MG	CA	1725	1/1	0.86	0.35	-	106,106,106,106	0
54	MG	DA	3432	1/1	0.87	0.51	-	91,91,91,91	0
54	MG	BA	3611	1/1	0.85	0.39	-	101,101,101,101	0
54	MG	BA	3623	1/1	0.93	0.19	-	86,86,86,86	0
54	MG	BA	3321	1/1	0.87	0.23	-	71,71,71,71	0
54	MG	BA	3439	1/1	0.85	0.40	-	109,109,109,109	0
54	MG	AA	1737	1/1	0.97	0.51	-	132,132,132,132	0
54	MG	DA	3324	1/1	0.75	0.23	-	109,109,109,109	0
54	MG	BA	3296	1/1	0.76	0.47	-	93,93,93,93	0
54	MG	CA	1762	1/1	0.83	0.37	-	116,116,116,116	0
54	MG	BA	3448	1/1	0.65	0.28	-	95,95,95,95	0
54	MG	BA	3576	1/1	0.70	0.48	-	120,120,120,120	0
54	MG	BA	3609	1/1	0.92	0.20	-	102,102,102,102	0
54	MG	BA	3294	1/1	0.84	0.50	-	79,79,79,79	0
54	MG	CA	1748	1/1	0.89	0.12	-	81,81,81,81	0
54	MG	DA	3036	1/1	0.90	0.23	-	108,108,108,108	0
54	MG	BA	3571	1/1	0.82	0.43	-	85,85,85,85	0
54	MG	BA	3396	1/1	0.75	0.48	-	101,101,101,101	0
54	MG	BA	3481	1/1	0.63	0.39	-	99,99,99,99	0
54	MG	DA	3342	1/1	0.95	0.24	-	114,114,114,114	0
54	MG	BA	3511	1/1	0.84	0.25	-	80,80,80,80	0
54	MG	DA	3028	1/1	0.85	0.31	-	122,122,122,122	0
54	MG	DA	3379	1/1	0.96	0.46	-	64,64,64,64	0
54	MG	DA	3026	1/1	0.92	0.13	-	122,122,122,122	0
54	MG	DA	3448	1/1	0.94	0.16	-	89,89,89,89	0
54	MG	AA	1646	1/1	0.90	0.07	-	150,150,150,150	0
54	MG	BA	3213	1/1	0.98	0.25	-	69,69,69,69	0
54	MG	BA	3261	1/1	0.91	0.13	-	90,90,90,90	0
54	MG	CA	1682	1/1	0.90	0.25	-	101,101,101,101	0
54	MG	BA	3435	1/1	0.96	0.10	-	109,109,109,109	0
54	MG	CA	1620	1/1	0.90	0.22	-	73,73,73,73	0
54	MG	CA	1619	1/1	0.89	0.24	-	111,111,111,111	0
54	MG	AA	1728	1/1	0.81	0.11	-	85,85,85,85	0
54	MG	AA	1698	1/1	0.98	0.39	-	132,132,132,132	0
54	MG	CA	1764	1/1	0.89	0.29	-	110,110,110,110	0
54	MG	DA	3457	1/1	0.93	0.16	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1689	1/1	0.81	0.23	-	153,153,153,153	0
54	MG	BA	3190	1/1	0.90	0.30	-	93,93,93,93	0
54	MG	AA	1641	1/1	0.87	0.21	-	90,90,90,90	0
54	MG	CA	1731	1/1	0.68	0.52	-	110,110,110,110	0
54	MG	AA	1786	1/1	0.79	0.31	-	131,131,131,131	0
54	MG	BA	3534	1/1	0.76	0.40	-	95,95,95,95	0
54	MG	AA	1612	1/1	0.89	0.23	-	135,135,135,135	0
54	MG	DA	3391	1/1	0.84	0.13	-	94,94,94,94	0
54	MG	DA	3347	1/1	0.91	0.36	-	116,116,116,116	0
54	MG	BA	3613	1/1	0.98	0.15	-	111,111,111,111	0
54	MG	AJ	201	1/1	0.86	0.76	-	108,108,108,108	0
54	MG	DA	3291	1/1	0.78	0.41	-	85,85,85,85	0
54	MG	DA	3380	1/1	0.90	0.31	-	94,94,94,94	0
54	MG	AA	1692	1/1	0.77	0.29	-	108,108,108,108	0
54	MG	CA	1707	1/1	0.75	0.46	-	109,109,109,109	0
54	MG	DA	3196	1/1	0.86	0.18	-	101,101,101,101	0
54	MG	AA	1679	1/1	0.94	0.28	-	105,105,105,105	0
54	MG	DA	3113	1/1	0.88	0.27	-	105,105,105,105	0
54	MG	BA	3019	1/1	0.95	0.25	-	49,49,49,49	0
54	MG	DA	3372	1/1	0.80	0.25	-	101,101,101,101	0
54	MG	BA	3170	1/1	0.93	0.33	-	90,90,90,90	0
54	MG	AA	1703	1/1	0.95	0.23	-	87,87,87,87	0
54	MG	BA	3188	1/1	0.68	0.59	-	120,120,120,120	0
54	MG	BA	3383	1/1	0.72	0.38	-	95,95,95,95	0
54	MG	DA	3451	1/1	0.87	0.28	-	90,90,90,90	0
54	MG	BA	3135	1/1	0.87	0.24	-	90,90,90,90	0
54	MG	CA	1732	1/1	0.93	0.30	-	144,144,144,144	0
54	MG	DA	3425	1/1	0.80	0.23	-	122,122,122,122	0
54	MG	BA	3529	1/1	0.95	0.29	-	89,89,89,89	0
54	MG	AA	1775	1/1	0.88	0.25	-	80,80,80,80	0
54	MG	BA	3326	1/1	0.90	0.38	-	89,89,89,89	0
54	MG	BA	3203	1/1	0.93	0.34	-	86,86,86,86	0
54	MG	BA	3236	1/1	0.83	0.45	-	97,97,97,97	0
54	MG	AA	1752	1/1	0.63	0.58	-	121,121,121,121	0
54	MG	DA	3210	1/1	0.95	0.23	-	63,63,63,63	0
54	MG	AA	1624	1/1	0.98	0.10	-	98,98,98,98	0
54	MG	CA	1642	1/1	0.58	0.15	-	105,105,105,105	0
54	MG	BB	211	1/1	0.24	0.42	-	102,102,102,102	0
54	MG	DA	3191	1/1	0.83	0.29	-	103,103,103,103	0
54	MG	DA	3160	1/1	0.92	0.42	-	84,84,84,84	0
54	MG	BA	3470	1/1	0.59	0.39	-	117,117,117,117	0
54	MG	BA	3195	1/1	0.99	0.13	-	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3511	1/1	0.90	0.84	-	111,111,111,111	0
54	MG	AA	1617	1/1	0.84	0.35	-	91,91,91,91	0
54	MG	BA	3355	1/1	0.82	0.52	-	90,90,90,90	0
54	MG	BA	3447	1/1	0.12	0.32	-	116,116,116,116	0
54	MG	BA	3327	1/1	0.97	0.21	-	117,117,117,117	0
54	MG	AA	1748	1/1	0.77	0.96	-	130,130,130,130	0
54	MG	DB	212	1/1	0.91	0.70	-	102,102,102,102	0
54	MG	BA	3255	1/1	0.88	0.74	-	110,110,110,110	0
54	MG	CA	1759	1/1	0.97	0.09	-	157,157,157,157	0
54	MG	DA	3135	1/1	0.79	0.45	-	99,99,99,99	0
54	MG	AA	1684	1/1	0.81	0.40	-	123,123,123,123	0
54	MG	AA	1761	1/1	0.91	0.08	-	152,152,152,152	0
54	MG	BA	3231	1/1	0.84	0.46	-	93,93,93,93	0
54	MG	BA	3427	1/1	0.94	0.44	-	91,91,91,91	0
54	MG	DA	3137	1/1	0.93	0.16	-	74,74,74,74	0
54	MG	BA	3323	1/1	0.82	0.35	-	116,116,116,116	0
54	MG	BA	3620	1/1	0.97	0.14	-	72,72,72,72	0
54	MG	DZ	102	1/1	0.91	0.17	-	88,88,88,88	0
54	MG	DA	3022	1/1	0.72	0.22	-	86,86,86,86	0
54	MG	AA	1616	1/1	1.00	0.30	-	158,158,158,158	0
54	MG	BB	204	1/1	0.85	0.50	-	86,86,86,86	0
54	MG	CA	1792	1/1	0.63	0.15	-	160,160,160,160	0
54	MG	DA	3077	1/1	0.94	0.15	-	96,96,96,96	0
54	MG	BA	3112	1/1	0.84	0.30	-	97,97,97,97	0
54	MG	DB	203	1/1	0.91	0.20	-	95,95,95,95	0
54	MG	DA	3490	1/1	0.95	0.20	-	120,120,120,120	0
54	MG	DA	3284	1/1	0.94	0.32	-	100,100,100,100	0
54	MG	BA	3604	1/1	0.93	0.22	-	97,97,97,97	0
54	MG	DA	3251	1/1	0.94	0.12	-	91,91,91,91	0
54	MG	BA	3037	1/1	0.96	0.39	-	71,71,71,71	0
54	MG	AA	1783	1/1	0.99	0.13	-	125,125,125,125	0
54	MG	CA	1667	1/1	0.90	0.25	-	139,139,139,139	0
54	MG	BA	3084	1/1	0.48	0.99	-	110,110,110,110	0
54	MG	BA	3450	1/1	0.78	0.29	-	99,99,99,99	0
54	MG	BA	3482	1/1	0.83	0.43	-	88,88,88,88	0
54	MG	BA	3459	1/1	0.74	0.34	-	91,91,91,91	0
54	MG	CA	1785	1/1	0.90	0.26	-	83,83,83,83	0
54	MG	BA	3085	1/1	0.84	0.47	-	95,95,95,95	0
54	MG	BA	3263	1/1	0.96	0.30	-	50,50,50,50	0
54	MG	AA	1777	1/1	0.97	0.06	-	141,141,141,141	0
54	MG	BA	3478	1/1	0.90	0.13	-	155,155,155,155	0
54	MG	BA	3318	1/1	0.91	0.32	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3564	1/1	0.70	0.58	-	116,116,116,116	0
54	MG	BA	3518	1/1	0.88	0.19	-	86,86,86,86	0
54	MG	CA	1613	1/1	0.86	0.36	-	94,94,94,94	0
54	MG	DA	3174	1/1	0.97	0.16	-	81,81,81,81	0
54	MG	AA	1710	1/1	0.58	0.30	-	116,116,116,116	0
54	MG	CA	1788	1/1	0.93	0.32	-	87,87,87,87	0
54	MG	DA	3285	1/1	0.87	0.13	-	67,67,67,67	0
54	MG	AA	1704	1/1	0.82	0.42	-	112,112,112,112	0
54	MG	BA	3559	1/1	0.86	0.99	-	105,105,105,105	0
54	MG	DA	3488	1/1	0.91	0.71	-	105,105,105,105	0
54	MG	BA	3521	1/1	0.52	0.21	-	123,123,123,123	0
54	MG	AA	1828	1/1	0.82	0.32	-	94,94,94,94	0
54	MG	BA	3458	1/1	0.74	0.47	-	96,96,96,96	0
54	MG	DA	3303	1/1	0.91	0.42	-	140,140,140,140	0
54	MG	BA	3372	1/1	0.87	0.66	-	99,99,99,99	0
54	MG	CA	1688	1/1	0.72	0.37	-	101,101,101,101	0
54	MG	BA	3492	1/1	0.92	0.44	-	76,76,76,76	0
54	MG	BA	3173	1/1	0.98	0.30	-	62,62,62,62	0
54	MG	CA	1775	1/1	0.84	0.17	-	90,90,90,90	0
54	MG	BA	3365	1/1	0.64	0.58	-	104,104,104,104	0
54	MG	DA	3202	1/1	0.94	0.23	-	88,88,88,88	0
54	MG	DA	3385	1/1	0.78	0.19	-	95,95,95,95	0
54	MG	CA	1684	1/1	0.62	0.25	-	115,115,115,115	0
54	MG	BA	3407	1/1	0.71	0.42	-	105,105,105,105	0
54	MG	DA	3329	1/1	0.88	0.33	-	110,110,110,110	0
54	MG	AA	1653	1/1	0.98	0.22	-	91,91,91,91	0
54	MG	DA	3017	1/1	0.64	0.28	-	111,111,111,111	0
54	MG	AA	1810	1/1	0.47	0.55	-	126,126,126,126	0
54	MG	AA	1693	1/1	0.61	0.38	-	123,123,123,123	0
54	MG	BA	3304	1/1	0.92	0.29	-	90,90,90,90	0
54	MG	DA	3059	1/1	0.96	0.19	-	68,68,68,68	0
54	MG	DA	3444	1/1	0.82	0.32	-	100,100,100,100	0
54	MG	AA	1683	1/1	0.40	0.41	-	116,116,116,116	0
54	MG	BA	3253	1/1	0.91	0.20	-	89,89,89,89	0
54	MG	BA	3452	1/1	0.76	0.27	-	131,131,131,131	0
54	MG	DA	3417	1/1	0.78	0.20	-	110,110,110,110	0
54	MG	DB	209	1/1	0.73	0.28	-	131,131,131,131	0
54	MG	BA	3359	1/1	0.89	0.15	-	92,92,92,92	0
54	MG	DA	3107	1/1	0.94	0.20	-	100,100,100,100	0
54	MG	BA	3017	1/1	0.98	0.26	-	67,67,67,67	0
54	MG	BA	3584	1/1	0.97	0.31	-	100,100,100,100	0
54	MG	DA	3442	1/1	0.95	0.12	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1795	1/1	0.85	0.13	-	102,102,102,102	0
54	MG	DA	3472	1/1	0.86	0.62	-	102,102,102,102	0
54	MG	AA	1739	1/1	0.90	0.56	-	99,99,99,99	0
54	MG	BA	3108	1/1	0.84	0.45	-	82,82,82,82	0
54	MG	BA	3316	1/1	0.95	0.29	-	82,82,82,82	0
54	MG	DA	3500	1/1	0.98	0.09	-	88,88,88,88	0
54	MG	AA	1732	1/1	0.89	0.40	-	112,112,112,112	0
54	MG	DB	214	1/1	0.79	0.09	-	118,118,118,118	0
54	MG	DA	3175	1/1	0.91	0.16	-	101,101,101,101	0
54	MG	DA	3334	1/1	0.92	0.10	-	136,136,136,136	0
54	MG	BA	3444	1/1	0.95	0.09	-	186,186,186,186	0
54	MG	BA	3107	1/1	0.83	0.50	-	76,76,76,76	0
54	MG	BA	3483	1/1	0.86	0.18	-	89,89,89,89	0
54	MG	CA	1603	1/1	0.97	0.56	-	93,93,93,93	0
54	MG	DA	3052	1/1	0.91	0.36	-	120,120,120,120	0
54	MG	DA	3388	1/1	0.94	0.11	-	152,152,152,152	0
54	MG	DA	3447	1/1	0.87	0.12	-	87,87,87,87	0
54	MG	BA	3535	1/1	0.72	0.44	-	116,116,116,116	0
54	MG	BA	3362	1/1	0.94	0.58	-	70,70,70,70	0
54	MG	AA	1702	1/1	0.94	0.32	-	77,77,77,77	0
54	MG	AA	1784	1/1	0.88	0.39	-	91,91,91,91	0
54	MG	CA	1630	1/1	0.70	0.43	-	120,120,120,120	0
54	MG	DA	3249	1/1	0.93	0.30	-	65,65,65,65	0
54	MG	AA	1824	1/1	0.87	0.16	-	120,120,120,120	0
54	MG	AA	1797	1/1	0.90	0.30	-	82,82,82,82	0
54	MG	DA	3302	1/1	0.93	0.34	-	79,79,79,79	0
54	MG	DA	3279	1/1	0.40	0.23	-	125,125,125,125	0
54	MG	DA	3454	1/1	0.82	0.17	-	94,94,94,94	0
54	MG	CA	1708	1/1	0.93	0.29	-	143,143,143,143	0
54	MG	DA	3243	1/1	0.98	0.18	-	86,86,86,86	0
54	MG	DA	3043	1/1	0.94	0.27	-	106,106,106,106	0
54	MG	DA	3142	1/1	0.91	0.14	-	99,99,99,99	0
54	MG	DA	3378	1/1	0.89	0.22	-	100,100,100,100	0
54	MG	BA	3035	1/1	0.97	0.23	-	70,70,70,70	0
54	MG	DA	3148	1/1	0.80	0.20	-	70,70,70,70	0
54	MG	DA	3333	1/1	0.43	0.50	-	128,128,128,128	0
54	MG	AA	1643	1/1	0.75	0.12	-	112,112,112,112	0
54	MG	BA	3397	1/1	0.90	0.37	-	92,92,92,92	0
54	MG	BA	3436	1/1	0.91	0.27	-	118,118,118,118	0
54	MG	DA	3125	1/1	0.75	0.20	-	105,105,105,105	0
54	MG	DA	3348	1/1	0.78	0.17	-	108,108,108,108	0
54	MG	DA	3509	1/1	0.81	0.18	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1737	1/1	0.94	0.38	-	97,97,97,97	0
54	MG	BA	3395	1/1	0.01	0.59	-	105,105,105,105	0
54	MG	BA	3293	1/1	0.92	0.41	-	77,77,77,77	0
54	MG	BA	3145	1/1	0.95	0.41	-	83,83,83,83	0
54	MG	BA	3423	1/1	0.92	0.58	-	89,89,89,89	0
54	MG	CA	1796	1/1	0.85	0.26	-	115,115,115,115	0
54	MG	BA	3298	1/1	0.91	0.33	-	73,73,73,73	0
54	MG	BA	3340	1/1	0.76	0.63	-	95,95,95,95	0
54	MG	AA	1809	1/1	0.70	0.40	-	108,108,108,108	0
54	MG	DA	3483	1/1	0.84	0.25	-	88,88,88,88	0
54	MG	DA	3275	1/1	0.94	0.20	-	93,93,93,93	0
54	MG	BA	3457	1/1	0.61	0.30	-	112,112,112,112	0
54	MG	AA	1733	1/1	0.86	0.21	-	120,120,120,120	0
54	MG	DA	3145	1/1	0.94	0.23	-	110,110,110,110	0
54	MG	BA	3044	1/1	0.96	0.14	-	58,58,58,58	0
54	MG	AA	1832	1/1	0.84	0.21	-	102,102,102,102	0
54	MG	AA	1771	1/1	0.87	0.23	-	117,117,117,117	0
54	MG	DA	3126	1/1	0.99	0.09	-	58,58,58,58	0
54	MG	BA	3348	1/1	0.86	0.36	-	90,90,90,90	0
54	MG	DA	3097	1/1	0.98	0.39	-	74,74,74,74	0
54	MG	DA	3412	1/1	0.60	0.14	-	110,110,110,110	0
54	MG	DA	3484	1/1	0.82	0.19	-	81,81,81,81	0
54	MG	AA	1751	1/1	0.60	0.66	-	102,102,102,102	0
54	MG	DA	3288	1/1	0.95	0.23	-	95,95,95,95	0
54	MG	DA	3100	1/1	0.86	0.34	-	100,100,100,100	0
54	MG	BA	3217	1/1	0.84	0.18	-	92,92,92,92	0
54	MG	AA	1730	1/1	0.15	2.51	-	116,116,116,116	0
54	MG	BA	3568	1/1	0.83	0.93	-	105,105,105,105	0
54	MG	BA	3024	1/1	0.87	0.20	-	81,81,81,81	0
54	MG	CA	1680	1/1	0.88	0.26	-	94,94,94,94	0
54	MG	BA	3532	1/1	0.79	0.35	-	100,100,100,100	0
54	MG	BA	3301	1/1	0.83	0.23	-	85,85,85,85	0
54	MG	BA	3331	1/1	0.97	0.42	-	74,74,74,74	0
54	MG	DE	301	1/1	0.90	0.17	-	73,73,73,73	0
54	MG	DA	3480	1/1	0.88	0.19	-	84,84,84,84	0
54	MG	DA	3430	1/1	0.65	0.23	-	105,105,105,105	0
54	MG	BA	3466	1/1	0.87	0.31	-	92,92,92,92	0
54	MG	BA	3366	1/1	0.94	0.34	-	95,95,95,95	0
54	MG	AA	1762	1/1	0.94	0.15	-	124,124,124,124	0
54	MG	CA	1778	1/1	0.76	0.42	-	118,118,118,118	0
54	MG	BA	3472	1/1	0.48	0.28	-	114,114,114,114	0
54	MG	AA	1661	1/1	0.93	0.35	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3268	1/1	0.93	0.28	-	87,87,87,87	0
54	MG	BA	3572	1/1	0.92	0.17	-	113,113,113,113	0
54	MG	DA	3094	1/1	0.99	0.14	-	85,85,85,85	0
54	MG	CA	1655	1/1	0.93	0.44	-	125,125,125,125	0
54	MG	BA	3199	1/1	0.95	0.14	-	78,78,78,78	0
54	MG	AA	1714	1/1	0.93	0.18	-	115,115,115,115	0
54	MG	AA	1814	1/1	0.95	0.11	-	152,152,152,152	0
54	MG	AA	1699	1/1	0.78	0.18	-	122,122,122,122	0
54	MG	BA	3453	1/1	0.84	0.39	-	85,85,85,85	0
54	MG	BA	3347	1/1	0.94	0.29	-	72,72,72,72	0
54	MG	BA	3376	1/1	0.76	0.52	-	96,96,96,96	0
54	MG	BA	3281	1/1	0.94	0.83	-	106,106,106,106	0
54	MG	DA	3070	1/1	0.93	0.31	-	76,76,76,76	0
54	MG	DA	3128	1/1	0.94	0.24	-	65,65,65,65	0
54	MG	BA	3148	1/1	0.88	0.20	-	59,59,59,59	0
54	MG	DA	3519	1/1	0.76	0.22	-	94,94,94,94	0
54	MG	DA	3272	1/1	0.75	0.24	-	92,92,92,92	0
54	MG	DA	3124	1/1	0.99	0.23	-	69,69,69,69	0
54	MG	BA	3146	1/1	0.96	0.48	-	82,82,82,82	0
54	MG	BA	3254	1/1	0.97	0.30	-	70,70,70,70	0
54	MG	DA	3256	1/1	0.65	1.59	-	103,103,103,103	0
54	MG	AA	1736	1/1	0.95	0.11	-	122,122,122,122	0
54	MG	BA	3066	1/1	0.69	0.38	-	97,97,97,97	0
54	MG	BA	3055	1/1	0.94	0.51	-	69,69,69,69	0
54	MG	BA	3126	1/1	0.92	0.13	-	89,89,89,89	0
54	MG	DA	3492	1/1	0.86	0.19	-	111,111,111,111	0
54	MG	DA	3054	1/1	0.93	0.36	-	88,88,88,88	0
54	MG	AA	1659	1/1	0.93	0.14	-	71,71,71,71	0
54	MG	AA	1691	1/1	0.86	0.35	-	105,105,105,105	0
54	MG	CA	1782	1/1	0.93	0.37	-	98,98,98,98	0
54	MG	AA	1725	1/1	0.84	0.31	-	111,111,111,111	0
54	MG	CA	1666	1/1	0.80	0.34	-	120,120,120,120	0
54	MG	CA	1755	1/1	0.75	0.19	-	97,97,97,97	0
54	MG	BA	3621	1/1	0.93	0.31	-	66,66,66,66	0
54	MG	DA	3410	1/1	0.67	0.53	-	118,118,118,118	0
54	MG	BA	3563	1/1	0.87	0.45	-	96,96,96,96	0
54	MG	BA	3488	1/1	0.89	0.50	-	109,109,109,109	0
54	MG	CC	105	1/1	0.98	0.27	-	125,125,125,125	0
54	MG	DA	3307	1/1	0.82	0.50	-	102,102,102,102	0
54	MG	CA	1795	1/1	0.96	0.23	-	112,112,112,112	0
54	MG	DA	3419	1/1	0.62	0.27	-	100,100,100,100	0
54	MG	BA	3074	1/1	0.98	0.13	-	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3160	1/1	0.82	0.54	-	109,109,109,109	0
54	MG	CA	1726	1/1	0.91	0.28	-	111,111,111,111	0
54	MG	BA	3361	1/1	0.78	0.59	-	123,123,123,123	0
54	MG	DA	3328	1/1	0.97	0.04	-	138,138,138,138	0
54	MG	CA	1718	1/1	0.83	0.60	-	114,114,114,114	0
54	MG	BA	3392	1/1	0.82	0.35	-	110,110,110,110	0
54	MG	DA	3422	1/1	0.83	0.27	-	93,93,93,93	0
54	MG	BA	3328	1/1	0.98	0.23	-	119,119,119,119	0
54	MG	DA	3187	1/1	0.95	0.18	-	70,70,70,70	0
54	MG	BA	3092	1/1	0.82	0.62	-	111,111,111,111	0
54	MG	DA	3146	1/1	0.94	0.60	-	87,87,87,87	0
54	MG	DA	3121	1/1	0.90	0.15	-	68,68,68,68	0
54	MG	BA	3132	1/1	0.78	0.37	-	127,127,127,127	0
54	MG	DA	3396	1/1	0.54	0.21	-	95,95,95,95	0
54	MG	BA	3192	1/1	0.99	0.28	-	67,67,67,67	0
54	MG	AA	1652	1/1	0.82	0.35	-	91,91,91,91	0
54	MG	AA	1675	1/1	0.82	0.13	-	93,93,93,93	0
54	MG	DA	3489	1/1	0.92	0.16	-	98,98,98,98	0
54	MG	BA	3520	1/1	0.96	0.41	-	129,129,129,129	0
54	MG	DA	3282	1/1	0.95	0.16	-	88,88,88,88	0
54	MG	AA	1711	1/1	0.88	0.25	-	118,118,118,118	0
54	MG	DA	3080	1/1	0.70	0.18	-	114,114,114,114	0
54	MG	BU	201	1/1	0.95	0.14	-	105,105,105,105	0
54	MG	BA	3585	1/1	0.97	0.18	-	62,62,62,62	0
54	MG	DA	3024	1/1	0.81	0.11	-	112,112,112,112	0
54	MG	BA	3059	1/1	0.98	0.09	-	144,144,144,144	0
54	MG	AA	1640	1/1	0.99	0.20	-	82,82,82,82	0
54	MG	AA	1708	1/1	0.81	0.37	-	104,104,104,104	0
54	MG	DA	3320	1/1	0.74	0.71	-	110,110,110,110	0
54	MG	AC	105	1/1	0.87	0.14	-	107,107,107,107	0
54	MG	DA	3264	1/1	0.99	0.28	-	80,80,80,80	0
54	MG	BA	3497	1/1	0.90	0.40	-	78,78,78,78	0
54	MG	DA	3293	1/1	0.45	1.85	-	112,112,112,112	0
54	MG	BA	3522	1/1	0.81	0.12	-	106,106,106,106	0
54	MG	BA	3555	1/1	0.96	0.19	-	67,67,67,67	0
54	MG	B3	101	1/1	0.83	0.34	-	77,77,77,77	0
54	MG	DA	3314	1/1	0.87	0.21	-	83,83,83,83	0
54	MG	BA	3516	1/1	0.94	0.24	-	80,80,80,80	0
54	MG	CA	1761	1/1	0.76	0.21	-	170,170,170,170	0
54	MG	AA	1686	1/1	0.43	0.21	-	120,120,120,120	0
54	MG	DA	3166	1/1	0.98	0.27	-	65,65,65,65	0
54	MG	AA	1830	1/1	0.88	0.10	-	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3494	1/1	0.96	0.31	-	45,45,45,45	0
54	MG	DA	3518	1/1	0.81	0.49	-	94,94,94,94	0
54	MG	BA	3523	1/1	0.91	0.17	-	64,64,64,64	0
54	MG	DA	3013	1/1	0.98	0.24	-	69,69,69,69	0
54	MG	DA	3136	1/1	0.95	0.24	-	64,64,64,64	0
54	MG	BA	3129	1/1	0.82	0.22	-	92,92,92,92	0
54	MG	DA	3206	1/1	0.94	0.39	-	58,58,58,58	0
54	MG	DA	3315	1/1	0.84	0.18	-	125,125,125,125	0
54	MG	AA	1697	1/1	0.92	0.50	-	143,143,143,143	0
54	MG	AA	1760	1/1	0.94	0.21	-	122,122,122,122	0
54	MG	CA	1627	1/1	0.81	0.47	-	112,112,112,112	0
54	MG	BA	3064	1/1	0.95	0.26	-	113,113,113,113	0
54	MG	AA	1829	1/1	0.73	0.34	-	112,112,112,112	0
54	MG	BA	3341	1/1	0.96	0.36	-	71,71,71,71	0
54	MG	CA	1777	1/1	0.93	0.28	-	133,133,133,133	0
54	MG	AH	202	1/1	0.77	0.14	-	108,108,108,108	0
54	MG	AA	1812	1/1	0.79	0.23	-	124,124,124,124	0
54	MG	DA	3411	1/1	0.88	0.17	-	68,68,68,68	0
54	MG	DA	3374	1/1	0.61	0.19	-	106,106,106,106	0
54	MG	DA	3259	1/1	0.95	0.36	-	76,76,76,76	0
54	MG	BA	3183	1/1	0.79	0.19	-	110,110,110,110	0
54	MG	BA	3335	1/1	0.93	0.28	-	96,96,96,96	0
54	MG	DA	3032	1/1	0.47	0.37	-	127,127,127,127	0
54	MG	BA	3284	1/1	0.93	0.11	-	121,121,121,121	0
54	MG	DA	3076	1/1	0.95	0.30	-	75,75,75,75	0
54	MG	BA	3536	1/1	0.38	0.39	-	96,96,96,96	0
54	MG	AA	1811	1/1	0.79	0.15	-	154,154,154,154	0
54	MG	BA	3101	1/1	0.98	0.42	-	58,58,58,58	0
54	MG	AA	1638	1/1	0.96	0.38	-	104,104,104,104	0
54	MG	AA	1627	1/1	0.96	0.29	-	87,87,87,87	0
54	MG	DA	3514	1/1	0.94	0.13	-	71,71,71,71	0
54	MG	CA	1730	1/1	0.91	0.42	-	121,121,121,121	0
54	MG	BA	3121	1/1	0.98	0.28	-	87,87,87,87	0
54	MG	BA	3306	1/1	0.87	0.27	-	81,81,81,81	0
54	MG	DA	3027	1/1	0.75	0.12	-	115,115,115,115	0
54	MG	DA	3350	1/1	0.96	0.29	-	82,82,82,82	0
54	MG	AA	1800	1/1	0.88	0.40	-	92,92,92,92	0
54	MG	DA	3101	1/1	0.89	0.39	-	94,94,94,94	0
54	MG	AA	1645	1/1	0.90	0.25	-	93,93,93,93	0
54	MG	CA	1738	1/1	-0.03	0.23	-	114,114,114,114	0
54	MG	DA	3050	1/1	0.95	0.16	-	108,108,108,108	0
54	MG	BA	3531	1/1	0.96	0.38	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3283	1/1	0.89	0.20	-	108,108,108,108	0
54	MG	CA	1713	1/1	0.54	0.13	-	137,137,137,137	0
54	MG	DA	3309	1/1	0.96	0.07	-	145,145,145,145	0
54	MG	BA	3551	1/1	0.40	0.34	-	105,105,105,105	0
54	MG	BA	3558	1/1	0.87	0.39	-	118,118,118,118	0
54	MG	AA	1604	1/1	0.98	0.13	-	135,135,135,135	0
54	MG	BA	3446	1/1	0.56	0.55	-	127,127,127,127	0
54	MG	CA	1715	1/1	0.93	0.37	-	128,128,128,128	0
54	MG	BA	3525	1/1	0.85	0.25	-	96,96,96,96	0
54	MG	DA	3066	1/1	0.89	0.20	-	79,79,79,79	0
54	MG	BA	3042	1/1	0.95	0.18	-	94,94,94,94	0
54	MG	CC	107	1/1	0.82	1.17	-	120,120,120,120	0
54	MG	BA	3227	1/1	0.97	0.32	-	82,82,82,82	0
54	MG	DA	3195	1/1	0.75	0.22	-	104,104,104,104	0
54	MG	CA	1786	1/1	0.87	0.07	-	192,192,192,192	0
54	MG	DA	3355	1/1	0.82	0.15	-	89,89,89,89	0
54	MG	DA	3406	1/1	0.94	0.23	-	103,103,103,103	0
54	MG	BA	3379	1/1	0.76	0.34	-	106,106,106,106	0
54	MG	BA	3307	1/1	0.85	0.21	-	90,90,90,90	0
54	MG	DA	3035	1/1	0.95	0.12	-	93,93,93,93	0
54	MG	DA	3130	1/1	0.96	0.32	-	92,92,92,92	0
54	MG	AA	1656	1/1	0.98	0.23	-	71,71,71,71	0
54	MG	DA	3502	1/1	0.93	0.25	-	64,64,64,64	0
54	MG	DA	3397	1/1	0.62	0.24	-	96,96,96,96	0
54	MG	CA	1729	1/1	0.91	0.32	-	115,115,115,115	0
54	MG	AA	1726	1/1	-0.01	0.31	-	132,132,132,132	0
54	MG	BA	3339	1/1	0.13	0.30	-	115,115,115,115	0
54	MG	BA	3248	1/1	0.90	0.36	-	74,74,74,74	0
54	MG	DA	3415	1/1	0.88	0.11	-	84,84,84,84	0
54	MG	CA	1709	1/1	0.95	0.35	-	110,110,110,110	0
54	MG	CA	1750	1/1	0.78	0.47	-	122,122,122,122	0
54	MG	CA	1719	1/1	0.96	0.12	-	116,116,116,116	0
54	MG	DA	3167	1/1	0.99	0.07	-	75,75,75,75	0
54	MG	BA	3565	1/1	0.79	0.22	-	86,86,86,86	0
54	MG	AA	1793	1/1	0.86	0.37	-	103,103,103,103	0
54	MG	BA	3068	1/1	0.96	0.16	-	71,71,71,71	0
54	MG	B5	102	1/1	0.92	0.11	-	92,92,92,92	0
54	MG	DA	3312	1/1	0.92	0.19	-	87,87,87,87	0
54	MG	DA	3401	1/1	0.90	0.27	-	103,103,103,103	0
54	MG	BA	3500	1/1	0.96	0.18	-	129,129,129,129	0
54	MG	DA	3371	1/1	0.64	0.28	-	111,111,111,111	0
54	MG	DA	3063	1/1	0.93	0.20	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3257	1/1	0.92	0.34	-	88,88,88,88	0
54	MG	DA	3403	1/1	0.94	0.18	-	84,84,84,84	0
54	MG	BA	3104	1/1	0.99	0.33	-	70,70,70,70	0
54	MG	BA	3371	1/1	0.91	0.39	-	81,81,81,81	0
54	MG	DA	3280	1/1	0.68	0.25	-	94,94,94,94	0
54	MG	AA	1807	1/1	0.65	0.22	-	101,101,101,101	0
54	MG	BA	3001	1/1	0.88	0.44	-	53,53,53,53	0
54	MG	AA	1765	1/1	0.73	0.15	-	137,137,137,137	0
54	MG	BA	3388	1/1	0.85	0.52	-	100,100,100,100	0
54	MG	AA	1602	1/1	0.98	0.23	-	95,95,95,95	0
54	MG	DA	3093	1/1	0.63	0.22	-	106,106,106,106	0
54	MG	BA	3513	1/1	0.76	0.22	-	112,112,112,112	0
54	MG	CA	1698	1/1	0.70	0.24	-	96,96,96,96	0
54	MG	BA	3514	1/1	0.85	0.53	-	90,90,90,90	0
54	MG	AA	1648	1/1	0.95	0.31	-	123,123,123,123	0
54	MG	AA	1651	1/1	0.85	0.21	-	108,108,108,108	0
54	MG	BA	3490	1/1	0.83	0.43	-	100,100,100,100	0
54	MG	AA	1742	1/1	0.89	0.24	-	108,108,108,108	0
54	MG	CA	1618	1/1	0.84	0.57	-	123,123,123,123	0
54	MG	BA	3612	1/1	0.58	0.43	-	99,99,99,99	0
54	MG	BA	3437	1/1	0.68	0.27	-	81,81,81,81	0
54	MG	DA	3453	1/1	0.73	0.20	-	104,104,104,104	0
54	MG	CA	1720	1/1	0.95	0.29	-	98,98,98,98	0
54	MG	DA	3273	1/1	0.88	0.32	-	83,83,83,83	0
54	MG	DA	3246	1/1	0.94	0.10	-	103,103,103,103	0
54	MG	BA	3618	1/1	0.54	0.80	-	107,107,107,107	0
54	MG	AA	1790	1/1	0.54	0.51	-	115,115,115,115	0
54	MG	CA	1702	1/1	0.86	0.26	-	156,156,156,156	0
54	MG	DA	3008	1/1	0.80	0.55	-	93,93,93,93	0
54	MG	DA	3240	1/1	0.86	0.20	-	89,89,89,89	0
54	MG	BA	3082	1/1	0.87	0.41	-	109,109,109,109	0
54	MG	CA	1637	1/1	0.91	0.21	-	121,121,121,121	0
54	MG	DA	3261	1/1	0.97	0.15	-	78,78,78,78	0
54	MG	BA	3370	1/1	0.61	0.42	-	111,111,111,111	0
54	MG	DA	3213	1/1	0.95	0.24	-	67,67,67,67	0
54	MG	BA	3586	1/1	0.92	0.37	-	62,62,62,62	0
54	MG	DA	3458	1/1	0.92	0.09	-	115,115,115,115	0
54	MG	DA	3386	1/1	0.42	0.35	-	102,102,102,102	0
54	MG	DA	3229	1/1	0.96	0.27	-	94,94,94,94	0
54	MG	DA	3065	1/1	0.94	0.26	-	103,103,103,103	0
54	MG	BA	3390	1/1	0.78	0.25	-	81,81,81,81	0
54	MG	DA	3508	1/1	0.96	0.24	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3188	1/1	0.92	0.34	-	69,69,69,69	0
54	MG	BA	3007	1/1	0.98	0.18	-	63,63,63,63	0
54	MG	AA	1804	1/1	0.95	0.10	-	130,130,130,130	0
54	MG	DB	205	1/1	0.92	0.17	-	85,85,85,85	0
54	MG	AC	106	1/1	0.91	0.32	-	119,119,119,119	0
54	MG	BA	3053	1/1	0.93	0.64	-	92,92,92,92	0
54	MG	DA	3426	1/1	0.95	0.14	-	159,159,159,159	0
54	MG	BB	201	1/1	0.81	0.39	-	99,99,99,99	0
54	MG	DA	3006	1/1	0.94	0.41	-	69,69,69,69	0
54	MG	BA	3389	1/1	0.84	0.23	-	102,102,102,102	0
54	MG	BA	3578	1/1	0.96	0.16	-	88,88,88,88	0
54	MG	BA	3226	1/1	0.90	0.44	-	87,87,87,87	0
54	MG	BA	3081	1/1	0.98	0.27	-	88,88,88,88	0
54	MG	DA	3387	1/1	0.87	0.23	-	106,106,106,106	0
54	MG	BA	3133	1/1	0.90	0.38	-	92,92,92,92	0
54	MG	BA	3356	1/1	0.92	0.23	-	128,128,128,128	0
54	MG	BA	3404	1/1	0.81	0.28	-	93,93,93,93	0
54	MG	DA	3108	1/1	0.97	0.23	-	67,67,67,67	0
54	MG	CA	1664	1/1	0.89	0.32	-	110,110,110,110	0
54	MG	DA	3144	1/1	0.83	0.42	-	85,85,85,85	0
54	MG	AH	201	1/1	0.95	0.18	-	118,118,118,118	0
54	MG	BA	3468	1/1	0.89	0.18	-	84,84,84,84	0
54	MG	AG	302	1/1	0.90	0.24	-	162,162,162,162	0
54	MG	BA	3419	1/1	0.87	0.17	-	129,129,129,129	0
54	MG	BA	3083	1/1	0.98	0.30	-	108,108,108,108	0
54	MG	BA	3412	1/1	0.86	0.25	-	94,94,94,94	0
54	MG	BA	3546	1/1	0.90	0.27	-	97,97,97,97	0
54	MG	DR	201	1/1	0.81	0.65	-	86,86,86,86	0
54	MG	BA	3266	1/1	0.89	0.30	-	77,77,77,77	0
54	MG	DA	3381	1/1	0.88	0.30	-	97,97,97,97	0
54	MG	DA	3226	1/1	0.96	0.27	-	81,81,81,81	0
54	MG	BA	3191	1/1	0.54	0.67	-	111,111,111,111	0
54	MG	DA	3287	1/1	0.96	0.23	-	67,67,67,67	0
54	MG	AA	1636	1/1	0.65	0.34	-	92,92,92,92	0
54	MG	CA	1757	1/1	0.83	0.10	-	149,149,149,149	0
54	MG	BA	3408	1/1	0.98	0.13	-	109,109,109,109	0
54	MG	DA	3392	1/1	0.86	1.30	-	97,97,97,97	0
54	MG	BA	3494	1/1	0.70	0.23	-	97,97,97,97	0
54	MG	BA	3058	1/1	0.97	0.25	-	103,103,103,103	0
54	MG	CA	1607	1/1	0.95	0.41	-	83,83,83,83	0
54	MG	DA	3354	1/1	0.79	0.84	-	105,105,105,105	0
54	MG	DA	3278	1/1	0.97	0.12	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3401	1/1	0.79	0.34	-	91,91,91,91	0
54	MG	DA	3460	1/1	0.76	0.19	-	96,96,96,96	0
54	MG	AA	1798	1/1	0.97	0.41	-	100,100,100,100	0
54	MG	BA	3354	1/1	0.78	0.42	-	113,113,113,113	0
54	MG	CA	1746	1/1	0.92	0.34	-	92,92,92,92	0
54	MG	DA	3073	1/1	0.97	0.11	-	102,102,102,102	0
54	MG	AA	1801	1/1	0.75	0.21	-	97,97,97,97	0
54	MG	AA	1660	1/1	0.96	0.15	-	126,126,126,126	0
54	MG	AA	1647	1/1	0.83	0.36	-	96,96,96,96	0
54	MG	DA	3253	1/1	0.85	0.15	-	103,103,103,103	0
54	MG	CA	1710	1/1	0.84	0.36	-	104,104,104,104	0
54	MG	BA	3414	1/1	0.77	0.20	-	98,98,98,98	0
54	MG	CA	1645	1/1	0.81	0.13	-	103,103,103,103	0
54	MG	BA	3464	1/1	0.88	0.40	-	80,80,80,80	0
54	MG	BA	3368	1/1	0.75	0.43	-	93,93,93,93	0
54	MG	BA	3503	1/1	0.85	0.22	-	105,105,105,105	0
54	MG	BA	3360	1/1	0.78	0.30	-	110,110,110,110	0
54	MG	DA	3025	1/1	0.92	0.35	-	88,88,88,88	0
54	MG	BA	3508	1/1	0.86	0.48	-	85,85,85,85	0
54	MG	DA	3301	1/1	0.78	1.10	-	124,124,124,124	0
54	MG	CA	1774	1/1	0.73	0.34	-	110,110,110,110	0
54	MG	CA	1783	1/1	0.95	0.43	-	97,97,97,97	0
54	MG	AA	1813	1/1	0.88	0.17	-	131,131,131,131	0
54	MG	BA	3550	1/1	0.91	0.27	-	99,99,99,99	0
54	MG	BO	201	1/1	0.96	0.16	-	90,90,90,90	0
54	MG	DA	3474	1/1	0.76	0.34	-	107,107,107,107	0
54	MG	BA	3489	1/1	0.78	0.28	-	104,104,104,104	0
54	MG	CA	1653	1/1	0.98	0.27	-	122,122,122,122	0
54	MG	CA	1615	1/1	0.91	0.24	-	106,106,106,106	0
54	MG	BA	3071	1/1	0.74	0.28	-	103,103,103,103	0
54	MG	CA	1741	1/1	0.92	0.19	-	136,136,136,136	0
54	MG	BA	3329	1/1	0.70	0.45	-	106,106,106,106	0
54	MG	BA	3228	1/1	0.72	0.55	-	85,85,85,85	0
54	MG	CA	1743	1/1	0.95	0.35	-	117,117,117,117	0
54	MG	AA	1688	1/1	0.67	0.10	-	146,146,146,146	0
54	MG	AA	1729	1/1	0.86	0.41	-	108,108,108,108	0
54	MG	CA	1695	1/1	0.75	0.43	-	111,111,111,111	0
54	MG	DA	3159	1/1	0.97	0.10	-	128,128,128,128	0
54	MG	DA	3203	1/1	0.75	0.24	-	90,90,90,90	0
54	MG	CA	1722	1/1	0.94	0.09	-	109,109,109,109	0
54	MG	BA	3238	1/1	0.94	0.49	-	112,112,112,112	0
54	MG	AA	1607	1/1	0.95	0.39	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1695	1/1	0.97	0.09	-	152,152,152,152	0
54	MG	BA	3533	1/1	0.92	0.63	-	106,106,106,106	0
54	MG	DA	3088	1/1	0.82	0.12	-	99,99,99,99	0
54	MG	BA	3277	1/1	0.92	0.20	-	97,97,97,97	0
54	MG	CA	1766	1/1	0.53	0.24	-	107,107,107,107	0
54	MG	BA	3030	1/1	0.88	0.26	-	66,66,66,66	0
54	MG	DA	3197	1/1	0.93	0.28	-	103,103,103,103	0
54	MG	DA	3168	1/1	0.75	0.17	-	95,95,95,95	0
54	MG	DA	3405	1/1	0.86	0.24	-	121,121,121,121	0
54	MG	BA	3506	1/1	0.57	0.21	-	92,92,92,92	0
54	MG	BA	3233	1/1	0.83	0.33	-	106,106,106,106	0
54	MG	DA	3345	1/1	0.89	0.34	-	107,107,107,107	0
54	MG	DA	3358	1/1	0.98	0.35	-	73,73,73,73	0
54	MG	BA	3333	1/1	0.91	0.39	-	99,99,99,99	0
54	MG	CA	1727	1/1	0.51	0.19	-	113,113,113,113	0
54	MG	DA	3434	1/1	0.74	0.34	-	110,110,110,110	0
54	MG	CA	1673	1/1	0.93	0.12	-	89,89,89,89	0
54	MG	DA	3098	1/1	0.66	0.17	-	139,139,139,139	0
54	MG	DA	3523	1/1	0.56	0.67	-	100,100,100,100	0
54	MG	AA	1779	1/1	0.86	0.43	-	88,88,88,88	0
54	MG	CA	1733	1/1	0.97	0.34	-	124,124,124,124	0
54	MG	DA	3219	1/1	0.97	0.28	-	71,71,71,71	0
54	MG	CA	1697	1/1	0.96	0.16	-	185,185,185,185	0
54	MG	CA	1651	1/1	0.97	0.21	-	116,116,116,116	0
54	MG	DP	201	1/1	0.85	0.29	-	102,102,102,102	0
54	MG	DA	3111	1/1	0.99	0.18	-	64,64,64,64	0
54	MG	DA	3157	1/1	0.83	0.18	-	90,90,90,90	0
54	MG	CA	1752	1/1	0.85	0.38	-	106,106,106,106	0
54	MG	BA	3575	1/1	0.89	0.14	-	109,109,109,109	0
54	MG	CC	106	1/1	0.78	0.22	-	112,112,112,112	0
54	MG	AA	1694	1/1	0.78	0.84	-	105,105,105,105	0
54	MG	AA	1741	1/1	0.80	0.29	-	130,130,130,130	0
54	MG	DA	3245	1/1	0.91	0.35	-	83,83,83,83	0
54	MG	DA	3161	1/1	0.88	0.26	-	77,77,77,77	0
54	MG	DA	3178	1/1	0.58	0.24	-	100,100,100,100	0
54	MG	BA	3113	1/1	0.96	0.13	-	72,72,72,72	0
54	MG	DA	3485	1/1	0.61	0.18	-	104,104,104,104	0
54	MG	CA	1756	1/1	0.74	0.29	-	111,111,111,111	0
54	MG	CA	1771	1/1	0.92	0.26	-	92,92,92,92	0
54	MG	DA	3289	1/1	0.89	0.22	-	83,83,83,83	0
54	MG	DA	3138	1/1	0.90	0.21	-	79,79,79,79	0
54	MG	AA	1615	1/1	0.93	0.22	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1637	1/1	0.84	0.57	-	115,115,115,115	0
54	MG	BA	3477	1/1	0.69	0.39	-	93,93,93,93	0
54	MG	BA	3590	1/1	0.97	0.51	-	116,116,116,116	0
54	MG	BA	3320	1/1	0.75	0.32	-	104,104,104,104	0
54	MG	CA	1711	1/1	0.55	0.24	-	119,119,119,119	0
54	MG	BA	3102	1/1	0.64	0.30	-	98,98,98,98	0
54	MG	BB	216	1/1	0.93	0.29	-	111,111,111,111	0
54	MG	DA	3074	1/1	0.42	0.37	-	109,109,109,109	0
54	MG	BA	3159	1/1	0.98	0.23	-	101,101,101,101	0
54	MG	BA	3235	1/1	0.73	0.39	-	128,128,128,128	0
54	MG	BA	3519	1/1	0.88	0.36	-	75,75,75,75	0
54	MG	BA	3374	1/1	0.67	0.16	-	104,104,104,104	0
54	MG	DA	3414	1/1	0.92	0.10	-	95,95,95,95	0
54	MG	DA	3313	1/1	0.89	0.29	-	122,122,122,122	0
54	MG	DA	3456	1/1	0.84	0.25	-	138,138,138,138	0
54	MG	BA	3616	1/1	0.91	0.32	-	92,92,92,92	0
54	MG	DA	3152	1/1	0.93	0.17	-	112,112,112,112	0
54	MG	AA	1789	1/1	0.81	0.23	-	79,79,79,79	0
54	MG	CA	1772	1/1	0.81	0.24	-	109,109,109,109	0
54	MG	DA	3042	1/1	0.76	0.21	-	111,111,111,111	0
54	MG	DA	3478	1/1	0.54	0.41	-	114,114,114,114	0
54	MG	DA	3224	1/1	0.96	0.16	-	61,61,61,61	0
54	MG	DA	3129	1/1	0.86	0.22	-	115,115,115,115	0
54	MG	CA	1612	1/1	0.88	0.14	-	122,122,122,122	0
54	MG	BA	3234	1/1	0.90	0.45	-	84,84,84,84	0
54	MG	BA	3474	1/1	0.91	0.35	-	102,102,102,102	0
54	MG	BA	3100	1/1	0.41	0.51	-	100,100,100,100	0
54	MG	BA	3451	1/1	0.86	0.23	-	102,102,102,102	0
54	MG	BA	3538	1/1	0.80	0.68	-	111,111,111,111	0
54	MG	DA	3002	1/1	0.49	0.40	-	109,109,109,109	0
54	MG	DA	3343	1/1	0.66	0.35	-	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.